Full wwPDB X-ray Structure Validation Report (i)

Jan 5, 2024 – 12:12 am GMT

PDB ID	:	5FDV
Title	:	Crystal structure of the Pyrrhocoricin antimicrobial peptide bound to the Thermus thermophilus 70S ribosome
Authors	:	Seefeldt, A.C.; Graf, M.; Perebaskine, N.; Nguyen, F.; Arenz, S.; Mardirossian, M.; Scocchi, M.; Wilson, D.N.; Innis, C.A.
Deposited on	:	2015-12-16
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

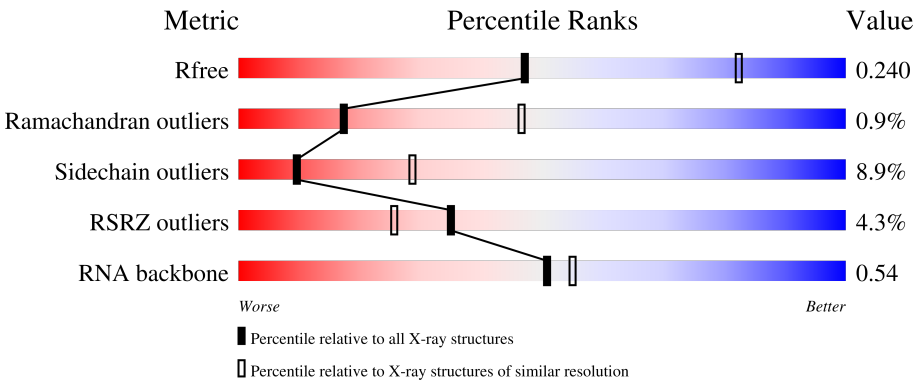
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 35% 54% 10% •
1	2A	2915	6% 54% 38% 7% •
2	1B	120	49% 50% •
2	2B	120	71% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1D	275	92% 8%
3	2D	275	91% 9%
4	1E	204	91% 8%
4	2E	204	91% 9%
5	1F	203	% 87% 13%
5	2F	203	91% 9%
6	1G	181	% 92% 7%
6	2G	181	8% 93% 7%
7	1H	174	% 93% 7%
7	2H	174	16% 92% 7%
8	1I	147	88% 11%
8	2I	147	3% 90% 8%
9	1N	140	88% 12%
9	2N	140	90% 10%
10	1O	122	92% 7%
10	2O	122	93% 7%
11	1P	149	94% 6%
11	2P	149	2% 93% 7%
12	1Q	141	94% 6%
12	2Q	141	% 94% 6%
13	1R	118	87% 11%
13	2R	118	87% 13%
14	1S	110	88% 11%
14	2S	110	3% 91% 9%
15	1T	131	% 92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	131	95% 5%
16	1U	116	85% 14%
16	2U	116	95% 5%
17	1V	101	90% 8%
17	2V	101	91% 8%
18	1W	112	2% 90% 8%
18	2W	112	93% 6%
19	1X	95	94% 6%
19	2X	95	% 94% 5%
20	1Y	107	% 94% 6%
20	2Y	107	11% 95% 5%
21	1Z	203	91% 9%
21	2Z	203	% 91% 8%
22	10	77	91% 9%
22	20	77	3% 94% 6%
23	11	97	% 93% 7%
23	21	97	% 91% 7%
24	12	70	94% 6%
24	22	70	99%
25	13	59	95% 5%
25	23	59	3% 93% 7%
26	14	69	17% 84% 14%
26	24	69	30% 81% 19%
27	15	59	86% 12%
27	25	59	92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	16	53	83% 17%
28	26	53	92% 8%
29	17	48	92% 6%
29	27	48	96%
30	18	64	84% 16%
30	28	64	92% 8%
31	19	37	92% 5%
31	29	37	3% 100%
32	1a	1521	4% 52% 38% 8%
32	2a	1521	4% 57% 35% 8%
33	1x	97	% 95% 5%
33	2x	97	41% 89% 10%
34	1b	231	8% 84% 14%
34	2b	231	6% 87% 12%
35	1c	206	6% 98%
35	2c	206	8% 91% 9%
36	1d	208	% 91% 9%
36	2d	208	% 91% 9%
37	1e	148	93% 7%
37	2e	148	94% 6%
38	1f	100	96%
38	2f	100	94% 6%
39	1g	155	3% 95% 5%
39	2g	155	9% 94% 6%
40	1h	137	% 94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	2h	137	96%
41	1i	127	6% 92% 8%
41	2i	127	27% 90% 9%
42	1j	97	21% 91% 9%
42	2j	97	20% 92% 7%
43	1k	114	96%
43	2k	114	% 91% 9%
44	1l	122	2% 95% 5%
44	2l	122	% 90% 8%
45	1m	116	7% 91% 9%
45	2m	116	9% 88% 10%
46	1n	60	7% 90% 8%
46	2n	60	17% 95%
47	1o	88	% 93% 7%
47	2o	88	% 93% 7%
48	1p	82	4% 89% 11%
48	2p	82	2% 87% 13%
49	1q	99	2% 96%
49	2q	99	93% 6%
50	1r	68	7% 91% 9%
50	2r	68	3% 94% 6%
51	1s	83	19% 88% 12%
51	2s	83	39% 90% 8%
52	1t	98	3% 90% 7%
52	2t	98	% 89% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1u	23	22% 87% 13%
53	2u	23	39% 96%
54	1y	16	12% 94% 6%
54	2y	16	31% 88% 12%

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
55	MG	1A	3062	-	-	-	X
55	MG	1A	3095	-	-	-	X
55	MG	1A	3174	-	-	-	X
55	MG	1A	3213	-	-	-	X
55	MG	1A	3219	-	-	-	X
55	MG	1A	3254	-	-	-	X
55	MG	1A	3514	-	-	-	X
55	MG	1A	3700	-	-	-	X
55	MG	1A	3724	-	-	-	X
55	MG	1A	3757	-	-	-	X
55	MG	1A	3758	-	-	-	X
55	MG	1A	3898	-	-	-	X
55	MG	1A	3904	-	-	-	X
55	MG	1D	303	-	-	-	X
55	MG	1a	3038	-	-	-	X
55	MG	1a	3039	-	-	-	X
55	MG	1a	3049	-	-	-	X
55	MG	1a	3057	-	-	-	X
55	MG	1a	3058	-	-	-	X
55	MG	1a	3063	-	-	-	X
55	MG	1a	3074	-	-	-	X
55	MG	1a	3077	-	-	-	X
55	MG	1a	3078	-	-	-	X
55	MG	1a	3136	-	-	-	X
55	MG	28	101	-	-	-	X
55	MG	2A	3011	-	-	-	X
55	MG	2A	3028	-	-	-	X
55	MG	2A	3041	-	-	-	X
55	MG	2A	3042	-	-	-	X
55	MG	2A	3049	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2A	3109	-	-	-	X
55	MG	2A	3128	-	-	-	X
55	MG	2A	3131	-	-	-	X
55	MG	2A	3132	-	-	-	X
55	MG	2A	3133	-	-	-	X
55	MG	2A	3136	-	-	-	X
55	MG	2A	3138	-	-	-	X
55	MG	2A	3141	-	-	-	X
55	MG	2A	3151	-	-	-	X
55	MG	2A	3183	-	-	-	X
55	MG	2A	3188	-	-	-	X
55	MG	2A	3255	-	-	-	X
55	MG	2A	3411	-	-	-	X
55	MG	2A	3416	-	-	-	X
55	MG	2A	3454	-	-	-	X
55	MG	2A	3475	-	-	-	X
55	MG	2A	3506	-	-	-	X
55	MG	2A	3513	-	-	-	X
55	MG	2A	3533	-	-	-	X
55	MG	2A	3549	-	-	-	X
55	MG	2A	3554	-	-	-	X
55	MG	2A	3555	-	-	-	X
55	MG	2A	3562	-	-	-	X
55	MG	2A	3631	-	-	-	X
55	MG	2A	3727	-	-	-	X
55	MG	2A	3752	-	-	-	X
55	MG	2A	3765	-	-	-	X
55	MG	2A	3791	-	-	-	X
55	MG	2A	3795	-	-	-	X
55	MG	2A	3811	-	-	-	X
55	MG	2A	3813	-	-	-	X
55	MG	2A	3815	-	-	-	X
55	MG	2D	304	-	-	-	X
55	MG	2N	201	-	-	-	X
55	MG	2Q	204	-	-	-	X
55	MG	2X	102	-	-	-	X
55	MG	2a	1603	-	-	-	X
55	MG	2a	1620	-	-	-	X
55	MG	2a	1641	-	-	-	X
55	MG	2a	1654	-	-	-	X
55	MG	2a	1733	-	-	-	X
55	MG	2a	1741	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2l	201	-	-	-	X
55	MG	2n	502	-	-	-	X
58	A	2A	3816	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 293583 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2872	61862	27535	11569	19886	2872	0	0	0
1	2A	2867	61751	27486	11547	19852	2866	0	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	2575	1145	476	834	120	0	0	0
2	2B	120	2571	1146	476	831	118	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	2131	1346	422	360	3	0	0	0
3	2D	275	2136	1349	423	361	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	1E	204	1559	985	298	270	6	0	0	0
4	2E	204	1559	985	298	270	6	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	1F	203	1584	1009	298	275	2	0	0	1
5	2F	203	1580	1007	297	274	2	0	0	1

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	1G	181	1426	916	253	253	4	0	0	0
6	2G	181	1424	912	259	249	4	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	1H	174	1330	845	248	236	1	0	0	0
7	2H	173	1324	842	247	234	1	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	1I	147	1094	699	191	203	1	0	0	0
8	2I	146	1076	687	186	202	1	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	1N	140	1121	722	208	187	4	0	0	0
9	2N	140	1117	719	207	187	4	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1O	122	933	588	171	170	4	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	2O	122	933	588	171	170	4	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	1P	149	1135	706	230	196	3	0	0	0
			Total	C	N	O	S			
11	2P	149	1135	706	230	196	3	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	1Q	141	1122	715	212	188	7	0	0	0
			Total	C	N	O	S			
12	2Q	141	1122	715	212	188	7	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	1R	118	968	604	203	160	1	0	0	0
			Total	C	N	O	S			
13	2R	118	968	604	203	160	1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	1S	110	877	553	175	149	0	0	0
			Total	C	N	O			
14	2S	110	870	549	173	148	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	1T	131	1091	680	225	185	1	0	0	0
			Total	C	N	O	S			
15	2T	131	1083	675	224	183	1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	1U	116	959	608	201	149	1	0	0	0
16	2U	116	959	608	201	149	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	1V	101	775	498	141	135	1	0	0	0
17	2V	101	771	495	140	135	1	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	1W	112	886	557	174	153	2	0	0	0
18	2W	112	886	557	174	153	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	1X	95	750	488	135	126	1	0	0	0
19	2X	95	750	488	135	126	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	1Y	107	810	520	153	131	6	0	0	0
20	2Y	107	810	519	153	132	6	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	1Z	203	1587	1011	282	292	2	0	0	0
21	2Z	201	1557	995	274	286	2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	10	77	608	375	129	103	1	0	0	0
22	20	77	608	375	129	103	1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	11	97	754	475	148	130	1	0	0	0
23	21	97	759	478	149	131	1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	12	70	588	365	118	103	2	0	0	0
24	22	70	592	368	119	103	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
25	13	59	469	298	90	81	0	0	0
25	23	59	464	296	90	78	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	14	69	546	346	96	99	5	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	24	69	536	342	98	91	5	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	15	59	459	288	90	76	5	0	0	0
			Total	C	N	O	S			
27	25	59	455	285	89	76	5	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	16	53	453	281	91	77	4	0	0	0
			Total	C	N	O	S			
28	26	53	449	279	91	75	4	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	17	48	418	257	104	55	2	0	0	0
			Total	C	N	O	S			
29	27	48	418	257	104	55	2	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	18	64	517	331	102	82	2	0	0	0
			Total	C	N	O	S			
30	28	64	517	331	102	82	2	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	19	37	307	188	68	47	4	0	0	0
			Total	C	N	O	S			
31	29	37	307	188	68	47	4	0	0	0

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
32	1a	1500	32246	14358	5975	10413	1500	0	0	0
32	2a	1504	32331	14396	5990	10441	1504	0	0	0

- Molecule 33 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	2x	96	749	468	141	137	3	0	0	0
33	1x	97	764	478	144	139	3	0	0	0

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	1b	231	1842	1175	330	332	5	0	0	0
34	2b	231	1825	1167	326	327	5	0	0	0

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	1c	206	1558	979	305	273	1	0	0	0
35	2c	206	1542	968	300	273	1	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	1d	208	1665	1043	329	286	7	0	0	0
36	2d	208	1668	1047	330	284	7	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	1e	148	1133	716	214	199	4	0	0	0
37	2e	148	1133	716	214	199	4	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	1f	100	814	516	144	151	3	0	0	0
38	2f	100	816	516	146	151	3	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	1g	155	1235	769	244	216	6	0	0	0
39	2g	155	1229	766	241	216	6	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	1h	137	1098	694	210	192	2	0	0	0
40	2h	137	1088	689	206	191	2	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
41	1i	127	986	625	193	168	0	0	0
41	2i	126	966	613	186	167	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	1j	97	719	446	142	131	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	2j	96	710	442	137	131	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	1k	114	834	520	156	155	3	0	0	0
43	2k	114	833	519	156	155	3	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1l	122	932	586	185	159	2	0	0	0
44	2l	122	932	586	185	159	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1m	116	914	564	189	159	2	0	0	0
45	2m	114	895	550	186	157	2	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1n	60	492	312	104	72	4	0	0	0
46	2n	60	492	312	104	72	4	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1o	88	728	456	144	126	2	0	0	0
47	2o	88	728	456	144	126	2	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	1p	82	681	433	134	113	1	0	0	0
48	2p	82	677	430	133	113	1	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	1q	99	823	528	151	142	2	0	0	0
49	2q	99	823	528	151	142	2	0	0	0

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
50	1r	68	555	355	108	92	0	0	0
50	2r	68	555	355	108	92	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	1s	83	648	415	120	111	2	0	0	0
51	2s	83	645	410	118	115	2	0	0	0

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	1t	96	732	449	157	124	2	0	0	0
52	2t	98	733	451	154	126	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
53	1u	23	199	122	48	29	0	0	0
53	2u	23	199	122	48	29	0	0	0

- Molecule 54 is a protein called Pyrrhocoricin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
54	1y	16	120	79	20	21	0	0	0
54	2y	16	120	79	20	21	0	0	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
55	1A	945	945	945	0	0
55	1B	26	26	26	0	0
55	1D	14	14	14	0	0
55	1E	5	5	5	0	0
55	1F	12	12	12	0	0
55	1G	3	3	3	0	0
55	1H	2	2	2	0	0
55	1N	4	4	4	0	0
55	1P	2	2	2	0	0
55	1Q	4	4	4	0	0
55	1R	3	3	3	0	0
55	1U	3	3	3	0	0
55	1V	1	1	1	0	0
55	1W	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
55	1X	1	1	1	0	0
55	1Y	1	1	1	0	0
55	10	7	7	7	0	0
55	11	3	3	3	0	0
55	13	1	1	1	0	0
55	15	4	4	4	0	0
55	17	2	2	2	0	0
55	18	3	3	3	0	0
55	19	2	2	2	0	0
55	1a	226	226	226	0	0
55	1b	1	1	1	0	0
55	1d	5	5	5	0	0
55	1e	1	1	1	0	0
55	1f	1	1	1	0	0
55	1g	1	1	1	0	0
55	1h	2	2	2	0	0
55	1k	1	1	1	0	0
55	1l	1	1	1	0	0
55	1o	1	1	1	0	0
55	1t	1	1	1	0	0
55	1y	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
55	2A	837	837	837	0	0
55	2B	18	18	18	0	0
55	2D	10	10	10	0	0
55	2E	4	4	4	0	0
55	2F	9	9	9	0	0
55	2G	3	3	3	0	0
55	2H	1	1	1	0	0
55	2N	1	1	1	0	0
55	2P	2	2	2	0	0
55	2Q	5	5	5	0	0
55	2R	2	2	2	0	0
55	2S	1	1	1	0	0
55	2U	2	2	2	0	0
55	2V	3	3	3	0	0
55	2W	1	1	1	0	0
55	2X	3	3	3	0	0
55	20	5	5	5	0	0
55	21	2	2	2	0	0
55	25	3	3	3	0	0
55	27	2	2	2	0	0
55	28	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	2a	197	Total Mg 197 197	0	0
55	2b	1	Total Mg 1 1	0	0
55	2d	3	Total Mg 3 3	0	0
55	2e	2	Total Mg 2 2	0	0
55	2f	1	Total Mg 1 1	0	0
55	2g	1	Total Mg 1 1	0	0
55	2h	2	Total Mg 2 2	0	0
55	2l	2	Total Mg 2 2	0	0
55	2n	1	Total Mg 1 1	0	0
55	2o	1	Total Mg 1 1	0	0
55	2q	1	Total Mg 1 1	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

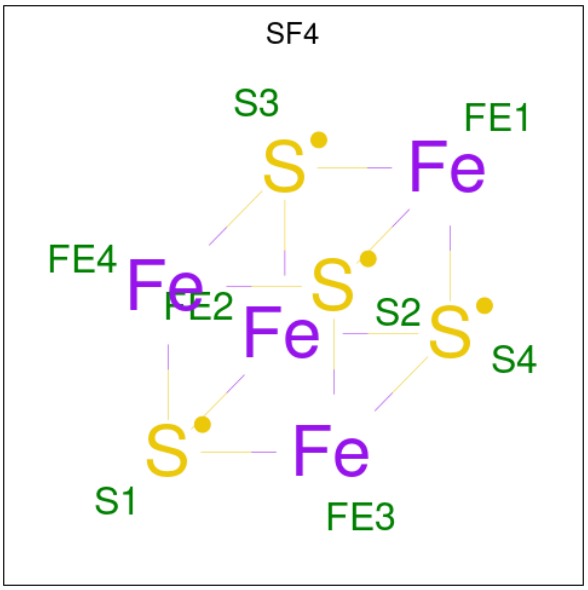
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1Y	1	Total Zn 1 1	0	0
56	14	1	Total Zn 1 1	0	0
56	15	1	Total Zn 1 1	0	0
56	16	1	Total Zn 1 1	0	0
56	19	1	Total Zn 1 1	0	0
56	1n	1	Total Zn 1 1	0	0
56	2Y	1	Total Zn 1 1	0	0
56	24	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

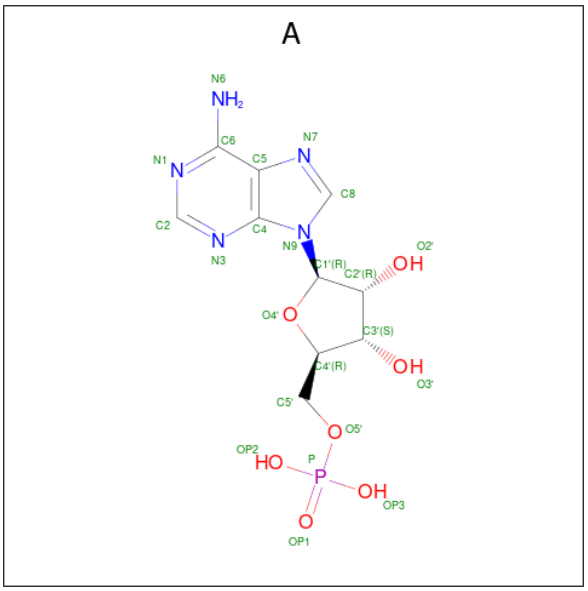
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	25	1	Total Zn 1 1	0	0
56	26	1	Total Zn 1 1	0	0
56	29	1	Total Zn 1 1	0	0
56	2n	1	Total Zn 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1d	1	Total Fe S 8 4 4	0	0
57	2d	1	Total Fe S 8 4 4	0	0

- Molecule 58 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2A	1	Total P 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1740	Total O 1740 1740	0	0
59	1B	43	Total O 43 43	0	0
59	1D	16	Total O 16 16	0	0
59	1E	17	Total O 17 17	0	0
59	1F	9	Total O 9 9	0	0
59	1G	2	Total O 2 2	0	0
59	1H	3	Total O 3 3	0	0
59	1N	8	Total O 8 8	0	0
59	1P	13	Total O 13 13	0	0
59	1Q	7	Total O 7 7	0	0
59	1R	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1T	5	Total O 5 5	0	0
59	1U	5	Total O 5 5	0	0
59	1V	3	Total O 3 3	0	0
59	1W	2	Total O 2 2	0	0
59	1X	4	Total O 4 4	0	0
59	1Y	4	Total O 4 4	0	0
59	10	5	Total O 5 5	0	0
59	11	3	Total O 3 3	0	0
59	13	1	Total O 1 1	0	0
59	15	2	Total O 2 2	0	0
59	16	2	Total O 2 2	0	0
59	17	2	Total O 2 2	0	0
59	18	9	Total O 9 9	0	0
59	19	2	Total O 2 2	0	0
59	1a	395	Total O 395 395	0	0
59	1d	10	Total O 10 10	0	0
59	1e	2	Total O 2 2	0	0
59	1f	1	Total O 1 1	0	0
59	1h	1	Total O 1 1	0	0
59	1j	1	Total O 1 1	0	0
59	1l	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1m	2	Total O 2 2	0	0
59	1n	1	Total O 1 1	0	0
59	1p	1	Total O 1 1	0	0
59	1q	1	Total O 1 1	0	0
59	1t	1	Total O 1 1	0	0
59	1y	2	Total O 2 2	0	0
59	2A	1667	Total O 1667 1667	0	0
59	2B	35	Total O 35 35	0	0
59	2D	14	Total O 14 14	0	0
59	2E	16	Total O 16 16	0	0
59	2F	11	Total O 11 11	0	0
59	2G	2	Total O 2 2	0	0
59	2H	2	Total O 2 2	0	0
59	2N	2	Total O 2 2	0	0
59	2P	11	Total O 11 11	0	0
59	2Q	4	Total O 4 4	0	0
59	2R	4	Total O 4 4	0	0
59	2T	2	Total O 2 2	0	0
59	2U	2	Total O 2 2	0	0
59	2V	2	Total O 2 2	0	0
59	2W	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

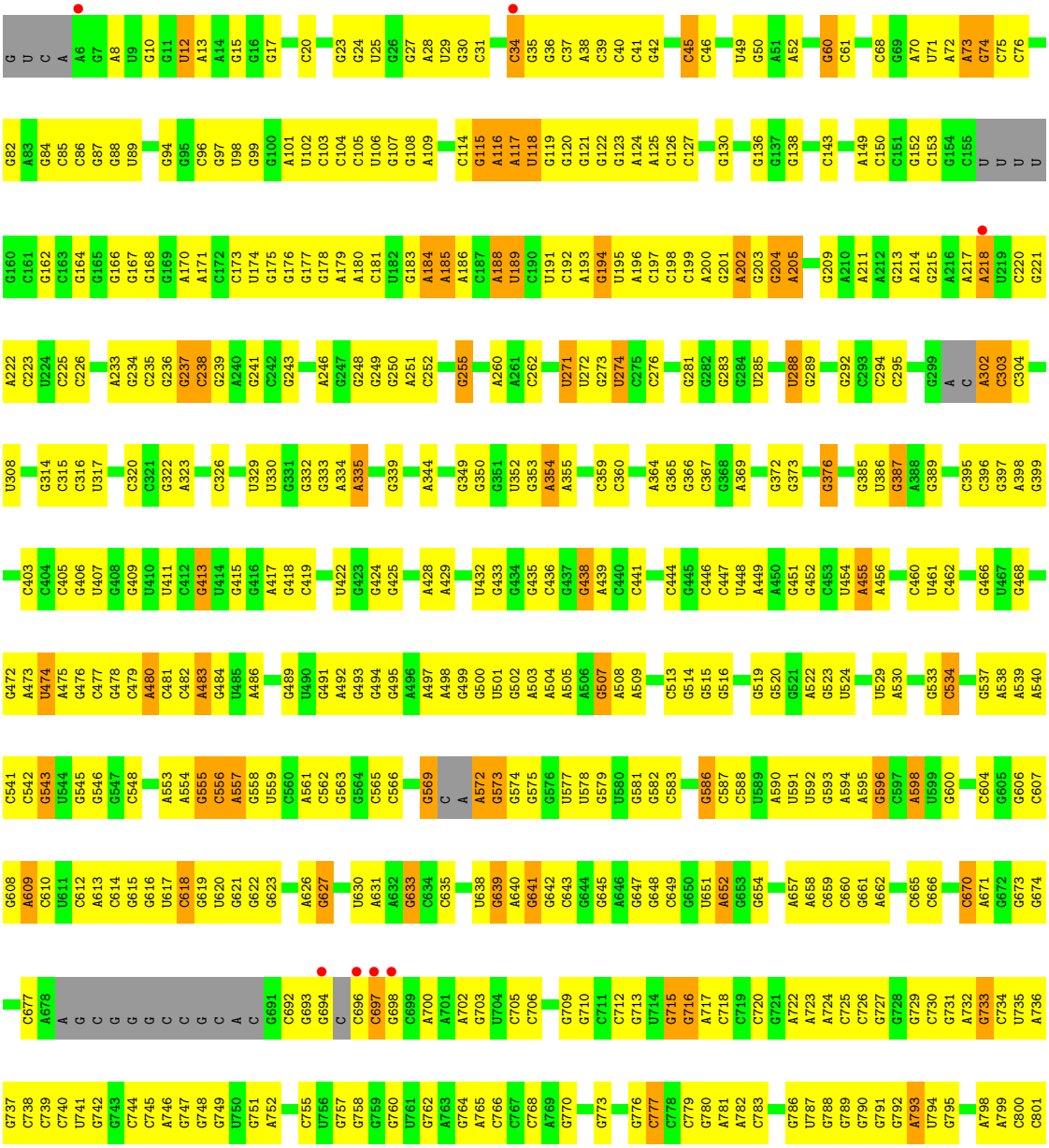
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2X	5	Total O 5 5	0	0
59	2Y	3	Total O 3 3	0	0
59	20	7	Total O 7 7	0	0
59	21	2	Total O 2 2	0	0
59	23	2	Total O 2 2	0	0
59	25	1	Total O 1 1	0	0
59	26	2	Total O 2 2	0	0
59	27	1	Total O 1 1	0	0
59	28	6	Total O 6 6	0	0
59	2a	387	Total O 387 387	0	0
59	2c	1	Total O 1 1	0	0
59	2d	6	Total O 6 6	0	0
59	2e	4	Total O 4 4	0	0
59	2f	1	Total O 1 1	0	0
59	2h	1	Total O 1 1	0	0
59	2j	1	Total O 1 1	0	0
59	2l	3	Total O 3 3	0	0
59	2m	2	Total O 2 2	0	0
59	2o	1	Total O 1 1	0	0
59	2t	1	Total O 1 1	0	0
59	2y	1	Total O 1 1	0	0

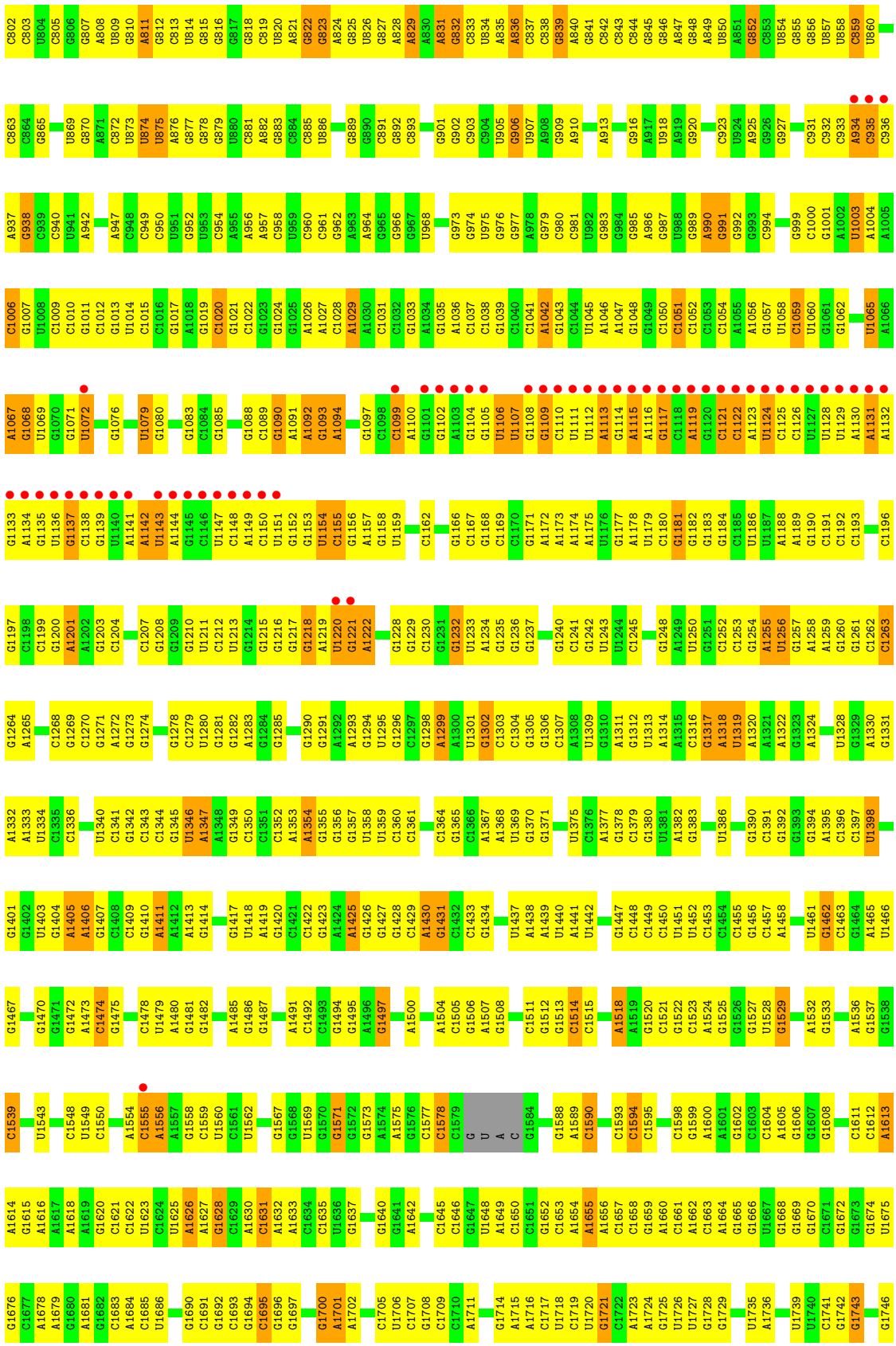
3 Residue-property plots (i)

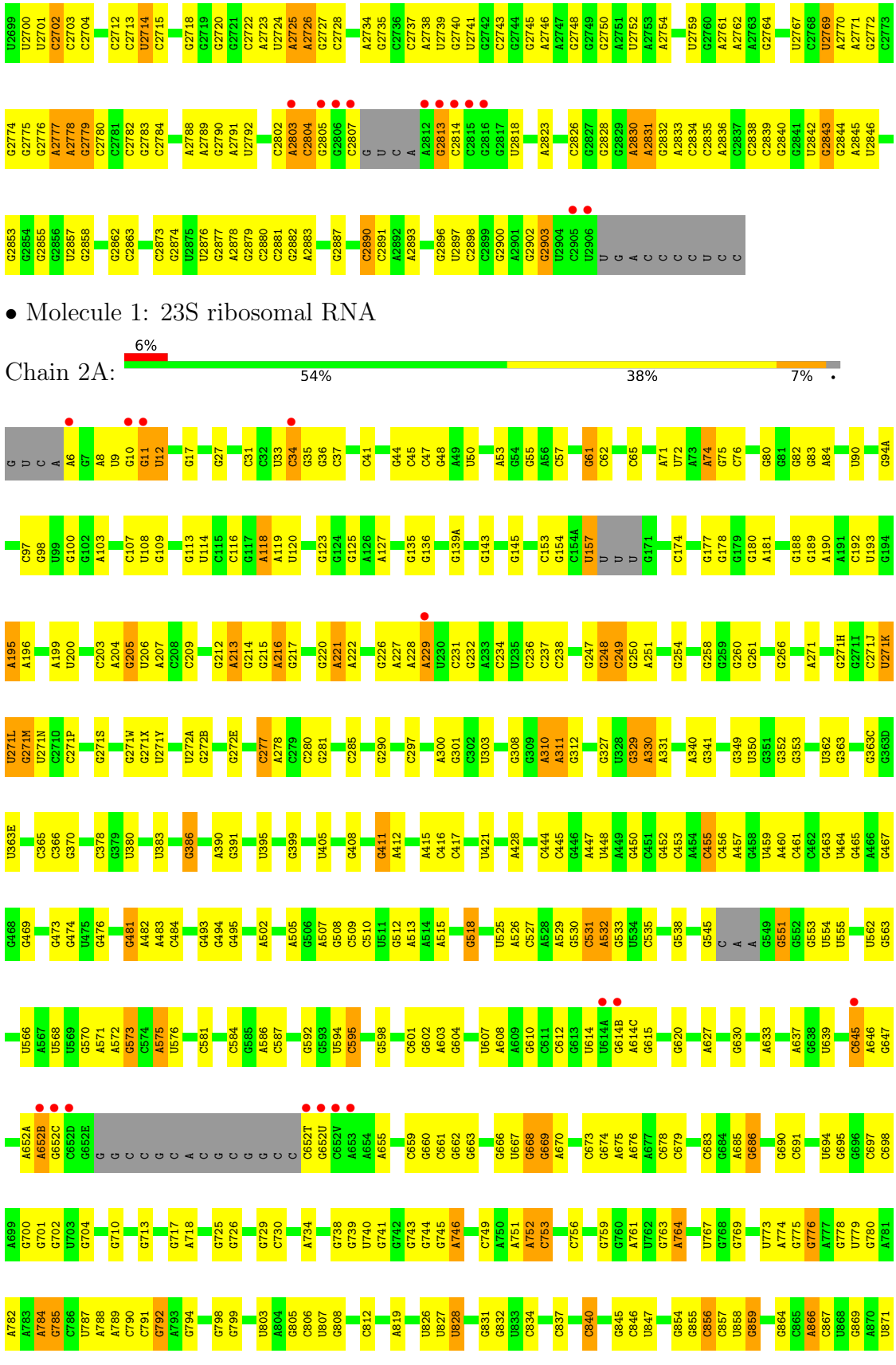
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: 23S ribosomal RNA

Chain 1A:

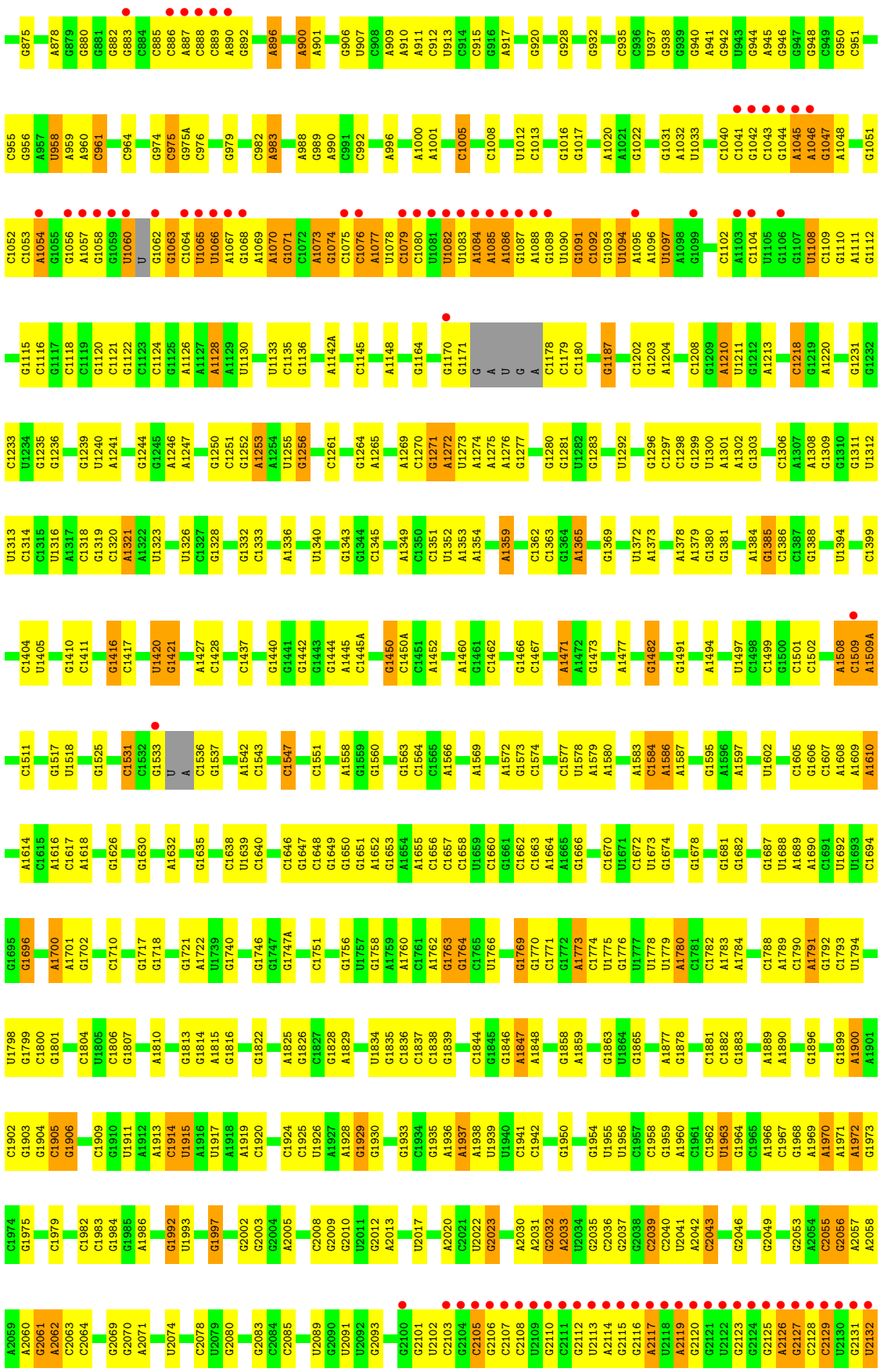


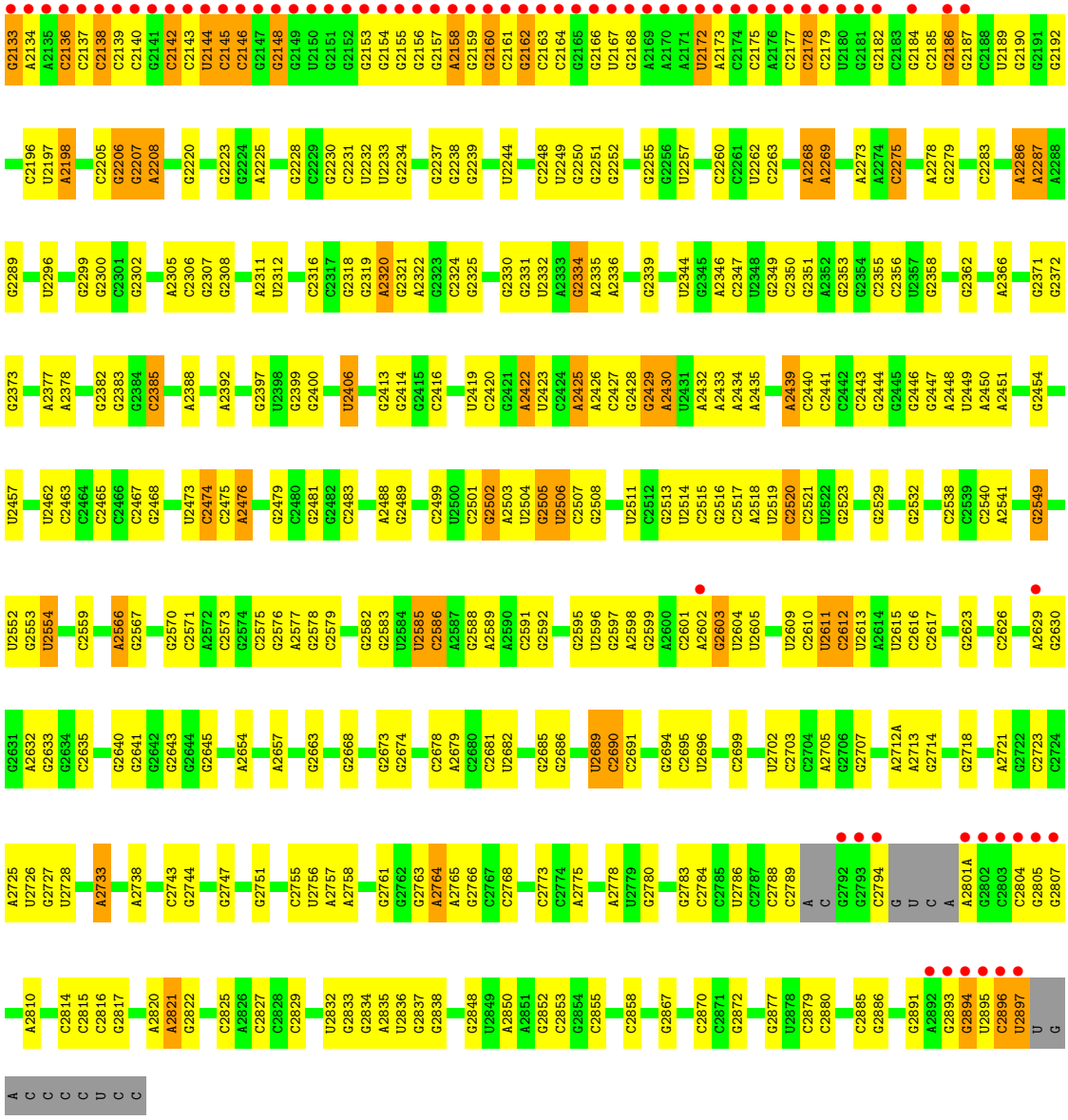

C802 C803 U804 C805 G806 G807 A808 U809 G810 A811 G812 C813 U814 G815 G816 G817 G818 C819 U820 A821 G822 G823 A824 G825 U826 G827 A828 A829 A830 A831 G832 C833 U834 A835 A836 C837 C838 G839 A840 G841 C842 C843 C844 G845 G846 A847 G848 A849 U850 A851 G852 C853 U854 G855 G856 U857 U858 C859 U860
C863 C864 G865 U869 G870 A871 C872 U873 U874 U875 A876 G877 G878 G879 U880 C881 A882 G883 C884 C885 U886 G889 G890 C891 G892 C893 G901 G902 C903 C904 U905 G906 U907 A908 G909 A910 A913 G916 A917 U918 A919 G920 C923 U924 A925 G926 G927 C931 C932 C933 A934 C935 C936
A937 G938 C939 C940 U941 A942 A947 C948 C949 C950 U951 G952 U953 C954 A955 A956 A957 C958 U959 C960 C961 G962 A963 A964 G965 G966 G967 U968 G973 G974 U975 G976 G977 A978 G979 C980 C981 U982 G983 G984 G985 A986 G987 U988 G989 A990 G991 G992 G993 C994 G999 C1000 G1001 A1002 U1003 A1004 A1005
C1006 G1007 U1008 C1009 C1010 G1011 C1012 G1013 U1014 C1015 C1016 G1017 A1018 G1019 C1020 G1021 C1022 G1023 G1024 G1025 A1026 A1027 C1028 A1029 A1030 C1031 C1032 G1033 A1034 G1035 A1036 C1037 C1038 G1039 C1040 C1041 A1042 G1043 C1044 U1045 A1046 A1047 G1048 G1049 C1050 C1051 C1052 C1053 C1054 A1055 A1056 G1057 U1058 C1059 G1061 G1062 U1065 A1066
A1067 G1068 U1069 G1070 G1071 U1072 G1076 U1079 G1080 G1083 C1084 G1085 G1088 C1089 G1090 A1091 A1092 G1093 A1094 G1097 C1098 C1099 A1100 G1101 G1102 A1103 G1104 G1105 U1106 U1107 G1108 G1109 C1110 U1111 U1112 A1113 G1114 A1115 A1116 G1117 C1118 A1119 G1120 C1121 C1122 A1123 U1124 C1125 C1126 U1127 U1128 U1129 A1130 A1131 A1132
G1133 A1134 G1135 U1136 G1137 C1138 G1139 U1140 A1141 A1142 U1143 A1144 G1145 C1146 U1147 C1148 A1149 C1150 U1151 G1152 G1153 U1154 C1155 G1156 A1157 G1158 U1159 C1162 G1166 C1167 G1168 C1169 C1170 G1171 A1172 A1173 A1174 A1175 U1176 G1177 A1178 U1179 C1180 G1181 G1182 G1183 G1184 C1185 U1186 U1187 A1188 A1189 G1190 C1191 C1192 C1193 C1196
G1197 C1198 C1199 G1200 A1201 A1202 G1203 C1204 C1207 G1208 G1209 G1210 U1211 C1212 U1213 G1214 G1215 G1216 G1217 G1218 A1219 U1220 G1221 A1222 G1228 G1229 C1230 G1231 G1232 U1233 A1234 G1235 G1236 G1237 G1240 C1241 G1242 U1243 U1244 C1245 G1248 A1249 U1250 G1251 C1252 C1253 G1254 A1255 U1256 G1257 A1258 A1259 G1260 C1261 C1262 C1263
G1264 A1265 C1268 G1269 C1270 G1271 A1272 G1273 G1274 G1278 C1279 U1280 G1281 G1282 A1283 G1284 G1285 G1290 G1291 A1292 A1293 G1294 U1295 G1296 C1297 G1298 A1299 A1300 U1301 G1302 C1303 C1304 G1305 G1306 C1307 A1308 U1309 G1310 A1311 G1312 U1313 A1314 A1315 C1316 G1317 A1318 U1319 A1320 A1321 A1322 G1323 A1324 U1328 G1329 A1330 G1331
A1332 A1333 U1334 C1335 C1336 U1340 C1341 G1342 C1343 C1344 G1345 U1346 A1347 A1348 G1349 C1350 C1351 C1352 A1353 A1354 G1355 G1356 G1357 U1358 U1359 C1360 C1361 C1364 G1365 C1366 A1367 A1368 U1369 G1370 G1371 U1375 C1376 A1377 G1378 C1379 G1380 U1381 A1382 G1383 U1386 G1390 C1391 G1392 G1393 G1394 A1395 C1396 C1397 U1398
G1401 G1402 U1403 G1404 A1405 A1406 G1407 C1408 C1409 G1410 A1411 A1412 A1413 G1414 G1417 U1418 A1419 G1420 C1421 C1422 G1423 A1424 A1425 G1426 G1427 G1428 C1429 A1430 G1431 C1432 C1433 G1434 U1437 A1438 A1439 A1440 A1441 U1442 G1447 C1448 C1449 C1450 U1451 U1452 C1453 C1454 C1455 G1456 C1457 A1458 U1461 G1462 C1463 G1464 A1465 U1466
G1467 G1470 G1471 G1472 A1473 C1474 G1475 C1478 U1479 A1480 G1481 G1482 A1485 G1486 G1487 A1491 C1492 C1493 G1494 G1495 A1496 G1497 A1500 A1504 C1505 G1506 A1507 G1508 C1511 G1512 G1513 C1514 C1515 A1518 A1519 G1520 C1521 G1522 C1523 A1524 G1525 G1526 G1527 U1528 G1529 A1532 G1533 A1536 G1537 G1538
C1539 U1543 C1548 U1549 C1550 A1554 C1555 A1556 A1557 G1558 C1559 U1560 C1561 U1562 G1567 G1568 U1569 G1570 G1571 G1572 G1573 A1574 A1575 G1576 C1577 C1578 C1579 G U A C G1584 G1588 A1589 C1590 C1593 C1594 C1595 C1598 G1599 A1600 A1601 G1602 G1603 C1604 A1605 G1606 G1607 G1608 C1611 C1612 A1613
A1614 G1615 A1616 A1617 A1618 A1619 G1620 C1621 C1622 U1623 C1624 U1625 A1626 A1627 G1628 C1629 A1630 C1631 A1632 A1633 C1634 C1635 U1636 G1637 G1640 G1641 A1642 C1645 C1646 G1647 U1648 A1649 C1650 C1651 G1652 C1653 A1654 A1655 A1656 C1657 C1658 G1659 A1660 C1661 A1662 C1663 A1664 G1665 G1666 U1667 G1668 G1669 G1670 C1671 G1672 G1673 G1674 U1675
G1676 C1677 A1678 A1679 G1680 A1681 G1682 C1683 A1684 C1685 U1686 G1690 C1691 G1692 C1693 G1694 C1695 G1696 G1697 G1700 A1701 A1702 C1705 U1706 C1707 G1708 C1709 C1710 A1711 G1714 A1715 A1716 C1717 U1718 C1719 U1720 G1721 C1722 A1723 A1724 G1725 U1726 U1727 G1728 G1729 U1735 A1736 U1739 U1740 C1741 G1742 G1743 G1746



• Molecule 1: 23S ribosomal RNA

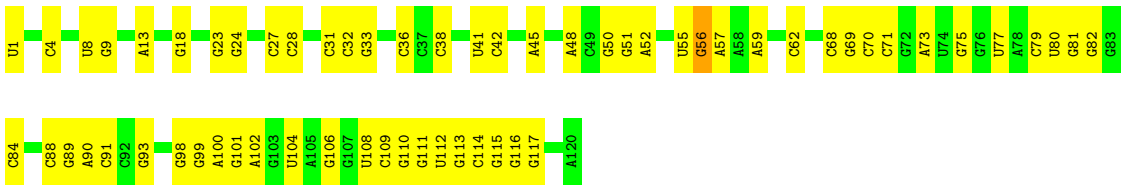
Chain 2A: 6% 54% 38% 7%


G875
A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892
A896
A900 A901
G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917
G920
G928
G932
C935 C936 U937 G938 G939 G940 A941 G942 U943 G944 A945 G946 G947 G948 C949 G950 C951
C955 G956 A957 U958 A959 A960 C961 C964 G974 C975 G975A C976 G979 C982 A983 A988 G989 A990 C991 C992 A996 A1000 A1001 C1005 C1008 U1012 C1013 G1016 G1017 A1020 A1021 G1022 G1031 A1032 U1033 C1040 C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 G1051
C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112
G1115 C1116 G1117 C1118 C1119 G1120 C1121 G1122 C1123 C1124 G1125 A1126 A1127 A1128 A1129 U1130 U1133 C1135 G1136 A1142A C1145 A1148 G1164 G1170 G1171 G A U G A C1178 C1179 C1180 G1187 C1202 G1203 A1204 C1208 G1209 A1210 U1211 G1212 A1213 C1218 G1219 A1220 G1231 G1232
C1233 U1234 G1235 G1236 G1239 U1240 A1241 G1244 G1245 A1246 A1247 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1261 G1264 A1265 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 G1280 G1281 U1282 G1283 U1292 G1296 C1297 C1298 G1299 U1300 A1301 A1302 G1303 C1306 A1307 A1308 G1309 G1310 G1311 U1312
U1313 C1314 C1315 U1316 A1317 C1318 G1319 C1320 A1321 A1322 U1323 U1326 C1327 G1328 G1332 C1333 A1336 U1340 G1343 G1344 C1345 A1349 C1350 C1351 U1352 A1353 A1354 A1359 C1362 C1363 G1364 A1365 G1369 U1372 A1373 A1378 A1379 G1380 G1381 A1384 G1385 C1386 C1387 G1388 U1394 C1399
C1404 U1405 G1410 C1411 G1416 C1417 U1420 G1421 A1427 C1428 C1437 G1440 G1441 G1442 G1443 G1444 A1445 C1445A G1450 C1450A C1451 A1452 A1460 G1461 C1462 G1466 C1467 A1471 A1472 G1473 A1477 G1482 G1491 A1494 U1497 C1498 C1499 G1500 C1501 C1502 A1508 C1509 A1509A
C1511 G1517 U1518 G1525 C1531 C1532 G1533 U A C1536 G1537 A1542 C1543 C1547 C1551 A1558 G1559 G1560 G1563 C1564 C1565 A1566 A1569 A1572 G1573 C1574 C1577 U1578 A1579 A1580 A1583 C1584 A1586 A1587 G1595 A1596 A1597 U1602 C1605 G1606 C1607 A1608 A1609 A1610
A1614 C1615 A1616 C1617 A1618 G1626 G1630 A1632 G1635 C1638 U1639 C1640 C1646 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 U1659 C1660 G1661 C1662 C1663 A1664 A1665 G1666 C1670 U1671 C1672 U1673 G1674 G1678 G1681 G1682 G1687 U1688 A1689 A1690 C1691 U1692 U1693 C1694
G1695 G1696 A1700 A1701 G1702 C1710 G1717 G1718 G1721 A1722 U1739 G1740 G1746 G1747 G1747A C1751 C1756 U1757 C1758 A1759 A1760 C1761 A1762 G1763 G1764 C1765 U1766 C1769 G1770 C1771 G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 C1788 A1789 C1790 A1791 G1792 C1793 U1794
U1798 G1799 C1800 G1801 C1804 U1805 C1806 G1807 A1810 G1813 A1814 A1815 G1816 G1822 A1825 G1826 C1827 G1828 A1829 U1834 G1835 C1836 C1837 C1838 G1839 C1844 G1845 G1846 A1847 A1848 G1858 A1859 G1863 U1864 G1865 A1877 G1878 C1881 C1882 G1883 A1889 A1890 G1896 G1899 A1900 A1901
C1902 G1903 G1904 C1905 G1906 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 C1924 C1925 U1926 A1927 G1928 A1929 G1929 G1930 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 G1950 G1954 U1955 U1956 C1957 C1958 G1959 A1960 C1961 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973
C1974 G1975 C1979 C1982 C1983 G1984 G1985 A1986 G1992 U1993 G1997 G2002 G2003 G2004 A2005 C2008 G2009 G2010 U2011 G2012 A2013 U2017 A2020 C2021 U2022 G2023 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2046 G2049 G2053 A2054 C2055 G2056 A2057 A2058
A2059 A2060 G2061 A2062 C2063 C2064 G2069 G2070 A2071 U2074 C2078 U2079 G2080 C2083 C2084 C2085 U2089 G2090 U2091 U2092 G2093 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132



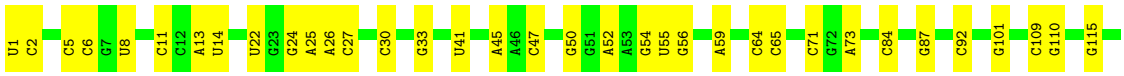
- Molecule 2: 5S ribosomal RNA

Chain 1B:



- Molecule 2: 5S ribosomal RNA

Chain 2B:



• Molecule 3: 50S ribosomal protein L2

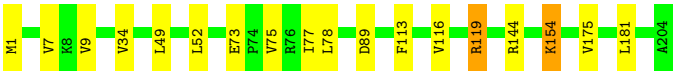
Chain 1D:

• Molecule 3: 50S ribosomal protein L2

Chain 2D:

• Molecule 4: 50S ribosomal protein L3

Chain 1E:

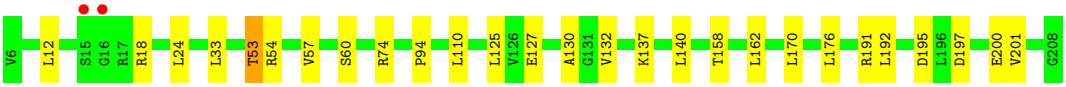


• Molecule 4: 50S ribosomal protein L3

Chain 2E:

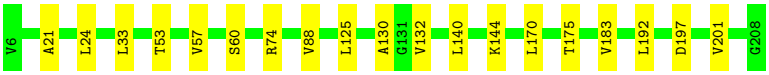
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



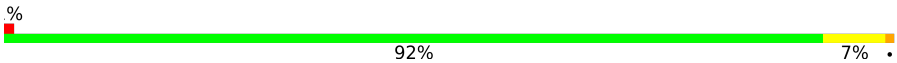
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



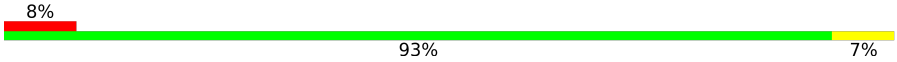
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



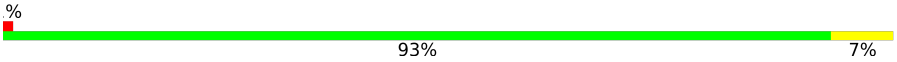
• Molecule 6: 50S ribosomal protein L5

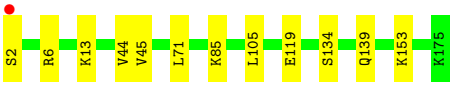
Chain 2G:



• Molecule 7: 50S ribosomal protein L6

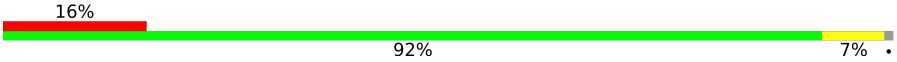
Chain 1H:

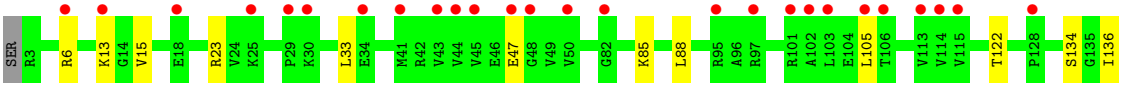




• Molecule 7: 50S ribosomal protein L6

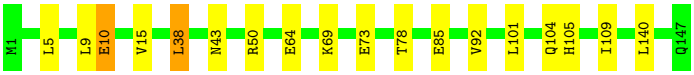
Chain 2H:





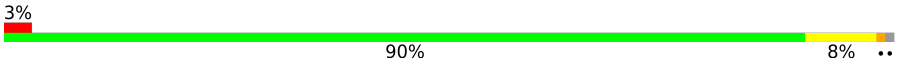
• Molecule 8: 50S ribosomal protein L9

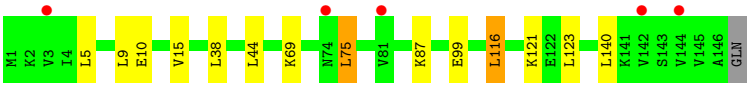
Chain 1I:



• Molecule 8: 50S ribosomal protein L9

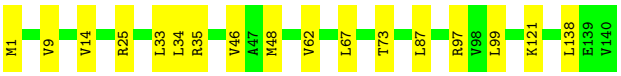
Chain 2I:





• Molecule 9: 50S ribosomal protein L13

Chain 1N:



• Molecule 9: 50S ribosomal protein L13

Chain 2N: 90% 10%

M1 R12 T28 L33 L34 V46 A47 M48 K59 V62 L67 E68 T73 L87 R97 V98 L99 V140

• Molecule 10: 50S ribosomal protein L14

Chain 1O: 92% 7%

M1 Q5 L8 E9 V10 M20 R64 R94 R104 R107 E108 K113 L122

• Molecule 10: 50S ribosomal protein L14

Chain 2O: 93% 7%

M1 Q5 V10 R23 V24 K66 Q90 V98 E108 L122

• Molecule 11: 50S ribosomal protein L15

Chain 1P: 94% 6%

M1 K2 L3 K39 S40 R41 L59 V83 L99 L112 V125 E149

• Molecule 11: 50S ribosomal protein L15

Chain 2P: 2% 93% 7%

M1 K2 L3 K29 T30 A31 T32 L59 K76 V83 F91 L99 L112 P122 V125 E149

• Molecule 12: 50S ribosomal protein L16

Chain 1Q: 94% 6%

M1 L2 R6 M7 K18 R59 T75 V109 K130 R133 Q141

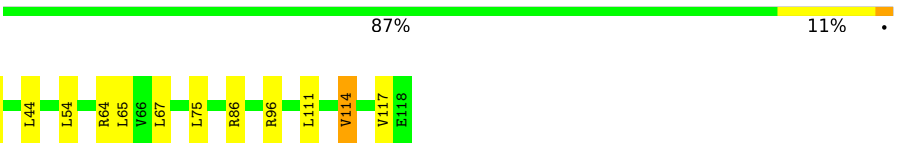
• Molecule 12: 50S ribosomal protein L16

Chain 2Q: % 94% 6%

M1 L2 R5 R6 M7 R16 L17 K18 T21 K22 R59 T75 V106 Q141

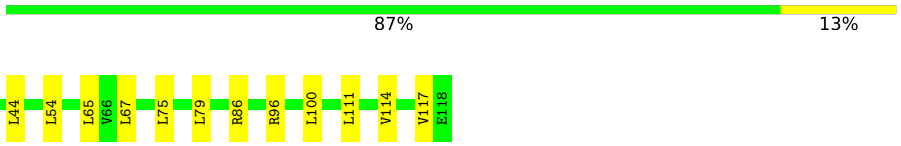
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



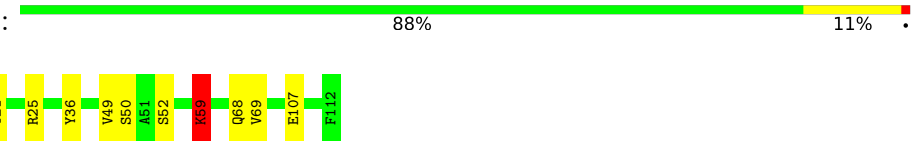
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



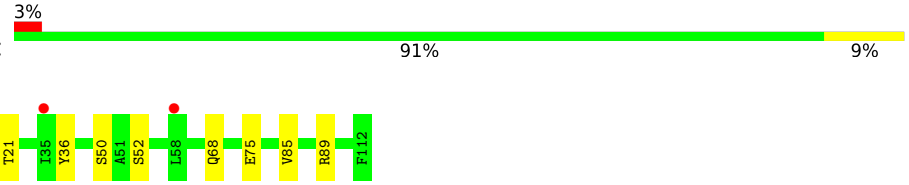
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



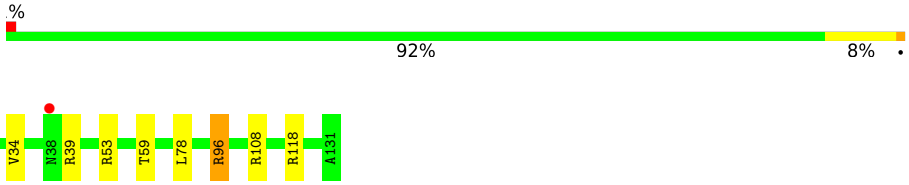
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



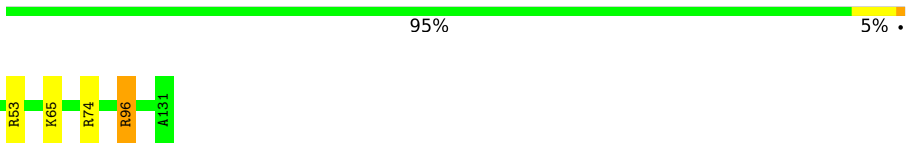
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



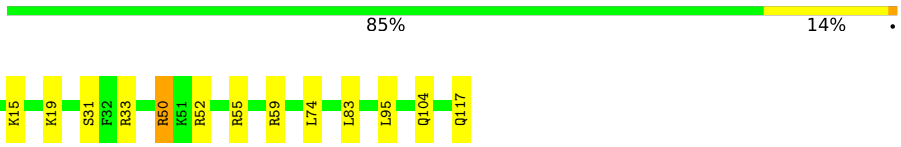
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



• Molecule 16: 50S ribosomal protein L20

Chain 1U:



• Molecule 16: 50S ribosomal protein L20

Chain 2U: 95% 5%

P2 K5 S31 R59 L74 L83 E89 Q117

• Molecule 17: 50S ribosomal protein L21

Chain 1V: 90% 8%

M1 E28 L35 V46 V61 L62 V72 S73 V79 R82 R100 G101

• Molecule 17: 50S ribosomal protein L21

Chain 2V: 91% 8%

M1 L35 V46 V51 V52 E53 V72 V79 R82 E98 G101

• Molecule 18: 50S ribosomal protein L22

Chain 1W: 2% 90% 8%

M1 R11 R15 K16 V17 R18 L19 L23 K27 D67 K83 R92 T100 L107 H111 G112

• Molecule 18: 50S ribosomal protein L22

Chain 2W: 93% 6%

M1 R11 R15 K16 V17 R18 L19 L23 K27 T100 L107 G112

• Molecule 19: 50S ribosomal protein L23

Chain 1X: 94% 6%

M1 T45 L57 L66 R73 K88 E93 G94 L95

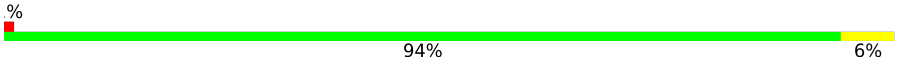
• Molecule 19: 50S ribosomal protein L23

Chain 2X: % 94% 5%

M1 I8 L57 L66 G67 R68 K88 L92 E93 G94 L95

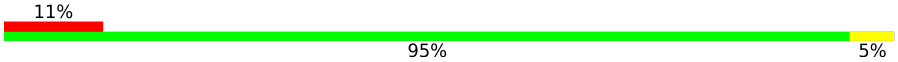
• Molecule 20: 50S ribosomal protein L24

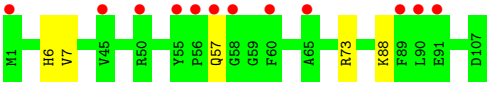
Chain 1Y:



• Molecule 20: 50S ribosomal protein L24

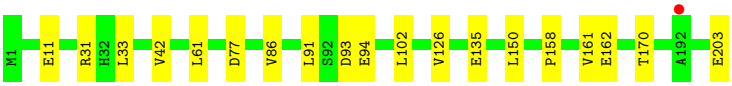
Chain 2Y:





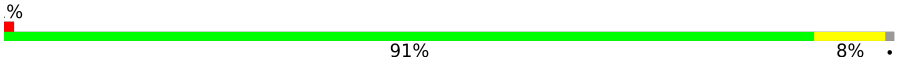
• Molecule 21: 50S ribosomal protein L25

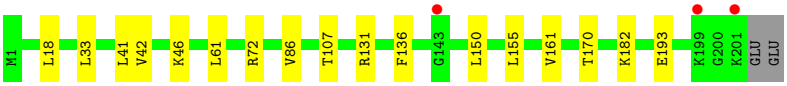
Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



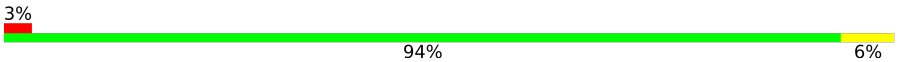


• Molecule 22: 50S ribosomal protein L27

Chain 10:

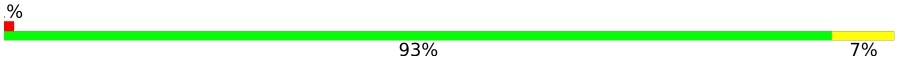
• Molecule 22: 50S ribosomal protein L27

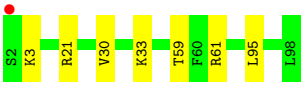
Chain 20:



• Molecule 23: 50S ribosomal protein L28

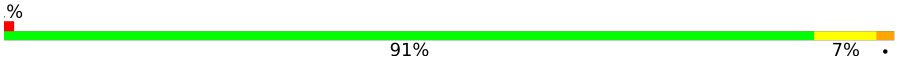
Chain 11:





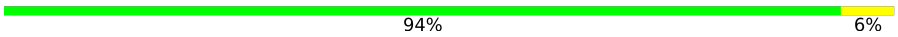
• Molecule 23: 50S ribosomal protein L28

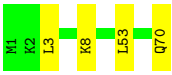
Chain 21:



• Molecule 24: 50S ribosomal protein L29

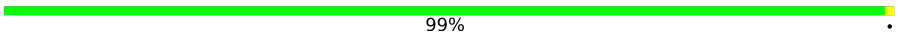
Chain 12:





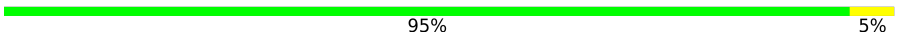
• Molecule 24: 50S ribosomal protein L29

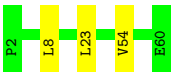
Chain 22:



• Molecule 25: 50S ribosomal protein L30

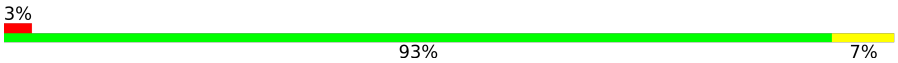
Chain 13:

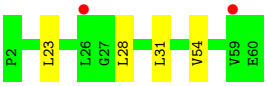




• Molecule 25: 50S ribosomal protein L30

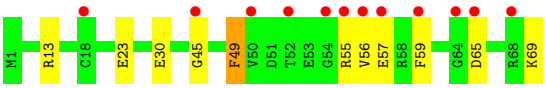
Chain 23:





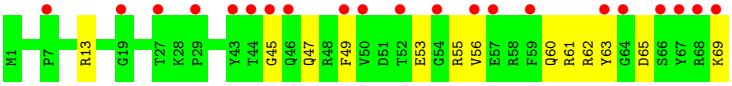
• Molecule 26: 50S ribosomal protein L31

Chain 14:



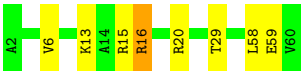
• Molecule 26: 50S ribosomal protein L31

Chain 24:



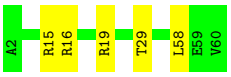
• Molecule 27: 50S ribosomal protein L32

Chain 15:



• Molecule 27: 50S ribosomal protein L32

Chain 25:



• Molecule 28: 50S ribosomal protein L33

Chain 16:

• Molecule 28: 50S ribosomal protein L33

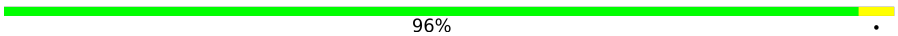
Chain 26:

• Molecule 29: 50S ribosomal protein L34

Chain 17:

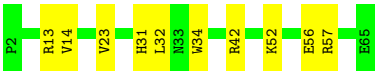
• Molecule 29: 50S ribosomal protein L34

Chain 27:



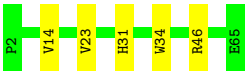
• Molecule 30: 50S ribosomal protein L35

Chain 18:



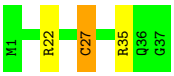
• Molecule 30: 50S ribosomal protein L35

Chain 28:



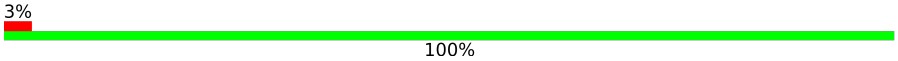
• Molecule 31: 50S ribosomal protein L36

Chain 19:



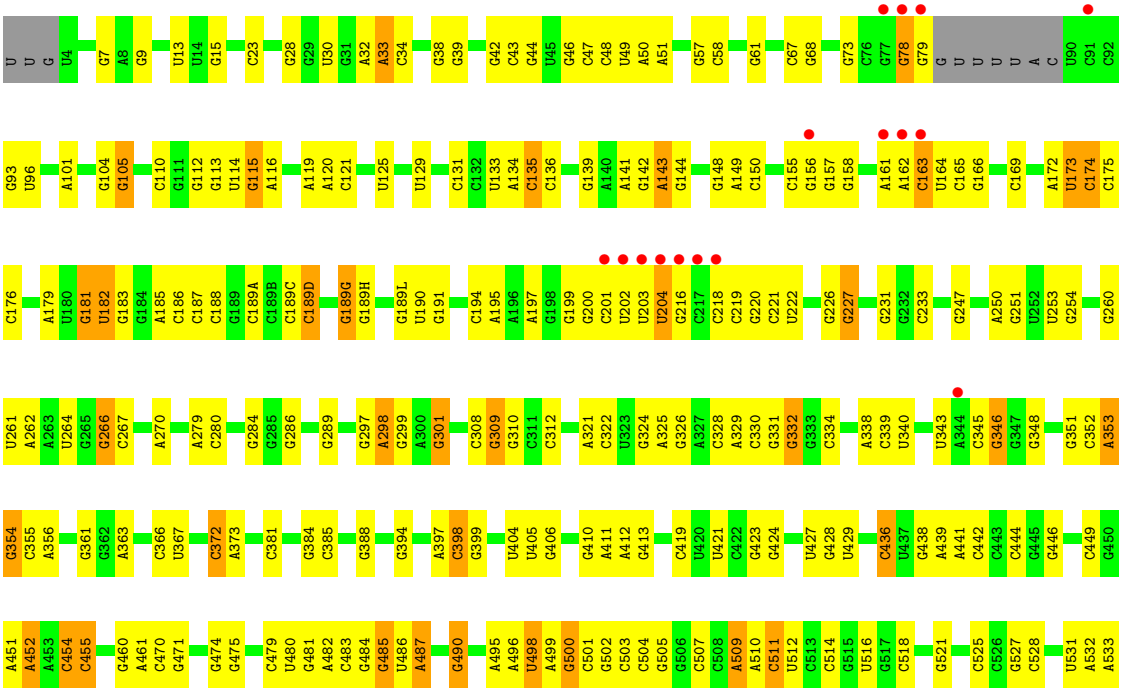
• Molecule 31: 50S ribosomal protein L36

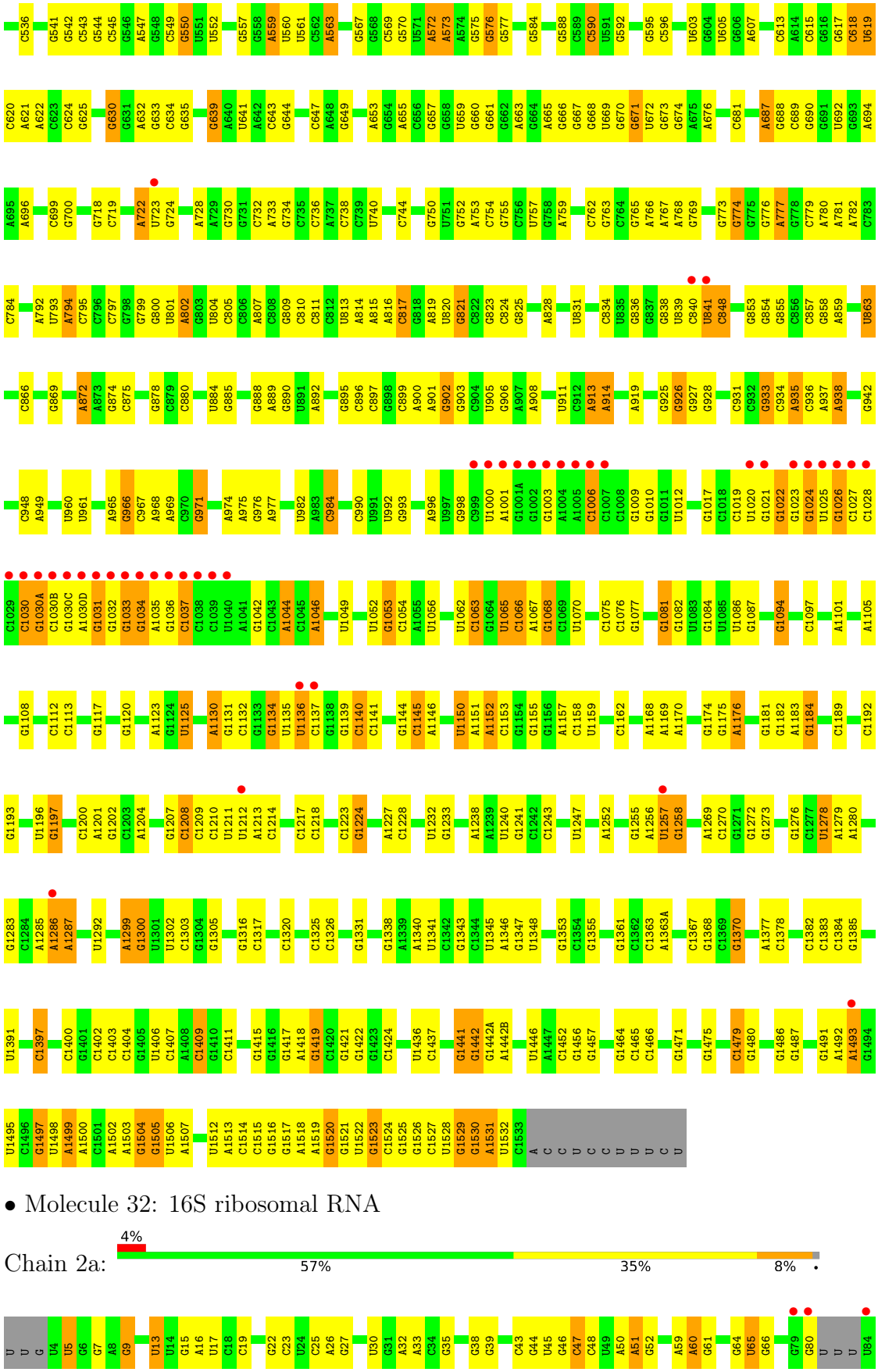
Chain 29:



• Molecule 32: 16S ribosomal RNA

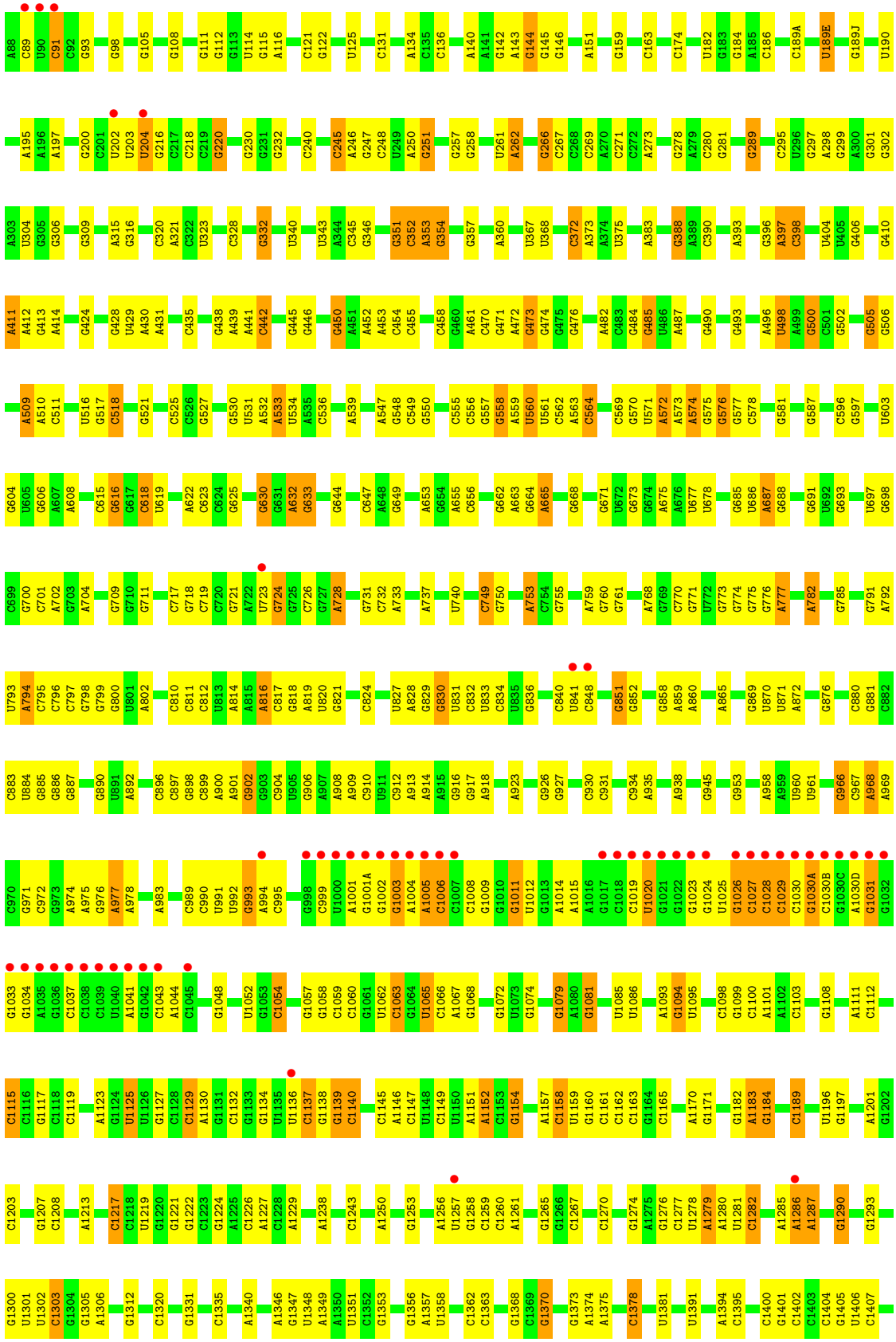
Chain 1a:

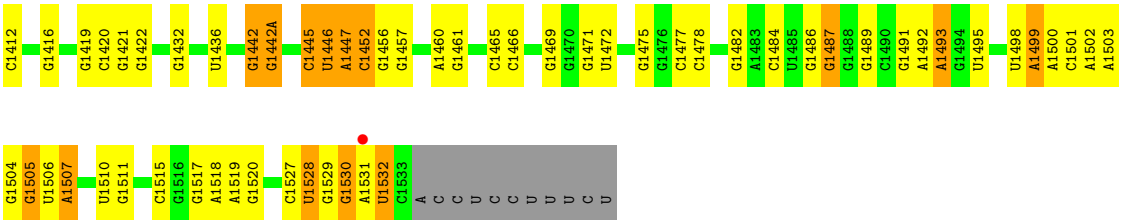




• Molecule 32: 16S ribosomal RNA

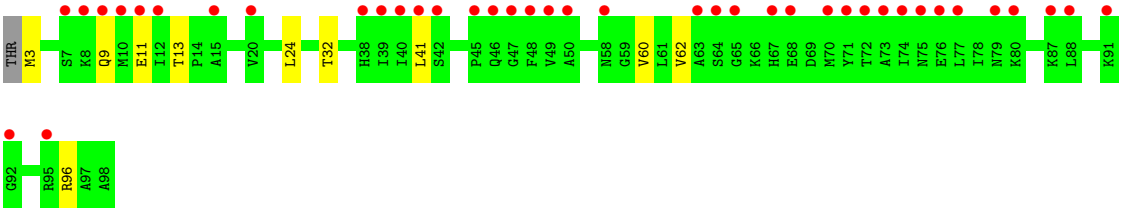
Chain 2a:


A88 C89 U90 C91 C92 G93 G98 G105 G108 G111 G112 G113 U114 G115 A116 C121 G122 U125 C131 A134 C135 C136 A140 A141 G142 A143 G144 G145 G146 A151 G159 C163 C174 U182 G183 G184 A185 C186 C189A U189E G189J U190
A195 A196 A197 G200 C201 U202 U203 U204 G216 C217 C218 C219 G220 G230 G231 G232 C240 C245 A246 G247 C248 U249 A250 G251 G257 G258 U261 A262 G266 C267 C268 C269 A270 C271 C272 A273 G278 A279 C280 G281 G289 C295 U296 G297 A298 G299 A300 G301 G302
A303 U304 G305 G306 G309 A315 G316 C320 A321 C322 U323 C328 G332 U340 U343 A344 C345 G346 G351 C352 A353 G354 G357 A360 U367 U368 C372 A373 A374 U375 A383 G388 A389 C390 A393 G396 A397 C398 U404 U405 G406 G410
A411 A412 G413 A414 G424 G428 U429 A430 A431 C435 G438 A439 A441 C442 G445 G446 G450 A451 A452 A453 C454 C455 C458 G460 A461 C470 G471 A472 G473 G474 G475 G476 A482 G483 G484 G485 U486 A487 G490 G493 A496 U498 A499 G500 C501 G502 G505 G506
A509 A510 C511 U516 G517 C518 G521 C525 C526 G527 G530 U531 A532 A533 U534 A535 C536 A539 A547 G548 C549 G550 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 C569 G570 U571 A572 A573 A574 G575 G576 G577 C578 G581 G587 C596 G597 U603
G604 U605 G606 A607 A608 C615 G616 G617 C618 U619 A622 C623 C624 G625 G630 G631 A632 G633 G644 C647 A648 G649 A653 G654 A655 C656 G662 A663 G664 A665 G668 G671 U672 G673 G674 A675 A676 U677 U678 G685 U686 A687 G688 G691 U692 G693 U697 G698
C699 G700 C701 A702 G703 A704 G709 G710 G711 C717 G718 C719 C720 G721 A722 U723 G724 G725 C726 G727 A728 G731 C732 A733 A737 U740 C749 G750 A753 C754 G755 A759 G760 G761 A768 G769 C770 G771 U772 G773 G774 G775 G776 A777 A782 G785 G791 A792
U793 A794 C795 C796 C797 G798 G799 G800 U801 A802 C810 C811 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C824 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 C840 U841 C848 G851 G852 G858 A859 A860 A865 G869 U870 U871 A872 G876 C880 G881 C882
C883 U884 G885 G886 G887 G890 U891 A892 C896 C897 G898 C899 A900 A901 G902 G903 C904 U905 G906 A907 A908 A909 C910 U911 C912 A913 A914 A915 G916 G917 A918 A923 G926 G927 C930 C931 C934 A935 A938 G945 G953 A958 A959 U960 U961 G966 C967 A968 A969
C970 G971 C972 G973 A974 A975 G976 A977 A978 A983 C989 C990 U991 U992 G993 A994 C995 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032
G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 G1048 U1052 G1053 C1054 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 G1072 U1073 G1074 G1079 A1080 G1081 U1085 U1086 A1093 G1094 U1095 C1098 G1099 C1100 A1101 A1102 C1103 G1108 A1111 C1112
C1115 C1116 G1117 C1118 C1119 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1164 C1165 A1170 G1171 G1182 G1183 G1184 C1189 U1196 G1197 A1201 G1202
C1203 G1207 C1208 A1213 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 A1238 C1243 A1250 G1253 A1256 U1257 G1258 C1259 C1260 A1261 G1265 G1266 C1267 C1270 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 A1285 A1286 A1287 G1290 G1293
G1300 U1301 U1302 C1303 G1304 G1305 A1306 G1312 C1320 G1331 C1335 A1340 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 G1356 A1357 U1358 C1362 C1363 G1368 C1369 G1370 G1373 A1374 A1375 C1378 U1381 U1391 A1394 C1395 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407



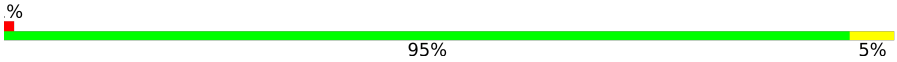
• Molecule 33: Ribosome-associated inhibitor A

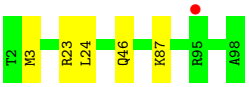
Chain 2x:



• Molecule 33: Ribosome-associated inhibitor A

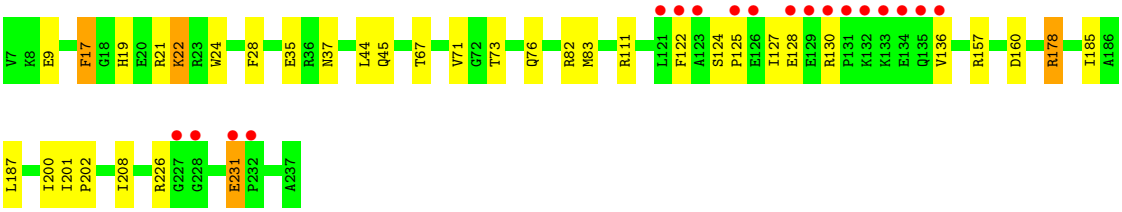
Chain 1x:





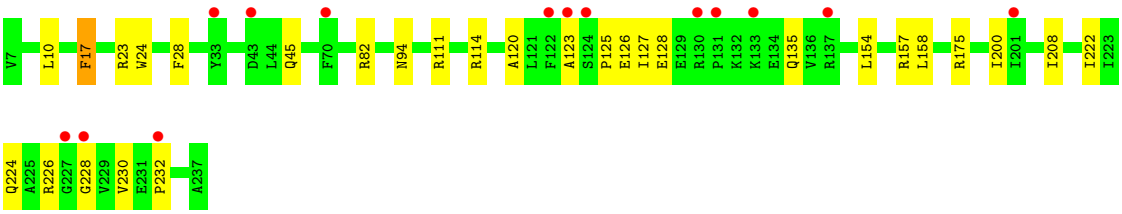
• Molecule 34: 30S ribosomal protein S2

Chain 1b:



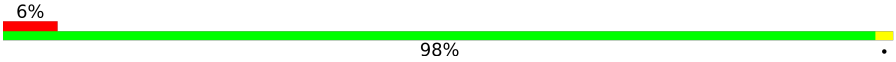
• Molecule 34: 30S ribosomal protein S2

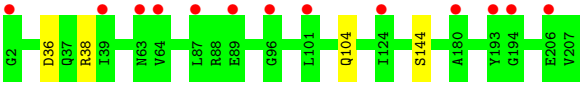
Chain 2b:



• Molecule 35: 30S ribosomal protein S3

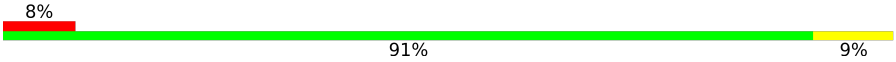
Chain 1c:

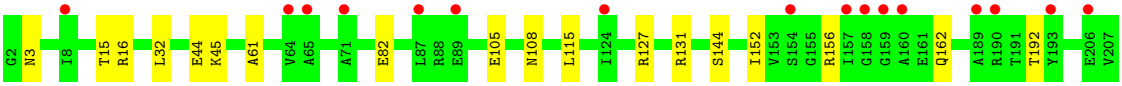




• Molecule 35: 30S ribosomal protein S3

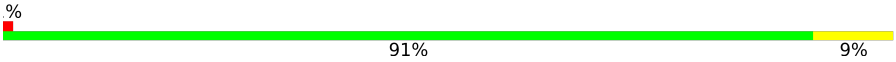
Chain 2c:





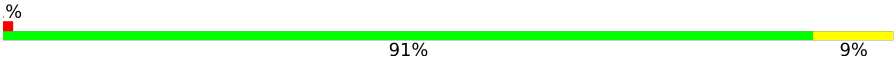
• Molecule 36: 30S ribosomal protein S4

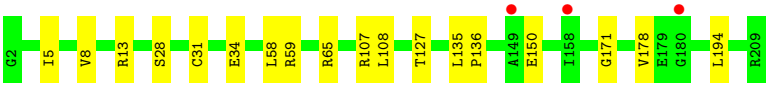
Chain 1d:



• Molecule 36: 30S ribosomal protein S4

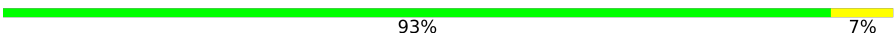
Chain 2d:





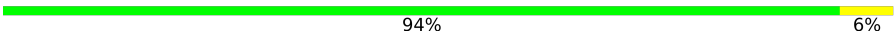
• Molecule 37: 30S ribosomal protein S5

Chain 1e:



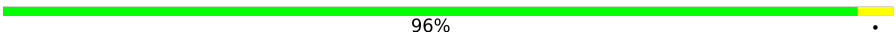
• Molecule 37: 30S ribosomal protein S5

Chain 2e:



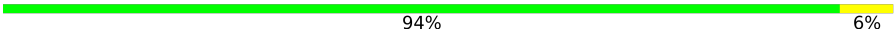
• Molecule 38: 30S ribosomal protein S6

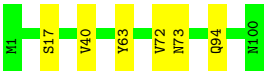
Chain 1f:



• Molecule 38: 30S ribosomal protein S6

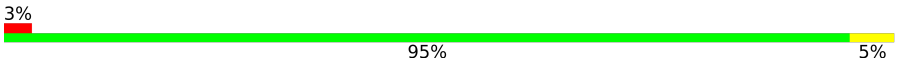
Chain 2f:

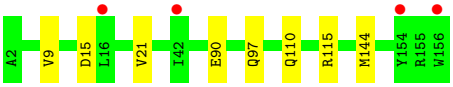




• Molecule 39: 30S ribosomal protein S7

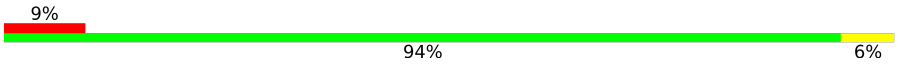
Chain 1g:

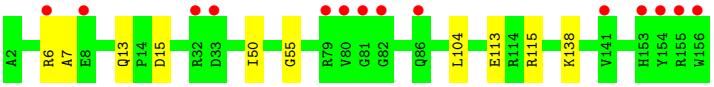




• Molecule 39: 30S ribosomal protein S7

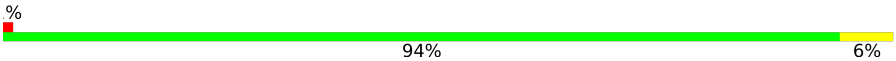
Chain 2g:

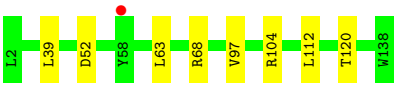




• Molecule 40: 30S ribosomal protein S8

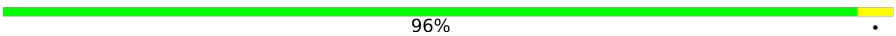
Chain 1h:





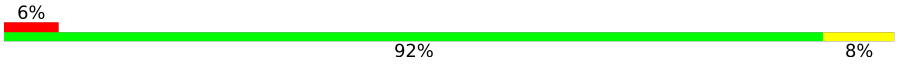
• Molecule 40: 30S ribosomal protein S8

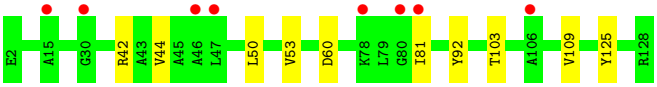
Chain 2h:



• Molecule 41: 30S ribosomal protein S9

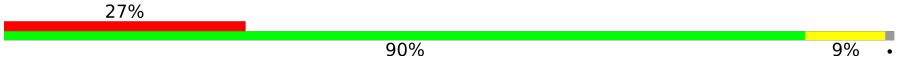
Chain 1i:

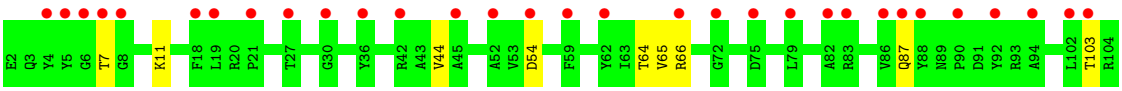


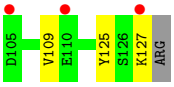


• Molecule 41: 30S ribosomal protein S9

Chain 2i:

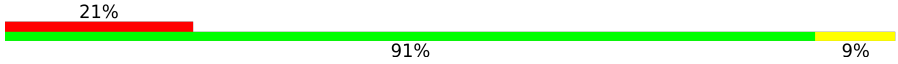






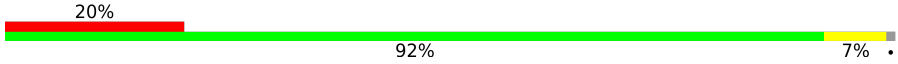
• Molecule 42: 30S ribosomal protein S10

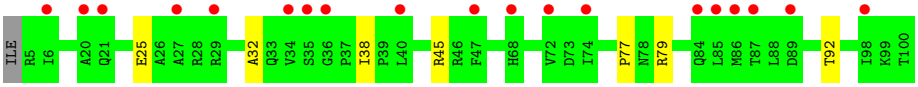
Chain 1j:



• Molecule 42: 30S ribosomal protein S10

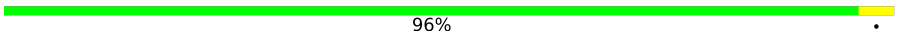
Chain 2j:

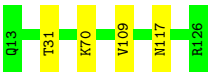




• Molecule 43: 30S ribosomal protein S11

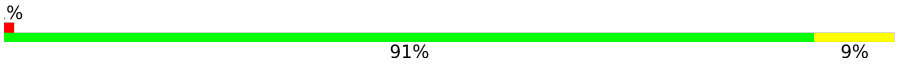
Chain 1k:

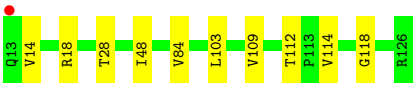




• Molecule 43: 30S ribosomal protein S11

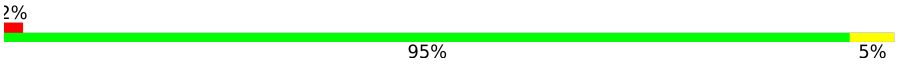
Chain 2k:

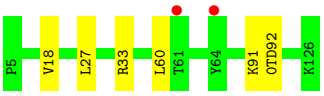




• Molecule 44: 30S ribosomal protein S12

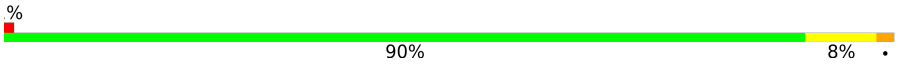
Chain 1l:

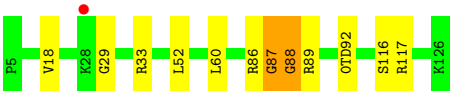




• Molecule 44: 30S ribosomal protein S12

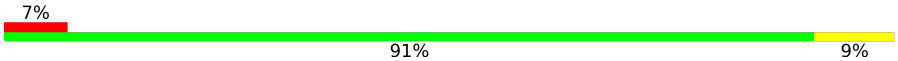
Chain 2l:





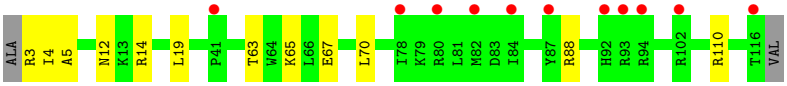
• Molecule 45: 30S ribosomal protein S13

Chain 1m:



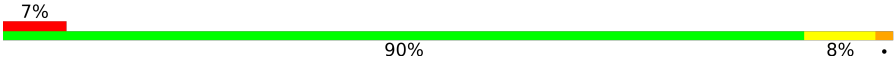
• Molecule 45: 30S ribosomal protein S13

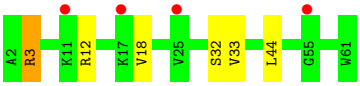
Chain 2m:



• Molecule 46: 30S ribosomal protein S14 type Z

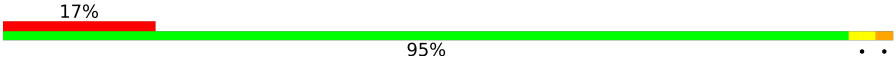
Chain 1n:

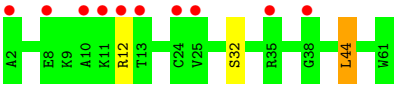




• Molecule 46: 30S ribosomal protein S14 type Z

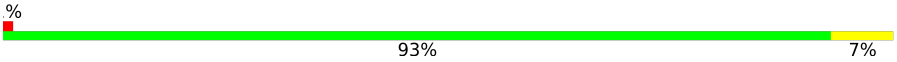
Chain 2n:

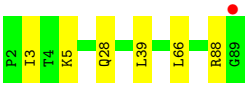




• Molecule 47: 30S ribosomal protein S15

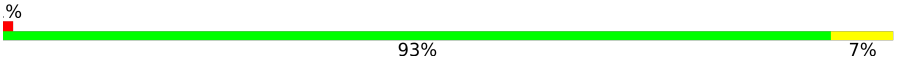
Chain 1o:





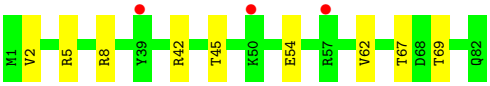
• Molecule 47: 30S ribosomal protein S15

Chain 2o:



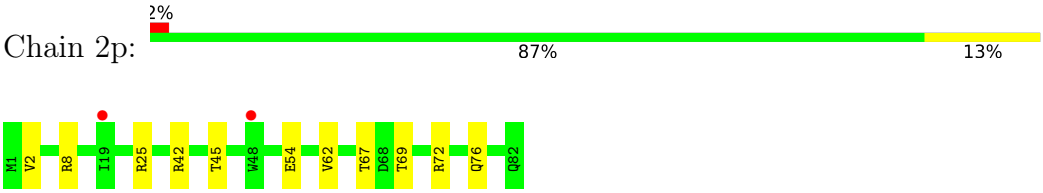
• Molecule 48: 30S ribosomal protein S16

Chain 1p:



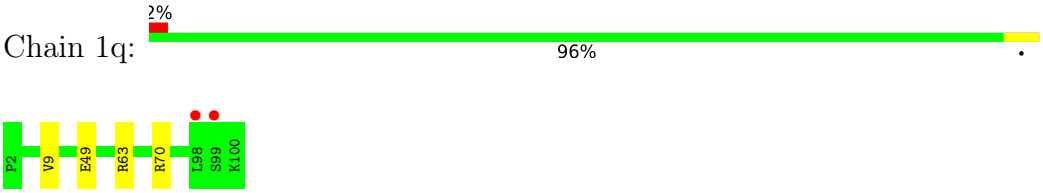
• Molecule 48: 30S ribosomal protein S16

Chain 2p:



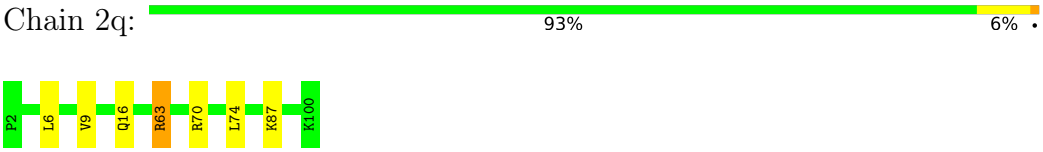
• Molecule 49: 30S ribosomal protein S17

Chain 1q:



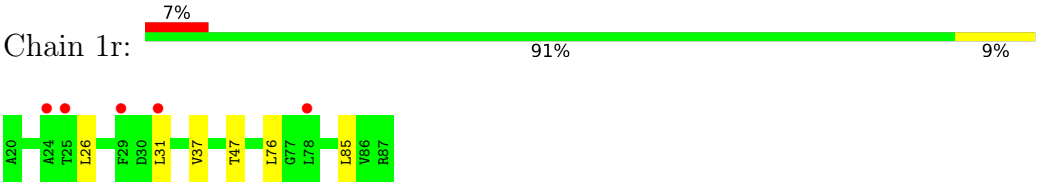
• Molecule 49: 30S ribosomal protein S17

Chain 2q:



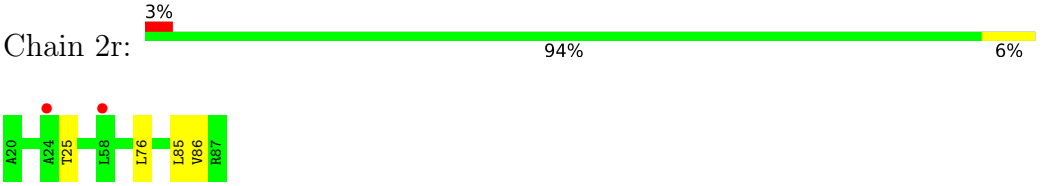
• Molecule 50: 30S ribosomal protein S18

Chain 1r:



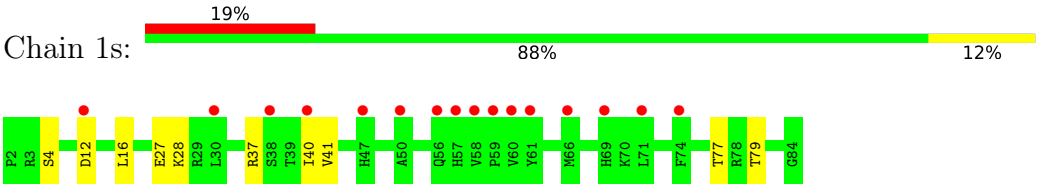
• Molecule 50: 30S ribosomal protein S18

Chain 2r:



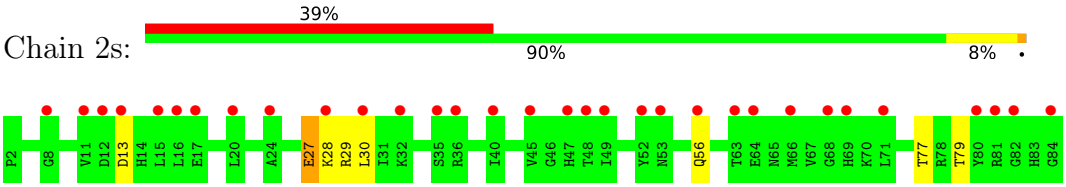
• Molecule 51: 30S ribosomal protein S19

Chain 1s:



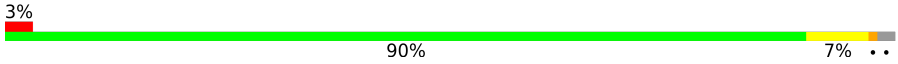
• Molecule 51: 30S ribosomal protein S19

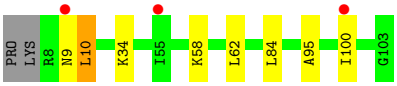
Chain 2s:



• Molecule 52: 30S ribosomal protein S20

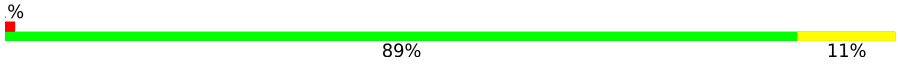
Chain 1t:

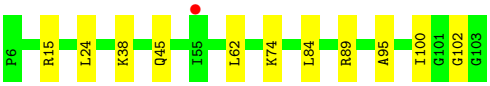




• Molecule 52: 30S ribosomal protein S20

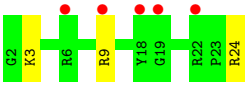
Chain 2t:





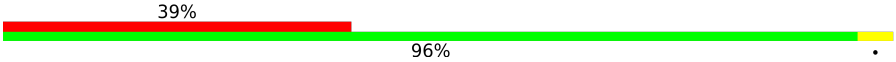
• Molecule 53: 30S ribosomal protein Thx

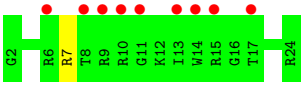
Chain 1u:



• Molecule 53: 30S ribosomal protein Thx

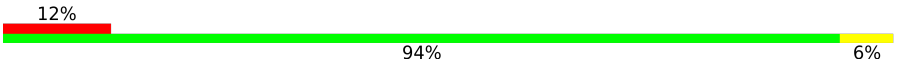
Chain 2u:

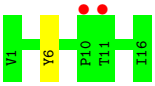




• Molecule 54: Pyrrhocoricin

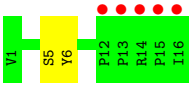
Chain 1y:





• Molecule 54: Pyrrhocoricin

Chain 2y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.94Å 450.10Å 622.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.81-2.80) 99.9 (49.81-2.59)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.189 , 0.240 0.190 , 0.240	Depositor DCC
R_{free} test set	88568 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	293583	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, MA6, PSU, OMC, M2G, UR3, 2MA, G7M, 0TD, OMU, 4OC, OMG, 5MC, ZN, 5MU, MG, SF4

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	1A	1.57	577/69022 (0.8%)	2.06	3825/107739 (3.6%)
1	2A	1.21	119/68893 (0.2%)	1.72	1783/107533 (1.7%)
2	1B	1.15	4/2879 (0.1%)	1.89	110/4490 (2.4%)
2	2B	1.02	1/2874 (0.0%)	1.58	50/4482 (1.1%)
3	1D	0.93	0/2181	1.00	4/2940 (0.1%)
3	2D	0.78	0/2186	0.87	1/2944 (0.0%)
4	1E	0.99	0/1592	1.02	3/2149 (0.1%)
4	2E	0.79	0/1592	0.91	2/2149 (0.1%)
5	1F	0.95	0/1619	0.96	4/2193 (0.2%)
5	2F	0.73	0/1615	0.85	0/2188
6	1G	0.70	0/1451	0.86	0/1961
6	2G	0.78	1/1449 (0.1%)	0.86	0/1957
7	1H	0.80	0/1356	0.89	0/1834
7	2H	0.77	0/1350	0.85	0/1826
8	1I	0.77	2/1109 (0.2%)	0.92	2/1512 (0.1%)
8	2I	0.67	0/1091	0.87	2/1490 (0.1%)
9	1N	0.93	1/1148 (0.1%)	0.97	3/1547 (0.2%)
9	2N	0.64	0/1144	0.83	0/1543
10	1O	1.02	0/943	1.00	2/1269 (0.2%)
10	2O	0.81	0/943	0.86	1/1269 (0.1%)
11	1P	0.89	0/1152	0.96	2/1533 (0.1%)
11	2P	0.68	0/1152	0.83	0/1533
12	1Q	0.94	0/1143	0.94	0/1527
12	2Q	0.68	0/1143	0.83	0/1527
13	1R	0.94	0/982	1.08	7/1312 (0.5%)
13	2R	0.70	0/982	0.90	1/1312 (0.1%)
14	1S	0.79	1/887 (0.1%)	0.98	2/1180 (0.2%)
14	2S	0.68	0/880	0.85	0/1172
15	1T	0.88	1/1105 (0.1%)	1.06	4/1477 (0.3%)
15	2T	0.73	0/1097	0.91	2/1468 (0.1%)
16	1U	1.08	2/977 (0.2%)	1.05	7/1301 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.73	0/977	0.83	0/1301
17	1V	0.94	0/786	0.98	2/1053 (0.2%)
17	2V	0.67	0/782	0.84	0/1049
18	1W	1.04	0/897	1.02	4/1205 (0.3%)
18	2W	0.83	0/897	0.84	1/1205 (0.1%)
19	1X	0.95	0/764	0.96	1/1025 (0.1%)
19	2X	0.76	0/764	0.86	2/1025 (0.2%)
20	1Y	0.86	0/823	0.96	1/1099 (0.1%)
20	2Y	0.79	0/823	0.92	0/1100
21	1Z	0.73	0/1620	0.83	1/2200 (0.0%)
21	2Z	0.70	0/1590	0.84	1/2162 (0.0%)
22	10	0.88	0/616	0.94	0/821
22	20	0.68	0/616	0.86	0/821
23	11	1.01	1/761 (0.1%)	0.96	1/1013 (0.1%)
23	21	0.79	0/766	0.92	2/1018 (0.2%)
24	12	0.87	0/590	0.94	0/781
24	22	0.77	0/594	0.81	0/785
25	13	0.92	0/474	0.94	0/635
25	23	0.62	0/469	0.80	1/630 (0.2%)
26	14	0.89	0/559	0.89	0/754
26	24	1.06	0/549	0.97	0/741
27	15	1.08	3/473 (0.6%)	1.07	6/639 (0.9%)
27	25	0.83	0/469	0.97	2/635 (0.3%)
28	16	0.98	2/460 (0.4%)	1.04	1/613 (0.2%)
28	26	0.68	0/456	0.80	0/608
29	17	1.08	0/426	1.08	1/561 (0.2%)
29	27	0.81	0/426	0.88	0/561
30	18	0.96	1/525 (0.2%)	0.95	2/691 (0.3%)
30	28	0.72	0/525	0.79	0/691
31	19	0.96	1/310 (0.3%)	1.09	2/407 (0.5%)
31	29	0.70	0/310	0.79	0/407
32	1a	1.14	55/35795 (0.2%)	1.70	881/55864 (1.6%)
32	2a	1.10	48/35890 (0.1%)	1.65	737/56012 (1.3%)
33	1x	0.66	0/776	0.79	0/1048
33	2x	0.72	0/761	0.79	0/1030
34	1b	0.77	0/1876	0.93	3/2533 (0.1%)
34	2b	0.78	0/1860	0.89	0/2518
35	1c	0.72	0/1582	0.80	0/2137
35	2c	0.81	0/1566	0.81	0/2119
36	1d	0.71	0/1695	0.84	0/2274
36	2d	0.70	0/1698	0.85	0/2277
37	1e	0.66	0/1149	0.88	0/1548
37	2e	0.68	0/1149	0.87	0/1548

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1f	0.72	0/827	0.81	0/1120
38	2f	0.70	0/829	0.84	0/1123
39	1g	0.71	1/1254 (0.1%)	0.77	0/1683
39	2g	0.73	0/1248	0.76	0/1676
40	1h	0.67	0/1118	0.83	0/1506
40	2h	0.61	0/1108	0.83	0/1494
41	1i	0.77	0/1005	0.82	0/1351
41	2i	0.84	0/985	0.88	0/1329
42	1j	0.79	0/732	0.84	0/993
42	2j	0.81	0/723	0.76	0/984
43	1k	0.73	0/849	0.85	0/1150
43	2k	0.67	0/848	0.86	1/1149 (0.1%)
44	1l	0.69	0/937	0.83	0/1260
44	2l	0.68	0/937	0.95	3/1260 (0.2%)
45	1m	0.68	0/924	0.83	0/1242
45	2m	0.76	0/905	0.82	0/1217
46	1n	0.74	0/501	0.93	2/664 (0.3%)
46	2n	0.75	0/501	0.82	1/664 (0.2%)
47	1o	0.72	0/739	0.86	0/985
47	2o	0.65	0/739	0.79	0/985
48	1p	0.69	0/697	0.85	0/939
48	2p	0.70	0/693	0.90	0/935
49	1q	0.73	0/836	0.86	0/1117
49	2q	0.67	0/836	0.85	1/1117 (0.1%)
50	1r	0.70	0/560	0.87	1/746 (0.1%)
50	2r	0.70	0/560	0.81	0/746
51	1s	0.73	0/663	0.81	0/895
51	2s	0.81	0/660	0.79	1/893 (0.1%)
52	1t	0.68	0/734	0.86	0/969
52	2t	0.64	0/736	0.85	0/976
53	1u	0.69	0/203	0.83	0/266
53	2u	0.73	0/203	0.87	0/266
54	1y	0.83	0/125	0.82	0/173
54	2y	0.69	0/125	0.74	0/173
All	All	1.17	821/310171 (0.3%)	1.62	7479/463547 (1.6%)

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
19	1X	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
30	18	0	1
44	2l	0	1
All	All	0	4

All (821) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2026	G	N7-C5	-11.28	1.32	1.39
1	1A	2040	G	P-OP2	-11.24	1.29	1.49
1	1A	354	A	N9-C4	-10.67	1.31	1.37
1	1A	1814	A	N3-C4	-10.29	1.28	1.34
1	2A	1046	A	N9-C4	9.81	1.43	1.37
1	1A	2040	G	P-OP1	-9.48	1.32	1.49
32	2a	1034	G	C6-N1	9.40	1.46	1.39
28	16	13	CYS	CB-SG	9.24	1.98	1.82
32	2a	343	U	C2-N3	-9.16	1.31	1.37
1	1A	1820	A	N9-C4	-9.09	1.32	1.37
1	1A	854	U	C2-N3	8.70	1.43	1.37
1	1A	782	A	N3-C4	-8.47	1.29	1.34
1	1A	572	A	N9-C4	8.29	1.42	1.37
1	1A	1994	A	N9-C4	-8.23	1.32	1.37
1	1A	2042	A	C6-N6	-8.23	1.27	1.33
1	1A	2803	A	N9-C4	8.22	1.42	1.37
1	1A	1092	A	N9-C4	8.18	1.42	1.37
32	1a	1493	A	N9-C4	8.12	1.42	1.37
32	2a	1003	G	N9-C4	8.09	1.44	1.38
1	1A	1132	A	N9-C4	8.05	1.42	1.37
1	1A	492	A	C6-N6	-8.03	1.27	1.33
1	1A	835	A	N7-C5	-8.01	1.34	1.39
1	1A	1144	A	N9-C4	7.92	1.42	1.37
1	1A	1280	U	C2-N3	-7.87	1.32	1.37
1	1A	13	A	N7-C5	-7.86	1.34	1.39
1	1A	1272	A	N9-C4	-7.83	1.33	1.37
32	1a	250	A	N9-C4	7.71	1.42	1.37
1	1A	251	A	N9-C4	-7.70	1.33	1.37
1	1A	609	A	N3-C4	-7.62	1.30	1.34
1	1A	2803	A	N3-C4	7.56	1.39	1.34
1	1A	813	C	N1-C6	-7.56	1.32	1.37
1	1A	986	A	N7-C5	-7.55	1.34	1.39
28	16	16	CYS	CB-SG	-7.53	1.69	1.82
1	1A	1222	A	N9-C4	7.52	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2612	A	C6-N1	-7.50	1.30	1.35
1	1A	2272	C	N3-C4	-7.46	1.28	1.33
32	1a	163	C	N1-C6	7.43	1.41	1.37
1	1A	1846	A	N3-C4	-7.42	1.30	1.34
1	1A	886	U	C4-O4	-7.41	1.17	1.23
1	1A	2697	G	C6-N1	-7.41	1.34	1.39
1	1A	2331	G	N9-C4	-7.41	1.32	1.38
1	1A	731	G	C6-N1	-7.36	1.34	1.39
1	1A	537	G	C5-C4	-7.36	1.33	1.38
1	1A	716	G	C2-N3	-7.34	1.26	1.32
1	1A	1283	A	N3-C4	-7.34	1.30	1.34
1	1A	1795	G	N7-C5	-7.34	1.34	1.39
1	1A	409	G	C6-N1	-7.33	1.34	1.39
1	1A	752	A	C5-C6	-7.27	1.34	1.41
32	1a	161	A	N9-C4	7.25	1.42	1.37
32	2a	1034	G	N9-C4	7.25	1.43	1.38
1	1A	2778	A	N7-C5	-7.24	1.34	1.39
1	1A	1001	G	C6-N1	-7.23	1.34	1.39
1	2A	2805	G	N9-C4	7.23	1.43	1.38
1	1A	36	G	N7-C5	-7.22	1.34	1.39
1	1A	700	A	N3-C4	7.20	1.39	1.34
32	1a	1003	G	N9-C4	7.19	1.43	1.38
32	2a	1279	A	N9-C4	7.18	1.42	1.37
1	1A	989	G	C6-N1	-7.16	1.34	1.39
2	1B	1	U	C2-N3	7.16	1.42	1.37
1	1A	2454	C	N1-C2	-7.10	1.33	1.40
1	1A	827	G	N9-C8	-7.10	1.32	1.37
1	2A	2117	A	N9-C4	7.09	1.42	1.37
1	1A	476	G	C6-O6	-7.09	1.17	1.24
1	1A	2040	G	P-O5'	-7.08	1.52	1.59
1	1A	178	G	N7-C5	-7.03	1.35	1.39
1	1A	2630	G	N7-C5	-7.02	1.35	1.39
1	1A	724	A	C6-N1	-7.01	1.30	1.35
1	1A	1679	A	N7-C5	-6.99	1.35	1.39
1	1A	1377	A	N3-C4	-6.98	1.30	1.34
1	1A	2082	A	N9-C4	-6.97	1.33	1.37
1	1A	101	A	C6-N6	6.97	1.39	1.33
1	1A	2039	U	O3'-P	-6.96	1.52	1.61
1	1A	2633	A	C5-C6	-6.96	1.34	1.41
1	1A	1833	A	C5-C6	-6.94	1.34	1.41
1	2A	1091	G	N9-C4	6.94	1.43	1.38
1	1A	2331	G	N3-C4	-6.93	1.30	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1113	A	N9-C4	6.92	1.42	1.37
1	2A	529	A	N9-C4	-6.91	1.33	1.37
1	1A	1741	C	N1-C6	-6.91	1.33	1.37
1	1A	670	C	N1-C6	6.90	1.41	1.37
1	1A	1067	A	N3-C4	-6.89	1.30	1.34
2	1B	75	G	N1-C2	6.85	1.43	1.37
1	1A	2600	G	C6-N1	-6.85	1.34	1.39
1	1A	218	A	N9-C4	6.83	1.42	1.37
1	1A	776	G	N3-C4	-6.81	1.30	1.35
1	1A	199	C	C2-N3	-6.80	1.30	1.35
1	1A	554	A	C6-N1	6.80	1.40	1.35
1	1A	2600	G	N3-C4	-6.78	1.30	1.35
1	1A	1834	A	N3-C4	-6.78	1.30	1.34
32	1a	148	G	N9-C4	6.78	1.43	1.38
1	1A	1130	A	C5-C6	6.77	1.47	1.41
1	1A	27	G	C6-N1	-6.77	1.34	1.39
1	1A	987	G	N7-C5	-6.77	1.35	1.39
1	1A	2591	C	N1-C6	-6.76	1.33	1.37
1	1A	186	A	C2-N3	-6.75	1.27	1.33
1	1A	731	G	N1-C2	-6.74	1.32	1.37
1	1A	1312	G	N7-C5	-6.74	1.35	1.39
1	1A	476	G	N9-C8	-6.72	1.33	1.37
1	1A	2697	G	N1-C2	-6.72	1.32	1.37
1	1A	1669	G	C6-N1	-6.71	1.34	1.39
32	2a	1030(D)	A	N9-C4	6.71	1.41	1.37
1	1A	2883	A	C6-N1	-6.71	1.30	1.35
32	2a	1034	G	C2-N3	6.70	1.38	1.32
1	1A	720	C	N3-C4	6.70	1.38	1.33
1	1A	1313	U	P-OP1	-6.70	1.37	1.49
1	1A	1822	A	N3-C4	-6.69	1.30	1.34
1	1A	2069	U	C4-O4	-6.68	1.18	1.23
1	1A	2106	C	N3-C4	-6.68	1.29	1.33
1	1A	2442	A	N9-C4	-6.67	1.33	1.37
1	1A	2251	G	N1-C2	-6.67	1.32	1.37
1	1A	1422	C	N3-C4	-6.65	1.29	1.33
1	1A	840	A	C5-C6	-6.62	1.35	1.41
1	2A	2805	G	N3-C4	6.62	1.40	1.35
1	1A	2658	C	N3-C4	-6.61	1.29	1.33
1	1A	2035	A	N7-C5	-6.61	1.35	1.39
1	1A	722	A	C5-C6	-6.60	1.35	1.41
1	2A	2030	A	N9-C4	-6.59	1.33	1.37
1	1A	1672	G	C6-N1	-6.58	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	848	G	C6-N1	-6.58	1.34	1.39
1	1A	835	A	N9-C8	-6.57	1.32	1.37
1	1A	717	A	N7-C5	-6.54	1.35	1.39
32	2a	1026	G	N9-C8	6.53	1.42	1.37
1	1A	823	G	C6-N1	-6.53	1.34	1.39
1	2A	1533	G	C5-C4	6.52	1.43	1.38
1	2A	1054	A	N9-C4	6.52	1.41	1.37
1	1A	1305	G	C6-N1	-6.51	1.34	1.39
1	1A	2460	A	C5-C4	-6.51	1.34	1.38
1	1A	1259	A	N9-C8	-6.49	1.32	1.37
1	1A	1135	G	N9-C4	6.49	1.43	1.38
1	1A	1130	A	N7-C5	6.48	1.43	1.39
32	2a	1436	U	C2-N3	6.48	1.42	1.37
1	1A	2006	G	C6-N1	-6.47	1.35	1.39
1	1A	1175	A	C6-N1	-6.46	1.31	1.35
1	1A	2510	C	N3-C4	-6.46	1.29	1.33
1	1A	1271	G	N3-C4	-6.46	1.30	1.35
1	1A	354	A	C5-C6	-6.45	1.35	1.41
32	2a	1034	G	N3-C4	6.44	1.40	1.35
1	1A	1405	A	N7-C5	6.43	1.43	1.39
1	1A	1822	A	N9-C4	-6.43	1.33	1.37
1	1A	1298	G	N9-C4	-6.42	1.32	1.38
1	1A	1113	A	N3-C4	6.41	1.38	1.34
1	1A	1838	G	N9-C4	-6.41	1.32	1.38
1	1A	1010	C	N3-C4	-6.40	1.29	1.33
1	1A	2260	C	C4-N4	-6.40	1.28	1.33
1	2A	1378	A	N9-C4	-6.39	1.34	1.37
1	1A	164	G	C2-N3	6.38	1.37	1.32
1	1A	1394	G	N9-C8	-6.38	1.33	1.37
1	1A	2261	U	C4-O4	-6.38	1.18	1.23
1	1A	1690	G	N3-C4	-6.38	1.30	1.35
1	1A	2777	A	N9-C4	-6.38	1.34	1.37
1	1A	742	G	N1-C2	-6.37	1.32	1.37
1	1A	1727	U	C4-O4	-6.34	1.18	1.23
32	1a	1492	A	N9-C4	6.34	1.41	1.37
1	1A	1822	A	C6-N1	-6.34	1.31	1.35
1	1A	2376	C	N1-C6	-6.33	1.33	1.37
1	1A	125	A	C6-N6	-6.32	1.28	1.33
32	1a	1493	A	N3-C4	6.32	1.38	1.34
2	2B	1	U	N1-C2	6.31	1.44	1.38
1	1A	557	A	C6-N1	-6.30	1.31	1.35
1	2A	1721	G	N3-C4	6.28	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	859	C	C4-N4	-6.28	1.28	1.33
1	1A	1091	A	C5-C6	6.27	1.46	1.41
1	2A	2897	U	C2-N3	6.27	1.42	1.37
1	2A	2775	A	N9-C4	-6.27	1.34	1.37
1	1A	1117	G	N9-C4	6.26	1.43	1.38
1	1A	1102	G	N3-C4	6.26	1.39	1.35
1	1A	1660	A	N7-C5	-6.26	1.35	1.39
1	1A	474	U	C4-O4	-6.26	1.18	1.23
1	1A	2033	U	C2-O2	-6.25	1.16	1.22
1	1A	1829	U	C4-O4	-6.25	1.18	1.23
1	1A	2034	G	C6-N1	-6.25	1.35	1.39
32	1a	1286	A	N9-C4	6.25	1.41	1.37
32	1a	1034	G	C6-N1	6.25	1.44	1.39
1	2A	1913	A	N9-C4	6.25	1.41	1.37
1	1A	839	G	C6-N1	-6.25	1.35	1.39
32	1a	204	U	N1-C2	6.24	1.44	1.38
1	2A	1070	A	N9-C4	6.23	1.41	1.37
1	1A	1701	A	C8-N7	-6.22	1.27	1.31
1	1A	2451	A	N7-C5	-6.22	1.35	1.39
1	1A	555	G	N1-C2	-6.22	1.32	1.37
1	2A	645	C	N1-C6	6.22	1.40	1.37
1	2A	1652	A	N9-C4	-6.21	1.34	1.37
1	1A	2554	A	N9-C4	-6.21	1.34	1.37
1	1A	598	A	N3-C4	-6.21	1.31	1.34
32	2a	759	A	N9-C4	-6.21	1.34	1.37
1	1A	815	G	N3-C4	-6.21	1.31	1.35
16	1U	9	VAL	CB-CG1	-6.21	1.39	1.52
1	1A	1653	C	N1-C6	-6.21	1.33	1.37
1	1A	1479	U	C4-O4	-6.20	1.18	1.23
1	2A	1345	C	N1-C6	-6.20	1.33	1.37
1	1A	2331	G	N9-C8	6.20	1.42	1.37
1	1A	731	G	C5-C4	-6.20	1.34	1.38
1	1A	2584	A	C5-C4	-6.20	1.34	1.38
1	1A	1148	C	N1-C2	6.19	1.46	1.40
1	1A	2073	A	N3-C4	-6.19	1.31	1.34
1	1A	1507	A	N3-C4	6.19	1.38	1.34
1	1A	537	G	N7-C5	-6.18	1.35	1.39
1	1A	1132	A	N3-C4	6.18	1.38	1.34
31	19	27	CYS	CB-SG	6.17	1.92	1.82
1	1A	2605	U	C2-N3	-6.17	1.33	1.37
1	2A	1963	U	N1-C2	6.17	1.44	1.38
1	1A	2187	G	N3-C4	6.17	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	827	G	N7-C5	-6.16	1.35	1.39
32	2a	1157	A	N9-C4	6.16	1.41	1.37
1	1A	2112	G	C6-N1	-6.15	1.35	1.39
1	1A	2443	U	N1-C6	-6.15	1.32	1.38
1	1A	1724	A	N3-C4	-6.14	1.31	1.34
1	1A	2134	G	N9-C4	6.13	1.42	1.38
1	2A	1794	U	C2-N3	-6.13	1.33	1.37
32	2a	1026	G	C8-N7	6.12	1.34	1.30
1	1A	1475	G	N1-C2	-6.12	1.32	1.37
1	1A	2453	C	N1-C6	-6.12	1.33	1.37
1	1A	1076	G	N7-C5	-6.11	1.35	1.39
1	1A	1658	C	N1-C6	-6.11	1.33	1.37
1	1A	1705	C	N1-C6	6.11	1.40	1.37
1	1A	2625	U	C2-N3	-6.11	1.33	1.37
32	1a	1044	A	N9-C4	6.10	1.41	1.37
1	1A	2280	A	N7-C5	-6.09	1.35	1.39
1	1A	2612	A	N3-C4	-6.08	1.31	1.34
1	1A	1718	U	C4-O4	-6.07	1.18	1.23
1	2A	1082	U	N1-C2	6.07	1.44	1.38
1	1A	1293	A	C6-N6	-6.06	1.29	1.33
1	1A	1356	G	N1-C2	-6.06	1.32	1.37
1	1A	2093	A	C5-C4	-6.06	1.34	1.38
1	1A	2294	G	C6-N1	-6.05	1.35	1.39
1	1A	878	G	C8-N7	-6.05	1.27	1.30
16	1U	15	LYS	CE-NZ	6.05	1.64	1.49
1	1A	1121	C	N1-C2	6.05	1.46	1.40
1	1A	1235	G	N7-C5	-6.04	1.35	1.39
1	1A	724	A	N7-C5	-6.03	1.35	1.39
1	1A	2836	A	C5-C6	-6.03	1.35	1.41
1	1A	1015	C	N3-C4	-6.03	1.29	1.33
1	1A	1026	A	N9-C4	-6.03	1.34	1.37
1	1A	2634	C	C4-N4	-6.02	1.28	1.33
1	1A	1304	C	N3-C4	-6.02	1.29	1.33
1	2A	2244	U	C2-N3	-6.01	1.33	1.37
1	1A	1711	A	N7-C5	-6.00	1.35	1.39
32	1a	1436	U	C2-N3	6.00	1.42	1.37
1	1A	1700	G	C6-N1	-6.00	1.35	1.39
1	1A	2024	G	C8-N7	-6.00	1.27	1.30
1	1A	729	G	C6-N1	-5.99	1.35	1.39
1	1A	1666	G	C6-N1	-5.99	1.35	1.39
1	1A	1221	G	N7-C5	5.99	1.42	1.39
1	1A	2828	G	C6-N1	-5.99	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2441	G	N7-C5	-5.98	1.35	1.39
1	1A	553	A	N9-C4	5.98	1.41	1.37
1	1A	554	A	C2-N3	5.98	1.39	1.33
1	1A	832	G	N9-C4	-5.97	1.33	1.38
1	1A	2775	G	C5-C4	-5.97	1.34	1.38
1	1A	2075	G	N7-C5	-5.97	1.35	1.39
1	1A	2738	A	N9-C4	-5.97	1.34	1.37
1	2A	792	G	N1-C2	-5.97	1.32	1.37
1	1A	2467	G	C2-N2	-5.96	1.28	1.34
1	1A	2517	G	C2-N3	-5.95	1.27	1.32
1	1A	1282	G	C5-C4	-5.95	1.34	1.38
1	1A	180	A	N9-C8	-5.94	1.32	1.37
1	2A	1721	G	C2-N3	5.94	1.37	1.32
1	2A	2153	G	C5-C4	5.94	1.42	1.38
1	1A	1853	G	C6-N1	-5.94	1.35	1.39
32	1a	1030(A)	G	N9-C4	5.93	1.42	1.38
1	1A	1690	G	C5-C4	-5.93	1.34	1.38
1	1A	833	C	N3-C4	-5.93	1.29	1.33
1	1A	876	A	N7-C5	-5.92	1.35	1.39
1	1A	2466	G	N7-C5	-5.92	1.35	1.39
8	1I	10	GLU	CB-CG	5.92	1.63	1.52
1	1A	2530	A	N7-C5	-5.92	1.35	1.39
1	1A	1368	A	N7-C5	-5.92	1.35	1.39
1	1A	1080	G	C5-C4	-5.91	1.34	1.38
1	1A	1109	G	N3-C4	5.91	1.39	1.35
1	1A	2342	G	C8-N7	5.91	1.34	1.30
6	2G	167	GLU	CG-CD	5.91	1.60	1.51
1	2A	570	G	C6-O6	-5.90	1.18	1.24
1	1A	2405	A	N7-C5	-5.90	1.35	1.39
1	1A	417	A	N9-C4	-5.90	1.34	1.37
1	1A	2611	G	N3-C4	-5.90	1.31	1.35
1	1A	2442	A	C8-N7	-5.90	1.27	1.31
1	1A	2006	G	C2-N3	-5.89	1.28	1.32
1	1A	952	G	C8-N7	5.89	1.34	1.30
1	1A	962	G	N7-C5	-5.89	1.35	1.39
1	1A	1014	U	C4-O4	-5.88	1.19	1.23
1	1A	1035	G	C5-C4	-5.88	1.34	1.38
1	1A	1299	A	C5-C4	-5.87	1.34	1.38
1	1A	2600	G	C5-C4	-5.86	1.34	1.38
1	1A	2358	A	N7-C5	-5.86	1.35	1.39
1	1A	2037	A	C8-N7	-5.85	1.27	1.31
1	1A	798	A	N7-C5	-5.85	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2506	G	C2-N3	-5.85	1.28	1.32
27	15	6	VAL	CB-CG2	-5.85	1.40	1.52
32	2a	1370	G	N3-C4	5.85	1.39	1.35
1	1A	2014	G	C5-C4	-5.85	1.34	1.38
1	1A	2780	C	N3-C4	-5.85	1.29	1.33
32	1a	1030(A)	G	C5-C4	5.84	1.42	1.38
32	1a	1030(A)	G	N3-C4	5.84	1.39	1.35
32	2a	404	U	N1-C2	5.84	1.43	1.38
1	1A	2251	G	C6-N1	-5.83	1.35	1.39
1	1A	2003	A	C6-N6	-5.83	1.29	1.33
1	2A	2578	G	N3-C4	-5.83	1.31	1.35
1	1A	709	G	N9-C8	-5.82	1.33	1.37
1	1A	2093	A	N7-C5	-5.82	1.35	1.39
1	1A	2451	A	C8-N7	-5.82	1.27	1.31
1	1A	1221	G	C6-N1	5.81	1.43	1.39
1	2A	2113	U	C2-N3	5.81	1.41	1.37
1	1A	2030	C	C2-O2	-5.81	1.19	1.24
1	2A	2805	G	C2-N3	5.81	1.37	1.32
1	1A	1417	G	N7-C5	-5.81	1.35	1.39
32	2a	1447	A	N9-C4	5.81	1.41	1.37
1	2A	1051	G	C6-N1	5.80	1.43	1.39
1	1A	2491	G	N7-C5	-5.80	1.35	1.39
1	1A	1411	A	N9-C8	-5.80	1.33	1.37
1	1A	2037	A	N9-C4	-5.80	1.34	1.37
1	1A	829	A	C5-C4	-5.79	1.34	1.38
1	1A	174	U	C2-O2	-5.79	1.17	1.22
1	2A	2821	A	N9-C4	-5.79	1.34	1.37
32	2a	1134	G	N9-C4	5.79	1.42	1.38
1	1A	515	G	N3-C4	-5.79	1.31	1.35
1	2A	652(B)	A	N9-C4	5.79	1.41	1.37
1	1A	1394	G	C5-C4	-5.79	1.34	1.38
1	1A	25	U	C4-C5	-5.79	1.38	1.43
1	1A	2004	C	N3-C4	-5.78	1.29	1.33
1	1A	1840	A	C6-N6	-5.78	1.29	1.33
1	1A	833	C	C4-N4	-5.77	1.28	1.33
1	1A	1301	U	C2-O2	-5.77	1.17	1.22
1	1A	1133	G	N3-C4	5.76	1.39	1.35
1	1A	1413	A	N7-C5	-5.76	1.35	1.39
1	1A	2828	G	N9-C8	-5.76	1.33	1.37
30	18	56	GLU	CG-CD	5.76	1.60	1.51
1	1A	731	G	C6-O6	-5.76	1.19	1.24
1	1A	800	C	N3-C4	-5.76	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	575	G	C6-N1	-5.75	1.35	1.39
1	1A	2187	G	N9-C4	5.75	1.42	1.38
32	1a	1024	G	N3-C4	5.75	1.39	1.35
1	1A	185	A	N3-C4	-5.75	1.31	1.34
1	1A	811	A	N3-C4	-5.75	1.31	1.34
1	2A	1041	C	N1-C6	5.75	1.40	1.37
32	1a	1035	A	N9-C4	5.75	1.41	1.37
1	2A	673	C	C2-N3	5.75	1.40	1.35
1	2A	2009	G	N3-C4	-5.75	1.31	1.35
1	1A	1829	U	C2-N3	-5.74	1.33	1.37
1	1A	495	G	N9-C8	-5.74	1.33	1.37
1	2A	1508	A	N3-C4	5.74	1.38	1.34
1	1A	239	G	N3-C4	-5.73	1.31	1.35
32	2a	791	G	N9-C4	-5.73	1.33	1.38
1	1A	505	A	N3-C4	-5.73	1.31	1.34
32	2a	848	C	N1-C6	5.73	1.40	1.37
1	1A	1394	G	N1-C2	-5.72	1.33	1.37
1	2A	776	G	N7-C5	-5.72	1.35	1.39
1	1A	354	A	N9-C8	5.71	1.42	1.37
1	1A	1427	G	N1-C2	-5.71	1.33	1.37
1	1A	2440	G	N7-C5	-5.71	1.35	1.39
1	1A	1149	A	N9-C4	5.71	1.41	1.37
1	1A	1720	U	N1-C2	-5.71	1.33	1.38
1	1A	645	G	N9-C8	-5.71	1.33	1.37
1	1A	986	A	N9-C4	-5.71	1.34	1.37
39	1g	90	GLU	CG-CD	5.71	1.60	1.51
1	1A	747	G	N9-C8	-5.71	1.33	1.37
1	1A	1537	G	N9-C8	-5.70	1.33	1.37
1	1A	836	A	N7-C5	-5.70	1.35	1.39
1	1A	1296	G	N1-C2	-5.70	1.33	1.37
1	1A	1248	G	N7-C5	-5.69	1.35	1.39
1	1A	225	C	C2-O2	-5.69	1.19	1.24
1	1A	460	C	N3-C4	-5.69	1.29	1.33
1	1A	2171	G	N7-C5	5.69	1.42	1.39
1	1A	713	G	C5-C4	-5.68	1.34	1.38
1	1A	2076	A	N7-C5	-5.68	1.35	1.39
32	2a	530	G	C2-N3	5.68	1.37	1.32
1	1A	2134	G	N3-C4	5.68	1.39	1.35
1	1A	1307	C	C4-N4	-5.68	1.28	1.33
1	1A	2187	G	N7-C5	5.68	1.42	1.39
1	1A	609	A	N9-C4	-5.68	1.34	1.37
1	1A	2134	G	C2-N3	5.68	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2579	G	N3-C4	-5.68	1.31	1.35
1	1A	473	A	N3-C4	-5.67	1.31	1.34
1	2A	2140	C	N1-C6	5.67	1.40	1.37
1	1A	218	A	C5-C4	5.67	1.42	1.38
32	2a	190	U	C2-N3	5.67	1.41	1.37
23	11	33	LYS	CE-NZ	5.67	1.63	1.49
1	1A	2638	C	C4-N4	-5.66	1.28	1.33
1	2A	741	G	N3-C4	-5.66	1.31	1.35
1	1A	2555	G	C6-N1	-5.65	1.35	1.39
1	1A	2579	G	C5-C4	-5.65	1.34	1.38
1	1A	2735	G	N3-C4	5.65	1.39	1.35
32	1a	821	G	N7-C5	-5.65	1.35	1.39
1	1A	2586	G	N1-C2	-5.65	1.33	1.37
1	2A	2160	G	C5-C4	5.65	1.42	1.38
1	1A	1807	G	C6-N1	-5.64	1.35	1.39
1	1A	2582	G	N9-C4	-5.64	1.33	1.38
1	2A	2119	A	N9-C4	5.64	1.41	1.37
1	1A	1600	A	N7-C5	-5.64	1.35	1.39
1	2A	2160	G	N9-C4	5.64	1.42	1.38
1	1A	1809	U	C4-O4	-5.64	1.19	1.23
32	1a	965	A	N9-C4	-5.63	1.34	1.37
32	1a	1030(D)	A	N9-C4	5.63	1.41	1.37
1	1A	2652	G	N3-C4	-5.63	1.31	1.35
1	1A	2443	U	N3-C4	-5.62	1.33	1.38
1	1A	1665	G	N9-C8	-5.62	1.33	1.37
1	1A	716	G	N1-C2	-5.62	1.33	1.37
1	1A	2191	A	N7-C5	5.62	1.42	1.39
1	1A	2587	C	C4-N4	-5.62	1.28	1.33
1	1A	700	A	N9-C4	5.61	1.41	1.37
1	1A	2102	G	N9-C8	-5.61	1.33	1.37
1	2A	639	U	C2-N3	-5.61	1.33	1.37
1	1A	2636	G	C2-N3	5.61	1.37	1.32
8	1I	10	GLU	CG-CD	5.61	1.60	1.51
1	1A	1395	A	N3-C4	5.61	1.38	1.34
1	1A	218	A	N3-C4	5.61	1.38	1.34
1	1A	932	C	N1-C6	5.61	1.40	1.37
1	1A	1375	U	C2-O2	-5.60	1.17	1.22
1	1A	561	A	N3-C4	-5.60	1.31	1.34
1	1A	1181	G	N9-C8	-5.60	1.33	1.37
1	2A	2589	A	N9-C4	-5.60	1.34	1.37
32	1a	346	G	N9-C4	5.60	1.42	1.38
1	2A	729	G	N3-C4	-5.60	1.31	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1091	A	N3-C4	5.59	1.38	1.34
1	1A	1674	G	N7-C5	-5.59	1.35	1.39
1	1A	2752	U	N1-C6	-5.59	1.32	1.38
1	1A	1305	G	C8-N7	5.59	1.34	1.30
1	1A	2086	C	N1-C6	-5.58	1.33	1.37
1	2A	2153	G	N3-C4	5.58	1.39	1.35
32	1a	814	A	N9-C4	-5.58	1.34	1.37
1	1A	1816	A	C6-N1	-5.58	1.31	1.35
1	1A	2654	G	N1-C2	-5.58	1.33	1.37
1	1A	215	G	C2-N3	-5.57	1.28	1.32
1	1A	2261	U	C2-O2	-5.57	1.17	1.22
1	1A	839	G	N1-C2	-5.57	1.33	1.37
1	1A	1241	C	N1-C6	-5.57	1.33	1.37
1	1A	1863	C	C2-O2	-5.57	1.19	1.24
1	1A	811	A	C5-C4	-5.56	1.34	1.38
1	1A	1112	U	C2-N3	5.56	1.41	1.37
32	1a	1026	G	C5-C4	5.56	1.42	1.38
1	2A	1536	C	N3-C4	5.56	1.37	1.33
1	1A	1404	G	N7-C5	-5.55	1.35	1.39
32	2a	1405	G	N7-C5	-5.55	1.35	1.39
1	1A	1017	G	C8-N7	-5.55	1.27	1.30
1	2A	2249	U	C2-N3	-5.55	1.33	1.37
1	1A	2256	U	C2-N3	-5.54	1.33	1.37
1	1A	365	G	N1-C2	-5.54	1.33	1.37
1	1A	2426	G	N3-C4	-5.54	1.31	1.35
32	1a	346	G	N7-C5	5.54	1.42	1.39
1	2A	1274	A	N7-C5	-5.54	1.35	1.39
1	2A	1972	A	N9-C4	-5.54	1.34	1.37
32	1a	630	G	N3-C4	5.54	1.39	1.35
1	1A	1831	C	N1-C6	-5.54	1.33	1.37
1	1A	2561	G	N3-C4	-5.53	1.31	1.35
1	1A	594	A	C5-C4	-5.53	1.34	1.38
1	1A	1175	A	C6-N6	-5.53	1.29	1.33
32	2a	1029	C	N1-C6	5.53	1.40	1.37
1	1A	2446	A	N7-C5	-5.52	1.35	1.39
1	1A	2456	G	C8-N7	5.52	1.34	1.30
1	1A	109	A	C6-N6	-5.52	1.29	1.33
1	1A	2516	U	C4-O4	-5.51	1.19	1.23
32	2a	346	G	C6-N1	5.51	1.43	1.39
1	1A	607	C	C2-O2	-5.51	1.19	1.24
1	1A	556	C	P-OP2	-5.51	1.39	1.49
1	1A	860	U	C4-O4	-5.51	1.19	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	592	U	C2-O2	-5.51	1.17	1.22
1	1A	1873	G	C6-O6	-5.51	1.19	1.24
1	1A	2139	A	N9-C4	5.51	1.41	1.37
1	1A	1296	G	C6-N1	-5.50	1.35	1.39
32	1a	155	C	N1-C6	5.50	1.40	1.37
1	2A	1074	G	N7-C5	5.50	1.42	1.39
1	1A	2431	U	C2-N3	-5.50	1.33	1.37
32	2a	1026	G	C5-C4	5.50	1.42	1.38
1	1A	1441	A	C5-C6	-5.50	1.36	1.41
1	2A	1584	C	N3-C4	5.50	1.37	1.33
32	2a	1030(D)	A	C5-C4	5.50	1.42	1.38
1	1A	1786	A	N7-C5	-5.49	1.35	1.39
1	2A	1537	G	N9-C4	5.49	1.42	1.38
1	1A	2001	C	C2-O2	-5.49	1.19	1.24
1	2A	2106	G	C5-C4	5.49	1.42	1.38
1	1A	1952	G	C6-N1	-5.49	1.35	1.39
1	2A	450	G	C6-O6	-5.49	1.19	1.24
1	1A	456	A	C6-N1	-5.48	1.31	1.35
1	1A	1728	G	N3-C4	-5.48	1.31	1.35
32	2a	51	A	N7-C5	-5.48	1.35	1.39
1	1A	780	G	C6-N1	-5.47	1.35	1.39
1	2A	1086	A	N9-C4	5.47	1.41	1.37
1	1A	2448	G	C5-C4	-5.47	1.34	1.38
1	1A	694	G	C5-C4	5.47	1.42	1.38
1	1A	1092	A	N3-C4	5.47	1.38	1.34
1	1A	2738	A	N3-C4	-5.47	1.31	1.34
1	1A	1293	A	N9-C4	-5.46	1.34	1.37
1	1A	1394	G	N7-C5	-5.46	1.35	1.39
1	1A	1411	A	C8-N7	-5.46	1.27	1.31
1	1A	2157	A	N9-C4	5.46	1.41	1.37
32	1a	1003	G	C5-C4	5.46	1.42	1.38
1	1A	504	A	C6-N6	-5.46	1.29	1.33
1	1A	843	C	C2-O2	-5.46	1.19	1.24
1	1A	1427	G	C2-N3	-5.46	1.28	1.32
1	1A	1537	G	C5-C4	-5.46	1.34	1.38
1	1A	1313	U	C2-O2	-5.46	1.17	1.22
1	1A	1042	A	C5-C4	-5.45	1.34	1.38
1	2A	2106	G	N9-C4	5.45	1.42	1.38
1	1A	13	A	C8-N7	-5.45	1.27	1.31
1	1A	2082	A	C6-N1	-5.45	1.31	1.35
1	1A	934	A	N7-C5	5.45	1.42	1.39
1	1A	1661	C	C4-N4	-5.45	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	78	G	C6-N1	5.44	1.43	1.39
1	1A	215	G	N3-C4	-5.44	1.31	1.35
1	1A	1439	A	N3-C4	-5.44	1.31	1.34
1	1A	2017	U	N1-C2	-5.44	1.33	1.38
1	1A	2538	G	N9-C8	-5.44	1.34	1.37
1	2A	1359	A	N9-C4	5.44	1.41	1.37
1	1A	1012	C	C4-N4	-5.44	1.29	1.33
1	2A	2296	U	N1-C2	5.44	1.43	1.38
1	1A	2009	G	C2-N3	-5.43	1.28	1.32
1	2A	2319	G	N9-C8	5.43	1.41	1.37
1	1A	1080	G	N9-C8	-5.43	1.34	1.37
1	1A	2639	G	C5-C4	-5.43	1.34	1.38
1	1A	2057	G	N9-C4	-5.43	1.33	1.38
1	1A	237	G	N1-C2	-5.42	1.33	1.37
1	1A	2277	U	N1-C6	-5.42	1.33	1.38
1	1A	1993	A	N9-C4	-5.42	1.34	1.37
1	1A	2001	C	C4-N4	-5.42	1.29	1.33
1	1A	841	G	N9-C8	-5.42	1.34	1.37
1	1A	2601	A	N9-C4	-5.42	1.34	1.37
32	1a	346	G	C6-N1	5.42	1.43	1.39
1	1A	543	G	C8-N7	5.42	1.34	1.30
1	1A	724	A	N9-C8	-5.42	1.33	1.37
1	1A	1189	A	N3-C4	-5.41	1.31	1.34
1	1A	1507	A	N9-C4	5.41	1.41	1.37
1	1A	2639	G	N7-C5	-5.41	1.36	1.39
32	1a	1000	U	C2-N3	5.41	1.41	1.37
1	1A	2724	U	C4-C5	-5.40	1.38	1.43
1	1A	865	G	N7-C5	-5.40	1.36	1.39
1	1A	1382	A	N1-C2	-5.40	1.29	1.34
1	2A	2805	G	C5-C6	5.40	1.47	1.42
1	1A	1669	G	C5-C4	-5.40	1.34	1.38
32	1a	1134	G	C5-C4	5.39	1.42	1.38
1	1A	2883	A	C8-N7	-5.39	1.27	1.31
32	2a	1149	C	N1-C6	5.39	1.40	1.37
1	1A	1248	G	C5-C6	-5.39	1.36	1.42
1	2A	2893	G	N3-C4	5.39	1.39	1.35
32	2a	1001	A	C5-C6	5.39	1.45	1.41
1	2A	1076	C	N1-C2	5.39	1.45	1.40
32	2a	1030	C	N1-C2	5.39	1.45	1.40
1	1A	845	G	N1-C2	-5.39	1.33	1.37
1	1A	2740	G	N7-C5	-5.39	1.36	1.39
1	1A	38	A	C5-C4	-5.38	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1059	C	C4-N4	-5.38	1.29	1.33
1	1A	1119	A	N9-C4	5.38	1.41	1.37
1	1A	2454	C	C2-N3	-5.38	1.31	1.35
1	2A	1587	A	N9-C4	5.38	1.41	1.37
1	1A	2028	C	N1-C2	-5.38	1.34	1.40
1	1A	2752	U	N3-C4	-5.38	1.33	1.38
1	1A	168	G	N3-C4	-5.38	1.31	1.35
1	1A	2514	G	C6-N1	-5.38	1.35	1.39
1	1A	97	G	N7-C5	-5.38	1.36	1.39
32	1a	1257	U	N1-C2	5.37	1.43	1.38
1	2A	2450	A	N9-C4	-5.37	1.34	1.37
1	1A	1674	G	N1-C2	-5.37	1.33	1.37
1	1A	1814	A	N9-C4	-5.36	1.34	1.37
1	1A	2094	G	N7-C5	-5.36	1.36	1.39
1	2A	1846	G	N9-C4	-5.36	1.33	1.38
32	2a	1034	G	N7-C5	5.36	1.42	1.39
1	1A	2521	G	C5-C4	-5.36	1.34	1.38
1	2A	1626	G	C6-N1	-5.36	1.35	1.39
1	1A	2660	C	N1-C6	-5.35	1.33	1.37
1	1A	1752	G	C6-N1	-5.35	1.35	1.39
1	1A	2299	A	N9-C4	-5.35	1.34	1.37
1	2A	1074	G	N3-C4	5.35	1.39	1.35
32	2a	990	C	N1-C2	5.35	1.45	1.40
32	2a	1129	C	N3-C4	5.35	1.37	1.33
32	1a	1035	A	N3-C4	5.34	1.38	1.34
1	2A	2801(A)	A	N9-C4	5.34	1.41	1.37
1	1A	418	G	C5-C4	-5.33	1.34	1.38
1	1A	809	U	C4-O4	-5.33	1.19	1.23
1	1A	1232	G	C6-O6	-5.33	1.19	1.24
1	1A	2068	G	C5-C4	-5.33	1.34	1.38
1	1A	1403	U	C2-N3	-5.33	1.34	1.37
1	1A	1449	C	N1-C6	-5.33	1.33	1.37
1	1A	478	G	C5-C4	-5.33	1.34	1.38
1	1A	495	G	C2-N3	-5.32	1.28	1.32
1	1A	118	U	N1-C2	-5.32	1.33	1.38
1	1A	1707	C	N3-C4	-5.32	1.30	1.33
1	1A	1316	C	N3-C4	-5.32	1.30	1.33
1	1A	2041	A	N7-C5	-5.32	1.36	1.39
1	2A	1650	G	N1-C2	-5.32	1.33	1.37
1	1A	2179	G	C5-C6	5.32	1.47	1.42
1	1A	779	C	N3-C4	-5.31	1.30	1.33
1	1A	869	U	C2-O2	-5.31	1.17	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	840	A	C6-N1	-5.31	1.31	1.35
1	2A	1460	A	N9-C4	5.31	1.41	1.37
1	2A	2160	G	N3-C4	5.31	1.39	1.35
1	1A	1394	G	C6-N1	-5.31	1.35	1.39
27	15	59	GLU	CB-CG	5.30	1.62	1.52
32	2a	1530	G	N7-C5	5.30	1.42	1.39
1	1A	2633	A	C5-C4	-5.30	1.35	1.38
1	1A	2556	G	N3-C4	-5.30	1.31	1.35
32	1a	767	A	N9-C4	-5.29	1.34	1.37
32	1a	1003	G	N3-C4	5.29	1.39	1.35
1	1A	999	G	C6-N1	-5.29	1.35	1.39
32	2a	1014	A	N9-C4	5.28	1.41	1.37
1	1A	795	G	C6-N1	-5.28	1.35	1.39
1	2A	2129	C	N1-C6	5.27	1.40	1.37
1	1A	365	G	C6-N1	-5.27	1.35	1.39
1	1A	821	A	N1-C2	-5.27	1.29	1.34
1	1A	115	G	N9-C8	-5.27	1.34	1.37
32	2a	250	A	N9-C4	5.27	1.41	1.37
1	1A	178	G	C5-C4	-5.26	1.34	1.38
1	2A	213	A	N9-C4	-5.26	1.34	1.37
1	2A	1084	A	N3-C4	5.26	1.38	1.34
1	2A	2598	A	N3-C4	-5.26	1.31	1.34
1	1A	1398	U	C4-C5	-5.26	1.38	1.43
15	1T	5	ALA	CA-CB	-5.26	1.41	1.52
1	1A	1110	C	N1-C2	5.26	1.45	1.40
1	1A	2203	G	C6-N1	5.26	1.43	1.39
1	1A	2443	U	P-OP2	-5.26	1.40	1.49
32	1a	1036	G	N3-C4	5.26	1.39	1.35
1	2A	507	A	N7-C5	5.26	1.42	1.39
1	1A	825	G	N1-C2	-5.26	1.33	1.37
32	2a	1357	A	N9-C4	5.26	1.41	1.37
1	1A	123	G	N1-C2	-5.25	1.33	1.37
1	1A	791	G	N9-C8	-5.25	1.34	1.37
1	1A	591	U	C4-O4	-5.25	1.19	1.23
1	1A	2138	G	C5-C4	5.25	1.42	1.38
1	2A	686	G	N7-C5	-5.25	1.36	1.39
1	1A	398	A	N9-C4	-5.25	1.34	1.37
32	1a	1530	G	C6-N1	5.24	1.43	1.39
1	1A	582	G	N7-C5	-5.24	1.36	1.39
32	1a	250	A	C5-C4	5.24	1.42	1.38
1	2A	2177	C	N1-C6	5.24	1.40	1.37
32	1a	1030(C)	G	N9-C4	5.23	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2153	G	C6-N1	5.23	1.43	1.39
1	1A	2171	G	C6-N1	5.23	1.43	1.39
1	1A	2187	G	C2-N3	5.23	1.36	1.32
1	1A	540	A	N9-C4	-5.23	1.34	1.37
1	1A	446	C	C2-O2	-5.23	1.19	1.24
1	1A	1846	A	N9-C4	-5.23	1.34	1.37
1	1A	2245	U	C2-O2	-5.22	1.17	1.22
32	1a	156	G	N9-C8	5.22	1.41	1.37
1	2A	1536	C	C2-N3	5.22	1.40	1.35
1	2A	2162	G	C5-C4	5.22	1.42	1.38
1	1A	1255	A	C5-C4	-5.22	1.35	1.38
1	1A	2063	U	C2-O2	-5.22	1.17	1.22
1	1A	369	A	C6-N6	-5.22	1.29	1.33
1	1A	1149	A	N3-C4	5.21	1.38	1.34
1	1A	1112	U	N1-C6	5.21	1.42	1.38
1	1A	2068	G	N7-C5	-5.21	1.36	1.39
1	1A	221	G	N7-C5	-5.21	1.36	1.39
1	1A	1669	G	N1-C2	-5.21	1.33	1.37
32	2a	1030(A)	G	N3-C4	5.21	1.39	1.35
32	2a	1446	U	N1-C2	5.21	1.43	1.38
1	2A	1041	C	N1-C2	5.20	1.45	1.40
1	2A	1788	C	N1-C6	-5.20	1.34	1.37
1	1A	747	G	N1-C2	-5.20	1.33	1.37
1	1A	2129	C	N1-C6	5.20	1.40	1.37
1	1A	579	G	N3-C4	-5.20	1.31	1.35
1	1A	2453	C	N3-C4	-5.20	1.30	1.33
1	2A	6	A	N9-C4	5.20	1.41	1.37
1	2A	2613	U	C2-N3	-5.20	1.34	1.37
1	1A	538	A	N7-C5	-5.20	1.36	1.39
1	1A	2565	G	N9-C8	-5.20	1.34	1.37
1	1A	845	G	N7-C5	-5.19	1.36	1.39
1	1A	1665	G	C8-N7	-5.19	1.27	1.30
1	1A	2450	U	C4-O4	-5.19	1.19	1.23
1	1A	166	G	C6-N1	-5.19	1.35	1.39
1	2A	675	A	N9-C4	-5.19	1.34	1.37
1	1A	428	A	N3-C4	-5.19	1.31	1.34
1	2A	2132	U	C2-N3	5.19	1.41	1.37
1	1A	1304	C	C2-N3	-5.18	1.31	1.35
1	2A	229	A	C5-C4	5.18	1.42	1.38
1	2A	2517	C	N1-C6	-5.18	1.34	1.37
32	2a	1031	G	N9-C4	5.18	1.42	1.38
1	1A	1669	G	N3-C4	-5.18	1.31	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	484	G	C6-N1	-5.18	1.35	1.39
1	1A	23	G	C6-O6	5.18	1.28	1.24
1	2A	1092	C	N1-C6	5.18	1.40	1.37
1	1A	2623	U	C2-O2	-5.17	1.17	1.22
1	1A	2576	A	C5-C6	-5.17	1.36	1.41
1	2A	2064	C	C2-O2	-5.17	1.19	1.24
1	1A	2092	G	C6-N1	-5.17	1.35	1.39
1	1A	2137	G	N9-C4	5.17	1.42	1.38
1	1A	2258	G	N1-C2	-5.17	1.33	1.37
1	1A	2069	U	C2-N3	5.17	1.41	1.37
32	2a	1374	A	N9-C4	5.16	1.41	1.37
1	1A	2560	G	C8-N7	5.16	1.34	1.30
1	1A	1143	U	C2-N3	5.16	1.41	1.37
1	1A	2256	U	C2-O2	-5.16	1.17	1.22
1	1A	1846	A	C5-C4	-5.16	1.35	1.38
1	1A	2879	G	N7-C5	-5.16	1.36	1.39
32	1a	1024	G	N9-C4	5.16	1.42	1.38
1	2A	2167	U	N1-C2	5.15	1.43	1.38
1	1A	1390	G	C2-N3	-5.15	1.28	1.32
14	1S	107	GLU	CG-CD	5.15	1.59	1.51
32	1a	144	G	N9-C4	5.15	1.42	1.38
1	1A	323	A	C6-N1	-5.15	1.31	1.35
1	1A	1141	A	C5-C4	5.15	1.42	1.38
32	1a	1276	G	C5-C4	5.15	1.42	1.38
1	2A	2113	U	N1-C2	5.15	1.43	1.38
1	1A	176	G	N7-C5	-5.14	1.36	1.39
1	1A	794	U	C4-O4	5.14	1.27	1.23
1	2A	2177	C	C2-N3	5.14	1.39	1.35
32	1a	1026	G	N3-C4	5.14	1.39	1.35
1	1A	1356	G	C6-N1	-5.14	1.35	1.39
1	1A	1959	A	N3-C4	-5.14	1.31	1.34
1	1A	751	G	N3-C4	-5.13	1.31	1.35
1	1A	1666	G	N1-C2	-5.13	1.33	1.37
1	1A	1873	G	C6-N1	-5.13	1.35	1.39
1	2A	1655	A	N9-C8	-5.13	1.33	1.37
1	1A	2828	G	C5-C4	-5.13	1.34	1.38
1	2A	883	G	N7-C5	5.13	1.42	1.39
32	2a	204	U	N1-C2	5.12	1.43	1.38
1	1A	1371	G	N9-C8	-5.12	1.34	1.37
1	1A	2834	C	C4-C5	-5.12	1.38	1.43
1	2A	2635	C	N1-C6	-5.12	1.34	1.37
1	1A	891	C	N1-C6	-5.12	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1306	G	N3-C4	-5.12	1.31	1.35
1	1A	1816	A	C5-C6	-5.12	1.36	1.41
1	1A	29	U	C2-N3	-5.12	1.34	1.37
1	1A	255	G	C5-C6	-5.12	1.37	1.42
1	1A	1690	G	C2-N3	-5.12	1.28	1.32
32	2a	1033	G	C6-N1	5.12	1.43	1.39
1	1A	2689	G	N1-C2	-5.12	1.33	1.37
1	1A	608	G	C8-N7	5.12	1.34	1.30
1	1A	2271	G	N1-C2	-5.12	1.33	1.37
1	2A	792	G	C5-C4	-5.12	1.34	1.38
1	1A	1668	G	O3'-P	-5.11	1.55	1.61
1	1A	617	U	C2-N3	-5.11	1.34	1.37
1	1A	1177	G	C6-N1	-5.11	1.35	1.39
1	2A	2454	G	C6-N1	-5.11	1.35	1.39
1	1A	2639	G	C5-C6	-5.11	1.37	1.42
1	1A	2071	G	N1-C2	-5.11	1.33	1.37
1	1A	2440	G	C8-N7	5.11	1.34	1.30
32	2a	306	G	N7-C5	5.11	1.42	1.39
1	1A	1993	A	C6-N1	-5.10	1.31	1.35
1	1A	2348	A	C8-N7	-5.10	1.27	1.31
9	1N	14	VAL	CB-CG1	-5.10	1.42	1.52
1	2A	568	U	C4-O4	-5.10	1.19	1.23
1	2A	1509	C	N1-C2	5.10	1.45	1.40
1	1A	792	G	N1-C2	-5.10	1.33	1.37
1	2A	1079	C	N1-C2	5.10	1.45	1.40
1	2A	2114	A	C5-C4	5.10	1.42	1.38
1	1A	1109	G	N7-C5	5.10	1.42	1.39
1	1A	1133	G	N9-C4	5.10	1.42	1.38
1	1A	1475	G	C2-N3	-5.10	1.28	1.32
1	1A	2061	C	C4-C5	-5.10	1.38	1.43
1	1A	2857	U	C2-N3	-5.10	1.34	1.37
32	2a	1027	C	N1-C2	5.09	1.45	1.40
1	1A	495	G	N7-C5	-5.09	1.36	1.39
1	1A	1726	U	C2-O2	-5.09	1.17	1.22
1	1A	1997	G	C8-N7	-5.09	1.27	1.30
1	1A	271	U	N1-C6	5.08	1.42	1.38
1	1A	631	A	N3-C4	-5.08	1.31	1.34
1	1A	1724	A	C8-N7	-5.08	1.27	1.31
1	1A	2158	C	N1-C2	5.08	1.45	1.40
32	1a	189(L)	G	N9-C4	5.08	1.42	1.38
1	1A	122	G	N1-C2	-5.08	1.33	1.37
1	1A	885	C	C2-O2	-5.08	1.19	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2042	A	N9-C4	-5.08	1.34	1.37
1	1A	2341	G	N9-C4	-5.08	1.33	1.38
1	1A	2205	C	N1-C6	5.07	1.40	1.37
1	2A	2727	G	N7-C5	-5.07	1.36	1.39
32	2a	908	A	N7-C5	-5.07	1.36	1.39
1	1A	541	C	N1-C2	-5.07	1.35	1.40
1	1A	933	C	N1-C2	5.07	1.45	1.40
1	1A	1357	G	N1-C2	-5.07	1.33	1.37
1	1A	2113	U	C2-O2	-5.07	1.17	1.22
1	2A	459	U	C2-N3	-5.07	1.34	1.37
1	1A	1702	A	C8-N7	5.07	1.35	1.31
1	1A	848	G	P-OP2	-5.07	1.40	1.49
1	1A	1172	A	C5-C4	-5.06	1.35	1.38
1	1A	2187	G	C5-C6	5.06	1.47	1.42
1	1A	2724	U	N1-C6	-5.06	1.33	1.38
1	1A	479	C	C4-C5	5.06	1.47	1.43
1	1A	872	C	C4-C5	-5.06	1.39	1.43
1	1A	2823	A	C6-N1	-5.05	1.32	1.35
1	1A	810	G	N1-C2	-5.05	1.33	1.37
32	1a	156	G	N9-C4	5.05	1.42	1.38
32	1a	1285	A	C5-C4	5.05	1.42	1.38
1	1A	1203	G	C8-N7	-5.05	1.27	1.30
1	2A	744	G	N1-C2	-5.05	1.33	1.37
1	2A	2553	G	N9-C8	-5.05	1.34	1.37
27	15	59	GLU	CG-CD	5.04	1.59	1.51
32	1a	1286	A	C5-C4	5.04	1.42	1.38
1	1A	123	G	N3-C4	-5.04	1.31	1.35
1	2A	2128	C	N3-C4	5.04	1.37	1.33
1	1A	1197	G	N7-C5	5.04	1.42	1.39
32	1a	1001	A	C5-C4	5.04	1.42	1.38
1	2A	1950	G	N7-C5	-5.04	1.36	1.39
1	1A	1117	G	C5-C4	5.04	1.41	1.38
1	1A	1240	G	N3-C4	-5.04	1.31	1.35
32	1a	1525	G	C8-N7	5.04	1.33	1.30
1	1A	1380	G	N3-C4	-5.04	1.31	1.35
1	1A	477	C	C2-O2	-5.03	1.20	1.24
1	1A	715	G	N9-C8	-5.03	1.34	1.37
1	1A	2093	A	C6-N1	-5.03	1.32	1.35
1	1A	1676	G	C2-N3	-5.03	1.28	1.32
1	2A	2156	G	N9-C4	5.03	1.42	1.38
1	1A	1650	C	N1-C6	-5.03	1.34	1.37
1	1A	2013	U	N1-C2	-5.03	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2457	G	C6-N1	-5.03	1.36	1.39
1	1A	2610	A	C5-C4	-5.03	1.35	1.38
2	1B	98	G	N7-C5	-5.03	1.36	1.39
1	2A	652(A)	A	N9-C4	5.03	1.40	1.37
1	1A	1555	C	N1-C6	5.03	1.40	1.37
32	1a	1134	G	N9-C4	5.03	1.42	1.38
1	1A	1970	G	C2-N3	-5.02	1.28	1.32
1	1A	2043	C	N1-C6	-5.02	1.34	1.37
1	2A	2604	U	C2-N3	-5.02	1.34	1.37
32	2a	993	G	N9-C4	5.02	1.42	1.38
1	1A	1330	A	N3-C4	5.02	1.37	1.34
32	1a	298	A	N3-C4	-5.02	1.31	1.34
1	2A	1678	G	N7-C5	-5.02	1.36	1.39
1	1A	1661	C	N3-C4	-5.02	1.30	1.33
1	1A	1092	A	C5-C4	5.01	1.42	1.38
1	2A	1256	G	C8-N7	-5.01	1.27	1.30
1	1A	104	C	N3-C4	-5.01	1.30	1.33
1	1A	2006	G	N1-C2	-5.01	1.33	1.37
1	2A	741	G	N1-C2	-5.01	1.33	1.37
32	2a	1030(A)	G	C6-N1	5.01	1.43	1.39
1	1A	872	C	N3-C4	-5.01	1.30	1.33
1	1A	2818	U	N3-C4	5.01	1.43	1.38
2	1B	1	U	N3-C4	5.01	1.43	1.38
32	1a	73	G	N7-C5	5.01	1.42	1.39
1	1A	2048	C	N1-C6	-5.01	1.34	1.37
1	1A	2535	G	C6-N1	-5.01	1.36	1.39
1	1A	2818	U	C2-N3	5.01	1.41	1.37
1	2A	2160	G	C6-N1	5.01	1.43	1.39
1	2A	2794	C	N1-C6	5.01	1.40	1.37
32	1a	1278	U	N1-C6	5.00	1.42	1.38
1	1A	2180	A	N7-C5	5.00	1.42	1.39

All (7479) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1208	C	O5'-P-OP1	-33.37	70.65	110.70
32	1a	1520	G	O5'-P-OP1	-31.38	73.04	110.70
32	1a	1520	G	O5'-P-OP2	26.23	142.18	110.70
32	1a	1520	G	OP1-P-OP2	-24.67	82.60	119.60
32	2a	1208	C	OP1-P-OP2	-24.65	82.62	119.60
1	1A	354	A	C2-N3-C4	-20.05	100.57	110.60
1	1A	543	G	O5'-P-OP2	-18.52	88.47	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1208	C	O5'-P-OP2	17.85	132.12	110.70
1	1A	2045	G	O5'-P-OP1	-17.16	90.10	110.70
1	1A	2624	C	O5'-P-OP2	-16.87	90.45	110.70
1	1A	1847	G	O5'-P-OP1	-16.84	90.49	110.70
1	1A	2091	G	O5'-P-OP2	-16.80	90.54	110.70
32	2a	343	U	N3-C4-O4	-16.62	107.77	119.40
1	1A	991	G	O5'-P-OP1	-16.43	90.91	105.70
1	1A	2596	U	O5'-P-OP2	-16.28	91.05	105.70
32	2a	438	G	O5'-P-OP2	-16.24	91.09	105.70
1	2A	2603	G	O5'-P-OP2	-16.23	91.10	105.70
1	1A	1006	C	O5'-P-OP2	-16.15	91.17	105.70
32	2a	343	U	C2-N1-C1'	-15.59	98.99	117.70
32	1a	343	U	C2-N1-C1'	-14.61	100.17	117.70
1	2A	2554	U	O5'-P-OP1	-14.55	92.60	105.70
32	1a	533	A	N1-C6-N6	14.45	127.27	118.60
1	1A	834	U	O5'-P-OP1	-14.30	92.83	105.70
1	1A	2453	C	C2-N3-C4	-14.22	112.79	119.90
32	2a	404	U	N1-C2-O2	14.19	132.74	122.80
1	1A	1562	U	O5'-P-OP2	-14.19	92.93	105.70
1	1A	2331	G	N3-C4-N9	-14.14	117.52	126.00
1	1A	2598	C	N1-C2-O2	-13.95	110.53	118.90
1	1A	295	C	O5'-P-OP2	-13.93	93.16	105.70
1	2A	1272	A	O5'-P-OP2	-13.86	93.23	105.70
32	1a	343	U	N3-C4-O4	-13.78	109.76	119.40
1	1A	1054	C	C6-N1-C2	-13.75	114.80	120.30
32	1a	1530	G	C5-C6-O6	-13.73	120.36	128.60
1	1A	832	G	O5'-P-OP2	-13.72	93.35	105.70
32	2a	1207	2MG	OP2-P-O3'	-13.67	75.14	105.20
32	2a	1207	2MG	OP1-P-O3'	13.64	135.22	105.20
1	1A	1042	A	O5'-P-OP1	-13.50	93.55	105.70
1	1A	2194	U	C5-C4-O4	13.40	133.94	125.90
32	2a	1003	G	N3-C4-C5	-13.39	121.91	128.60
32	2a	1034	G	C5-C6-O6	-13.38	120.57	128.60
1	1A	2697	G	N1-C6-O6	-13.35	111.89	119.90
1	1A	82	G	N9-C4-C5	-13.35	100.06	105.40
32	1a	1530	G	N1-C6-O6	13.23	127.83	119.90
1	1A	2639	G	C5-C6-O6	-13.22	120.67	128.60
1	1A	1316	C	C6-N1-C2	13.10	125.54	120.30
32	1a	404	U	N1-C2-O2	13.07	131.95	122.80
1	1A	2620	G	C5-C6-O6	-12.86	120.88	128.60
1	1A	918	U	C5-C4-O4	-12.86	118.19	125.90
1	1A	2331	G	N3-C4-C5	12.86	135.03	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	194	G	C8-N9-C4	12.81	111.52	106.40
1	1A	354	A	N3-C4-C5	12.75	135.72	126.80
1	2A	2413	G	O5'-P-OP2	-12.60	94.36	105.70
32	2a	1003	G	C8-N9-C4	-12.59	101.36	106.40
1	1A	205	A	O5'-P-OP1	-12.50	94.45	105.70
1	2A	518	G	O5'-P-OP2	-12.46	94.49	105.70
1	1A	641	G	O5'-P-OP2	-12.43	94.52	105.70
1	1A	537	G	O4'-C1'-N9	12.33	118.07	108.20
32	1a	902	G	O5'-P-OP2	-12.29	94.64	105.70
1	1A	2102	G	O5'-P-OP2	-12.21	94.71	105.70
1	1A	1571	G	O5'-P-OP2	-12.19	94.73	105.70
1	1A	2566	U	O5'-P-OP1	-12.12	94.80	105.70
1	1A	2402	U	O5'-P-OP1	-12.07	94.84	105.70
1	1A	575	G	N1-C6-O6	-12.05	112.67	119.90
1	1A	1743	G	O5'-P-OP2	-12.04	94.86	105.70
1	1A	2440	G	C8-N9-C4	-12.03	101.59	106.40
1	1A	1695	C	O5'-P-OP1	-12.02	94.88	105.70
1	2A	1639	U	O5'-P-OP2	-12.02	94.88	105.70
32	2a	343	U	C5-C4-O4	12.01	133.10	125.90
32	2a	404	U	N3-C2-O2	-12.01	113.80	122.20
1	2A	2566	A	O5'-P-OP2	-11.96	94.94	105.70
1	2A	1063	G	C8-N9-C4	-11.95	101.62	106.40
1	1A	1425	A	N1-C6-N6	11.95	125.77	118.60
1	1A	1237	G	C8-N9-C4	11.95	111.18	106.40
1	2A	906	G	C5-C6-O6	11.94	135.76	128.60
2	1B	108	U	O5'-P-OP2	-11.93	94.97	105.70
1	1A	1666	G	N1-C6-O6	-11.92	112.75	119.90
1	1A	2331	G	C5-N7-C8	-11.87	98.36	104.30
1	2A	2575	C	O5'-P-OP2	-11.87	95.02	105.70
1	2A	2378	A	N1-C6-N6	11.86	125.72	118.60
32	1a	42	G	O5'-P-OP1	-11.81	95.07	105.70
32	1a	533	A	C5-C6-N6	-11.77	114.29	123.70
1	1A	2027	A	O5'-P-OP1	-11.77	95.11	105.70
1	1A	1318	A	O5'-P-OP2	-11.76	95.12	105.70
1	1A	2436	C	O5'-P-OP2	-11.76	95.11	105.70
2	1B	75	G	C6-N1-C2	-11.75	118.05	125.10
1	2A	1071	G	C8-N9-C4	-11.71	101.72	106.40
1	2A	481	G	O5'-P-OP2	-11.69	95.18	105.70
1	2A	1597	A	O5'-P-OP2	-11.68	95.18	105.70
2	1B	56	G	O5'-P-OP2	-11.68	95.19	105.70
1	1A	1986	G	N9-C4-C5	-11.67	100.73	105.40
1	2A	2145	C	C5-C6-N1	11.65	126.83	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	266	G	C8-N9-C4	-11.64	101.74	106.40
32	2a	299	G	C5-C6-O6	-11.62	121.63	128.60
32	1a	1137	C	C6-N1-C2	-11.62	115.65	120.30
2	1B	57	A	N9-C4-C5	-11.59	101.17	105.80
1	1A	2599	A	O5'-P-OP2	-11.58	95.28	105.70
1	1A	322	G	O5'-P-OP2	-11.52	95.33	105.70
1	2A	751	A	O5'-P-OP1	-11.49	95.36	105.70
1	1A	1787	G	O5'-P-OP2	-11.46	95.39	105.70
1	1A	1270	C	C6-N1-C2	11.40	124.86	120.30
1	1A	1358	U	C5-C4-O4	11.40	132.74	125.90
1	1A	36	G	O5'-P-OP2	-11.40	95.44	105.70
32	1a	343	U	C5-C4-O4	11.40	132.74	125.90
1	1A	2612	A	N1-C6-N6	-11.35	111.79	118.60
32	2a	1003	G	C2-N3-C4	11.34	117.57	111.90
1	2A	2612	C	C6-N1-C2	11.34	124.84	120.30
1	1A	2443	U	C5-C6-N1	-11.30	117.05	122.70
1	1A	49	U	O5'-P-OP1	-11.30	95.53	105.70
1	1A	2735	G	C8-N9-C4	11.28	110.91	106.40
32	2a	343	U	C6-N1-C1'	11.24	136.93	121.20
1	1A	1298	G	O5'-P-OP1	-11.23	95.59	105.70
1	1A	2640	C	C6-N1-C2	11.21	124.78	120.30
1	1A	2511	C	N3-C4-C5	-11.20	117.42	121.90
1	1A	2331	G	C2-N3-C4	-11.20	106.30	111.90
1	1A	1442	U	O5'-P-OP1	-11.17	95.64	105.70
1	1A	2586	G	N1-C6-O6	-11.17	113.20	119.90
1	2A	467	G	C8-N9-C4	11.13	110.85	106.40
1	2A	555	U	O5'-P-OP2	-11.12	95.70	105.70
1	1A	2067	C	C5-C6-N1	-11.11	115.44	121.00
1	1A	1237	G	N7-C8-N9	-11.09	107.56	113.10
1	1A	1720	U	N1-C2-O2	-11.05	115.06	122.80
1	1A	418	G	C6-N1-C2	-11.04	118.48	125.10
1	1A	575	G	C5-C6-O6	11.03	135.22	128.60
1	1A	2578	A	O5'-P-OP2	-11.03	95.78	105.70
1	1A	2014	G	N7-C8-N9	-11.01	107.60	113.10
32	1a	855	G	O5'-P-OP1	-11.00	95.80	105.70
1	1A	2006	G	C5-C6-O6	10.98	135.19	128.60
1	1A	1015	C	C5-C6-N1	-10.97	115.51	121.00
1	1A	1434	G	O5'-P-OP2	-10.95	95.85	105.70
1	1A	720	C	C2-N3-C4	-10.93	114.44	119.90
1	1A	2326	C	O5'-P-OP2	-10.92	95.87	105.70
1	1A	101	A	C5-C6-N1	-10.92	112.24	117.70
1	2A	205	G	O5'-P-OP2	-10.88	95.91	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	194	G	N9-C4-C5	-10.86	101.06	105.40
1	1A	1382	A	O5'-P-OP2	-10.85	95.93	105.70
1	1A	1569	U	O5'-P-OP2	10.85	123.72	110.70
2	1B	55	U	O5'-P-OP1	-10.85	95.94	105.70
1	1A	841	G	N1-C6-O6	-10.84	113.39	119.90
1	1A	2475	C	N3-C4-C5	10.83	126.23	121.90
1	2A	1673	U	O5'-P-OP1	-10.83	95.95	105.70
1	2A	752	A	P-O3'-C3'	10.78	132.63	119.70
1	2A	807	U	C2-N3-C4	-10.75	120.55	127.00
1	1A	2014	G	C8-N9-C4	10.74	110.69	106.40
1	1A	1700	G	C5-C6-O6	10.72	135.03	128.60
1	1A	2623	U	O5'-P-OP1	-10.71	96.06	105.70
28	16	13	CYS	CA-CB-SG	10.69	133.24	114.00
1	1A	1425	A	N9-C4-C5	-10.67	101.53	105.80
1	1A	1569	U	O5'-P-OP1	-10.66	96.10	105.70
1	1A	652	A	O5'-P-OP2	-10.66	96.11	105.70
1	2A	2023	G	O5'-P-OP1	-10.66	96.11	105.70
1	1A	101	A	C4-C5-C6	10.63	122.31	117.00
1	2A	1992	G	N3-C4-C5	-10.62	123.29	128.60
32	1a	226	G	C8-N9-C4	10.61	110.64	106.40
1	1A	2348	A	C8-N9-C4	10.60	110.04	105.80
1	1A	409	G	N1-C6-O6	-10.59	113.55	119.90
1	1A	1069	U	O5'-P-OP2	-10.59	96.17	105.70
1	1A	581	G	C5-C6-O6	10.56	134.94	128.60
1	1A	2348	A	N9-C4-C5	-10.56	101.58	105.80
32	1a	343	U	C6-N1-C1'	10.56	135.99	121.20
32	2a	697	U	O5'-P-OP2	-10.56	96.19	105.70
2	1B	75	G	N3-C2-N2	-10.54	112.53	119.90
32	1a	442	C	C6-N1-C2	-10.53	116.09	120.30
32	1a	1465	C	C2-N3-C4	-10.53	114.64	119.90
1	1A	537	G	N1-C6-O6	10.49	126.19	119.90
1	1A	449	A	O5'-P-OP2	-10.48	96.27	105.70
1	1A	1472	G	C5-C6-O6	-10.47	122.32	128.60
1	2A	912	C	C6-N1-C2	-10.46	116.11	120.30
1	2A	869	G	O5'-P-OP2	-10.44	96.30	105.70
1	1A	436	C	O5'-P-OP1	-10.44	96.31	105.70
1	1A	101	A	C2-N3-C4	-10.43	105.39	110.60
1	1A	2257	U	C2-N3-C4	-10.43	120.74	127.00
32	1a	1436	U	C2-N3-C4	-10.43	120.74	127.00
1	1A	1995	G	O5'-P-OP2	-10.41	96.33	105.70
32	1a	533	A	C6-C5-N7	-10.40	125.02	132.30
1	1A	2521	G	N1-C6-O6	-10.39	113.67	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1753	U	O5'-P-OP1	-10.37	96.36	105.70
1	1A	82	G	C4-C5-N7	10.35	114.94	110.80
1	2A	467	G	N7-C8-N9	-10.34	107.93	113.10
1	2A	2145	C	C6-N1-C2	-10.33	116.17	120.30
32	2a	1028	C	C6-N1-C2	-10.33	116.17	120.30
1	2A	510	C	O5'-P-OP2	-10.32	96.41	105.70
1	1A	2464	C	N1-C2-O2	-10.31	112.71	118.90
1	1A	1291	G	N1-C6-O6	-10.31	113.72	119.90
1	1A	1700	G	N1-C6-O6	-10.29	113.73	119.90
1	1A	2735	G	N9-C4-C5	-10.29	101.28	105.40
1	1A	849	A	O5'-P-OP1	-10.29	96.44	105.70
1	1A	2858	G	O4'-C1'-N9	10.28	116.42	108.20
32	2a	1530	G	C8-N9-C4	10.28	110.51	106.40
1	2A	2318	G	O4'-C1'-N9	10.27	116.42	108.20
1	1A	1052	C	C5-C6-N1	-10.25	115.87	121.00
1	1A	255	G	C5-C6-O6	-10.25	122.45	128.60
1	1A	354	A	C5-N7-C8	-10.24	98.78	103.90
1	2A	1071	G	N7-C8-N9	10.23	118.22	113.10
1	2A	2467	C	C6-N1-C2	-10.23	116.21	120.30
1	2A	749	C	O5'-P-OP2	-10.23	96.50	105.70
1	1A	1035	G	C5-C6-N1	10.22	116.61	111.50
1	2A	2549	G	O5'-P-OP2	-10.21	96.51	105.70
1	1A	593	G	C5-C6-O6	-10.21	122.47	128.60
1	1A	1099	C	C2-N3-C4	10.20	125.00	119.90
1	1A	1210	G	C5-C6-O6	10.19	134.71	128.60
1	1A	1216	G	C8-N9-C4	-10.19	102.33	106.40
1	1A	1621	C	O5'-P-OP2	-10.18	96.53	105.70
1	2A	1063	G	N7-C8-N9	10.18	118.19	113.10
1	1A	1425	A	C8-N9-C4	10.17	109.87	105.80
1	1A	2100	C	C2-N3-C4	-10.17	114.81	119.90
1	1A	1093	G	O5'-P-OP2	-10.16	96.56	105.70
1	1A	1386	U	C2-N3-C4	-10.14	120.91	127.00
32	1a	1502	A	O5'-P-OP2	-10.13	96.58	105.70
1	1A	31	C	O5'-P-OP1	-10.12	96.59	105.70
1	1A	1319	U	N3-C4-O4	-10.12	112.32	119.40
1	1A	1959	A	N1-C2-N3	10.11	134.35	129.30
1	1A	2582	G	C5-C6-O6	10.10	134.66	128.60
1	1A	1847	G	O5'-P-OP2	10.10	122.82	110.70
1	1A	1959	A	N1-C6-N6	-10.09	112.55	118.60
1	1A	2697	G	C5-C6-O6	10.09	134.66	128.60
1	2A	1187	G	O5'-P-OP2	-10.08	96.63	105.70
1	2A	948	G	O5'-P-OP1	-10.06	96.65	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2576	G	O5'-P-OP1	-10.04	96.66	105.70
1	2A	807	U	C5-C4-O4	-10.03	119.88	125.90
1	1A	2335	G	C4-C5-N7	10.03	114.81	110.80
1	1A	1425	A	C5-C6-N6	-10.02	115.68	123.70
2	2B	115	G	C8-N9-C4	10.02	110.41	106.40
1	1A	848	G	C5-C6-O6	10.01	134.61	128.60
1	2A	1092	C	N1-C2-O2	10.01	124.91	118.90
1	1A	1620	G	C5-C6-O6	-10.01	122.60	128.60
1	1A	2638	C	N3-C4-C5	9.99	125.90	121.90
32	1a	1137	C	C5-C6-N1	9.98	125.99	121.00
1	1A	2440	G	N9-C4-C5	9.97	109.39	105.40
1	1A	40	C	N1-C2-O2	-9.97	112.92	118.90
1	1A	45	C	O5'-P-OP1	-9.97	96.73	105.70
1	1A	1299	A	C5-N7-C8	9.95	108.88	103.90
1	1A	1723	A	N7-C8-N9	-9.95	108.82	113.80
32	2a	266	G	N3-C4-C5	-9.95	123.62	128.60
1	1A	1766	G	C4-C5-N7	9.95	114.78	110.80
1	1A	856	G	N1-C6-O6	-9.94	113.94	119.90
1	1A	952	G	N9-C4-C5	9.94	109.37	105.40
1	2A	856	C	C6-N1-C2	-9.93	116.33	120.30
1	1A	1245	C	N1-C2-O2	-9.93	112.94	118.90
1	1A	2610	A	N7-C8-N9	-9.93	108.84	113.80
1	2A	2105	C	C5-C6-N1	9.93	125.96	121.00
1	2A	2105	C	C6-N1-C2	-9.92	116.33	120.30
1	1A	1347	A	O5'-P-OP2	-9.91	96.78	105.70
32	2a	246	A	O5'-P-OP2	-9.91	96.78	105.70
1	1A	2596	U	C5-C4-O4	9.91	131.84	125.90
1	2A	1913	A	C8-N9-C4	-9.90	101.84	105.80
1	2A	2172	U	O4'-C1'-N1	9.90	116.12	108.20
1	1A	472	G	C4-C5-N7	9.90	114.76	110.80
1	1A	1048	G	O5'-P-OP2	-9.89	96.80	105.70
1	1A	2453	C	N3-C4-C5	9.89	125.85	121.90
1	2A	2430	A	O5'-P-OP2	-9.88	96.81	105.70
1	1A	874	U	C5-C6-N1	-9.87	117.77	122.70
1	1A	2439	C	C6-N1-C2	9.87	124.25	120.30
1	2A	2554	U	O5'-P-OP2	9.86	122.53	110.70
1	1A	1669	G	N1-C6-O6	-9.86	113.98	119.90
1	1A	752	A	N1-C6-N6	9.85	124.51	118.60
1	1A	1357	G	O5'-P-OP2	-9.85	96.84	105.70
1	2A	1536	C	N3-C4-C5	-9.84	117.96	121.90
32	2a	30	U	O5'-P-OP2	-9.81	96.87	105.70
1	1A	1148	C	N1-C2-O2	9.80	124.78	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2022	U	O5'-P-OP1	-9.79	96.89	105.70
1	1A	1439	A	N1-C6-N6	-9.78	112.73	118.60
1	1A	2383	G	C5-C6-O6	-9.78	122.73	128.60
1	1A	1316	C	C5-C6-N1	-9.78	116.11	121.00
1	1A	2238	C	C6-N1-C2	9.77	124.21	120.30
1	1A	1299	A	N7-C8-N9	-9.77	108.92	113.80
2	2B	24	G	C5-C6-O6	-9.77	122.74	128.60
1	1A	101	A	N1-C2-N3	9.77	134.18	129.30
1	1A	1181	G	C8-N9-C4	9.76	110.31	106.40
32	2a	1158	C	C6-N1-C2	-9.75	116.40	120.30
1	2A	673	C	C2-N3-C4	-9.75	115.03	119.90
32	2a	295	C	C6-N1-C2	9.75	124.20	120.30
1	1A	2257	U	N3-C4-C5	9.73	120.44	114.60
1	1A	2029	C	N3-C4-N4	-9.72	111.20	118.00
1	1A	2521	G	C5-C6-O6	9.72	134.43	128.60
1	1A	2630	G	N9-C4-C5	9.70	109.28	105.40
1	1A	2702	C	O5'-P-OP1	-9.70	96.97	105.70
32	2a	1495	U	N1-C2-O2	9.70	129.59	122.80
1	1A	1995	G	N1-C6-O6	-9.69	114.09	119.90
2	2B	6	C	C6-N1-C2	9.69	124.18	120.30
32	1a	1512	U	C5-C4-O4	9.68	131.71	125.90
32	2a	1034	G	C2-N3-C4	9.68	116.74	111.90
1	1A	1218	G	O4'-C1'-N9	9.67	115.94	108.20
1	1A	1294	G	N9-C4-C5	-9.67	101.53	105.40
1	1A	842	C	N1-C2-O2	9.67	124.70	118.90
1	2A	529	A	C5-N7-C8	-9.66	99.07	103.90
1	1A	537	G	C5-C6-O6	-9.66	122.81	128.60
1	1A	843	C	C2-N3-C4	-9.65	115.07	119.90
1	1A	246	A	O5'-P-OP2	-9.65	97.02	105.70
1	1A	790	G	N1-C6-O6	-9.64	114.11	119.90
32	1a	366	C	O5'-P-OP2	-9.64	97.02	105.70
32	2a	558	G	O5'-P-OP1	-9.64	97.03	105.70
1	1A	127	C	O5'-P-OP2	-9.62	97.04	105.70
1	1A	2272	C	C5-C6-N1	-9.62	116.19	121.00
1	1A	735	U	C5-C6-N1	-9.61	117.90	122.70
1	1A	2434	A	C8-N9-C4	-9.60	101.96	105.80
1	1A	417	A	C8-N9-C4	9.60	109.64	105.80
32	2a	1125	U	C5-C4-O4	9.59	131.65	125.90
1	1A	354	A	N3-C4-N9	-9.59	119.73	127.40
1	1A	1665	G	C8-N9-C4	9.57	110.23	106.40
1	1A	2258	G	C8-N9-C4	9.57	110.23	106.40
1	2A	512	G	O4'-C1'-N9	9.57	115.85	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2112	G	N1-C6-O6	-9.56	114.16	119.90
1	1A	1807	G	O5'-P-OP2	-9.55	97.10	105.70
1	1A	1750	G	O5'-P-OP2	-9.55	97.11	105.70
1	1A	1150	C	C6-N1-C2	-9.54	116.48	120.30
1	1A	2630	G	C4-C5-N7	-9.53	106.99	110.80
32	1a	115	G	O5'-P-OP2	-9.51	97.14	105.70
1	1A	1707	C	O5'-P-OP2	-9.51	97.14	105.70
1	1A	2382	G	O5'-P-OP2	-9.50	97.15	105.70
1	1A	195	U	C5-C6-N1	-9.49	117.95	122.70
1	2A	2177	C	C5-C6-N1	9.48	125.74	121.00
1	1A	2703	C	C6-N1-C2	9.47	124.09	120.30
1	1A	1860	A	O5'-P-OP2	-9.47	97.18	105.70
32	2a	1034	G	N3-C4-N9	9.47	131.68	126.00
32	2a	1034	G	C5-C6-N1	9.46	116.23	111.50
1	1A	831	A	C8-N9-C4	9.46	109.58	105.80
1	1A	903	C	C6-N1-C2	-9.46	116.52	120.30
1	1A	20	C	C5-C6-N1	-9.46	116.27	121.00
1	1A	760	G	C2-N3-C4	-9.46	107.17	111.90
1	1A	1450	C	O5'-P-OP2	-9.46	97.19	105.70
32	2a	1420	C	C6-N1-C2	-9.46	116.52	120.30
1	1A	748	G	O5'-P-OP2	-9.45	97.20	105.70
1	1A	641	G	N1-C6-O6	-9.43	114.24	119.90
1	1A	765	A	N1-C6-N6	9.42	124.25	118.60
1	1A	702	A	C8-N9-C4	-9.42	102.03	105.80
1	1A	1216	G	N7-C8-N9	9.42	117.81	113.10
1	1A	1803	G	C8-N9-C4	9.42	110.17	106.40
1	1A	1015	C	C6-N1-C2	9.41	124.07	120.30
1	1A	1772	C	C6-N1-C2	-9.41	116.53	120.30
1	1A	1419	A	O5'-P-OP1	9.41	122.00	110.70
1	1A	726	C	O5'-P-OP1	-9.41	97.23	105.70
1	1A	1409	C	O5'-P-OP2	-9.40	97.24	105.70
32	1a	819	A	N1-C6-N6	9.40	124.24	118.60
1	1A	2088	C	C6-N1-C2	-9.40	116.54	120.30
1	1A	419	C	O5'-P-OP1	-9.39	97.25	105.70
32	1a	1424	C	O5'-P-OP2	-9.39	97.25	105.70
32	2a	902	G	O5'-P-OP2	-9.38	97.26	105.70
34	1b	178	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	1A	170	A	N1-C6-N6	-9.38	112.97	118.60
1	1A	2606	C	C5-C6-N1	-9.36	116.32	121.00
1	1A	1669	G	C5-C6-O6	9.36	134.22	128.60
1	1A	952	G	C5-C6-O6	9.36	134.21	128.60
1	1A	752	A	N9-C4-C5	-9.35	102.06	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	812	C	C6-N1-C2	-9.35	116.56	120.30
1	1A	98	U	N1-C2-O2	9.34	129.34	122.80
1	1A	710	G	O5'-P-OP2	-9.34	97.30	105.70
1	1A	2607	G	C5-C6-O6	9.33	134.20	128.60
1	1A	1724	A	N1-C2-N3	9.33	133.97	129.30
1	1A	2535	G	N1-C6-O6	-9.33	114.30	119.90
1	1A	405	C	N3-C4-C5	9.31	125.62	121.90
1	1A	183	G	C5-C6-O6	9.30	134.18	128.60
1	1A	1666	G	C5-C6-O6	9.30	134.18	128.60
32	1a	768	A	C8-N9-C4	9.30	109.52	105.80
1	1A	749	G	O5'-P-OP2	-9.30	97.33	105.70
1	1A	1865	U	O5'-P-OP1	-9.30	97.33	105.70
32	2a	1465	C	C2-N3-C4	-9.30	115.25	119.90
1	2A	249	C	C6-N1-C2	9.29	124.02	120.30
1	2A	474	G	C8-N9-C4	-9.29	102.68	106.40
1	1A	2030	C	C4-C5-C6	9.29	122.05	117.40
1	1A	1071	G	O5'-P-OP1	-9.28	97.35	105.70
2	1B	13	A	O5'-P-OP2	-9.28	97.35	105.70
1	1A	810	G	N3-C2-N2	9.28	126.39	119.90
1	2A	1780	A	O5'-P-OP1	-9.27	97.35	105.70
32	2a	297	G	O5'-P-OP2	-9.27	97.36	105.70
32	1a	533	A	N9-C4-C5	-9.27	102.09	105.80
1	1A	2700	U	N3-C4-O4	9.26	125.88	119.40
32	1a	204	U	C2-N1-C1'	9.26	128.81	117.70
1	1A	472	G	C5-C6-O6	-9.25	123.05	128.60
1	1A	1316	C	N3-C4-C5	9.25	125.60	121.90
1	1A	1354	A	O5'-P-OP2	-9.24	97.38	105.70
1	1A	1821	C	C5-C4-N4	-9.23	113.73	120.20
1	1A	716	G	C8-N9-C4	9.23	110.09	106.40
1	1A	1856	A	N1-C6-N6	-9.23	113.06	118.60
1	1A	2582	G	N1-C6-O6	-9.22	114.37	119.90
1	1A	241	G	C8-N9-C4	-9.21	102.71	106.40
1	1A	799	A	C2-N3-C4	-9.21	106.00	110.60
1	1A	852	G	C5-C6-N1	9.21	116.10	111.50
1	2A	2827	C	C6-N1-C2	9.21	123.98	120.30
1	2A	154	G	C8-N9-C4	9.21	110.08	106.40
1	1A	2450	U	C5-C6-N1	-9.20	118.10	122.70
1	1A	1462	G	O4'-C1'-N9	9.20	115.56	108.20
1	2A	1071	G	C6-C5-N7	-9.19	124.89	130.40
32	2a	1406	U	C2-N3-C4	-9.19	121.49	127.00
32	2a	299	G	C4-C5-N7	9.18	114.47	110.80
1	1A	109	A	N1-C6-N6	-9.18	113.09	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	751	G	C5-C6-O6	-9.18	123.09	128.60
1	1A	1766	G	C5-N7-C8	-9.16	99.72	104.30
1	1A	2025	G	N1-C6-O6	-9.16	114.40	119.90
1	2A	1076	C	N1-C2-O2	9.16	124.40	118.90
1	2A	1992	G	C8-N9-C4	-9.15	102.74	106.40
1	2A	2805	G	N3-C4-C5	-9.14	124.03	128.60
1	1A	365	G	C5-C6-O6	9.14	134.09	128.60
1	1A	2902	G	N1-C2-N3	-9.13	118.42	123.90
1	1A	642	G	O5'-P-OP2	-9.13	97.49	105.70
1	1A	238	C	C6-N1-C2	9.12	123.95	120.30
1	1A	1021	G	O5'-P-OP2	-9.12	97.49	105.70
1	1A	1995	G	C5-C6-O6	9.12	134.07	128.60
32	1a	1136	U	C5-C6-N1	9.12	127.26	122.70
1	1A	891	C	C5-C6-N1	-9.12	116.44	121.00
1	1A	1237	G	C5-N7-C8	9.12	108.86	104.30
1	1A	1701	A	N9-C4-C5	-9.11	102.16	105.80
1	1A	2331	G	O4'-C1'-N9	9.11	115.48	108.20
1	1A	1003	U	C6-N1-C2	-9.10	115.54	121.00
1	1A	125	A	C5-C6-N1	9.09	122.25	117.70
1	1A	82	G	C8-N9-C4	9.08	110.03	106.40
32	2a	665	A	O5'-P-OP2	-9.08	97.53	105.70
1	1A	1803	G	N7-C8-N9	-9.07	108.56	113.10
32	1a	884	U	O5'-P-OP2	-9.07	97.54	105.70
32	1a	1495	U	N1-C2-O2	9.06	129.14	122.80
1	1A	1814	A	C2-N3-C4	9.05	115.13	110.60
1	1A	598	A	O5'-P-OP1	-9.05	97.56	105.70
1	2A	1914	C	C6-N1-C2	-9.05	116.68	120.30
1	1A	2876	U	N1-C2-O2	9.04	129.13	122.80
1	1A	2158	C	C6-N1-C2	-9.04	116.69	120.30
1	2A	9	U	C2-N3-C4	9.04	132.42	127.00
1	2A	773	U	O5'-P-OP1	-9.03	97.57	105.70
1	2A	2699	C	C6-N1-C2	9.04	123.91	120.30
1	1A	96	C	O5'-P-OP2	-9.03	97.57	105.70
1	1A	354	A	C4-C5-N7	9.03	115.22	110.70
1	1A	1690	G	N1-C6-O6	-9.03	114.48	119.90
1	1A	2069	U	C5-C4-O4	-9.03	120.48	125.90
32	2a	487	A	C8-N9-C4	9.03	109.41	105.80
1	2A	33	U	N3-C2-O2	-9.03	115.88	122.20
1	1A	1060	U	O5'-P-OP2	-9.02	97.58	105.70
1	1A	2067	C	C6-N1-C2	9.02	123.91	120.30
1	1A	1980	C	N3-C4-C5	-9.01	118.29	121.90
1	1A	932	C	C6-N1-C2	-9.01	116.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2258	G	N7-C8-N9	-9.01	108.60	113.10
1	1A	2608	U	N1-C2-O2	-9.00	116.50	122.80
1	1A	1986	G	C8-N9-C4	9.00	110.00	106.40
1	1A	1655	A	N7-C8-N9	-9.00	109.30	113.80
1	1A	1826	C	C2-N3-C4	-8.99	115.40	119.90
32	1a	1530	G	N3-C4-C5	8.99	133.09	128.60
1	1A	1282	G	C8-N9-C4	8.98	109.99	106.40
1	2A	2502	G	O5'-P-OP2	-8.98	97.62	105.70
1	1A	1505	C	N3-C2-O2	-8.98	115.62	121.90
1	1A	2596	U	O5'-P-OP1	8.98	121.47	110.70
1	2A	1696	G	O5'-P-OP2	-8.98	97.62	105.70
1	2A	2306	C	N1-C2-O2	8.97	124.28	118.90
1	1A	493	G	O5'-P-OP2	-8.97	97.63	105.70
1	1A	1723	A	C8-N9-C4	8.97	109.39	105.80
1	2A	1913	A	C4-C5-C6	8.97	121.48	117.00
32	2a	1024	G	C2-N3-C4	8.97	116.38	111.90
1	2A	1614	A	O5'-P-OP1	-8.96	97.64	105.70
1	2A	906	G	N9-C4-C5	8.96	108.98	105.40
1	1A	2802	C	C2-N1-C1'	-8.95	108.95	118.80
32	1a	699	C	C6-N1-C2	-8.95	116.72	120.30
1	1A	2316	G	O5'-P-OP1	-8.95	97.64	105.70
1	1A	519	G	C8-N9-C4	-8.95	102.82	106.40
1	1A	1001	G	C2-N3-C4	-8.95	107.43	111.90
1	1A	2574	U	N3-C2-O2	-8.94	115.94	122.20
1	1A	20	C	C2-N3-C4	-8.93	115.43	119.90
1	1A	952	G	N1-C6-O6	-8.93	114.54	119.90
1	1A	581	G	N1-C6-O6	-8.93	114.54	119.90
1	1A	1346	U	P-O3'-C3'	8.92	130.41	119.70
1	2A	1906	G	O5'-P-OP1	-8.92	97.67	105.70
32	2a	1465	C	C5-C4-N4	-8.92	113.95	120.20
1	1A	2828	G	N1-C6-O6	-8.92	114.55	119.90
16	1U	33	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	1A	2561	G	O5'-P-OP2	-8.92	97.67	105.70
1	1A	1177	G	C5-C6-O6	8.91	133.95	128.60
1	1A	96	C	C6-N1-C2	-8.91	116.73	120.30
1	1A	1992	A	O5'-P-OP2	8.91	121.39	110.70
1	1A	2069	U	N3-C4-C5	8.91	119.95	114.60
1	1A	1427	G	C5-C6-O6	8.91	133.94	128.60
32	1a	825	G	N1-C6-O6	-8.91	114.56	119.90
32	2a	1436	U	C2-N3-C4	-8.90	121.66	127.00
1	1A	223	C	N1-C2-O2	8.90	124.24	118.90
1	2A	774	A	O5'-P-OP2	-8.89	97.69	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1278	U	C5-C6-N1	8.89	127.14	122.70
1	1A	1663	C	N1-C2-O2	-8.88	113.57	118.90
1	1A	2065	C	N1-C2-O2	-8.88	113.58	118.90
1	2A	832	G	O5'-P-OP2	8.87	121.35	110.70
1	1A	474	U	O5'-P-OP2	-8.87	97.72	105.70
1	1A	1958	A	O4'-C1'-N9	8.87	115.29	108.20
32	1a	1384	C	C6-N1-C2	-8.86	116.75	120.30
1	1A	365	G	N1-C6-O6	-8.86	114.58	119.90
1	1A	1148	C	O5'-P-OP1	8.86	121.33	110.70
1	2A	2855	C	C6-N1-C2	-8.85	116.76	120.30
1	1A	2630	G	C8-N9-C4	-8.84	102.86	106.40
1	1A	1705	C	C6-N1-C2	-8.84	116.76	120.30
1	1A	554	A	C6-N1-C2	-8.84	113.30	118.60
1	2A	1690	A	N1-C6-N6	8.84	123.90	118.60
1	1A	45	C	N3-C4-N4	-8.83	111.82	118.00
1	1A	2331	G	C8-N9-C4	-8.83	102.87	106.40
32	2a	1530	G	N3-C4-C5	8.82	133.01	128.60
1	1A	2251	G	N1-C6-O6	-8.82	114.61	119.90
1	2A	1776	G	O5'-P-OP2	-8.82	97.76	105.70
1	1A	733	G	C8-N9-C4	8.82	109.93	106.40
1	2A	2207	G	C6-C5-N7	-8.82	125.11	130.40
1	1A	848	G	N1-C6-O6	-8.81	114.61	119.90
32	2a	1495	U	N3-C2-O2	-8.81	116.03	122.20
1	1A	1747	A	O5'-P-OP1	-8.81	97.77	105.70
1	1A	121	G	O5'-P-OP2	-8.80	97.78	105.70
32	2a	472	A	C8-N9-C4	-8.80	102.28	105.80
1	1A	731	G	N1-C6-O6	-8.80	114.62	119.90
1	2A	1793	C	N3-C4-C5	8.80	125.42	121.90
1	1A	731	G	C2-N3-C4	8.80	116.30	111.90
1	1A	2858	G	C4-C5-N7	-8.80	107.28	110.80
32	1a	1530	G	C4-C5-N7	8.79	114.32	110.80
1	1A	874	U	C2-N3-C4	-8.79	121.73	127.00
1	1A	475	A	C8-N9-C4	8.78	109.31	105.80
1	2A	476	G	O5'-P-OP2	-8.78	97.80	105.70
1	1A	934	A	O4'-C1'-N9	8.78	115.22	108.20
1	1A	2611	G	N1-C6-O6	-8.78	114.64	119.90
1	2A	484	C	O5'-P-OP2	-8.78	97.80	105.70
1	2A	2167	U	N3-C2-O2	-8.77	116.06	122.20
32	1a	460	G	C8-N9-C4	-8.77	102.89	106.40
1	1A	799	A	C8-N9-C4	8.76	109.31	105.80
1	2A	2523	G	O5'-P-OP2	-8.76	97.82	105.70
1	1A	2674	A	C8-N9-C4	-8.76	102.30	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2245	U	N1-C2-N3	8.75	120.15	114.90
1	1A	2586	G	C5-C6-O6	8.75	133.85	128.60
1	2A	2207	G	N7-C8-N9	8.75	117.47	113.10
1	1A	1505	C	N1-C2-O2	8.74	124.14	118.90
1	1A	829	A	O5'-P-OP1	-8.73	97.84	105.70
32	1a	158	G	N9-C4-C5	8.73	108.89	105.40
1	1A	2034	G	C5-C6-O6	8.72	133.84	128.60
1	1A	809	U	C5-C4-O4	-8.72	120.67	125.90
1	2A	1187	G	C5-C6-O6	8.72	133.83	128.60
32	2a	884	U	O5'-P-OP2	-8.72	97.85	105.70
1	1A	1151	U	N1-C2-N3	-8.72	109.67	114.90
1	1A	2001	C	C2-N3-C4	-8.72	115.54	119.90
1	1A	1296	G	N1-C6-O6	-8.72	114.67	119.90
1	2A	1204	A	C8-N9-C4	8.71	109.28	105.80
1	1A	2425	G	O5'-P-OP2	-8.71	97.86	105.70
1	1A	1567	G	C8-N9-C4	-8.69	102.92	106.40
32	1a	404	U	N3-C2-O2	-8.69	116.11	122.20
1	2A	415	A	O5'-P-OP2	-8.69	97.88	105.70
1	1A	491	G	C6-N1-C2	-8.68	119.89	125.10
32	2a	530	G	N3-C4-C5	-8.68	124.26	128.60
1	1A	1725	G	C8-N9-C4	-8.68	102.93	106.40
1	1A	37	C	O5'-P-OP2	-8.67	97.89	105.70
1	1A	702	A	C5-N7-C8	-8.67	99.56	103.90
1	1A	1167	C	C6-N1-C2	-8.67	116.83	120.30
1	1A	102	U	C5-C4-O4	-8.67	120.70	125.90
1	1A	1769	G	N1-C6-O6	-8.67	114.70	119.90
1	1A	2047	C	N1-C2-O2	-8.66	113.70	118.90
1	1A	2046	G	C8-N9-C4	8.65	109.86	106.40
1	1A	2331	G	N7-C8-N9	8.65	117.43	113.10
1	2A	1926	U	C5-C4-O4	8.65	131.09	125.90
32	2a	1034	G	N3-C4-C5	-8.65	124.28	128.60
1	1A	1846	A	C6-N1-C2	-8.64	113.41	118.60
1	2A	1351	C	OP1-P-O3'	8.64	124.22	105.20
1	1A	735	U	C2-N3-C4	-8.64	121.81	127.00
2	2B	5	C	C6-N1-C2	8.64	123.76	120.30
1	1A	130	G	C4-C5-N7	-8.63	107.35	110.80
1	1A	1392	G	C5-C6-O6	8.63	133.78	128.60
1	1A	638	U	O5'-P-OP2	-8.62	97.94	105.70
32	1a	148	G	N3-C4-C5	-8.63	124.29	128.60
1	1A	747	G	N1-C6-O6	-8.62	114.73	119.90
1	1A	2579	G	N7-C8-N9	-8.62	108.79	113.10
1	1A	472	G	N1-C6-O6	8.61	125.07	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2612	A	C5-C6-N6	8.61	130.59	123.70
32	1a	135	C	O5'-P-OP1	8.61	121.03	110.70
1	1A	1245	C	C2-N3-C4	-8.61	115.60	119.90
1	1A	1620	G	N1-C6-O6	8.61	125.06	119.90
2	1B	70	C	O5'-P-OP2	-8.61	97.95	105.70
1	2A	2207	G	N1-C6-O6	8.61	125.07	119.90
32	1a	498	U	C5-C4-O4	8.60	131.06	125.90
1	2A	566	U	OP2-P-O3'	8.60	124.12	105.20
1	2A	1694	C	O5'-P-OP1	-8.60	97.96	105.70
1	1A	2802	C	N1-C2-O2	-8.60	113.74	118.90
1	2A	718	A	N1-C6-N6	8.60	123.76	118.60
1	1A	592	U	N1-C2-O2	-8.60	116.78	122.80
1	1A	1986	G	N3-C2-N2	8.59	125.92	119.90
1	1A	2780	C	N3-C2-O2	-8.59	115.89	121.90
1	1A	494	G	C5-C6-O6	8.59	133.75	128.60
32	2a	993	G	N3-C4-N9	8.59	131.15	126.00
1	1A	2452	C	C6-N1-C2	8.58	123.73	120.30
1	1A	2430	A	C2-N3-C4	8.58	114.89	110.60
1	2A	35	G	C5-C6-O6	8.57	133.74	128.60
1	1A	1130	A	N1-C6-N6	-8.57	113.46	118.60
1	1A	2587	C	N3-C4-C5	8.57	125.33	121.90
1	1A	1474	C	C2-N1-C1'	-8.56	109.38	118.80
1	2A	1087	G	N3-C4-N9	-8.56	120.86	126.00
1	2A	645	C	C5-C6-N1	8.56	125.28	121.00
1	1A	1259	A	C5-N7-C8	8.56	108.18	103.90
1	2A	1992	G	C6-N1-C2	-8.56	119.97	125.10
32	2a	1370	G	N9-C4-C5	-8.55	101.98	105.40
1	1A	554	A	C5-C6-N6	-8.55	116.86	123.70
1	2A	1265	A	O5'-P-OP2	-8.55	98.00	105.70
1	1A	1821	C	N1-C2-O2	-8.55	113.77	118.90
1	1A	2606	C	C4-C5-C6	8.55	121.67	117.40
1	1A	641	G	N3-C2-N2	8.55	125.88	119.90
13	1R	2	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	1A	2630	G	C5-N7-C8	8.54	108.57	104.30
1	1A	1050	C	C2-N3-C4	-8.53	115.63	119.90
32	2a	791	G	N3-C4-C5	8.53	132.87	128.60
1	1A	34	C	O4'-C1'-N1	8.53	115.02	108.20
1	2A	1097	U	C2-N1-C1'	8.53	127.93	117.70
1	1A	2134	G	N3-C4-C5	-8.53	124.34	128.60
32	2a	299	G	N1-C6-O6	8.53	125.02	119.90
1	1A	720	C	N3-C4-C5	8.52	125.31	121.90
1	1A	2840	G	O5'-P-OP2	-8.52	98.03	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1187	G	N1-C6-O6	-8.52	114.79	119.90
32	2a	1027	C	N1-C2-O2	8.52	124.01	118.90
1	1A	1099	C	C5-C6-N1	8.51	125.26	121.00
1	1A	1024	G	C5-C6-O6	8.51	133.70	128.60
1	1A	1291	G	C5-C6-O6	8.51	133.70	128.60
1	1A	859	C	O5'-P-OP1	-8.50	98.05	105.70
32	1a	355	C	C6-N1-C2	-8.50	116.90	120.30
1	1A	398	A	N1-C6-N6	8.50	123.70	118.60
1	1A	1824	C	C2-N3-C4	-8.50	115.65	119.90
32	1a	158	G	N3-C4-N9	-8.49	120.91	126.00
1	2A	527	C	N1-C2-O2	-8.49	113.81	118.90
1	2A	341	G	O5'-P-OP2	-8.49	98.06	105.70
1	1A	1826	C	N3-C4-C5	8.49	125.30	121.90
1	1A	2234	G	C8-N9-C4	8.48	109.79	106.40
1	2A	1913	A	N1-C2-N3	8.48	133.54	129.30
1	1A	731	G	C5-C6-N1	8.47	115.74	111.50
1	1A	1341	C	N3-C2-O2	-8.47	115.97	121.90
32	2a	709	G	C8-N9-C4	-8.47	103.01	106.40
1	1A	181	C	N1-C2-O2	-8.46	113.82	118.90
1	1A	735	U	N1-C2-N3	8.46	119.98	114.90
32	1a	888	G	O5'-P-OP2	-8.46	98.08	105.70
32	1a	1067	A	P-O3'-C3'	8.46	129.85	119.70
1	1A	1518	A	O5'-P-OP1	-8.46	98.09	105.70
1	1A	2024	G	C5-N7-C8	8.46	108.53	104.30
1	1A	854	U	C2-N3-C4	-8.46	121.93	127.00
1	2A	2319	G	N3-C4-C5	8.45	132.83	128.60
32	2a	266	G	C4-N9-C1'	8.45	137.49	126.50
1	1A	1831	C	N3-C4-C5	-8.45	118.52	121.90
1	1A	809	U	C2-N1-C1'	8.45	127.84	117.70
1	2A	958	U	C6-N1-C2	-8.44	115.93	121.00
1	1A	837	C	O5'-P-OP2	-8.44	98.10	105.70
32	2a	1054	C	C2-N1-C1'	8.44	128.08	118.80
1	2A	1471	A	C8-N9-C4	-8.44	102.42	105.80
32	2a	266	G	P-O3'-C3'	8.43	129.82	119.70
1	1A	902	G	N3-C2-N2	8.43	125.80	119.90
1	1A	952	G	C8-N9-C4	-8.43	103.03	106.40
32	2a	1034	G	C6-N1-C2	-8.43	120.04	125.10
1	1A	591	U	C2-N3-C4	-8.43	121.94	127.00
32	1a	479	C	N3-C4-C5	-8.42	118.53	121.90
2	1B	50	G	N1-C6-O6	-8.42	114.85	119.90
1	2A	214	G	O4'-C1'-N9	8.42	114.94	108.20
1	1A	214	A	O5'-P-OP2	-8.41	98.13	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	841	G	C5-C6-O6	8.41	133.65	128.60
1	1A	2056	U	N3-C4-O4	-8.41	113.51	119.40
1	1A	2063	U	C2-N3-C4	-8.41	121.96	127.00
1	1A	2607	G	N1-C6-O6	-8.40	114.86	119.90
1	2A	1834	U	N3-C2-O2	-8.40	116.32	122.20
1	1A	660	C	C6-N1-C2	-8.39	116.94	120.30
1	1A	39	C	O5'-P-OP2	-8.39	98.15	105.70
1	1A	2277	U	C4-C5-C6	8.39	124.73	119.70
32	2a	656	C	C5-C6-N1	8.39	125.19	121.00
1	1A	1301	U	O5'-P-OP2	-8.38	98.16	105.70
1	1A	1474	C	C6-N1-C2	8.38	123.65	120.30
1	1A	2702	C	N1-C2-O2	-8.38	113.87	118.90
1	1A	793	A	O4'-C1'-N9	8.37	114.90	108.20
1	1A	2639	G	C5-C6-N1	8.37	115.69	111.50
32	1a	874	G	C8-N9-C4	8.37	109.75	106.40
1	1A	2510	C	C5-C4-N4	8.37	126.06	120.20
1	1A	403	C	N3-C2-O2	-8.36	116.05	121.90
32	2a	1030	C	C2-N1-C1'	8.36	128.00	118.80
32	2a	1003	G	C4-N9-C1'	8.36	137.37	126.50
32	1a	781	A	N9-C4-C5	-8.36	102.46	105.80
1	1A	809	U	O5'-P-OP1	-8.35	98.18	105.70
32	2a	1422	G	O5'-P-OP2	-8.35	98.19	105.70
32	1a	914	A	C8-N9-C4	-8.33	102.47	105.80
1	2A	2850	A	C8-N9-C4	-8.33	102.47	105.80
1	1A	2627	U	N3-C2-O2	-8.33	116.37	122.20
1	1A	1859	G	C5-C6-N1	-8.33	107.34	111.50
1	1A	582	G	N7-C8-N9	8.32	117.26	113.10
1	1A	2883	A	O5'-P-OP2	-8.32	98.21	105.70
32	2a	1125	U	C2-N1-C1'	8.32	127.69	117.70
32	1a	204	U	C5-C6-N1	8.32	126.86	122.70
1	1A	405	C	C5-C4-N4	-8.32	114.38	120.20
1	1A	1092	A	O4'-C1'-N9	8.32	114.85	108.20
1	1A	2193	A	N1-C6-N6	8.32	123.59	118.60
1	2A	741	G	C5-C6-O6	8.32	133.59	128.60
1	1A	2320	G	C4-C5-N7	8.31	114.12	110.80
1	1A	2383	G	C5-C6-N1	8.31	115.66	111.50
32	1a	750	G	O5'-P-OP1	-8.31	98.22	105.70
1	1A	499	G	N1-C6-O6	-8.31	114.92	119.90
1	1A	494	G	C4-C5-N7	-8.30	107.48	110.80
1	1A	1282	G	N7-C8-N9	-8.30	108.95	113.10
32	2a	1003	G	N7-C8-N9	8.30	117.25	113.10
1	1A	433	G	O5'-P-OP1	-8.30	98.23	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	251	A	C2-N3-C4	-8.29	106.45	110.60
1	2A	2467	C	N3-C4-C5	-8.29	118.58	121.90
32	2a	375	U	O5'-P-OP1	-8.29	98.24	105.70
1	1A	1559	C	O5'-P-OP1	-8.28	98.25	105.70
1	1A	2277	U	N3-C4-O4	8.28	125.19	119.40
1	2A	1778	U	C5-C6-N1	-8.28	118.56	122.70
1	1A	2700	U	N1-C2-O2	-8.27	117.01	122.80
1	1A	2397	C	O5'-P-OP1	-8.26	98.26	105.70
32	1a	1077	G	O5'-P-OP2	-8.26	98.27	105.70
1	2A	2427	C	O5'-P-OP1	-8.26	98.27	105.70
1	2A	2629	A	O4'-C1'-N9	8.26	114.81	108.20
1	1A	2598	C	N3-C2-O2	8.24	127.67	121.90
1	1A	1056	A	C8-N9-C4	8.24	109.10	105.80
1	1A	1092	A	C8-N9-C4	-8.24	102.50	105.80
1	1A	591	U	C5-C4-O4	-8.24	120.96	125.90
32	1a	1422	G	O5'-P-OP2	-8.23	98.29	105.70
1	1A	495	G	C4-C5-N7	-8.23	107.51	110.80
1	1A	1539	C	N3-C2-O2	-8.23	116.14	121.90
1	1A	2439	C	C5-C6-N1	-8.23	116.89	121.00
1	2A	2596	U	C2-N3-C4	-8.23	122.06	127.00
1	1A	98	U	N3-C2-O2	-8.23	116.44	122.20
1	1A	1862	G	C5-C6-N1	-8.23	107.39	111.50
2	1B	31	C	O5'-P-OP2	-8.23	98.30	105.70
1	1A	991	G	O5'-P-OP2	8.22	120.57	110.70
1	1A	2244	U	C5-C6-N1	-8.22	118.59	122.70
1	2A	992	C	C6-N1-C2	-8.22	117.01	120.30
1	2A	1983	C	N1-C2-O2	-8.22	113.97	118.90
1	1A	422	U	N1-C2-O2	8.22	128.55	122.80
1	1A	2620	G	N1-C6-O6	8.22	124.83	119.90
32	1a	165	C	C6-N1-C2	-8.21	117.01	120.30
1	2A	892	G	O5'-P-OP1	-8.21	98.31	105.70
32	1a	299	G	C5-C6-N1	8.21	115.61	111.50
1	1A	836	A	O5'-P-OP2	8.21	120.55	110.70
1	1A	2331	G	N3-C2-N2	-8.21	114.15	119.90
1	1A	2067	C	C4-C5-C6	8.21	121.50	117.40
1	2A	2319	G	N3-C4-N9	-8.20	121.08	126.00
1	2A	1992	G	C2-N3-C4	8.19	116.00	111.90
1	2A	416	C	O5'-P-OP1	8.19	120.53	110.70
32	2a	750	G	O5'-P-OP1	-8.19	98.33	105.70
1	1A	2111	U	C5-C4-O4	-8.19	120.99	125.90
32	1a	174	C	C6-N1-C2	-8.19	117.03	120.30
1	1A	486	A	N1-C6-N6	-8.18	113.69	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2839	C	C6-N1-C2	-8.18	117.03	120.30
1	1A	1294	G	N3-C2-N2	8.18	125.63	119.90
32	2a	830	G	N1-C6-O6	8.18	124.81	119.90
1	1A	2526	U	O5'-P-OP1	-8.18	98.34	105.70
1	1A	665	C	O5'-P-OP2	-8.18	98.34	105.70
1	1A	1522	G	N3-C2-N2	-8.18	114.18	119.90
32	2a	1027	C	C6-N1-C2	-8.18	117.03	120.30
1	1A	665	C	N3-C2-O2	8.17	127.62	121.90
1	1A	2639	G	C8-N9-C4	8.17	109.67	106.40
1	1A	2372	A	O5'-P-OP2	-8.16	98.35	105.70
32	2a	346	G	C6-N1-C2	-8.16	120.20	125.10
1	2A	1210	A	P-O3'-C3'	8.16	129.49	119.70
32	2a	726	C	O5'-P-OP1	-8.16	98.36	105.70
1	1A	215	G	O4'-C1'-N9	8.15	114.72	108.20
1	1A	592	U	C5-C6-N1	-8.15	118.62	122.70
1	1A	472	G	C6-C5-N7	-8.15	125.51	130.40
32	1a	1276	G	C8-N9-C4	-8.15	103.14	106.40
1	1A	355	A	N1-C6-N6	8.14	123.49	118.60
32	2a	904	C	N3-C4-N4	8.14	123.70	118.00
1	1A	1453	C	C5-C6-N1	-8.13	116.94	121.00
32	2a	299	G	N9-C4-C5	-8.13	102.15	105.40
1	1A	2034	G	N1-C6-O6	-8.12	115.03	119.90
1	1A	2598	C	C5-C4-N4	-8.12	114.51	120.20
1	1A	1716	A	N1-C2-N3	8.12	133.36	129.30
14	1S	3	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	2A	1380	G	O5'-P-OP2	-8.12	98.39	105.70
1	2A	2257	U	O5'-P-OP1	-8.12	98.39	105.70
1	1A	495	G	N3-C2-N2	-8.12	114.22	119.90
1	1A	873	U	C5-C6-N1	-8.12	118.64	122.70
1	1A	1986	G	N1-C2-N2	-8.12	108.90	116.20
1	1A	2193	A	C5-C6-N6	-8.12	117.21	123.70
1	1A	2227	G	C4-N9-C1'	-8.12	115.95	126.50
1	2A	961	C	C6-N1-C2	8.12	123.55	120.30
1	1A	2386	C	C6-N1-C2	8.11	123.55	120.30
1	1A	958	C	C6-N1-C2	-8.11	117.06	120.30
32	2a	115	G	C8-N9-C4	-8.11	103.16	106.40
1	1A	1863	C	C6-N1-C2	-8.11	117.06	120.30
1	2A	248	G	C8-N9-C4	-8.11	103.16	106.40
1	2A	2032	G	C5-N7-C8	8.11	108.36	104.30
1	2A	450	G	N1-C6-O6	-8.11	115.04	119.90
1	2A	1984	G	C8-N9-C4	-8.11	103.16	106.40
32	1a	1512	U	N3-C4-O4	-8.10	113.73	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1233	G	N1-C6-O6	-8.09	115.05	119.90
32	2a	5	U	C5-C6-N1	8.09	126.75	122.70
1	1A	827	G	N1-C2-N3	8.09	128.75	123.90
1	2A	11	G	N7-C8-N9	8.09	117.14	113.10
27	25	58	LEU	CA-CB-CG	8.09	133.90	115.30
32	2a	1158	C	C2-N1-C1'	8.09	127.69	118.80
1	1A	2033	U	C6-N1-C2	-8.08	116.15	121.00
1	1A	189	U	O5'-P-OP2	-8.08	98.43	105.70
1	1A	192	C	C6-N1-C2	8.08	123.53	120.30
1	1A	1606	G	O5'-P-OP2	-8.08	98.43	105.70
1	1A	883	G	C8-N9-C4	-8.07	103.17	106.40
1	1A	1418	U	N3-C4-O4	8.07	125.05	119.40
1	1A	2598	C	C2-N3-C4	-8.07	115.86	119.90
1	1A	2823	A	N1-C6-N6	-8.07	113.76	118.60
1	1A	1701	A	C8-N9-C4	8.07	109.03	105.80
1	1A	1104	G	N9-C4-C5	-8.06	102.17	105.40
1	2A	391	G	C6-N1-C2	-8.06	120.26	125.10
1	1A	2587	C	C2-N3-C4	-8.06	115.87	119.90
32	1a	250	A	C8-N9-C4	-8.06	102.58	105.80
1	1A	2375	C	C6-N1-C2	8.06	123.52	120.30
1	1A	1681	A	N9-C4-C5	8.05	109.02	105.80
1	2A	1881	C	O5'-P-OP1	-8.05	98.45	105.70
1	2A	2008	C	O5'-P-OP2	-8.05	98.45	105.70
1	1A	1411	A	C8-N9-C4	8.05	109.02	105.80
1	1A	1379	C	N3-C4-C5	8.04	125.12	121.90
1	1A	1341	C	C2-N3-C4	-8.04	115.88	119.90
1	1A	2618	C	N1-C2-O2	-8.04	114.08	118.90
32	1a	841	U	C2-N1-C1'	8.04	127.34	117.70
1	2A	2017	U	C5-C6-N1	-8.04	118.68	122.70
1	1A	2442	A	N1-C6-N6	-8.03	113.78	118.60
32	1a	175	C	O5'-P-OP1	-8.03	98.47	105.70
1	2A	912	C	C5-C6-N1	8.03	125.02	121.00
1	2A	1372	U	C5-C4-O4	-8.03	121.08	125.90
1	1A	2171	G	C4-N9-C1'	-8.03	116.06	126.50
1	1A	2596	U	N3-C4-O4	-8.03	113.78	119.40
1	2A	12	U	N3-C2-O2	-8.03	116.58	122.20
1	1A	1758	C	OP1-P-OP2	-8.03	107.56	119.60
1	1A	1270	C	C5-C6-N1	-8.03	116.99	121.00
32	1a	297	G	C2-N3-C4	-8.03	107.89	111.90
1	1A	1155	C	N3-C4-N4	8.02	123.61	118.00
1	1A	2804	C	C6-N1-C2	-8.02	117.09	120.30
1	1A	838	C	C6-N1-C2	8.01	123.50	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1573	G	N3-C2-N2	-8.01	114.29	119.90
1	2A	2071	A	O5'-P-OP1	-8.01	98.49	105.70
1	1A	2200	C	C6-N1-C2	-8.01	117.10	120.30
32	2a	1026	G	C8-N9-C4	-8.01	103.20	106.40
1	1A	515	G	N3-C2-N2	-8.00	114.30	119.90
1	1A	2082	A	N1-C6-N6	-8.00	113.80	118.60
32	2a	913	A	P-O3'-C3'	8.00	129.30	119.70
1	1A	1065	U	O5'-P-OP2	-8.00	98.50	105.70
1	1A	1232	G	O5'-P-OP1	8.00	120.30	110.70
1	1A	1973	U	C5-C6-N1	-7.99	118.70	122.70
32	2a	625	G	C8-N9-C4	-7.99	103.20	106.40
1	1A	1043	G	OP1-P-OP2	-7.99	107.61	119.60
1	2A	1975	G	O5'-P-OP2	-7.99	98.51	105.70
1	1A	501	U	O5'-P-OP1	-7.99	98.51	105.70
1	2A	11	G	C6-C5-N7	-7.99	125.61	130.40
1	1A	2404	A	O5'-P-OP1	-7.99	98.51	105.70
1	2A	469	G	C5-C6-O6	-7.99	123.81	128.60
1	2A	2611	U	O5'-P-OP1	-7.99	98.51	105.70
1	1A	1418	U	C5-C4-O4	-7.97	121.11	125.90
2	2B	54	G	N3-C2-N2	-7.97	114.32	119.90
1	2A	1764	G	N1-C6-O6	-7.97	115.12	119.90
1	1A	752	A	C5-C6-N6	-7.97	117.32	123.70
1	1A	2084	A	O5'-P-OP1	-7.97	98.53	105.70
1	1A	1330	A	O5'-P-OP2	-7.97	98.53	105.70
1	1A	2257	U	C5-C4-O4	-7.97	121.12	125.90
2	2B	59	A	C6-N1-C2	-7.97	113.82	118.60
1	2A	1900	A	O5'-P-OP1	-7.96	98.53	105.70
1	1A	2638	C	C2-N3-C4	-7.96	115.92	119.90
1	1A	1121	C	N1-C2-O2	7.96	123.67	118.90
1	2A	976	C	N1-C2-O2	7.96	123.67	118.90
1	1A	1472	G	N1-C6-O6	7.96	124.67	119.90
1	1A	1377	A	N9-C4-C5	7.96	108.98	105.80
1	1A	2091	G	C5-C6-N1	7.95	115.48	111.50
1	1A	2030	C	C2-N3-C4	-7.95	115.92	119.90
1	2A	277	C	N1-C2-O2	7.95	123.67	118.90
1	2A	1968	G	N1-C6-O6	7.95	124.67	119.90
32	1a	183	G	C8-N9-C4	-7.95	103.22	106.40
1	2A	1662	C	N3-C4-C5	7.95	125.08	121.90
1	1A	766	C	N3-C4-C5	7.95	125.08	121.90
1	1A	735	U	C4-C5-C6	7.94	124.46	119.70
1	1A	1430	A	C8-N9-C4	-7.94	102.62	105.80
1	2A	447	A	C8-N9-C4	7.93	108.97	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	533	A	C4-C5-C6	7.93	120.97	117.00
1	2A	1079	C	O4'-C1'-N1	7.93	114.54	108.20
1	1A	2595	G	C8-N9-C4	7.93	109.57	106.40
1	2A	1692	U	O5'-P-OP2	-7.93	98.57	105.70
1	1A	466	G	C5-C6-N1	-7.92	107.54	111.50
1	1A	579	G	N9-C4-C5	7.92	108.57	105.40
32	2a	1482	G	C5-C6-O6	7.92	133.35	128.60
1	1A	1426	G	N1-C6-O6	7.92	124.65	119.90
1	1A	52	A	C8-N9-C4	-7.92	102.63	105.80
1	1A	1735	U	OP1-P-OP2	7.91	131.47	119.60
1	1A	2042	A	N1-C2-N3	-7.91	125.34	129.30
1	1A	241	G	N9-C4-C5	7.91	108.56	105.40
1	1A	2006	G	N1-C6-O6	-7.91	115.15	119.90
32	1a	343	U	O4'-C1'-N1	7.91	114.53	108.20
1	1A	233	A	O5'-P-OP2	-7.91	98.58	105.70
1	1A	952	G	N3-C4-N9	-7.91	121.25	126.00
1	2A	2080	G	O5'-P-OP2	-7.91	98.58	105.70
1	1A	1179	U	O5'-P-OP2	-7.91	98.58	105.70
1	1A	1303	C	C4-C5-C6	7.91	121.35	117.40
1	2A	2597	G	O5'-P-OP2	-7.91	98.58	105.70
32	2a	316	G	O5'-P-OP2	-7.91	98.58	105.70
1	1A	553	A	O5'-P-OP1	7.91	120.19	110.70
1	1A	1365	G	C8-N9-C4	-7.91	103.24	106.40
1	1A	2624	C	C6-N1-C2	7.90	123.46	120.30
1	2A	529	A	C4-C5-N7	7.90	114.65	110.70
1	1A	1240	G	N1-C6-O6	-7.90	115.16	119.90
1	2A	11	G	N1-C6-O6	7.90	124.64	119.90
1	2A	2626	C	C6-N1-C2	7.90	123.46	120.30
1	1A	1193	C	O5'-P-OP2	-7.90	98.59	105.70
1	1A	1681	A	C8-N9-C4	-7.89	102.64	105.80
32	1a	186	C	C6-N1-C2	-7.89	117.14	120.30
32	1a	533	A	N3-C4-N9	7.89	133.71	127.40
1	2A	1758	G	O5'-P-OP1	-7.89	98.60	105.70
1	1A	2158	C	N1-C2-O2	7.89	123.63	118.90
1	1A	1719	C	C6-N1-C2	-7.89	117.14	120.30
32	1a	560	U	C6-N1-C2	-7.89	116.27	121.00
32	2a	266	G	N7-C8-N9	7.89	117.04	113.10
1	1A	847	A	N1-C6-N6	-7.89	113.87	118.60
1	1A	1833	A	O5'-P-OP1	-7.89	98.60	105.70
1	2A	1936	A	O4'-C1'-N9	7.89	114.51	108.20
1	1A	1826	C	C5-C6-N1	-7.89	117.06	121.00
1	2A	2269	A	O5'-P-OP1	-7.89	98.60	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	857	C	O5'-P-OP2	-7.88	98.60	105.70
1	1A	569	G	C8-N9-C4	-7.88	103.25	106.40
2	1B	33	G	O5'-P-OP2	-7.88	98.61	105.70
1	1A	2576	A	N1-C6-N6	7.87	123.32	118.60
32	1a	174	C	C2-N1-C1'	7.87	127.46	118.80
1	2A	1790	C	C6-N1-C2	7.87	123.45	120.30
1	1A	742	G	N1-C6-O6	-7.87	115.18	119.90
1	1A	835	A	C5-N7-C8	7.87	107.83	103.90
1	1A	2638	C	C5-C4-N4	-7.87	114.69	120.20
1	2A	1664	A	O5'-P-OP2	-7.87	98.62	105.70
1	2A	1791	A	C8-N9-C4	-7.87	102.65	105.80
32	1a	576	G	N3-C4-N9	7.86	130.72	126.00
1	2A	1251	C	N3-C4-N4	7.86	123.50	118.00
1	1A	2257	U	C6-N1-C2	7.86	125.72	121.00
1	1A	1012	C	N3-C4-C5	7.86	125.04	121.90
1	1A	1264	G	C2-N3-C4	-7.86	107.97	111.90
32	1a	1513	A	C2-N3-C4	7.86	114.53	110.60
1	1A	932	C	C5-C6-N1	7.86	124.93	121.00
1	1A	918	U	N3-C4-O4	7.86	124.90	119.40
32	1a	670	G	N1-C6-O6	-7.86	115.19	119.90
1	1A	891	C	C6-N1-C2	7.86	123.44	120.30
1	1A	2014	G	C5-N7-C8	7.85	108.23	104.30
1	1A	1800	G	O5'-P-OP2	-7.85	98.63	105.70
1	1A	2572	C	C2-N3-C4	-7.85	115.97	119.90
19	2X	57	LEU	CA-CB-CG	7.85	133.36	115.30
1	1A	1177	G	N1-C6-O6	-7.85	115.19	119.90
1	2A	72	U	O5'-P-OP1	-7.84	98.64	105.70
1	1A	369	A	C5-C6-N6	-7.84	117.43	123.70
1	1A	1364	C	O5'-P-OP2	7.84	120.11	110.70
1	1A	35	G	N1-C6-O6	-7.83	115.20	119.90
1	1A	1486	G	O5'-P-OP2	-7.83	98.65	105.70
1	2A	601	C	C6-N1-C2	-7.83	117.17	120.30
1	1A	751	G	O4'-C1'-N9	7.83	114.46	108.20
1	1A	892	G	O4'-C1'-N9	7.82	114.46	108.20
1	2A	1771	C	N3-C4-C5	7.82	125.03	121.90
32	1a	156	G	C8-N9-C4	-7.82	103.27	106.40
1	2A	1298	C	O5'-P-OP2	-7.82	98.66	105.70
1	1A	618	C	O5'-P-OP2	-7.82	98.67	105.70
1	2A	1630	G	N9-C4-C5	7.82	108.53	105.40
1	1A	101	A	N1-C6-N6	7.82	123.29	118.60
1	1A	271	U	C5-C4-O4	7.81	130.59	125.90
1	1A	1175	A	OP1-P-OP2	7.81	131.32	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	316	C	O5'-P-OP1	-7.81	98.67	105.70
1	1A	1916	C	C6-N1-C2	-7.81	117.18	120.30
1	1A	2624	C	OP1-P-OP2	7.81	131.31	119.60
1	1A	813	C	C4-C5-C6	7.80	121.30	117.40
1	2A	744	G	O5'-P-OP2	-7.80	98.67	105.70
8	1I	38	LEU	CA-CB-CG	7.80	133.25	115.30
1	2A	633	A	O5'-P-OP1	-7.80	98.68	105.70
1	2A	2032	G	N7-C8-N9	-7.80	109.20	113.10
32	2a	1432	G	N1-C6-O6	-7.80	115.22	119.90
1	1A	191	U	C2-N3-C4	-7.80	122.32	127.00
1	2A	956	G	N1-C6-O6	7.80	124.58	119.90
32	2a	1125	U	N3-C4-O4	-7.80	113.94	119.40
1	1A	184	A	P-O3'-C3'	7.79	129.05	119.70
1	2A	463	G	C5-C6-O6	7.79	133.28	128.60
1	1A	2639	G	N9-C4-C5	-7.79	102.28	105.40
1	1A	2738	A	C2-N3-C4	-7.79	106.71	110.60
1	1A	1213	U	O5'-P-OP2	-7.79	98.69	105.70
1	1A	2335	G	C5-N7-C8	-7.79	100.41	104.30
1	1A	2610	A	C8-N9-C4	7.79	108.91	105.80
1	1A	1262	C	N1-C2-O2	-7.78	114.23	118.90
1	1A	1317	G	OP1-P-OP2	-7.78	107.93	119.60
1	1A	2403	G	O5'-P-OP2	-7.78	98.70	105.70
1	1A	2804	C	N3-C4-C5	-7.78	118.79	121.90
1	2A	2689	U	P-O3'-C3'	7.78	129.03	119.70
1	2A	906	G	C8-N9-C4	-7.78	103.29	106.40
32	1a	1003	G	N3-C4-C5	-7.77	124.71	128.60
1	1A	556	C	C2-N3-C4	-7.77	116.01	119.90
1	2A	1848	A	C8-N9-C4	7.77	108.91	105.80
1	1A	2220	A	O4'-C1'-N9	7.77	114.42	108.20
1	2A	794	G	O5'-P-OP2	-7.77	98.71	105.70
1	1A	2551	C	C5-C6-N1	-7.76	117.12	121.00
1	2A	568	U	C5-C4-O4	-7.76	121.24	125.90
1	1A	1036	A	N1-C2-N3	-7.76	125.42	129.30
32	1a	57	G	C8-N9-C4	-7.76	103.30	106.40
1	2A	780	G	C5-C6-O6	-7.76	123.94	128.60
1	1A	2256	U	C2-N3-C4	-7.76	122.34	127.00
32	1a	1158	C	C4-C5-C6	7.76	121.28	117.40
1	1A	1958	A	C5-N7-C8	-7.75	100.02	103.90
1	1A	779	C	C6-N1-C2	-7.75	117.20	120.30
1	1A	1959	A	C5-C6-N6	7.75	129.90	123.70
32	2a	1335	C	N1-C2-O2	7.75	123.55	118.90
32	2a	346	G	N3-C4-C5	-7.75	124.72	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	189(D)	C	C2-N1-C1'	7.75	127.33	118.80
32	1a	354	G	O5'-P-OP2	-7.75	98.73	105.70
1	1A	702	A	N7-C8-N9	7.74	117.67	113.80
1	2A	906	G	N3-C4-N9	-7.74	121.36	126.00
1	2A	2063	C	O5'-P-OP2	-7.74	98.74	105.70
32	2a	834	C	O5'-P-OP2	-7.74	98.74	105.70
32	1a	460	G	N7-C8-N9	7.73	116.97	113.10
1	2A	153	C	O5'-P-OP2	-7.73	98.74	105.70
1	2A	1721	G	N3-C4-N9	7.73	130.64	126.00
1	1A	2658	C	N3-C4-N4	-7.73	112.59	118.00
1	1A	1661	C	N3-C2-O2	-7.73	116.49	121.90
32	2a	1495	U	C2-N1-C1'	7.73	126.98	117.70
1	1A	415	G	C8-N9-C4	7.73	109.49	106.40
1	1A	1232	G	O5'-P-OP2	-7.73	98.75	105.70
1	1A	1966	U	C2-N3-C4	-7.73	122.36	127.00
1	1A	2137	G	C8-N9-C4	-7.73	103.31	106.40
1	1A	2689	G	N1-C6-O6	-7.73	115.26	119.90
1	1A	2537	G	O5'-P-OP2	-7.73	98.75	105.70
32	2a	142	G	C8-N9-C4	-7.72	103.31	106.40
1	1A	413	G	C8-N9-C4	-7.72	103.31	106.40
1	1A	1007	G	C8-N9-C4	-7.72	103.31	106.40
1	1A	2188	G	N3-C4-N9	-7.72	121.37	126.00
1	1A	2194	U	N3-C2-O2	-7.72	116.80	122.20
1	2A	979	G	O5'-P-OP1	-7.72	98.75	105.70
32	2a	142	G	N3-C4-C5	-7.72	124.74	128.60
1	1A	2767	U	N1-C2-O2	7.72	128.20	122.80
1	1A	1831	C	C6-N1-C2	-7.72	117.21	120.30
1	1A	718	C	C5-C4-N4	7.71	125.60	120.20
1	1A	1411	A	N9-C4-C5	-7.71	102.71	105.80
1	1A	1668	G	O5'-P-OP2	-7.71	98.76	105.70
32	2a	458	C	C6-N1-C2	-7.71	117.22	120.30
1	1A	2453	C	N1-C2-N3	7.71	124.60	119.20
1	1A	2510	C	N3-C4-N4	-7.71	112.60	118.00
1	1A	2517	G	C5-C6-N1	-7.71	107.64	111.50
1	1A	2624	C	O5'-P-OP1	-7.71	98.76	105.70
1	1A	1811	A	C8-N9-C4	-7.71	102.72	105.80
1	2A	2362	G	C4-C5-N7	7.71	113.88	110.80
1	1A	1377	A	OP1-P-O3'	-7.70	88.26	105.20
1	1A	1702	A	N1-C6-N6	-7.70	113.98	118.60
1	1A	2277	U	OP1-P-OP2	-7.70	108.05	119.60
1	1A	2292	G	N1-C6-O6	-7.70	115.28	119.90
32	1a	635	G	O5'-P-OP2	7.70	119.94	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1689	A	N1-C6-N6	7.70	123.22	118.60
1	2A	2041	U	C5-C4-O4	-7.70	121.28	125.90
1	2A	2805	G	N3-C4-N9	7.70	130.62	126.00
1	1A	591	U	N3-C4-C5	7.70	119.22	114.60
1	1A	2752	U	C5-C6-N1	-7.70	118.85	122.70
32	2a	472	A	N7-C8-N9	7.70	117.65	113.80
1	1A	191	U	N3-C4-C5	7.69	119.22	114.60
1	1A	271	U	C6-N1-C1'	7.69	131.97	121.20
1	1A	122	G	N3-C2-N2	7.69	125.28	119.90
1	2A	9	U	C5-C6-N1	7.69	126.55	122.70
1	1A	1000	C	N3-C4-N4	-7.69	112.62	118.00
32	1a	795	C	N1-C2-O2	-7.69	114.29	118.90
1	1A	519	G	N7-C8-N9	7.68	116.94	113.10
1	1A	2505	U	OP2-P-O3'	7.68	122.11	105.20
1	1A	2262	G	OP1-P-OP2	7.68	131.12	119.60
1	1A	405	C	C2-N3-C4	-7.68	116.06	119.90
1	2A	1774	C	C5-C6-N1	7.68	124.84	121.00
1	1A	2630	G	C5-C6-O6	7.68	133.21	128.60
1	1A	725	C	C2-N3-C4	-7.67	116.06	119.90
1	2A	383	U	N1-C2-O2	7.67	128.17	122.80
1	2A	988	A	N1-C6-N6	7.67	123.20	118.60
1	2A	2362	G	C5-C6-O6	-7.67	124.00	128.60
1	1A	1497	G	O5'-P-OP2	-7.67	98.79	105.70
1	1A	1571	G	OP1-P-OP2	7.67	131.11	119.60
1	1A	195	U	C2-N3-C4	-7.67	122.40	127.00
32	2a	686	U	N1-C2-N3	7.67	119.50	114.90
32	2a	908	A	O5'-P-OP2	-7.67	98.80	105.70
1	1A	223	C	N3-C2-O2	-7.67	116.53	121.90
32	1a	615	C	C6-N1-C2	-7.67	117.23	120.30
32	2a	1003	G	N3-C4-N9	7.67	130.60	126.00
1	1A	1155	C	C2-N1-C1'	7.66	127.23	118.80
1	1A	2278	A	O5'-P-OP1	-7.66	98.80	105.70
32	2a	993	G	N3-C4-C5	-7.66	124.77	128.60
1	1A	1766	G	N7-C8-N9	7.66	116.93	113.10
1	1A	354	A	N1-C2-N3	7.66	133.13	129.30
1	1A	733	G	N9-C4-C5	-7.66	102.34	105.40
1	2A	1836	C	O5'-P-OP1	7.66	119.89	110.70
1	2A	2177	C	C6-N1-C2	-7.65	117.24	120.30
1	1A	832	G	C5-C6-O6	7.65	133.19	128.60
1	1A	1052	C	C4-C5-C6	7.65	121.22	117.40
1	2A	1639	U	O5'-P-OP1	7.65	119.88	110.70
1	1A	957	A	OP1-P-OP2	7.64	131.07	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	474	U	C2-N3-C4	-7.64	122.41	127.00
1	1A	150	C	N3-C4-N4	-7.64	112.65	118.00
1	1A	447	C	C6-N1-C2	7.64	123.36	120.30
1	1A	10	G	N1-C6-O6	-7.64	115.32	119.90
1	1A	1099	C	N3-C4-C5	-7.64	118.84	121.90
1	1A	1147	U	N1-C2-O2	7.64	128.15	122.80
32	2a	16	A	N1-C6-N6	-7.64	114.02	118.60
1	1A	1199	C	N1-C2-O2	-7.63	114.32	118.90
1	1A	1630	A	O5'-P-OP2	-7.63	98.83	105.70
1	2A	2691	C	O5'-P-OP1	-7.63	98.83	105.70
32	2a	404	U	C2-N1-C1'	7.63	126.86	117.70
1	2A	2578	G	O5'-P-OP1	-7.63	98.83	105.70
1	2A	2827	C	C5-C4-N4	-7.63	114.86	120.20
1	1A	752	A	C4-C5-N7	7.63	114.52	110.70
1	1A	782	A	N9-C4-C5	7.63	108.85	105.80
1	1A	2284	U	N1-C2-N3	7.63	119.48	114.90
1	2A	1008	C	N1-C2-O2	7.63	123.48	118.90
1	2A	2399	G	N1-C6-O6	-7.63	115.32	119.90
1	1A	1319	U	C5-C4-O4	7.62	130.47	125.90
1	1A	409	G	C5-C6-O6	7.62	133.17	128.60
13	1R	2	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	1A	429	A	O5'-P-OP1	7.62	119.84	110.70
1	1A	2735	G	N7-C8-N9	-7.62	109.29	113.10
1	2A	2585	U	C5-C6-N1	-7.62	118.89	122.70
32	2a	791	G	N3-C4-N9	-7.62	121.43	126.00
1	2A	1082	U	C2-N1-C1'	7.62	126.84	117.70
1	1A	918	U	N3-C2-O2	7.62	127.53	122.20
1	1A	1453	C	C2-N3-C4	-7.61	116.09	119.90
1	2A	2896	C	C5-C6-N1	7.61	124.81	121.00
1	2A	1721	G	N3-C2-N2	7.61	125.23	119.90
1	1A	507	G	O5'-P-OP2	-7.61	98.85	105.70
1	1A	575	G	N1-C2-N2	-7.61	109.35	116.20
1	1A	1455	C	OP2-P-O3'	7.61	121.94	105.20
1	1A	2331	G	C4-C5-N7	7.61	113.84	110.80
1	1A	2597	U	C5-C4-O4	7.61	130.47	125.90
1	2A	2513	G	C8-N9-C4	-7.61	103.36	106.40
1	1A	1013	G	C5-C6-O6	7.61	133.16	128.60
1	1A	1128	U	C5-C6-N1	7.61	126.50	122.70
1	1A	2091	G	N1-C6-O6	-7.61	115.33	119.90
2	1B	32	C	N3-C4-C5	7.61	124.94	121.90
1	1A	335	A	OP1-P-OP2	-7.61	108.19	119.60
1	2A	221	A	O5'-P-OP1	-7.60	98.86	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	332	G	C8-N9-C4	7.60	109.44	106.40
1	1A	2448	G	N1-C6-O6	-7.60	115.34	119.90
32	2a	1028	C	C5-C6-N1	7.60	124.80	121.00
1	1A	202	A	OP2-P-O3'	7.60	121.92	105.20
1	1A	793	A	N7-C8-N9	7.60	117.60	113.80
1	1A	847	A	N9-C4-C5	7.60	108.84	105.80
1	1A	1816	A	C5-N7-C8	-7.59	100.10	103.90
1	2A	1617	C	N1-C2-O2	-7.59	114.34	118.90
1	1A	592	U	C2-N3-C4	-7.59	122.45	127.00
1	2A	2893	G	N3-C4-N9	7.59	130.55	126.00
1	1A	780	G	C5-N7-C8	7.58	108.09	104.30
1	1A	2080	A	N1-C2-N3	7.58	133.09	129.30
32	1a	181	G	C8-N9-C4	-7.58	103.37	106.40
32	1a	768	A	N7-C8-N9	-7.58	110.01	113.80
1	2A	1511	C	C6-N1-C2	-7.58	117.27	120.30
1	1A	2390	A	C4-C5-C6	7.58	120.79	117.00
32	2a	245	C	O5'-P-OP1	-7.58	98.88	105.70
1	1A	554	A	C5-C6-N1	7.58	121.49	117.70
1	1A	1807	G	N3-C4-N9	7.58	130.55	126.00
1	1A	2625	U	N3-C2-O2	-7.58	116.89	122.20
1	1A	1261	G	OP1-P-OP2	-7.58	108.24	119.60
1	1A	2591	C	C2-N3-C4	-7.58	116.11	119.90
1	2A	837	C	N1-C2-O2	-7.58	114.36	118.90
1	2A	2685	G	N1-C6-O6	-7.58	115.36	119.90
32	2a	5	U	C6-N1-C2	-7.58	116.45	121.00
1	1A	1822	A	O5'-P-OP2	7.57	119.78	110.70
1	1A	2718	G	C5-N7-C8	7.57	108.08	104.30
32	1a	58	C	O5'-P-OP1	-7.57	98.89	105.70
1	1A	2610	A	OP2-P-O3'	7.57	121.85	105.20
32	2a	530	G	N3-C4-N9	7.57	130.54	126.00
32	2a	1486	G	O5'-P-OP1	7.57	119.78	110.70
32	1a	46	G	O5'-P-OP2	7.57	119.78	110.70
1	1A	2593	G	N3-C2-N2	7.56	125.19	119.90
1	1A	1278	G	C4-C5-N7	-7.56	107.78	110.80
1	1A	2700	U	C4-C5-C6	7.56	124.24	119.70
1	1A	1054	C	N3-C2-O2	-7.56	116.61	121.90
2	1B	41	U	C5-C6-N1	-7.56	118.92	122.70
1	2A	659	C	C6-N1-C2	7.56	123.32	120.30
1	2A	1471	A	N7-C8-N9	7.56	117.58	113.80
1	1A	2354	C	O5'-P-OP2	7.55	119.76	110.70
1	2A	1903	G	N3-C2-N2	-7.55	114.61	119.90
32	2a	1183	A	P-O3'-C3'	7.55	128.76	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1823	G	C5-C6-O6	7.55	133.13	128.60
1	1A	2579	G	C4-C5-N7	-7.54	107.78	110.80
1	1A	494	G	C5-N7-C8	7.54	108.07	104.30
1	1A	2611	G	C5-C6-O6	7.54	133.12	128.60
1	1A	987	G	N1-C6-O6	-7.54	115.38	119.90
1	1A	1386	U	N3-C4-C5	7.54	119.12	114.60
1	2A	701	G	N3-C4-C5	7.54	132.37	128.60
32	2a	880	C	O5'-P-OP2	-7.54	98.92	105.70
1	1A	2636	G	N1-C6-O6	-7.54	115.38	119.90
32	1a	903	G	O5'-P-OP2	-7.53	98.92	105.70
32	2a	904	C	N1-C2-O2	-7.53	114.38	118.90
1	1A	1294	G	N1-C2-N2	-7.53	109.42	116.20
1	1A	738	C	C6-N1-C2	-7.53	117.29	120.30
1	1A	2134	G	C8-N9-C4	-7.53	103.39	106.40
1	1A	2576	A	C5-C6-N6	-7.53	117.68	123.70
1	1A	2657	G	C5-N7-C8	-7.53	100.54	104.30
1	2A	2378	A	N9-C4-C5	-7.53	102.79	105.80
1	1A	2640	C	N3-C4-C5	7.52	124.91	121.90
32	1a	799	G	C5-C6-O6	7.52	133.11	128.60
1	1A	88	G	C8-N9-C4	-7.52	103.39	106.40
1	1A	2111	U	N3-C4-C5	7.52	119.11	114.60
1	1A	2296	C	N3-C4-C5	-7.52	118.89	121.90
1	1A	1076	G	C2-N3-C4	-7.52	108.14	111.90
32	1a	543	C	C6-N1-C2	-7.52	117.29	120.30
1	2A	1145	C	C6-N1-C2	-7.52	117.29	120.30
32	2a	346	G	C2-N3-C4	7.52	115.66	111.90
1	1A	2704	C	C2-N3-C4	-7.51	116.14	119.90
1	1A	777	C	O5'-P-OP1	-7.51	98.94	105.70
1	1A	1359	U	O5'-P-OP2	7.51	119.72	110.70
1	2A	2355	C	O5'-P-OP1	-7.51	98.94	105.70
1	1A	1067	A	C6-N1-C2	-7.51	114.10	118.60
1	1A	1842	G	N1-C6-O6	-7.51	115.40	119.90
1	1A	1700	G	P-O3'-C3'	7.50	128.71	119.70
1	1A	1294	G	C4-C5-N7	7.50	113.80	110.80
1	2A	1066	U	N1-C2-N3	7.50	119.40	114.90
32	2a	343	U	N3-C4-C5	7.50	119.10	114.60
1	1A	810	G	N1-C2-N2	-7.50	109.45	116.20
32	1a	1515	C	O5'-P-OP2	-7.50	98.95	105.70
1	1A	1725	G	N3-C2-N2	-7.50	114.65	119.90
32	1a	1279	A	C8-N9-C4	-7.50	102.80	105.80
1	1A	1875	C	C6-N1-C2	7.50	123.30	120.30
1	2A	2794	C	C5-C6-N1	7.50	124.75	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2696	U	O5'-P-OP1	-7.49	98.95	105.70
1	1A	82	G	C2-N3-C4	-7.49	108.15	111.90
1	1A	2158	C	N3-C2-O2	-7.49	116.66	121.90
1	1A	1994	A	C5-N7-C8	-7.49	100.15	103.90
1	1A	1365	G	N7-C8-N9	7.49	116.84	113.10
1	1A	2024	G	N7-C8-N9	-7.49	109.36	113.10
32	2a	1378	C	C6-N1-C2	-7.49	117.31	120.30
1	1A	1330	A	OP1-P-OP2	7.49	130.83	119.60
1	1A	2428	C	N3-C4-N4	-7.49	112.76	118.00
1	1A	149	A	O5'-P-OP1	-7.48	98.97	105.70
1	1A	2625	U	N1-C2-O2	7.48	128.04	122.80
1	2A	251	A	N1-C2-N3	7.48	133.04	129.30
1	1A	859	C	N1-C2-O2	-7.48	114.41	118.90
1	1A	2060	G	C5-N7-C8	7.48	108.04	104.30
32	1a	639	G	C8-N9-C4	-7.48	103.41	106.40
1	2A	1046	A	C8-N9-C4	-7.48	102.81	105.80
1	1A	60	G	N3-C2-N2	-7.47	114.67	119.90
1	1A	990	A	O5'-P-OP1	7.47	119.67	110.70
1	2A	527	C	C2-N1-C1'	-7.47	110.58	118.80
1	2A	1253	A	C5-N7-C8	7.47	107.64	103.90
32	1a	299	G	C4-C5-N7	7.47	113.79	110.80
32	1a	804	U	O5'-P-OP1	7.47	119.67	110.70
1	2A	1983	C	N3-C2-O2	7.47	127.13	121.90
1	1A	2010	C	C2-N3-C4	-7.47	116.17	119.90
1	1A	2341	G	C5-C6-O6	-7.47	124.12	128.60
2	1B	1	U	C5-C6-N1	7.47	126.44	122.70
1	1A	1278	G	O5'-P-OP1	-7.46	98.98	105.70
32	1a	738	C	C6-N1-C2	-7.46	117.31	120.30
1	1A	1420	G	O5'-P-OP2	7.46	119.66	110.70
1	2A	1275	A	C8-N9-C4	7.46	108.78	105.80
32	2a	902	G	C5-N7-C8	7.46	108.03	104.30
1	1A	2618	C	C4-C5-C6	7.46	121.13	117.40
1	1A	2649	U	N3-C2-O2	-7.46	116.98	122.20
32	1a	863	U	C2-N1-C1'	-7.46	108.75	117.70
1	1A	315	C	O5'-P-OP1	-7.46	98.99	105.70
32	1a	914	A	O5'-P-OP1	-7.46	98.99	105.70
32	1a	1442	G	C2-N3-C4	7.46	115.63	111.90
1	1A	1965	U	C2-N3-C4	-7.45	122.53	127.00
1	1A	582	G	C8-N9-C4	-7.45	103.42	106.40
1	1A	2038	U	N3-C4-O4	-7.44	114.19	119.40
1	2A	697	C	N3-C4-C5	-7.44	118.92	121.90
1	2A	2185	C	N1-C2-O2	7.44	123.36	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1109	G	N1-C2-N3	-7.44	119.44	123.90
32	1a	1176	A	C8-N9-C4	-7.44	102.83	105.80
1	2A	572	A	C8-N9-C4	-7.44	102.83	105.80
1	1A	322	G	O5'-P-OP1	7.43	119.62	110.70
1	1A	2511	C	C2-N3-C4	7.43	123.62	119.90
32	1a	754	C	N1-C2-O2	7.43	123.36	118.90
32	1a	1522	U	OP1-P-OP2	7.43	130.75	119.60
2	1B	79	C	N3-C2-O2	-7.43	116.70	121.90
1	2A	990	A	O5'-P-OP2	-7.43	99.01	105.70
1	1A	826	U	N3-C4-O4	7.43	124.60	119.40
1	1A	1336	C	C6-N1-C2	-7.43	117.33	120.30
1	1A	1427	G	N1-C6-O6	-7.43	115.44	119.90
1	2A	35	G	N1-C6-O6	-7.43	115.44	119.90
1	1A	220	C	C4-C5-C6	7.43	121.11	117.40
1	1A	1855	G	O5'-P-OP2	-7.43	99.02	105.70
1	1A	2597	U	C5-C6-N1	-7.43	118.99	122.70
32	1a	174	C	N1-C2-O2	7.43	123.36	118.90
1	2A	1309	G	O5'-P-OP1	7.43	119.61	110.70
32	2a	1219	U	C5-C6-N1	7.43	126.41	122.70
1	1A	649	C	C2-N3-C4	-7.42	116.19	119.90
1	1A	702	A	N3-C4-N9	-7.42	121.46	127.40
1	1A	1992	A	O5'-P-OP1	-7.42	99.02	105.70
1	1A	2826	C	O5'-P-OP2	-7.42	99.02	105.70
1	1A	2673	G	N1-C6-O6	-7.42	115.45	119.90
32	1a	1486	G	N1-C6-O6	7.42	124.35	119.90
1	2A	271(K)	U	C6-N1-C2	-7.42	116.55	121.00
32	2a	493	G	O5'-P-OP1	-7.42	99.02	105.70
1	1A	2038	U	C5-C4-O4	7.42	130.35	125.90
1	2A	885	C	C5-C6-N1	7.42	124.71	121.00
32	2a	340	U	O5'-P-OP2	-7.42	99.02	105.70
32	1a	191	G	C8-N9-C4	-7.42	103.43	106.40
1	2A	1074	G	O5'-P-OP2	-7.42	99.02	105.70
1	1A	260	A	C8-N9-C4	7.42	108.77	105.80
1	1A	878	G	C2-N3-C4	-7.42	108.19	111.90
1	1A	1783	C	N1-C2-O2	-7.41	114.45	118.90
32	1a	1021	G	C2-N3-C4	7.41	115.61	111.90
1	2A	2451	A	C5-N7-C8	-7.41	100.19	103.90
32	2a	896	C	C6-N1-C2	7.41	123.26	120.30
1	2A	1051	G	N1-C6-O6	7.41	124.34	119.90
2	1B	50	G	O5'-P-OP2	-7.41	99.03	105.70
32	1a	897	C	O5'-P-OP2	-7.41	99.03	105.70
1	1A	2460	A	C5-C6-N1	7.41	121.40	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2550	C	N3-C4-C5	7.41	124.86	121.90
1	1A	2788	A	C8-N9-C4	7.40	108.76	105.80
32	1a	189(D)	C	N1-C2-O2	7.40	123.34	118.90
1	1A	641	G	C5-C6-O6	7.40	133.04	128.60
1	1A	1102	G	N9-C4-C5	-7.40	102.44	105.40
1	1A	2535	G	C5-C6-O6	7.40	133.04	128.60
32	1a	326	G	C4-C5-N7	-7.40	107.84	110.80
1	1A	1371	G	N9-C4-C5	7.40	108.36	105.40
1	1A	2194	U	C6-N1-C2	-7.40	116.56	121.00
1	1A	2272	C	C4-C5-C6	7.40	121.10	117.40
1	2A	673	C	N1-C2-O2	-7.40	114.46	118.90
1	1A	2598	C	N3-C4-N4	7.40	123.18	118.00
32	1a	996	A	C8-N9-C4	-7.40	102.84	105.80
1	1A	125	A	C2-N3-C4	7.39	114.30	110.60
1	1A	274	U	C5-C4-O4	-7.39	121.46	125.90
1	1A	451	G	C5-C6-N1	7.39	115.20	111.50
1	1A	1746	G	O5'-P-OP2	-7.39	99.05	105.70
1	1A	903	C	C5-C6-N1	7.39	124.69	121.00
32	2a	5	U	C2-N1-C1'	7.39	126.57	117.70
32	1a	577	G	OP2-P-O3'	7.39	121.45	105.20
1	2A	791	C	C2-N3-C4	-7.39	116.21	119.90
1	1A	2294	G	N3-C2-N2	7.38	125.07	119.90
32	1a	1211	U	C5-C6-N1	-7.38	119.01	122.70
1	1A	1210	G	C4-C5-N7	-7.38	107.85	110.80
32	1a	605	U	C5-C4-O4	7.38	130.33	125.90
1	1A	486	A	N9-C4-C5	7.38	108.75	105.80
1	1A	985	G	C5-N7-C8	7.38	107.99	104.30
1	1A	2780	C	C6-N1-C2	-7.38	117.35	120.30
1	2A	2699	C	C5-C6-N1	-7.38	117.31	121.00
1	1A	1341	C	N3-C4-C5	7.37	124.85	121.90
1	1A	1518	A	C8-N9-C4	-7.37	102.85	105.80
32	1a	172	A	C8-N9-C4	-7.37	102.85	105.80
1	1A	2063	U	N1-C2-N3	7.37	119.32	114.90
1	2A	2894	G	N3-C4-N9	-7.37	121.58	126.00
32	2a	65	U	P-O3'-C3'	7.37	128.54	119.70
1	1A	2832	G	C5-C6-O6	-7.37	124.18	128.60
1	2A	1271	G	C8-N9-C4	7.37	109.35	106.40
1	1A	2460	A	N7-C8-N9	-7.37	110.12	113.80
1	2A	1647	G	C5-C6-O6	-7.37	124.18	128.60
1	1A	881	C	N1-C2-O2	-7.37	114.48	118.90
1	1A	2548	G	C2-N3-C4	-7.37	108.22	111.90
32	1a	557	G	N3-C4-N9	7.37	130.42	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	574	A	N1-C6-N6	7.37	123.02	118.60
1	1A	2818	U	N3-C2-O2	7.36	127.36	122.20
32	2a	990	C	N1-C2-O2	7.36	123.32	118.90
1	2A	445	C	N1-C2-O2	-7.36	114.48	118.90
1	2A	2454	G	C5-C6-O6	7.36	133.02	128.60
1	1A	2188	G	C4-N9-C1'	-7.36	116.93	126.50
1	1A	2858	G	N3-C2-N2	-7.36	114.75	119.90
32	2a	428	G	O5'-P-OP2	-7.36	99.08	105.70
1	1A	492	A	N1-C6-N6	-7.36	114.19	118.60
1	1A	718	C	N3-C4-N4	-7.36	112.85	118.00
1	1A	751	G	N3-C2-N2	-7.36	114.75	119.90
1	1A	1255	A	P-O3'-C3'	7.36	128.53	119.70
32	1a	13	U	C5-C6-N1	-7.35	119.02	122.70
1	2A	2220	G	N3-C2-N2	-7.35	114.75	119.90
1	2A	785	G	O5'-P-OP2	-7.35	99.08	105.70
1	1A	2788	A	N7-C8-N9	-7.35	110.12	113.80
1	1A	1361	C	C2-N3-C4	-7.35	116.23	119.90
32	2a	909	A	N1-C6-N6	7.35	123.01	118.60
1	1A	648	G	N1-C6-O6	-7.34	115.49	119.90
1	1A	1013	G	N1-C6-O6	-7.34	115.49	119.90
1	1A	2487	C	N1-C2-O2	-7.34	114.49	118.90
1	1A	2260	C	N3-C4-C5	7.34	124.84	121.90
1	2A	135	G	OP2-P-O3'	7.34	121.35	105.20
1	2A	740	U	O5'-P-OP2	-7.34	99.09	105.70
1	1A	807	G	C2-N3-C4	-7.34	108.23	111.90
1	1A	975	U	C5-C4-O4	-7.34	121.50	125.90
1	1A	27	G	O4'-C1'-N9	7.34	114.07	108.20
1	1A	2459	G	OP2-P-O3'	7.34	121.34	105.20
1	1A	790	G	C5-C6-O6	7.34	133.00	128.60
32	1a	1505	G	N9-C4-C5	7.34	108.33	105.40
1	2A	1203	G	C4-C5-N7	7.34	113.73	110.80
1	2A	1969	A	OP1-P-O3'	7.34	121.34	105.20
32	2a	1132	C	C6-N1-C2	-7.34	117.36	120.30
1	1A	2890	C	OP1-P-OP2	7.33	130.60	119.60
1	1A	1846	A	N1-C2-N3	7.33	132.97	129.30
32	1a	841	U	C5-C6-N1	7.33	126.37	122.70
2	1B	102	A	C6-N1-C2	-7.33	114.20	118.60
1	1A	1686	U	O5'-P-OP2	-7.33	99.10	105.70
1	2A	1678	G	C8-N9-C4	-7.33	103.47	106.40
1	2A	2388	A	O5'-P-OP1	7.33	119.49	110.70
32	2a	332	G	O5'-P-OP1	-7.33	99.11	105.70
32	1a	1523	G	O5'-P-OP2	-7.33	99.11	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1108	G	N3-C4-N9	7.33	130.40	126.00
1	1A	539	A	OP1-P-OP2	7.32	130.58	119.60
1	1A	2089	G	C8-N9-C4	-7.32	103.47	106.40
32	1a	1495	U	C2-N1-C1'	7.32	126.48	117.70
32	2a	1515	C	O5'-P-OP2	-7.32	99.11	105.70
1	1A	1655	A	C8-N9-C4	7.32	108.73	105.80
1	2A	1963	U	N1-C2-O2	7.31	127.92	122.80
1	1A	2111	U	C2-N3-C4	-7.31	122.61	127.00
1	2A	2157	G	C8-N9-C4	-7.31	103.47	106.40
32	2a	487	A	N7-C8-N9	-7.31	110.14	113.80
32	1a	405	U	O5'-P-OP1	-7.31	99.12	105.70
1	1A	1007	G	C2-N3-C4	7.31	115.55	111.90
32	2a	560	U	C6-N1-C2	-7.31	116.62	121.00
1	1A	2290	A	OP2-P-O3'	7.30	121.27	105.20
1	1A	2595	G	N7-C8-N9	-7.30	109.45	113.10
1	2A	203	C	O5'-P-OP2	-7.30	99.13	105.70
32	1a	483	C	C6-N1-C2	7.30	123.22	120.30
1	1A	1742	G	C4-C5-N7	7.30	113.72	110.80
32	2a	1532	U	C5-C6-N1	7.30	126.35	122.70
32	2a	1478	C	C6-N1-C2	-7.29	117.38	120.30
1	1A	2443	U	N3-C2-O2	-7.29	117.10	122.20
1	2A	1170	G	N1-C6-O6	7.29	124.28	119.90
1	1A	373	G	O5'-P-OP2	-7.29	99.14	105.70
1	1A	2069	U	C2-N3-C4	-7.29	122.63	127.00
1	1A	2106	C	C5-C6-N1	-7.29	117.36	121.00
1	1A	2526	U	OP1-P-OP2	7.29	130.53	119.60
1	2A	1941	C	N1-C2-O2	-7.29	114.53	118.90
1	1A	2588	G	C2-N3-C4	7.29	115.54	111.90
1	1A	2833	A	C8-N9-C4	-7.29	102.89	105.80
32	2a	562	C	C5-C4-N4	-7.29	115.10	120.20
1	1A	1394	G	N1-C6-O6	-7.28	115.53	119.90
1	1A	1720	U	N3-C2-O2	7.28	127.30	122.20
1	1A	217	A	C8-N9-C1'	7.28	140.80	127.70
2	1B	36	C	N1-C2-O2	-7.28	114.53	118.90
1	1A	1453	C	N1-C2-O2	-7.28	114.53	118.90
1	1A	1852	A	C2-N3-C4	7.28	114.24	110.60
1	2A	906	G	C4-C5-N7	-7.28	107.89	110.80
32	2a	797	C	O5'-P-OP2	7.28	119.43	110.70
1	1A	198	C	C2-N3-C4	-7.28	116.26	119.90
1	1A	1093	G	N3-C4-C5	-7.28	124.96	128.60
1	1A	1724	A	C2-N3-C4	-7.28	106.96	110.60
32	1a	825	G	OP2-P-O3'	7.28	121.21	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	913	A	P-O3'-C3'	7.28	128.43	119.70
1	1A	2138	G	C4-N9-C1'	7.27	135.96	126.50
1	1A	2689	G	C5-C6-O6	7.27	132.96	128.60
1	2A	834	C	N3-C2-O2	-7.27	116.81	121.90
1	1A	661	G	N1-C6-O6	7.27	124.26	119.90
1	1A	1437	U	C5-C4-O4	-7.27	121.54	125.90
1	1A	2883	A	OP1-P-OP2	7.27	130.51	119.60
1	2A	1075	C	C6-N1-C2	-7.27	117.39	120.30
1	1A	2517	G	C6-N1-C2	7.27	129.46	125.10
32	2a	1406	U	N1-C2-N3	7.27	119.26	114.90
1	1A	553	A	N3-C4-C5	-7.27	121.71	126.80
1	2A	2207	G	C4-N9-C1'	7.27	135.95	126.50
32	2a	1067	A	P-O3'-C3'	7.27	128.42	119.70
32	1a	784	C	C6-N1-C2	7.26	123.20	120.30
32	1a	1442	G	N3-C4-C5	-7.26	124.97	128.60
8	2I	116	LEU	CA-CB-CG	7.26	132.00	115.30
1	1A	1264	G	O5'-P-OP2	-7.26	99.17	105.70
32	2a	1505	G	O5'-P-OP2	-7.26	99.17	105.70
1	1A	1270	C	C2-N3-C4	-7.26	116.27	119.90
32	1a	560	U	N3-C2-O2	-7.26	117.12	122.20
1	1A	722	A	N1-C6-N6	7.25	122.95	118.60
1	1A	848	G	C8-N9-C4	-7.25	103.50	106.40
1	2A	2427	C	N1-C2-O2	-7.25	114.55	118.90
32	2a	506	G	O5'-P-OP1	-7.25	99.17	105.70
1	2A	912	C	N1-C2-O2	7.25	123.25	118.90
1	1A	98	U	C2-N1-C1'	7.25	126.40	117.70
1	1A	852	G	N3-C2-N2	7.25	124.97	119.90
1	1A	1456	G	N3-C4-C5	7.25	132.22	128.60
1	2A	2385	C	O5'-P-OP1	-7.25	99.18	105.70
1	1A	1618	A	O5'-P-OP2	-7.24	99.18	105.70
1	2A	1838	C	C6-N1-C2	-7.24	117.40	120.30
1	2A	2821	A	C8-N9-C4	7.24	108.70	105.80
32	1a	1217	C	O5'-P-OP2	-7.24	99.18	105.70
32	1a	343	U	C5-C6-N1	-7.24	119.08	122.70
32	1a	817	C	O5'-P-OP1	-7.24	99.18	105.70
1	1A	2033	U	N1-C2-N3	7.24	119.24	114.90
32	2a	1054	C	C6-N1-C1'	-7.24	112.11	120.80
1	1A	1783	C	N3-C2-O2	7.24	126.96	121.90
1	1A	2525	G	C2-N3-C4	-7.24	108.28	111.90
1	2A	856	C	P-O3'-C3'	7.24	128.38	119.70
1	2A	1925	C	N1-C2-O2	-7.24	114.56	118.90
1	1A	2604	G	C5-C6-O6	7.23	132.94	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	514	G	C5-C6-O6	7.23	132.94	128.60
1	2A	2511	U	N1-C2-O2	-7.23	117.74	122.80
1	1A	243	G	C5-C6-O6	7.23	132.94	128.60
1	1A	1269	G	N1-C6-O6	-7.23	115.56	119.90
1	1A	1807	G	C4-C5-N7	7.23	113.69	110.80
1	2A	247	G	C2-N3-C4	-7.23	108.28	111.90
1	2A	1902	C	O5'-P-OP2	7.23	119.37	110.70
1	2A	2041	U	N1-C2-O2	-7.23	117.74	122.80
1	2A	236	C	C5-C6-N1	-7.22	117.39	121.00
1	2A	2049	G	C5-C6-O6	7.22	132.94	128.60
32	2a	1158	C	N3-C2-O2	-7.22	116.84	121.90
1	1A	702	A	C2-N3-C4	-7.22	106.99	110.60
1	1A	1167	C	N3-C2-O2	-7.22	116.84	121.90
32	1a	841	U	C6-N1-C2	-7.22	116.67	121.00
32	1a	913	A	N9-C4-C5	7.22	108.69	105.80
32	1a	925	G	O5'-P-OP2	-7.22	99.20	105.70
1	2A	807	U	N1-C2-N3	7.22	119.23	114.90
32	2a	398	C	N3-C4-N4	-7.22	112.94	118.00
1	1A	504	A	C8-N9-C4	-7.22	102.91	105.80
1	2A	312	G	C5-C6-O6	-7.22	124.27	128.60
32	2a	1287	A	C5-C6-N6	7.22	129.47	123.70
1	2A	1236	G	O5'-P-OP1	-7.22	99.20	105.70
1	1A	820	U	C5-C6-N1	-7.21	119.09	122.70
1	1A	821	A	C8-N9-C4	-7.21	102.91	105.80
32	1a	889	A	OP1-P-OP2	7.21	130.42	119.60
32	2a	44	G	C2-N3-C4	-7.21	108.29	111.90
1	1A	215	G	N9-C4-C5	7.21	108.28	105.40
32	1a	667	G	O5'-P-OP1	7.21	119.36	110.70
1	1A	45	C	N3-C4-C5	7.21	124.78	121.90
1	1A	1832	G	O5'-P-OP1	-7.21	99.21	105.70
1	2A	353	G	N1-C6-O6	7.21	124.23	119.90
1	2A	474	G	N9-C4-C5	7.21	108.28	105.40
1	1A	1278	G	O5'-P-OP2	7.21	119.35	110.70
1	2A	792	G	O4'-C1'-N9	-7.21	102.43	108.20
1	2A	1046	A	C2-N3-C4	7.21	114.20	110.60
1	2A	1848	A	N7-C8-N9	-7.21	110.20	113.80
1	2A	2300	G	C8-N9-C4	-7.21	103.52	106.40
1	1A	50	G	O5'-P-OP2	-7.21	99.21	105.70
1	1A	725	C	C5-C6-N1	-7.21	117.40	121.00
1	1A	2023	A	N9-C4-C5	7.21	108.68	105.80
32	2a	485	G	N3-C4-C5	-7.21	125.00	128.60
1	1A	399	G	O4'-C1'-N9	7.20	113.96	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	444	C	C6-N1-C2	7.20	123.18	120.30
1	1A	903	C	N3-C4-C5	-7.20	119.02	121.90
1	2A	2505	G	C5-C6-O6	7.20	132.92	128.60
1	1A	1707	C	N3-C2-O2	-7.20	116.86	121.90
32	1a	888	G	C4-C5-N7	7.20	113.68	110.80
1	2A	608	A	C8-N9-C4	-7.20	102.92	105.80
1	1A	2516	U	N3-C4-C5	7.20	118.92	114.60
1	2A	2157	G	N7-C8-N9	7.20	116.70	113.10
1	1A	2240	G	C8-N9-C4	-7.19	103.52	106.40
1	2A	1984	G	N7-C8-N9	7.19	116.70	113.10
1	1A	330	U	N3-C4-C5	-7.19	110.28	114.60
1	1A	1853	G	N3-C2-N2	7.19	124.94	119.90
1	2A	1992	G	C5-C6-N1	7.19	115.09	111.50
1	2A	2378	A	C6-C5-N7	-7.19	127.27	132.30
1	1A	1181	G	N9-C4-C5	-7.19	102.53	105.40
1	1A	1396	C	N3-C4-C5	7.19	124.78	121.90
1	1A	2724	U	C5-C4-O4	-7.19	121.59	125.90
1	1A	472	G	C5-N7-C8	-7.19	100.71	104.30
1	2A	1979	C	C6-N1-C2	-7.19	117.42	120.30
1	1A	1035	G	C2-N3-C4	7.19	115.49	111.90
1	1A	1420	G	OP1-P-OP2	-7.18	108.83	119.60
1	2A	2138	C	C5-C6-N1	7.18	124.59	121.00
1	1A	2467	G	N1-C2-N2	-7.18	109.74	116.20
32	1a	57	G	O5'-P-OP1	-7.18	99.24	105.70
1	2A	668	G	O5'-P-OP1	-7.18	99.24	105.70
1	1A	832	G	N1-C6-O6	-7.18	115.59	119.90
1	1A	217	A	C4-C5-C6	-7.18	113.41	117.00
1	1A	666	C	C6-N1-C2	-7.18	117.43	120.30
1	1A	1917	C	C6-N1-C2	-7.18	117.43	120.30
1	1A	2453	C	C5-C6-N1	-7.18	117.41	121.00
32	1a	1067	A	C8-N9-C4	-7.18	102.93	105.80
1	2A	741	G	N9-C4-C5	7.18	108.27	105.40
32	2a	1163	C	C5-C6-N1	7.18	124.59	121.00
1	1A	184	A	C5-C6-N1	-7.17	114.11	117.70
1	1A	192	C	N3-C4-N4	-7.17	112.98	118.00
1	1A	677	C	N3-C4-C5	7.17	124.77	121.90
1	2A	598	G	N1-C6-O6	-7.17	115.59	119.90
1	1A	127	C	N1-C2-O2	-7.17	114.60	118.90
1	1A	2637	G	N1-C6-O6	-7.17	115.60	119.90
1	1A	2183	C	C6-N1-C2	-7.17	117.43	120.30
2	1B	28	C	O5'-P-OP2	-7.17	99.25	105.70
32	1a	183	G	N7-C8-N9	7.17	116.69	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1184	G	C5-C6-O6	-7.17	124.30	128.60
1	1A	1718	U	N3-C4-C5	7.17	118.90	114.60
10	1O	8	LEU	CA-CB-CG	7.17	131.79	115.30
1	2A	1783	A	O4'-C1'-N9	-7.17	102.47	108.20
1	1A	82	G	C6-C5-N7	-7.17	126.10	130.40
1	1A	923	C	O5'-P-OP1	-7.16	99.25	105.70
32	1a	763	G	O5'-P-OP2	-7.16	99.25	105.70
32	1a	1030	C	C5-C6-N1	7.16	124.58	121.00
32	1a	781	A	N1-C2-N3	-7.16	125.72	129.30
32	1a	1054	C	N3-C2-O2	-7.16	116.89	121.90
32	2a	912	C	C6-N1-C2	7.16	123.17	120.30
1	1A	2610	A	C5-N7-C8	7.16	107.48	103.90
32	2a	15	G	C8-N9-C4	-7.16	103.54	106.40
1	1A	716	G	N3-C4-C5	7.16	132.18	128.60
1	1A	2834	C	C2-N3-C4	7.16	123.48	119.90
32	2a	983	A	O5'-P-OP1	-7.16	99.26	105.70
32	2a	1499	A	C8-N9-C4	7.16	108.66	105.80
1	2A	1992	G	C2'-C3'-O3'	7.16	125.25	109.50
32	2a	218	C	N3-C4-C5	-7.16	119.04	121.90
1	1A	500	G	N1-C2-N2	-7.16	109.76	116.20
1	1A	2194	U	N3-C4-O4	-7.16	114.39	119.40
1	2A	1890	A	C8-N9-C4	7.16	108.66	105.80
32	2a	1027	C	N3-C2-O2	-7.16	116.89	121.90
1	1A	1210	G	C5-N7-C8	7.15	107.88	104.30
1	1A	126	C	N1-C2-O2	-7.15	114.61	118.90
1	1A	1804	A	N1-C6-N6	7.15	122.89	118.60
1	1A	905	U	O5'-P-OP2	-7.15	99.26	105.70
1	1A	2004	C	C5-C4-N4	7.15	125.20	120.20
1	2A	1992	G	P-O3'-C3'	7.15	128.28	119.70
1	1A	545	G	OP2-P-O3'	7.15	120.93	105.20
1	1A	2639	G	C6-N1-C2	-7.15	120.81	125.10
1	2A	482	A	O5'-P-OP2	-7.15	99.27	105.70
1	1A	1811	A	N7-C8-N9	7.14	117.37	113.80
1	1A	1827	U	C5-C6-N1	-7.14	119.13	122.70
1	1A	2173	G	N9-C1'-C2'	-7.14	104.14	112.00
32	2a	261	U	N1-C2-N3	7.14	119.19	114.90
1	1A	108	G	N1-C6-O6	-7.14	115.61	119.90
1	1A	2485	U	C2-N1-C1'	7.14	126.27	117.70
1	1A	2276	C	OP2-P-O3'	7.14	120.91	105.20
1	2A	507	A	C4-C5-C6	-7.14	113.43	117.00
1	2A	1008	C	N3-C2-O2	-7.14	116.90	121.90
1	1A	428	A	C8-N9-C4	-7.14	102.95	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2188	G	N3-C4-C5	7.14	132.17	128.60
27	15	58	LEU	CA-CB-CG	7.14	131.71	115.30
32	2a	299	G	C8-N9-C4	7.14	109.25	106.40
1	1A	1683	C	N1-C2-O2	7.13	123.18	118.90
1	1A	478	G	C5-C6-N1	7.13	115.07	111.50
1	1A	2833	A	N9-C4-C5	7.13	108.65	105.80
1	1A	1842	G	N9-C4-C5	7.13	108.25	105.40
1	1A	2201	C	C6-N1-C2	-7.13	117.45	120.30
1	1A	1428	G	N1-C6-O6	7.13	124.18	119.90
1	2A	988	A	C5-N7-C8	-7.13	100.34	103.90
1	1A	1130	A	C5-C6-N6	7.12	129.40	123.70
32	1a	158	G	N3-C2-N2	-7.12	114.91	119.90
32	1a	888	G	N3-C2-N2	7.12	124.89	119.90
32	2a	23	C	O5'-P-OP2	7.12	119.25	110.70
1	1A	436	C	C6-N1-C2	7.12	123.15	120.30
1	2A	1240	U	N3-C4-O4	7.12	124.39	119.40
1	2A	1605	C	C4-C5-C6	7.12	120.96	117.40
1	2A	1416	G	O4'-C1'-N9	7.12	113.90	108.20
1	1A	196	A	N1-C6-N6	7.12	122.87	118.60
1	1A	660	C	N3-C2-O2	-7.12	116.92	121.90
1	1A	194	G	N3-C2-N2	7.12	124.88	119.90
1	1A	883	G	N7-C8-N9	7.12	116.66	113.10
1	1A	1549	U	N1-C2-O2	-7.12	117.82	122.80
1	2A	90	U	C5-C4-O4	7.11	130.17	125.90
1	2A	193	U	N1-C2-O2	-7.11	117.82	122.80
32	2a	1507	A	C8-N9-C4	7.11	108.64	105.80
1	1A	2778	A	C4-C5-C6	7.11	120.56	117.00
2	1B	114	C	N3-C4-C5	7.11	124.75	121.90
1	1A	554	A	O4'-C1'-N9	7.11	113.89	108.20
1	2A	1202	C	O5'-P-OP2	-7.11	99.30	105.70
1	2A	2596	U	N1-C2-O2	-7.11	117.83	122.80
1	1A	1294	G	C8-N9-C4	7.11	109.24	106.40
1	1A	2443	U	C2-N3-C4	-7.11	122.74	127.00
1	1A	283	G	N9-C4-C5	7.10	108.24	105.40
1	2A	2454	G	N1-C6-O6	-7.10	115.64	119.90
1	1A	1207	C	N1-C2-O2	-7.10	114.64	118.90
1	1A	2320	G	C5-N7-C8	-7.10	100.75	104.30
1	1A	2395	G	C5-C6-O6	7.10	132.86	128.60
32	1a	724	G	OP1-P-O3'	7.10	120.82	105.20
1	1A	2593	G	N9-C4-C5	-7.10	102.56	105.40
1	2A	683	C	O5'-P-OP1	-7.10	99.31	105.70
1	2A	912	C	N3-C2-O2	-7.10	116.93	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2250	G	OP1-P-OP2	7.10	130.25	119.60
32	2a	144	G	C8-N9-C4	-7.10	103.56	106.40
1	1A	188	A	N9-C4-C5	7.10	108.64	105.80
1	1A	543	G	N1-C6-O6	-7.10	115.64	119.90
1	1A	583	C	C5-C6-N1	-7.10	117.45	121.00
1	1A	760	G	N9-C4-C5	-7.10	102.56	105.40
1	1A	2387	G	C5-C6-O6	-7.10	124.34	128.60
1	1A	1360	C	O5'-P-OP1	-7.10	99.31	105.70
32	1a	1495	U	N3-C2-O2	-7.10	117.23	122.20
32	2a	902	G	N1-C6-O6	-7.09	115.64	119.90
1	1A	1627	A	N1-C6-N6	7.09	122.86	118.60
1	1A	2244	U	O5'-P-OP2	-7.09	99.32	105.70
1	1A	2301	G	N1-C6-O6	7.09	124.15	119.90
1	1A	874	U	N3-C4-O4	-7.09	114.44	119.40
1	1A	198	C	N3-C4-C5	7.09	124.73	121.90
1	1A	800	C	N3-C4-N4	-7.09	113.04	118.00
32	1a	1286	A	N1-C6-N6	-7.09	114.35	118.60
1	1A	1810	U	O4'-C1'-N1	7.08	113.87	108.20
1	1A	271	U	C2-N1-C1'	-7.08	109.20	117.70
1	1A	1006	C	C2-N3-C4	-7.08	116.36	119.90
1	1A	1240	G	N9-C4-C5	7.08	108.23	105.40
1	1A	1821	C	N3-C2-O2	7.08	126.86	121.90
1	2A	1690	A	C5-C6-N6	-7.08	118.03	123.70
1	2A	2356	C	N1-C2-O2	-7.08	114.65	118.90
1	1A	1069	U	OP1-P-OP2	7.08	130.22	119.60
1	1A	1431	G	O4'-C1'-N9	7.08	113.86	108.20
1	1A	2590	G	C5-C6-O6	7.07	132.84	128.60
32	1a	1528	U	O5'-P-OP2	-7.07	99.33	105.70
1	1A	999	G	C5-C6-O6	7.07	132.84	128.60
1	1A	217	A	C5-C6-N1	7.07	121.23	117.70
1	1A	735	U	N3-C2-O2	-7.07	117.25	122.20
1	1A	1054	C	C5-C6-N1	7.07	124.53	121.00
1	1A	1851	U	N3-C2-O2	-7.07	117.25	122.20
1	1A	35	G	C5-N7-C8	7.07	107.83	104.30
1	1A	2718	G	N7-C8-N9	-7.07	109.57	113.10
1	2A	1128	A	C8-N9-C4	7.07	108.63	105.80
1	2A	1079	C	C6-N1-C2	-7.06	117.47	120.30
1	2A	2499	C	N1-C2-O2	-7.06	114.66	118.90
1	2A	2848	G	O4'-C1'-N9	7.06	113.85	108.20
1	1A	1072	U	N1-C2-O2	7.06	127.74	122.80
1	1A	1257	G	O4'-C1'-N9	7.06	113.85	108.20
1	1A	1035	G	N1-C6-O6	-7.06	115.66	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	71	U	O5'-P-OP1	-7.06	99.35	105.70
1	1A	436	C	N3-C4-C5	7.06	124.72	121.90
1	2A	1639	U	C5-C6-N1	-7.06	119.17	122.70
1	1A	2858	G	C6-C5-N7	7.06	134.63	130.40
32	1a	310	G	O5'-P-OP2	7.06	119.17	110.70
1	1A	352	U	N3-C2-O2	-7.06	117.26	122.20
1	2A	975	C	O5'-P-OP1	-7.06	99.35	105.70
32	2a	719	C	N1-C2-O2	-7.06	114.67	118.90
1	1A	166	G	C5-C6-O6	7.05	132.83	128.60
1	1A	183	G	N1-C6-O6	-7.05	115.67	119.90
1	1A	322	G	C5-N7-C8	7.05	107.83	104.30
1	1A	859	C	N3-C4-C5	7.05	124.72	121.90
1	1A	1046	A	O5'-P-OP1	-7.05	99.35	105.70
32	1a	441	A	O5'-P-OP2	-7.05	99.35	105.70
1	2A	2447	G	C6-N1-C2	-7.05	120.87	125.10
32	2a	1125	U	N3-C2-O2	-7.05	117.26	122.20
1	1A	2023	A	C2-N3-C4	7.05	114.13	110.60
2	1B	32	C	C6-N1-C2	7.05	123.12	120.30
1	2A	2834	G	N1-C6-O6	-7.05	115.67	119.90
1	1A	194	G	N7-C8-N9	-7.05	109.58	113.10
32	2a	1030	C	N1-C2-O2	7.05	123.13	118.90
1	1A	1723	A	N1-C2-N3	-7.05	125.78	129.30
2	1B	77	U	C5-C4-O4	-7.05	121.67	125.90
1	2A	154	G	N7-C8-N9	-7.05	109.58	113.10
32	1a	254	G	O5'-P-OP1	-7.05	99.36	105.70
1	2A	1914	C	C5-C6-N1	7.04	124.52	121.00
1	1A	2421	G	O5'-P-OP2	-7.04	99.36	105.70
1	1A	1723	A	C5-N7-C8	7.04	107.42	103.90
1	1A	1124	U	O4'-C1'-N1	7.04	113.83	108.20
1	2A	1666	G	C5-C6-O6	7.04	132.82	128.60
1	2A	1087	G	C6-C5-N7	7.04	134.62	130.40
1	1A	1652	G	OP1-P-O3'	7.04	120.68	105.20
1	1A	1824	C	N3-C4-C5	7.04	124.71	121.90
1	1A	2451	A	N9-C4-C5	-7.04	102.99	105.80
1	1A	2723	A	O5'-P-OP2	-7.04	99.37	105.70
1	1A	2838	C	C6-N1-C2	-7.04	117.49	120.30
32	2a	27	G	C4-C5-N7	7.04	113.61	110.80
1	1A	1007	G	N3-C4-C5	-7.03	125.08	128.60
1	1A	1210	G	N1-C6-O6	-7.03	115.68	119.90
1	2A	562	U	N3-C2-O2	-7.03	117.28	122.20
32	2a	498	U	C5-C4-O4	7.03	130.12	125.90
1	1A	2449	U	C2-N3-C4	-7.03	122.78	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	855	G	N7-C8-N9	-7.03	109.58	113.10
1	1A	1823	G	C5-N7-C8	7.03	107.81	104.30
32	2a	1475	G	C8-N9-C4	-7.03	103.59	106.40
1	1A	1522	G	N1-C2-N2	7.02	122.52	116.20
1	1A	2622	C	C5-C4-N4	-7.02	115.28	120.20
32	1a	1522	U	O5'-P-OP1	-7.02	99.38	105.70
32	1a	569	C	N3-C4-C5	7.02	124.71	121.90
1	1A	654	G	C4-C5-N7	-7.02	107.99	110.80
1	1A	1117	G	C8-N9-C4	-7.02	103.59	106.40
1	1A	2030	C	N3-C2-O2	-7.02	116.99	121.90
1	1A	2527	C	N3-C4-C5	7.02	124.71	121.90
32	1a	1228	C	C6-N1-C2	-7.02	117.49	120.30
1	2A	2046	G	C8-N9-C4	7.02	109.21	106.40
1	2A	2140	C	C5-C6-N1	7.02	124.51	121.00
1	2A	2427	C	N3-C2-O2	7.02	126.81	121.90
32	2a	1531	A	N1-C6-N6	7.02	122.81	118.60
1	1A	607	C	OP1-P-O3'	7.02	120.64	105.20
1	1A	842	C	C5-C4-N4	7.02	125.11	120.20
1	1A	716	G	C4-C5-C6	-7.02	114.59	118.80
1	2A	2896	C	C2-N1-C1'	7.02	126.52	118.80
1	1A	1658	C	C6-N1-C2	7.01	123.11	120.30
1	1A	1692	G	C5-N7-C8	7.01	107.81	104.30
1	1A	2134	G	C5-C6-N1	7.01	115.01	111.50
1	1A	1259	A	N7-C8-N9	-7.01	110.30	113.80
32	2a	945	G	C5-C6-O6	-7.01	124.39	128.60
1	1A	838	C	C5-C6-N1	-7.01	117.50	121.00
1	1A	2060	G	C4-C5-N7	-7.01	108.00	110.80
1	2A	2679	A	N1-C6-N6	-7.01	114.39	118.60
32	2a	1452	C	C6-N1-C2	-7.01	117.50	120.30
1	2A	363(C)	G	C8-N9-C4	7.01	109.20	106.40
2	2B	59	A	C5-C6-N1	7.01	121.20	117.70
1	1A	2586	G	N3-C2-N2	7.00	124.80	119.90
1	1A	2902	G	C4-C5-N7	7.00	113.60	110.80
1	2A	213	A	C4-C5-C6	-7.00	113.50	117.00
1	1A	2511	C	N3-C2-O2	7.00	126.80	121.90
32	1a	68	G	C8-N9-C4	7.00	109.20	106.40
32	1a	613	C	C6-N1-C2	-7.00	117.50	120.30
1	2A	1983	C	C5-C4-N4	-7.00	115.30	120.20
1	1A	619	G	C8-N9-C4	7.00	109.20	106.40
1	1A	1539	C	C4-C5-C6	7.00	120.90	117.40
1	1A	1959	A	O4'-C1'-N9	7.00	113.80	108.20
1	1A	1982	A	N1-C2-N3	-7.00	125.80	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2611	G	N9-C4-C5	7.00	108.20	105.40
1	1A	2031	G	N3-C2-N2	-6.99	115.00	119.90
1	1A	2050	U	N3-C4-O4	-6.99	114.50	119.40
32	1a	187	C	C6-N1-C2	-6.99	117.50	120.30
32	1a	175	C	C6-N1-C2	-6.99	117.50	120.30
1	1A	1151	U	N3-C2-O2	6.99	127.09	122.20
32	2a	898	G	C8-N9-C4	6.99	109.20	106.40
1	1A	1094	A	C8-N9-C4	-6.99	103.00	105.80
1	1A	1593	C	O5'-P-OP2	6.99	119.08	110.70
32	1a	189(L)	G	N3-C4-N9	6.99	130.19	126.00
1	2A	744	G	N1-C6-O6	-6.99	115.71	119.90
1	2A	2037	G	C5-C6-O6	6.99	132.79	128.60
2	2B	65	C	O5'-P-OP2	6.99	119.09	110.70
2	2B	115	G	N3-C4-C5	6.99	132.09	128.60
1	1A	2463	A	C5-N7-C8	-6.99	100.41	103.90
1	2A	1073	A	N9-C1'-C2'	-6.99	104.32	112.00
1	2A	2041	U	N3-C4-O4	6.99	124.29	119.40
1	1A	2858	G	C5-N7-C8	6.98	107.79	104.30
1	2A	2144	U	N3-C2-O2	-6.98	117.31	122.20
1	1A	1307	C	C2-N3-C4	-6.98	116.41	119.90
1	1A	1382	A	N9-C4-C5	6.98	108.59	105.80
1	1A	1729	G	C5-C6-N1	6.98	114.99	111.50
1	1A	2330	G	N9-C1'-C2'	-6.98	104.32	112.00
1	2A	1652	A	C2-N3-C4	-6.98	107.11	110.60
32	2a	728	A	O5'-P-OP2	-6.98	99.42	105.70
32	1a	191	G	N9-C4-C5	6.98	108.19	105.40
1	2A	2237	G	N1-C6-O6	-6.98	115.71	119.90
1	1A	292	G	C2-N3-C4	-6.98	108.41	111.90
1	1A	555	G	O5'-P-OP1	-6.98	99.42	105.70
1	1A	2234	G	C2-N3-C4	-6.98	108.41	111.90
1	2A	913	U	O5'-P-OP2	-6.98	99.42	105.70
1	1A	1657	C	N3-C2-O2	-6.98	117.02	121.90
1	1A	1658	C	C5-C6-N1	-6.97	117.51	121.00
1	1A	2279	A	O5'-P-OP1	-6.97	99.42	105.70
1	1A	543	G	OP1-P-OP2	6.97	130.06	119.60
1	1A	985	G	C4-C5-N7	-6.97	108.01	110.80
1	1A	1294	G	C2-N3-C4	-6.97	108.41	111.90
1	2A	1655	A	C8-N9-C4	6.97	108.59	105.80
1	2A	2010	G	N1-C6-O6	6.97	124.08	119.90
1	1A	1407	G	N1-C6-O6	-6.97	115.72	119.90
32	1a	752	G	C8-N9-C4	6.97	109.19	106.40
32	1a	854	G	O5'-P-OP1	-6.97	99.43	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2133	G	N1-C6-O6	6.97	124.08	119.90
1	1A	1456	G	OP2-P-O3'	6.97	120.53	105.20
1	1A	2227	G	C8-N9-C1'	6.97	136.06	127.00
32	2a	615	C	C6-N1-C2	-6.97	117.51	120.30
1	1A	406	G	C8-N9-C4	6.96	109.19	106.40
1	2A	180	G	O5'-P-OP1	-6.96	99.43	105.70
1	1A	1700	G	O4'-C1'-N9	-6.96	102.63	108.20
1	2A	2318	G	C8-N9-C4	-6.96	103.61	106.40
1	1A	2579	G	C5-N7-C8	6.96	107.78	104.30
32	1a	1530	G	C8-N9-C4	6.96	109.18	106.40
2	2B	47	C	O5'-P-OP1	-6.96	99.44	105.70
1	1A	2266	C	N1-C2-O2	-6.96	114.72	118.90
32	1a	557	G	N3-C4-C5	-6.96	125.12	128.60
1	1A	225	C	C5-C6-N1	-6.96	117.52	121.00
1	2A	614	U	N1-C2-N3	6.96	119.07	114.90
1	1A	1859	G	C6-N1-C2	6.95	129.27	125.10
1	2A	271	A	O5'-P-OP2	-6.95	99.44	105.70
32	2a	289	G	O5'-P-OP2	6.95	119.04	110.70
1	1A	119	G	C8-N9-C4	6.95	109.18	106.40
1	1A	193	A	C2-N3-C4	6.95	114.08	110.60
1	2A	2070	G	N1-C6-O6	-6.95	115.73	119.90
32	2a	782	A	O5'-P-OP1	-6.95	99.44	105.70
1	1A	958	C	N3-C2-O2	-6.95	117.04	121.90
32	1a	676	A	C2-N3-C4	-6.95	107.13	110.60
32	2a	372	C	N1-C2-N3	-6.95	114.34	119.20
1	1A	1796	C	O5'-P-OP2	-6.95	99.45	105.70
1	1A	2638	C	N1-C2-O2	-6.95	114.73	118.90
32	1a	1003	G	N3-C4-N9	6.95	130.17	126.00
1	1A	619	G	N7-C8-N9	-6.95	109.63	113.10
1	1A	1451	U	N3-C4-O4	-6.95	114.54	119.40
2	1B	62	C	OP1-P-OP2	6.95	130.02	119.60
1	2A	906	G	N1-C6-O6	-6.95	115.73	119.90
1	1A	598	A	O5'-P-OP2	6.94	119.03	110.70
1	1A	316	C	C6-N1-C2	6.94	123.08	120.30
1	1A	1093	G	N3-C4-N9	6.94	130.16	126.00
1	1A	2560	G	C4-C5-N7	-6.94	108.02	110.80
1	2A	2577	A	C5-C6-N1	-6.94	114.23	117.70
1	1A	503	A	O5'-P-OP2	-6.94	99.45	105.70
1	1A	260	A	N7-C8-N9	-6.94	110.33	113.80
1	1A	295	C	N1-C2-O2	6.94	123.06	118.90
1	1A	1821	C	N3-C4-N4	6.94	122.86	118.00
1	1A	295	C	O5'-P-OP1	6.93	119.02	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	798	A	O5'-P-OP1	-6.93	99.46	105.70
32	1a	1504	G	N1-C6-O6	6.93	124.06	119.90
1	1A	826	U	C4-C5-C6	6.93	123.86	119.70
1	1A	2566	U	C5-C4-O4	-6.93	121.74	125.90
1	2A	2599	G	C5-C6-O6	6.93	132.76	128.60
32	1a	172	A	N7-C8-N9	6.93	117.27	113.80
1	2A	859	G	O4'-C1'-N9	-6.93	102.66	108.20
32	1a	1097	C	C6-N1-C2	-6.93	117.53	120.30
1	1A	2529	C	O4'-C1'-N1	6.93	113.74	108.20
1	2A	2611	U	N1-C2-O2	-6.93	117.95	122.80
1	2A	1933	G	C4-C5-N7	-6.92	108.03	110.80
1	2A	2399	G	C5-C6-O6	6.92	132.75	128.60
1	1A	1817	A	O5'-P-OP2	-6.92	99.47	105.70
1	1A	1829	U	N3-C4-C5	6.92	118.75	114.60
32	1a	188	C	N3-C2-O2	-6.92	117.06	121.90
1	2A	1092	C	N3-C2-O2	-6.92	117.06	121.90
32	2a	500	G	N1-C6-O6	6.92	124.05	119.90
1	1A	2577	A	C5-C6-N1	6.92	121.16	117.70
1	2A	2197	U	N3-C2-O2	-6.92	117.36	122.20
32	2a	368	U	O5'-P-OP1	-6.92	99.48	105.70
1	1A	1679	A	C5-N7-C8	6.91	107.36	103.90
1	2A	2511	U	N1-C2-N3	6.91	119.05	114.90
1	1A	474	U	C5-C6-N1	-6.91	119.25	122.70
1	1A	827	G	C5-N7-C8	6.91	107.75	104.30
1	2A	2164	C	C6-N1-C2	-6.91	117.54	120.30
1	1A	2006	G	C6-N1-C2	6.91	129.24	125.10
1	2A	1792	G	O5'-P-OP1	-6.91	99.48	105.70
32	1a	233	C	C6-N1-C2	-6.91	117.54	120.30
32	1a	913	A	C8-N9-C4	-6.91	103.04	105.80
1	2A	713	G	C2-N3-C4	-6.91	108.45	111.90
32	2a	1436	U	N1-C2-N3	6.91	119.04	114.90
32	2a	1493	A	C8-N9-C4	6.91	108.56	105.80
1	2A	83	G	O5'-P-OP2	-6.90	99.49	105.70
1	2A	2378	A	C4-C5-C6	6.90	120.45	117.00
1	1A	514	G	N1-C6-O6	-6.90	115.76	119.90
1	2A	2324	C	C6-N1-C2	6.90	123.06	120.30
32	2a	816	A	O5'-P-OP1	6.90	118.98	110.70
1	1A	842	C	N3-C2-O2	-6.90	117.07	121.90
1	1A	854	U	N1-C2-N3	6.89	119.04	114.90
1	1A	2171	G	C8-N9-C4	6.89	109.16	106.40
1	1A	1130	A	C6-C5-N7	6.89	137.12	132.30
1	1A	2234	G	C5-C6-N1	-6.89	108.05	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2246	G	N1-C6-O6	-6.89	115.77	119.90
1	1A	2633	A	OP1-P-OP2	6.89	129.94	119.60
32	2a	1027	C	C5-C6-N1	6.89	124.45	121.00
1	1A	2164	C	C5-C6-N1	6.89	124.44	121.00
1	1A	1451	U	C5-C6-N1	-6.89	119.25	122.70
1	1A	1665	G	N9-C4-C5	-6.89	102.64	105.40
32	1a	284	G	O5'-P-OP2	-6.89	99.50	105.70
1	1A	474	U	N3-C2-O2	-6.89	117.38	122.20
1	1A	1842	G	C5-C6-O6	6.89	132.73	128.60
1	1A	1843	A	O5'-P-OP1	-6.89	99.50	105.70
1	1A	1450	C	OP1-P-OP2	6.88	129.93	119.60
1	2A	1075	C	C5-C6-N1	6.88	124.44	121.00
1	2A	2378	A	C5-C6-N6	-6.88	118.19	123.70
1	1A	600	G	C5-N7-C8	6.88	107.74	104.30
1	1A	1028	C	N1-C2-O2	-6.88	114.77	118.90
1	1A	2082	A	N1-C2-N3	-6.88	125.86	129.30
1	1A	2003	A	C5-C6-N1	6.88	121.14	117.70
1	1A	243	G	N1-C6-O6	-6.88	115.78	119.90
1	1A	1991	A	OP1-P-O3'	6.88	120.33	105.20
1	2A	447	A	N7-C8-N9	-6.88	110.36	113.80
1	1A	1029	A	OP2-P-O3'	6.87	120.32	105.20
1	1A	1092	A	OP2-P-O3'	6.87	120.32	105.20
1	1A	149	A	N1-C2-N3	6.87	132.74	129.30
1	1A	2100	C	N3-C4-C5	6.87	124.65	121.90
1	1A	2580	C	C5-C4-N4	-6.87	115.39	120.20
1	2A	1071	G	C4-C5-C6	6.87	122.92	118.80
32	2a	904	C	C5-C4-N4	-6.87	115.39	120.20
1	2A	214	G	O5'-P-OP2	-6.87	99.52	105.70
1	1A	2632	C	N3-C4-N4	-6.87	113.19	118.00
32	1a	512	U	O5'-P-OP2	-6.87	99.52	105.70
1	2A	2867	G	C8-N9-C4	6.87	109.15	106.40
32	2a	442	C	C6-N1-C2	-6.86	117.56	120.30
1	1A	1304	C	C5-C6-N1	-6.86	117.57	121.00
32	1a	356	A	C2-N3-C4	6.86	114.03	110.60
32	1a	841	U	N3-C2-O2	-6.86	117.40	122.20
1	1A	2043	C	O5'-P-OP2	-6.86	99.53	105.70
16	1U	55	ARG	NE-CZ-NH1	-6.86	116.87	120.30
32	1a	1495	U	C2-N3-C4	6.86	131.11	127.00
1	2A	535	C	N1-C2-O2	-6.86	114.78	118.90
32	2a	346	G	C5-C6-N1	6.86	114.93	111.50
1	1A	2902	G	N3-C4-C5	6.86	132.03	128.60
32	1a	1184	G	N9-C4-C5	-6.86	102.66	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1119	C	C6-N1-C2	-6.86	117.56	120.30
1	1A	848	G	OP2-P-O3'	6.85	120.28	105.20
1	1A	2083	G	C8-N9-C4	-6.85	103.66	106.40
1	1A	2420	U	N3-C2-O2	-6.85	117.41	122.20
1	1A	2551	C	C2-N1-C1'	-6.85	111.27	118.80
1	2A	1769	G	C5-C6-O6	-6.85	124.49	128.60
32	2a	1026	G	N7-C8-N9	6.85	116.53	113.10
1	1A	235	C	O5'-P-OP1	-6.85	99.54	105.70
1	1A	2100	C	N1-C2-N3	6.85	123.99	119.20
32	1a	474	G	O5'-P-OP2	-6.85	99.54	105.70
1	1A	116	A	N9-C4-C5	6.84	108.54	105.80
1	1A	2449	U	N1-C2-N3	6.84	119.01	114.90
1	1A	856	G	C5-C6-N1	6.84	114.92	111.50
1	2A	739	G	O5'-P-OP1	-6.84	99.54	105.70
1	2A	2426	A	N1-C6-N6	6.84	122.70	118.60
1	1A	556	C	N3-C4-C5	6.84	124.64	121.90
1	1A	582	G	C5-N7-C8	-6.84	100.88	104.30
1	1A	1186	U	C6-N1-C2	-6.84	116.90	121.00
1	2A	1283	G	O5'-P-OP2	-6.84	99.55	105.70
1	2A	1399	C	OP2-P-O3'	6.84	120.24	105.20
1	1A	2453	C	N3-C2-O2	-6.83	117.12	121.90
1	2A	1890	A	N7-C8-N9	-6.83	110.38	113.80
1	1A	215	G	N3-C2-N2	-6.83	115.12	119.90
1	1A	2467	G	N1-C6-O6	-6.83	115.80	119.90
1	1A	23	G	N9-C4-C5	6.83	108.13	105.40
1	2A	189	G	C4-C5-N7	-6.83	108.07	110.80
1	1A	1043	G	N1-C6-O6	-6.83	115.80	119.90
1	1A	1812	C	C6-N1-C2	6.83	123.03	120.30
1	1A	1850	A	C5-C6-N1	-6.83	114.29	117.70
1	2A	2138	C	C6-N1-C2	-6.83	117.57	120.30
1	1A	1742	G	C6-C5-N7	-6.83	126.30	130.40
1	2A	2440	C	O5'-P-OP2	-6.83	99.56	105.70
1	2A	2010	G	N3-C2-N2	-6.83	115.12	119.90
1	2A	2186	G	N3-C2-N2	-6.83	115.12	119.90
5	1F	54	ARG	NE-CZ-NH2	-6.82	116.89	120.30
32	1a	819	A	N9-C4-C5	-6.82	103.07	105.80
32	1a	299	G	C5-C6-O6	-6.82	124.51	128.60
32	1a	858	G	C8-N9-C4	-6.82	103.67	106.40
1	1A	654	G	C5-N7-C8	6.82	107.71	104.30
1	1A	961	C	N1-C2-O2	6.82	122.99	118.90
1	1A	1324	A	OP1-P-OP2	-6.82	109.37	119.60
1	2A	421	U	OP2-P-O3'	-6.82	90.20	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2645	G	N3-C4-N9	-6.82	121.91	126.00
1	1A	573	G	N9-C4-C5	6.82	108.13	105.40
1	1A	815	G	N9-C4-C5	6.82	108.13	105.40
1	1A	2312	G	O5'-P-OP2	6.82	118.88	110.70
1	2A	2610	C	O5'-P-OP1	-6.82	99.56	105.70
1	1A	326	C	C6-N1-C2	-6.82	117.57	120.30
1	1A	1278	G	N9-C4-C5	6.81	108.13	105.40
1	1A	1298	G	N3-C4-C5	6.81	132.01	128.60
1	1A	1802	C	C5-C6-N1	-6.81	117.59	121.00
2	1B	108	U	O5'-P-OP1	6.81	118.88	110.70
1	1A	2427	G	OP1-P-OP2	-6.81	109.38	119.60
1	1A	1222	A	O5'-P-OP1	-6.81	99.57	105.70
1	1A	1245	C	N3-C4-C5	6.81	124.62	121.90
1	1A	2265	G	N3-C2-N2	-6.81	115.14	119.90
1	1A	2743	C	OP2-P-O3'	6.81	120.18	105.20
32	1a	576	G	N3-C4-C5	-6.81	125.20	128.60
1	2A	1118	C	C6-N1-C2	-6.81	117.58	120.30
1	2A	1261	C	O5'-P-OP1	-6.81	99.57	105.70
2	1B	13	A	N7-C8-N9	-6.81	110.40	113.80
1	1A	192	C	N1-C2-O2	6.80	122.98	118.90
32	1a	186	C	C5-C6-N1	6.80	124.40	121.00
1	1A	2020	G	C5-C6-O6	6.80	132.68	128.60
1	1A	891	C	C4-C5-C6	6.80	120.80	117.40
1	1A	2227	G	O4'-C1'-N9	6.80	113.64	108.20
1	2A	1062	G	C8-N9-C4	-6.80	103.68	106.40
1	1A	1067	A	O5'-P-OP1	-6.80	99.58	105.70
1	1A	1863	C	N3-C2-O2	-6.80	117.14	121.90
1	1A	1725	G	C5-C6-O6	-6.80	124.52	128.60
1	1A	1853	G	N7-C8-N9	-6.80	109.70	113.10
1	1A	2364	A	O5'-P-OP1	-6.80	99.58	105.70
32	1a	552	U	O5'-P-OP2	-6.80	99.58	105.70
32	2a	441	A	OP2-P-O3'	6.80	120.15	105.20
32	2a	1460	A	O5'-P-OP1	6.80	118.86	110.70
1	1A	2784	C	C2-N3-C4	-6.79	116.50	119.90
1	1A	2001	C	N3-C4-C5	6.79	124.62	121.90
1	1A	2881	C	C5-C4-N4	-6.79	115.44	120.20
1	1A	418	G	N7-C8-N9	-6.79	109.70	113.10
1	1A	1814	A	N1-C2-N3	-6.79	125.90	129.30
32	1a	1499	A	O5'-P-OP1	6.79	118.85	110.70
1	1A	476	G	C8-N9-C4	6.79	109.11	106.40
32	1a	397	A	OP2-P-O3'	6.79	120.14	105.20
1	1A	727	G	C8-N9-C4	-6.79	103.69	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1693	C	N1-C2-O2	-6.79	114.83	118.90
1	2A	1793	C	N3-C4-N4	-6.79	113.25	118.00
1	1A	171	A	O5'-P-OP1	-6.79	99.59	105.70
1	2A	718	A	C6-C5-N7	-6.79	127.55	132.30
1	2A	1281	G	O5'-P-OP1	-6.79	99.59	105.70
1	2A	1312	U	C5-C4-O4	6.79	129.97	125.90
32	2a	1527	C	O5'-P-OP2	-6.79	99.59	105.70
1	1A	1803	G	C5-N7-C8	6.78	107.69	104.30
1	1A	2286	A	C5-C6-N1	-6.78	114.31	117.70
1	2A	1966	A	N1-C6-N6	-6.78	114.53	118.60
1	1A	739	C	C4-C5-C6	-6.78	114.01	117.40
1	2A	2433	A	C5-C6-N1	6.78	121.09	117.70
1	1A	2835	C	C5-C6-N1	-6.78	117.61	121.00
32	2a	1149	C	C5-C6-N1	6.78	124.39	121.00
1	1A	1028	C	N3-C2-O2	6.78	126.64	121.90
1	1A	1637	G	N1-C6-O6	-6.78	115.83	119.90
1	1A	1995	G	C4-C5-N7	-6.78	108.09	110.80
1	1A	1178	A	OP2-P-O3'	6.77	120.10	105.20
1	1A	1135	G	N3-C4-C5	-6.77	125.21	128.60
1	1A	1470	G	C2-N3-C4	-6.77	108.51	111.90
1	1A	1786	A	C8-N9-C4	-6.77	103.09	105.80
1	1A	2256	U	C5-C6-N1	-6.77	119.31	122.70
32	1a	1417	G	C5-C6-N1	6.77	114.89	111.50
1	1A	557	A	N1-C6-N6	-6.77	114.54	118.60
1	1A	906	G	N7-C8-N9	-6.77	109.72	113.10
1	1A	1155	C	C5-C6-N1	6.77	124.39	121.00
1	1A	1243	U	N1-C2-N3	6.77	118.96	114.90
1	1A	2376	C	C6-N1-C2	6.77	123.01	120.30
32	1a	657	G	O5'-P-OP2	-6.77	99.61	105.70
1	1A	271	U	O4'-C1'-N1	6.77	113.61	108.20
32	1a	536	C	O5'-P-OP2	-6.77	99.61	105.70
1	1A	1314	A	C5-C6-N1	-6.76	114.32	117.70
2	1B	91	C	N3-C4-C5	6.76	124.61	121.90
1	2A	2447	G	C5-C6-O6	-6.76	124.54	128.60
1	1A	1813	C	C5-C6-N1	-6.76	117.62	121.00
1	2A	2848	G	C4-C5-N7	-6.76	108.09	110.80
1	1A	130	G	C5-N7-C8	6.76	107.68	104.30
1	1A	415	G	N9-C4-C5	-6.76	102.70	105.40
1	1A	1959	A	N9-C4-C5	6.76	108.50	105.80
2	1B	23	G	O5'-P-OP1	-6.76	99.61	105.70
32	2a	1062	U	N1-C2-O2	6.76	127.53	122.80
1	1A	1543	U	C2-N3-C4	-6.76	122.94	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1V	82	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	1A	729	G	O5'-P-OP1	-6.76	99.62	105.70
1	1A	2269	U	N3-C2-O2	-6.76	117.47	122.20
1	2A	1935	G	C5-C6-N1	6.76	114.88	111.50
2	2B	101	G	C5-C6-O6	-6.76	124.55	128.60
32	2a	1149	C	C6-N1-C2	-6.76	117.60	120.30
1	1A	444	C	C6-N1-C2	-6.75	117.60	120.30
1	2A	2827	C	N1-C2-O2	-6.75	114.85	118.90
1	1A	1221	G	C4-N9-C1'	-6.75	117.72	126.50
1	2A	290	G	O5'-P-OP1	-6.75	99.62	105.70
1	2A	882	G	C8-N9-C1'	6.75	135.78	127.00
1	1A	827	G	C4-C5-N7	-6.75	108.10	110.80
1	2A	834	C	C6-N1-C2	-6.75	117.60	120.30
1	1A	438	G	O5'-P-OP1	6.75	118.80	110.70
1	1A	849	A	C2-N3-C4	6.75	113.97	110.60
1	2A	1630	G	C8-N9-C4	-6.75	103.70	106.40
1	1A	2188	G	C8-N9-C1'	6.75	135.77	127.00
44	2l	87	GLY	N-CA-C	6.75	129.96	113.10
1	1A	2463	A	C5-C6-N1	6.74	121.07	117.70
32	1a	854	G	O5'-P-OP2	6.74	118.79	110.70
2	1B	52	A	C8-N9-C4	6.74	108.50	105.80
1	2A	238	C	N3-C4-C5	-6.74	119.20	121.90
1	2A	1710	C	O5'-P-OP1	6.74	118.79	110.70
32	2a	1125	U	O4'-C1'-N1	6.74	113.59	108.20
1	1A	561	A	O5'-P-OP2	-6.74	99.64	105.70
1	1A	2440	G	N3-C4-C5	-6.74	125.23	128.60
32	2a	848	C	C5-C6-N1	6.74	124.37	121.00
1	2A	1075	C	N1-C2-O2	6.74	122.94	118.90
1	1A	2439	C	O5'-P-OP1	-6.74	99.64	105.70
1	2A	743	G	C5-C6-O6	6.74	132.64	128.60
1	2A	1321	A	C8-N9-C4	6.74	108.49	105.80
1	2A	1618	A	C8-N9-C4	-6.74	103.11	105.80
1	2A	1681	G	N3-C4-C5	6.74	131.97	128.60
13	2R	67	LEU	CA-CB-CG	6.74	130.79	115.30
1	1A	2019	G	O5'-P-OP1	6.73	118.78	110.70
1	1A	1038	C	N3-C4-C5	6.73	124.59	121.90
1	1A	1986	G	C2-N3-C4	-6.73	108.53	111.90
32	1a	181	G	O4'-C1'-N9	6.73	113.58	108.20
1	2A	912	C	C2-N1-C1'	6.73	126.20	118.80
32	1a	863	U	C5-C4-O4	6.73	129.94	125.90
1	2A	1807	G	C8-N9-C4	6.73	109.09	106.40
1	2A	450	G	C5-C6-N1	6.73	114.86	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	662	G	O5'-P-OP2	6.72	118.77	110.70
1	2A	976	C	N3-C2-O2	-6.72	117.19	121.90
1	1A	1069	U	C2-N3-C4	-6.72	122.97	127.00
1	1A	1846	A	O5'-P-OP1	-6.72	99.65	105.70
1	1A	2320	G	C5-C6-O6	-6.72	124.57	128.60
1	1A	422	U	N3-C2-O2	-6.72	117.50	122.20
1	2A	1929	G	O5'-P-OP2	-6.72	99.65	105.70
1	2A	2893	G	C2-N3-C4	6.72	115.26	111.90
1	1A	23	G	C4-C5-N7	-6.72	108.11	110.80
1	1A	1769	G	C5-C6-O6	6.72	132.63	128.60
32	1a	1176	A	N9-C4-C5	6.72	108.49	105.80
1	1A	999	G	N1-C6-O6	-6.72	115.87	119.90
1	1A	673	G	C2-N3-C4	-6.72	108.54	111.90
1	1A	696	C	C6-N1-C2	-6.72	117.61	120.30
1	1A	1718	U	C5-C6-N1	-6.72	119.34	122.70
1	1A	1988	A	C8-N9-C4	6.72	108.49	105.80
2	1B	1	U	C2-N1-C1'	6.72	125.76	117.70
1	1A	486	A	C8-N9-C4	-6.71	103.11	105.80
1	1A	990	A	O4'-C1'-N9	-6.71	102.83	108.20
1	2A	1635	G	C8-N9-C4	6.71	109.09	106.40
1	1A	107	G	N1-C6-O6	-6.71	115.87	119.90
1	1A	1007	G	N9-C4-C5	6.71	108.08	105.40
1	1A	2083	G	N3-C4-C5	-6.71	125.24	128.60
1	2A	2425	A	C8-N9-C4	-6.71	103.11	105.80
1	1A	841	G	N3-C2-N2	6.71	124.60	119.90
1	2A	1763	G	N9-C4-C5	6.71	108.08	105.40
1	1A	344	A	C8-N9-C4	-6.71	103.12	105.80
1	1A	1181	G	C5-C6-O6	-6.71	124.58	128.60
1	1A	789	G	N7-C8-N9	-6.71	109.75	113.10
1	1A	2357	G	OP1-P-O3'	6.71	119.95	105.20
32	1a	557	G	OP1-P-O3'	6.71	119.96	105.20
1	2A	882	G	N3-C4-N9	-6.71	121.98	126.00
1	2A	1574	C	C4-C5-C6	-6.71	114.05	117.40
1	2A	1778	U	C6-N1-C2	6.71	125.02	121.00
32	2a	230	G	C4-C5-N7	-6.71	108.12	110.80
32	2a	881	G	C8-N9-C4	6.71	109.08	106.40
1	1A	572	A	C8-N9-C4	-6.70	103.12	105.80
1	1A	720	C	O5'-P-OP2	-6.70	99.67	105.70
1	1A	1341	C	N3-C4-N4	-6.70	113.31	118.00
1	1A	1991	A	OP1-P-OP2	-6.70	109.55	119.60
32	2a	1027	C	C2-N1-C1'	6.70	126.17	118.80
1	1A	592	U	N1-C2-N3	6.70	118.92	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1000	C	C5-C4-N4	6.70	124.89	120.20
1	1A	1045	U	O5'-P-OP2	-6.70	99.67	105.70
1	1A	2390	A	N1-C6-N6	6.70	122.62	118.60
2	1B	18	G	C5-C6-O6	-6.70	124.58	128.60
1	1A	1173	A	N1-C2-N3	-6.70	125.95	129.30
32	1a	1530	G	N9-C4-C5	-6.70	102.72	105.40
32	2a	776	G	O5'-P-OP2	-6.70	99.67	105.70
1	1A	1701	A	N7-C8-N9	-6.70	110.45	113.80
1	1A	2361	G	O5'-P-OP1	-6.70	99.67	105.70
1	2A	2612	C	O5'-P-OP2	-6.70	99.67	105.70
32	2a	550	G	O5'-P-OP1	-6.70	99.67	105.70
32	2a	1019	C	C6-N1-C2	-6.70	117.62	120.30
1	1A	706	C	N3-C4-C5	6.69	124.58	121.90
1	1A	809	U	C6-N1-C1'	-6.69	111.83	121.20
1	1A	1365	G	C5-N7-C8	-6.69	100.95	104.30
1	1A	2049	G	C2-N3-C4	6.69	115.25	111.90
1	1A	283	G	C8-N9-C4	-6.69	103.72	106.40
1	1A	2406	C	C2-N3-C4	-6.69	116.55	119.90
32	1a	896	C	C6-N1-C2	6.69	122.98	120.30
46	1n	3	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	1A	593	G	C5-C6-N1	6.69	114.84	111.50
1	1A	1298	G	N3-C4-N9	-6.69	121.99	126.00
1	1A	2074	G	N9-C4-C5	6.69	108.08	105.40
1	2A	614	U	C6-N1-C2	-6.69	116.99	121.00
1	2A	1681	G	N3-C4-N9	-6.69	121.99	126.00
1	1A	1346	U	N1-C2-N3	6.69	118.91	114.90
1	1A	793	A	C8-N9-C4	-6.68	103.13	105.80
1	1A	1669	G	C6-C5-N7	6.68	134.41	130.40
2	1B	115	G	C8-N9-C4	6.68	109.07	106.40
32	1a	204	U	C6-N1-C2	-6.68	116.99	121.00
32	2a	357	G	N3-C2-N2	-6.68	115.22	119.90
1	1A	1333	A	C8-N9-C4	-6.68	103.13	105.80
1	2A	94(A)	G	C8-N9-C4	-6.68	103.73	106.40
1	1A	1403	U	C5-C6-N1	-6.68	119.36	122.70
1	1A	1069	U	C5-C4-O4	-6.68	121.89	125.90
32	1a	115	G	P-O3'-C3'	6.68	127.72	119.70
32	1a	189(D)	C	N3-C2-O2	-6.68	117.22	121.90
1	2A	1828	G	O5'-P-OP1	-6.68	99.69	105.70
1	2A	2030	A	O5'-P-OP1	-6.68	99.69	105.70
1	1A	1178	A	N1-C2-N3	6.68	132.64	129.30
1	1A	1944	G	O5'-P-OP2	-6.68	99.69	105.70
1	1A	2183	C	C5-C6-N1	6.68	124.34	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	728	A	OP1-P-OP2	6.68	129.62	119.60
32	1a	807	A	C8-N9-C4	-6.68	103.13	105.80
1	2A	532	A	C8-N9-C4	-6.68	103.13	105.80
1	2A	2575	C	N3-C2-O2	-6.68	117.23	121.90
1	2A	2784	C	O5'-P-OP2	-6.68	99.69	105.70
3	2D	275	LYS	N-CA-C	-6.68	92.97	111.00
1	1A	2750	G	N1-C6-O6	-6.67	115.89	119.90
32	1a	690	G	OP1-P-OP2	6.67	129.61	119.60
1	2A	576	U	N1-C2-O2	-6.67	118.13	122.80
1	1A	802	C	C4-C5-C6	6.67	120.74	117.40
32	2a	431	A	O5'-P-OP1	-6.67	99.69	105.70
1	2A	572	A	N1-C6-N6	-6.67	114.60	118.60
1	1A	508	A	O5'-P-OP2	-6.67	99.70	105.70
1	1A	2358	A	N1-C2-N3	6.67	132.63	129.30
1	1A	2546	A	C5-C6-N6	-6.67	118.37	123.70
32	1a	326	G	N9-C4-C5	6.66	108.06	105.40
1	1A	314	G	O5'-P-OP1	-6.66	99.70	105.70
1	1A	15	G	C8-N9-C4	-6.66	103.74	106.40
1	1A	1621	C	N3-C4-C5	6.66	124.56	121.90
1	2A	679	C	N1-C2-O2	-6.66	114.90	118.90
1	2A	788	A	N1-C6-N6	6.66	122.60	118.60
1	2A	2237	G	C5-C6-O6	6.66	132.60	128.60
1	1A	590	A	N1-C2-N3	-6.66	125.97	129.30
1	1A	770	G	N1-C2-N2	-6.66	110.21	116.20
1	1A	1014	U	C4-C5-C6	-6.66	115.70	119.70
1	1A	1807	G	N3-C2-N2	6.66	124.56	119.90
1	1A	2020	G	N1-C6-O6	-6.66	115.91	119.90
1	1A	2503	U	C5-C4-O4	-6.66	121.91	125.90
32	1a	900	A	C2-N3-C4	6.66	113.93	110.60
32	1a	1243	C	C6-N1-C2	-6.66	117.64	120.30
32	1a	1486	G	C5-C6-O6	-6.66	124.61	128.60
1	2A	2773	C	C6-N1-C2	6.66	122.96	120.30
1	1A	107	G	N7-C8-N9	-6.65	109.77	113.10
32	2a	649	G	N3-C4-C5	6.65	131.93	128.60
1	1A	1237	G	C2-N3-C4	-6.65	108.57	111.90
1	1A	1422	C	N3-C4-N4	-6.65	113.34	118.00
1	1A	2284	U	OP2-P-O3'	6.65	119.83	105.20
1	1A	2592	U	C5-C6-N1	-6.65	119.37	122.70
32	1a	1169	A	C8-N9-C4	-6.65	103.14	105.80
1	2A	1363	C	O5'-P-OP2	-6.65	99.71	105.70
1	1A	2406	C	N1-C2-O2	-6.65	114.91	118.90
1	1A	2802	C	C2-N3-C4	-6.65	116.58	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1041	C	N1-C2-O2	6.65	122.89	118.90
1	1A	2010	C	C5-C6-N1	-6.65	117.68	121.00
1	1A	2568	C	N3-C4-C5	6.65	124.56	121.90
1	2A	271(P)	C	O5'-P-OP2	-6.65	99.72	105.70
1	1A	292	G	C4-C5-N7	6.65	113.46	110.80
1	1A	1822	A	OP1-P-OP2	-6.65	109.63	119.60
32	1a	1409	C	N1-C2-O2	6.65	122.89	118.90
1	2A	1253	A	N7-C8-N9	-6.65	110.48	113.80
1	1A	195	U	N1-C2-N3	6.64	118.89	114.90
1	1A	466	G	N1-C6-O6	6.64	123.89	119.90
1	1A	2457	G	OP1-P-OP2	6.64	129.57	119.60
1	2A	2783	G	N1-C6-O6	-6.64	115.91	119.90
1	1A	2447	A	O5'-P-OP1	-6.64	99.72	105.70
1	1A	1829	U	N3-C4-O4	-6.64	114.75	119.40
1	1A	436	C	O5'-P-OP2	6.64	118.67	110.70
1	2A	2058	A	C6-C5-N7	-6.64	127.65	132.30
1	1A	575	G	N3-C2-N2	6.64	124.55	119.90
1	1A	2291	G	C4-C5-N7	6.64	113.45	110.80
1	2A	1326	U	O5'-P-OP1	-6.64	99.73	105.70
1	2A	1652	A	O5'-P-OP1	-6.64	99.73	105.70
1	1A	2006	G	C6-C5-N7	6.63	134.38	130.40
1	1A	2375	C	N3-C4-N4	-6.63	113.36	118.00
32	1a	1479	C	OP1-P-O3'	6.63	119.80	105.20
1	2A	312	G	O5'-P-OP1	-6.63	99.73	105.70
1	1A	2839	C	C5-C6-N1	6.63	124.32	121.00
1	2A	2167	U	C6-N1-C2	-6.63	117.02	121.00
1	1A	302	A	P-O3'-C3'	6.63	127.66	119.70
1	1A	1186	U	N3-C2-O2	-6.63	117.56	122.20
32	1a	533	A	C4-C5-N7	6.63	114.01	110.70
1	2A	48	G	O5'-P-OP2	-6.63	99.73	105.70
1	1A	2358	A	C4-C5-C6	6.63	120.31	117.00
1	1A	747	G	N3-C2-N2	6.62	124.54	119.90
2	1B	100	A	OP1-P-OP2	6.62	129.54	119.60
1	2A	11	G	C4-C5-N7	6.62	113.45	110.80
32	2a	397	A	O5'-P-OP2	-6.62	99.74	105.70
1	1A	2576	A	C6-C5-N7	-6.62	127.66	132.30
1	2A	2385	C	N1-C2-O2	-6.62	114.93	118.90
32	2a	871	U	N1-C2-O2	6.62	127.44	122.80
1	1A	2225	U	C5-C6-N1	-6.62	119.39	122.70
32	1a	801	U	N1-C2-O2	6.62	127.44	122.80
32	1a	836	G	C4-C5-N7	6.62	113.45	110.80
1	2A	1087	G	C8-N9-C1'	6.62	135.61	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1365	G	N3-C2-N2	-6.62	115.27	119.90
1	1A	1181	G	N1-C6-O6	6.62	123.87	119.90
32	1a	204	U	N1-C2-O2	6.62	127.43	122.80
32	1a	1184	G	C4-C5-N7	6.62	113.45	110.80
1	2A	1076	C	C2-N1-C1'	6.62	126.08	118.80
32	2a	218	C	C6-N1-C2	-6.62	117.65	120.30
1	1A	1742	G	C5-N7-C8	-6.62	100.99	104.30
1	1A	1543	U	C5-C6-N1	-6.61	119.39	122.70
1	1A	2561	G	N3-C4-C5	-6.61	125.29	128.60
1	1A	2593	G	C4-C5-N7	6.61	113.44	110.80
32	1a	501	C	OP2-P-O3'	6.61	119.75	105.20
32	1a	1530	G	N1-C2-N2	6.61	122.15	116.20
1	2A	2679	A	OP2-P-O3'	6.61	119.75	105.20
1	1A	1831	C	N3-C2-O2	-6.61	117.27	121.90
1	1A	359	C	N3-C4-C5	-6.61	119.26	121.90
1	1A	418	G	C5-C6-N1	6.61	114.80	111.50
1	1A	1986	G	C4-C5-N7	6.61	113.44	110.80
1	1A	2284	U	C2-N3-C4	-6.61	123.04	127.00
1	2A	1073	A	P-O3'-C3'	6.61	127.63	119.70
1	1A	2217	C	OP1-P-O3'	6.60	119.73	105.20
1	1A	583	C	C4-C5-C6	6.60	120.70	117.40
1	1A	886	U	N3-C4-C5	6.60	118.56	114.60
2	1B	79	C	N3-C4-C5	6.60	124.54	121.90
32	2a	799	G	N1-C6-O6	-6.60	115.94	119.90
1	1A	790	G	N9-C4-C5	6.60	108.04	105.40
1	1A	1237	G	C4-C5-N7	-6.60	108.16	110.80
1	1A	1953	U	C4-C5-C6	-6.60	115.74	119.70
32	2a	618	C	OP1-P-O3'	6.60	119.72	105.20
32	1a	590	C	O5'-P-OP2	-6.60	99.76	105.70
1	1A	1611	C	C5-C4-N4	6.60	124.82	120.20
32	1a	563	A	N7-C8-N9	6.60	117.10	113.80
32	1a	769	G	OP2-P-O3'	6.60	119.72	105.20
32	2a	269	C	C6-N1-C2	6.60	122.94	120.30
1	1A	1708	G	N7-C8-N9	-6.60	109.80	113.10
1	1A	103	C	N3-C4-C5	6.59	124.54	121.90
1	1A	1700	G	OP1-P-O3'	6.59	119.71	105.20
32	1a	353	A	C5-N7-C8	-6.59	100.60	103.90
32	2a	898	G	N3-C4-C5	6.59	131.90	128.60
1	1A	1447	G	C5-C6-N1	-6.59	108.20	111.50
32	1a	804	U	C5-C4-O4	6.59	129.86	125.90
32	1a	819	A	C5-C6-N6	-6.59	118.43	123.70
2	2B	24	G	N1-C6-O6	6.59	123.86	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1333	A	N7-C8-N9	6.59	117.10	113.80
2	2B	14	U	O5'-P-OP2	-6.59	99.77	105.70
1	1A	1958	A	C4-C5-N7	6.59	113.99	110.70
1	2A	568	U	N3-C4-C5	6.59	118.55	114.60
1	2A	1904	G	O5'-P-OP2	-6.59	99.77	105.70
1	1A	428	A	N9-C4-C5	6.58	108.43	105.80
1	1A	1559	C	O5'-P-OP2	6.58	118.60	110.70
1	2A	2805	G	N1-C6-O6	-6.58	115.95	119.90
1	1A	1662	A	O5'-P-OP2	6.58	118.60	110.70
1	2A	1963	U	C2-N1-C1'	6.58	125.60	117.70
1	2A	2576	G	OP2-P-O3'	6.58	119.69	105.20
1	1A	2383	G	C2-N3-C4	6.58	115.19	111.90
1	1A	2432	C	N1-C2-O2	-6.58	114.95	118.90
1	2A	1244	G	C8-N9-C4	6.58	109.03	106.40
1	2A	1332	G	C5-C6-O6	-6.58	124.65	128.60
23	21	21	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	2A	1780	A	C8-N9-C4	-6.58	103.17	105.80
32	2a	831	U	OP1-P-OP2	-6.58	109.73	119.60
1	1A	901	G	C5-C6-O6	6.58	132.55	128.60
1	1A	2129	C	C6-N1-C2	-6.58	117.67	120.30
32	1a	1136	U	C6-N1-C2	-6.58	117.05	121.00
1	2A	36	G	O5'-P-OP2	-6.58	99.78	105.70
32	2a	581	G	N1-C6-O6	6.58	123.85	119.90
1	1A	1475	G	N1-C6-O6	-6.58	115.95	119.90
32	1a	1021	G	N1-C6-O6	-6.58	115.95	119.90
1	1A	1234	A	N1-C6-N6	6.58	122.55	118.60
1	2A	741	G	O5'-P-OP1	-6.58	99.78	105.70
1	2A	1836	C	O5'-P-OP2	-6.58	99.78	105.70
1	1A	604	C	N1-C2-O2	-6.57	114.96	118.90
1	1A	2017	U	C5-C6-N1	-6.57	119.41	122.70
1	1A	2596	U	C2-N1-C1'	-6.57	109.81	117.70
1	2A	188	G	O5'-P-OP2	-6.57	99.78	105.70
1	2A	1065	U	O4'-C1'-N1	6.57	113.46	108.20
1	2A	1783	A	C2-N3-C4	6.57	113.89	110.60
32	1a	148	G	N1-C6-O6	-6.57	115.96	119.90
1	2A	1666	G	N1-C2-N2	-6.57	110.28	116.20
1	1A	910	A	OP2-P-O3'	6.57	119.66	105.20
1	2A	312	G	N1-C6-O6	6.57	123.84	119.90
1	2A	655	A	C8-N9-C4	-6.57	103.17	105.80
1	1A	215	G	N1-C2-N2	6.57	122.11	116.20
32	1a	1176	A	N1-C6-N6	-6.57	114.66	118.60
1	2A	2773	C	C5-C6-N1	-6.57	117.72	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	483	A	C6-N1-C2	6.57	122.54	118.60
1	1A	1242	G	N1-C6-O6	-6.57	115.96	119.90
1	1A	1757	C	C6-N1-C2	6.57	122.93	120.30
1	2A	789	A	N1-C6-N6	6.57	122.54	118.60
32	2a	775	G	OP2-P-O3'	6.57	119.65	105.20
32	2a	824	C	N3-C4-C5	-6.57	119.27	121.90
1	1A	749	G	OP1-P-OP2	6.57	129.45	119.60
1	1A	418	G	C8-N9-C4	6.56	109.03	106.40
1	1A	593	G	C2-N3-C4	6.56	115.18	111.90
1	1A	1692	G	N7-C8-N9	-6.56	109.82	113.10
1	1A	1862	G	C5-C6-O6	6.56	132.54	128.60
1	1A	2523	U	C5-C6-N1	-6.56	119.42	122.70
32	1a	286	G	O5'-P-OP1	-6.56	99.79	105.70
1	1A	424	G	C8-N9-C4	6.56	109.03	106.40
1	1A	1302	G	N7-C8-N9	-6.56	109.82	113.10
1	1A	360	C	C6-N1-C2	-6.56	117.68	120.30
1	1A	1368	A	C6-N1-C2	6.56	122.54	118.60
1	1A	483	A	C5-C6-N1	-6.56	114.42	117.70
32	1a	1500	A	N1-C6-N6	-6.56	114.67	118.60
32	1a	1505	G	N3-C4-N9	-6.56	122.07	126.00
1	2A	2319	G	C5-N7-C8	-6.56	101.02	104.30
32	2a	572	A	C4-N9-C1'	-6.56	114.50	126.30
32	2a	871	U	N3-C2-O2	-6.56	117.61	122.20
1	1A	2030	C	N1-C2-N3	6.55	123.79	119.20
1	1A	2881	C	N3-C4-C5	6.55	124.52	121.90
1	2A	752	A	OP2-P-O3'	6.55	119.62	105.20
1	1A	554	A	C8-N9-C4	-6.55	103.18	105.80
32	1a	57	G	C5-C6-O6	6.55	132.53	128.60
32	1a	801	U	N3-C2-O2	-6.55	117.61	122.20
1	2A	108	U	O5'-P-OP2	-6.55	99.80	105.70
1	1A	2762	A	C5-C6-N1	6.55	120.98	117.70
1	1A	596	G	C5-C6-O6	-6.55	124.67	128.60
1	1A	1105	G	C8-N9-C4	6.55	109.02	106.40
1	1A	1377	A	OP2-P-O3'	6.55	119.61	105.20
1	1A	2440	G	C6-N1-C2	-6.55	121.17	125.10
32	2a	1378	C	N3-C4-C5	-6.55	119.28	121.90
1	2A	660	G	C5-C6-O6	6.55	132.53	128.60
32	2a	115	G	O5'-P-OP2	-6.55	99.81	105.70
32	2a	262	A	O5'-P-OP2	-6.55	99.81	105.70
32	2a	618	C	N3-C4-C5	-6.55	119.28	121.90
32	2a	1139	G	C4-C5-N7	-6.55	108.18	110.80
1	1A	891	C	C2-N3-C4	-6.54	116.63	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1379	C	C2-N3-C4	-6.54	116.63	119.90
1	1A	2639	G	N7-C8-N9	-6.54	109.83	113.10
2	1B	41	U	C5-C4-O4	6.54	129.83	125.90
1	2A	739	G	C5-C6-O6	-6.54	124.67	128.60
32	2a	717	C	O5'-P-OP2	6.54	118.55	110.70
32	2a	1011	G	C4-C5-N7	-6.54	108.18	110.80
1	1A	802	C	C6-N1-C2	-6.54	117.68	120.30
1	2A	663	G	C8-N9-C4	6.54	109.02	106.40
1	1A	1683	C	N3-C2-O2	-6.54	117.32	121.90
32	1a	134	A	N1-C6-N6	6.54	122.52	118.60
1	1A	2052	A	C5-N7-C8	-6.54	100.63	103.90
1	2A	2576	G	C8-N9-C4	6.54	109.02	106.40
1	1A	2100	C	C5-C6-N1	-6.54	117.73	121.00
1	1A	2353	G	C8-N9-C4	-6.54	103.79	106.40
1	1A	472	G	N9-C4-C5	-6.53	102.79	105.40
1	1A	652	A	C2-N3-C4	6.53	113.87	110.60
1	1A	2577	A	C6-N1-C2	-6.53	114.68	118.60
1	1A	2630	G	N1-C6-O6	-6.53	115.98	119.90
2	1B	57	A	C4-C5-C6	-6.53	113.73	117.00
32	1a	655	A	O5'-P-OP2	-6.53	99.82	105.70
1	1A	752	A	C8-N9-C4	6.53	108.41	105.80
1	1A	1752	G	C8-N9-C4	-6.53	103.79	106.40
1	2A	2515	C	N1-C2-O2	-6.53	114.98	118.90
1	1A	565	C	N3-C4-C5	6.53	124.51	121.90
1	1A	1655	A	C5-N7-C8	6.53	107.17	103.90
1	1A	1690	G	C6-C5-N7	6.53	134.32	130.40
1	1A	616	G	C5-C6-O6	6.53	132.52	128.60
1	2A	2002	G	C5-N7-C8	6.53	107.56	104.30
32	1a	928	G	O5'-P-OP1	-6.53	99.82	105.70
1	2A	2827	C	N3-C2-O2	6.53	126.47	121.90
32	2a	902	G	N7-C8-N9	-6.53	109.84	113.10
1	2A	1574	C	C5-C6-N1	6.53	124.26	121.00
1	2A	1937	A	O4'-C1'-N9	6.53	113.42	108.20
1	2A	1966	A	C5-C6-N6	6.53	128.92	123.70
1	1A	2229	A	O4'-C1'-N9	6.52	113.42	108.20
1	1A	848	G	N7-C8-N9	6.52	116.36	113.10
1	2A	1097	U	C6-N1-C1'	-6.52	112.07	121.20
32	2a	289	G	OP1-P-OP2	-6.52	109.82	119.60
1	1A	2080	A	C8-N9-C4	6.52	108.41	105.80
1	1A	874	U	OP1-P-OP2	-6.52	109.82	119.60
1	1A	1285	G	C5-C6-N1	-6.52	108.24	111.50
1	1A	2037	A	O5'-P-OP2	-6.52	99.83	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2283	G	N3-C4-C5	-6.52	125.34	128.60
32	1a	1465	C	N1-C2-O2	-6.52	114.99	118.90
1	2A	2058	A	N1-C6-N6	6.52	122.51	118.60
1	1A	1924	C	OP2-P-O3'	6.52	119.54	105.20
1	2A	573	G	OP1-P-O3'	6.52	119.54	105.20
32	2a	38	G	C8-N9-C4	6.52	109.01	106.40
1	1A	745	C	O5'-P-OP2	-6.52	99.84	105.70
1	2A	1618	A	N1-C6-N6	-6.52	114.69	118.60
1	2A	2488	A	N1-C6-N6	6.52	122.51	118.60
1	1A	1359	U	O5'-P-OP1	-6.51	99.84	105.70
1	1A	1853	G	N1-C6-O6	-6.51	115.99	119.90
1	2A	297	C	C6-N1-C2	-6.51	117.69	120.30
1	1A	1378	G	C6-C5-N7	-6.51	126.49	130.40
1	1A	106	U	N3-C4-C5	6.51	118.51	114.60
1	1A	204	G	O5'-P-OP2	6.51	118.51	110.70
1	1A	2244	U	OP1-P-OP2	6.51	129.37	119.60
1	1A	2877	G	N1-C6-O6	6.51	123.81	119.90
32	2a	190	U	C6-N1-C2	-6.51	117.09	121.00
1	1A	1057	G	O5'-P-OP2	-6.51	99.84	105.70
1	2A	1047	G	N3-C4-C5	-6.51	125.35	128.60
1	1A	1495	G	C8-N9-C4	6.50	109.00	106.40
1	1A	1482	G	C5-C6-O6	6.50	132.50	128.60
1	2A	1652	A	C8-N9-C4	6.50	108.40	105.80
1	1A	1700	G	C8-N9-C4	-6.50	103.80	106.40
1	1A	1911	A	C2-N3-C4	-6.50	107.35	110.60
32	1a	1279	A	N7-C8-N9	6.50	117.05	113.80
1	1A	1537	G	C5-N7-C8	6.50	107.55	104.30
32	1a	753	A	OP1-P-O3'	6.50	119.50	105.20
1	1A	2288	G	C5-C6-N1	6.50	114.75	111.50
2	1B	98	G	O5'-P-OP2	-6.50	99.85	105.70
1	2A	920	G	N9-C4-C5	6.50	108.00	105.40
1	2A	1650	G	C8-N9-C4	-6.50	103.80	106.40
32	2a	1099	G	N3-C2-N2	-6.50	115.35	119.90
32	1a	576	G	C4-N9-C1'	6.50	134.94	126.50
1	1A	1371	G	N3-C2-N2	-6.49	115.35	119.90
1	1A	2671	G	C2-N3-C4	-6.49	108.65	111.90
1	1A	2609	G	C8-N9-C4	-6.49	103.80	106.40
1	2A	2553	G	C8-N9-C4	6.49	109.00	106.40
1	1A	491	G	C5-C6-N1	6.49	114.75	111.50
1	1A	2095	C	N3-C4-C5	6.49	124.50	121.90
1	1A	2262	G	O5'-P-OP2	-6.49	99.86	105.70
1	2A	1087	G	C4-N9-C1'	-6.49	118.06	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	115	G	N3-C4-C5	-6.49	125.36	128.60
1	2A	11	G	C5-C6-O6	-6.49	124.71	128.60
1	2A	237	C	OP2-P-O3'	6.49	119.48	105.20
1	2A	1766	U	O5'-P-OP2	-6.49	99.86	105.70
1	1A	1650	C	C5-C4-N4	-6.49	115.66	120.20
1	2A	1968	G	C5-C6-O6	-6.49	124.71	128.60
2	2B	41	U	C6-N1-C2	-6.49	117.11	121.00
1	1A	892	G	O5'-P-OP2	-6.48	99.86	105.70
1	1A	2165	C	C5-C6-N1	6.48	124.24	121.00
1	1A	2476	C	N1-C2-O2	-6.48	115.01	118.90
1	1A	359	C	C2-N3-C4	6.48	123.14	119.90
1	1A	2102	G	N1-C6-O6	-6.48	116.01	119.90
1	2A	845	G	O4'-C1'-N9	6.48	113.38	108.20
1	1A	1033	G	N9-C4-C5	6.48	107.99	105.40
1	1A	1959	A	O5'-P-OP2	-6.48	99.87	105.70
32	1a	1276	G	N7-C8-N9	6.48	116.34	113.10
1	2A	1650	G	N1-C6-O6	-6.48	116.01	119.90
32	2a	1158	C	N1-C2-O2	6.48	122.79	118.90
1	1A	2272	C	O5'-P-OP2	-6.48	99.87	105.70
1	1A	2292	G	C5-C6-O6	6.48	132.49	128.60
2	2B	115	G	N7-C8-N9	-6.48	109.86	113.10
1	1A	1822	A	OP2-P-O3'	6.47	119.44	105.20
1	2A	1323	U	OP1-P-O3'	6.47	119.44	105.20
1	2A	2182	G	N9-C4-C5	6.47	107.99	105.40
32	2a	343	U	O4'-C1'-N1	6.47	113.38	108.20
1	1A	1951	G	O5'-P-OP2	-6.47	99.87	105.70
1	1A	2251	G	N3-C2-N2	6.47	124.43	119.90
1	1A	2361	G	C8-N9-C4	6.47	108.99	106.40
1	1A	2627	U	N3-C4-O4	-6.47	114.87	119.40
32	1a	1054	C	C5-C6-N1	-6.47	117.76	121.00
1	1A	1204	C	N3-C4-N4	-6.47	113.47	118.00
1	1A	107	G	C6-C5-N7	6.47	134.28	130.40
1	1A	1390	G	N3-C2-N2	-6.47	115.37	119.90
1	1A	2618	C	C2-N3-C4	-6.47	116.67	119.90
1	2A	1388	G	C8-N9-C4	6.47	108.99	106.40
1	1A	2754	A	OP1-P-OP2	6.47	129.30	119.60
1	2A	1784	A	O5'-P-OP2	-6.47	99.88	105.70
1	1A	849	A	N1-C6-N6	-6.47	114.72	118.60
1	1A	1255	A	C8-N9-C4	-6.47	103.21	105.80
1	1A	2266	C	C6-N1-C2	-6.47	117.71	120.30
1	1A	1867	C	N3-C2-O2	-6.46	117.38	121.90
1	1A	2195	A	N1-C2-N3	6.46	132.53	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	383	U	N3-C2-O2	-6.46	117.67	122.20
1	2A	2179	C	C6-N1-C2	-6.46	117.71	120.30
1	2A	2358	G	O5'-P-OP2	-6.46	99.88	105.70
32	2a	1015	A	C8-N9-C4	-6.46	103.21	105.80
32	2a	1024	G	N1-C2-N2	6.46	122.02	116.20
1	1A	575	G	OP1-P-OP2	-6.46	109.91	119.60
32	1a	836	G	C5-C6-O6	-6.46	124.72	128.60
1	2A	157	U	N1-C2-O2	6.46	127.32	122.80
1	2A	2041	U	N3-C2-O2	6.46	126.72	122.20
1	1A	403	C	N1-C2-O2	6.46	122.78	118.90
1	1A	755	C	N3-C4-C5	6.46	124.48	121.90
1	1A	2623	U	N1-C2-O2	-6.46	118.28	122.80
1	1A	2632	C	OP1-P-OP2	6.46	129.29	119.60
32	1a	221	C	C6-N1-C2	-6.46	117.72	120.30
1	2A	1531	C	C6-N1-C2	-6.46	117.72	120.30
1	1A	940	C	C6-N1-C2	-6.46	117.72	120.30
1	1A	1302	G	C8-N9-C4	6.46	108.98	106.40
1	2A	2541	A	N1-C6-N6	6.46	122.48	118.60
1	1A	841	G	N1-C2-N2	-6.46	110.39	116.20
1	1A	2319	G	N1-C6-O6	6.46	123.78	119.90
1	1A	2741	U	N3-C4-O4	-6.46	114.88	119.40
32	1a	875	C	OP1-P-O3'	6.46	119.41	105.20
1	1A	1831	C	N1-C2-N3	6.46	123.72	119.20
32	1a	105	G	C4-C5-N7	6.46	113.38	110.80
1	2A	1689	A	C4-C5-N7	6.46	113.93	110.70
1	1A	2620	G	O5'-P-OP2	-6.46	99.89	105.70
1	1A	1816	A	N7-C8-N9	6.45	117.03	113.80
1	2A	2599	G	N1-C6-O6	-6.45	116.03	119.90
1	2A	753	C	N3-C4-N4	-6.45	113.48	118.00
32	2a	890	G	O4'-C1'-N9	6.45	113.36	108.20
1	1A	621	G	N1-C6-O6	-6.45	116.03	119.90
1	1A	1093	G	C4-N9-C1'	6.45	134.89	126.50
1	1A	2348	A	C5-C6-N6	-6.45	118.54	123.70
1	2A	510	C	OP1-P-OP2	6.45	129.27	119.60
1	2A	1963	U	N3-C2-O2	-6.45	117.69	122.20
1	1A	1147	U	N3-C2-O2	-6.45	117.69	122.20
1	1A	1270	C	N3-C4-C5	6.45	124.48	121.90
1	1A	2612	A	N9-C4-C5	6.45	108.38	105.80
32	1a	1084	G	O5'-P-OP2	-6.45	99.90	105.70
32	1a	399	G	N1-C6-O6	6.45	123.77	119.90
1	1A	2269	U	N1-C2-N3	6.44	118.77	114.90
1	2A	2128	C	N1-C2-O2	6.44	122.77	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	28	A	O5'-P-OP2	-6.44	99.90	105.70
1	1A	786	G	OP2-P-O3'	-6.44	91.03	105.20
1	1A	966	G	C5-C6-O6	6.44	132.47	128.60
1	2A	792	G	C2-N3-C4	6.44	115.12	111.90
1	2A	882	G	C4-N9-C1'	-6.44	118.13	126.50
1	1A	1429	C	N1-C2-O2	-6.44	115.04	118.90
1	1A	1806	U	C2-N3-C4	-6.44	123.14	127.00
1	1A	2621	U	C5-C6-N1	-6.44	119.48	122.70
32	1a	511	C	N3-C2-O2	-6.44	117.39	121.90
1	1A	621	G	OP2-P-O3'	6.44	119.36	105.20
1	1A	1511	C	N1-C2-O2	-6.44	115.04	118.90
1	1A	2262	G	C5-C6-O6	6.44	132.46	128.60
1	1A	2346	G	C5-C6-O6	-6.44	124.74	128.60
1	1A	1438	A	OP2-P-O3'	6.43	119.36	105.20
1	1A	2043	C	C6-N1-C2	6.43	122.87	120.30
32	1a	500	G	OP2-P-O3'	6.43	119.36	105.20
1	2A	35	G	N3-C2-N2	6.43	124.40	119.90
1	2A	127	A	O5'-P-OP2	-6.43	99.91	105.70
1	2A	2207	G	C4-C5-C6	6.43	122.66	118.80
32	2a	539	A	C8-N9-C4	-6.43	103.23	105.80
1	1A	1809	U	C6-N1-C2	6.43	124.86	121.00
1	1A	2112	G	C5-C6-O6	6.43	132.46	128.60
1	2A	1318	C	N1-C2-O2	-6.43	115.04	118.90
32	2a	662	G	N1-C6-O6	6.43	123.76	119.90
1	1A	1311	A	C8-N9-C4	-6.43	103.23	105.80
1	1A	1690	G	C5-C6-O6	6.43	132.46	128.60
1	1A	2115	G	C8-N9-C4	6.43	108.97	106.40
1	2A	2570	G	C4-C5-N7	-6.43	108.23	110.80
1	1A	813	C	C5-C6-N1	-6.43	117.79	121.00
1	2A	1280	G	OP2-P-O3'	6.43	119.34	105.20
1	2A	1905	C	O5'-P-OP2	-6.43	99.92	105.70
1	1A	2019	G	OP1-P-OP2	-6.43	109.96	119.60
1	1A	98	U	C6-N1-C1'	-6.42	112.21	121.20
1	1A	2222	C	C2-N3-C4	-6.42	116.69	119.90
1	1A	2579	G	O5'-P-OP1	-6.42	99.92	105.70
1	2A	254	G	C2-N3-C4	-6.42	108.69	111.90
1	2A	1497	U	C5-C6-N1	-6.42	119.49	122.70
1	1A	916	G	O5'-P-OP2	-6.42	99.92	105.70
1	2A	1653	G	OP1-P-OP2	6.42	129.24	119.60
1	2A	2463	C	O5'-P-OP2	-6.42	99.92	105.70
32	2a	802	A	C8-N9-C4	-6.42	103.23	105.80
1	1A	1299	A	C2-N3-C4	6.42	113.81	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2609	G	O5'-P-OP2	-6.42	99.92	105.70
1	1A	879	G	O5'-P-OP2	-6.42	99.92	105.70
1	1A	2573	A	N1-C6-N6	-6.42	114.75	118.60
2	1B	71	C	C5-C6-N1	-6.42	117.79	121.00
1	1A	2451	A	C6-N1-C2	6.42	122.45	118.60
32	1a	134	A	C5-C6-N6	-6.42	118.56	123.70
32	1a	366	C	OP1-P-OP2	6.42	129.22	119.60
32	2a	773	G	N3-C4-C5	6.42	131.81	128.60
1	1A	1604	C	C6-N1-C2	6.42	122.87	120.30
1	1A	1886	G	OP2-P-O3'	6.42	119.31	105.20
1	1A	2107	C	C2-N3-C4	-6.42	116.69	119.90
32	1a	190	U	OP1-P-OP2	-6.42	109.98	119.60
2	1B	1	U	C5-C4-O4	-6.41	122.05	125.90
1	1A	803	C	C4-C5-C6	6.41	120.61	117.40
1	1A	1356	G	C5-C6-O6	6.41	132.45	128.60
1	1A	1377	A	C8-N9-C4	-6.41	103.23	105.80
1	2A	1066	U	N1-C2-O2	-6.41	118.31	122.80
1	1A	1299	A	C8-N9-C4	6.41	108.36	105.80
32	1a	935	A	O5'-P-OP1	-6.41	99.93	105.70
1	2A	1992	G	O5'-P-OP2	-6.41	99.93	105.70
1	2A	2178	C	C6-N1-C2	-6.41	117.74	120.30
1	1A	105	C	N1-C2-O2	-6.41	115.06	118.90
1	1A	497	A	C8-N9-C4	-6.41	103.24	105.80
1	1A	1442	U	OP1-P-OP2	6.41	129.21	119.60
1	1A	1543	U	N3-C4-C5	6.41	118.44	114.60
1	2A	467	G	C5-N7-C8	6.41	107.50	104.30
1	1A	1411	A	N1-C6-N6	6.41	122.44	118.60
32	1a	1382	C	N3-C2-O2	-6.41	117.42	121.90
1	2A	2612	C	N3-C4-C5	6.41	124.46	121.90
32	2a	899	C	C6-N1-C2	6.41	122.86	120.30
32	2a	1125	U	N1-C2-O2	6.41	127.28	122.80
32	1a	528	C	C6-N1-C2	-6.40	117.74	120.30
1	2A	1252	G	O4'-C1'-N9	-6.40	103.08	108.20
32	2a	372	C	C2-N3-C4	6.40	123.10	119.90
1	1A	1020	C	N3-C2-O2	-6.40	117.42	121.90
32	1a	158	G	C8-N9-C1'	6.40	135.32	127.00
1	2A	1583	A	O5'-P-OP2	-6.40	99.94	105.70
1	1A	985	G	N3-C4-C5	-6.40	125.40	128.60
32	1a	143	A	O5'-P-OP1	-6.40	99.94	105.70
1	1A	918	U	N1-C2-O2	-6.40	118.32	122.80
32	1a	567	G	C8-N9-C4	-6.40	103.84	106.40
32	1a	820	U	C4-C5-C6	6.40	123.54	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	830	G	C5-C6-O6	-6.40	124.76	128.60
1	1A	1260	G	C5-C6-N1	6.40	114.70	111.50
1	1A	1876	G	C5-C6-O6	6.40	132.44	128.60
1	1A	2604	G	N1-C6-O6	-6.40	116.06	119.90
1	2A	1517	G	C5-C6-N1	-6.40	108.30	111.50
1	1A	2272	C	N3-C2-O2	-6.40	117.42	121.90
1	2A	784	A	OP1-P-O3'	6.40	119.27	105.20
1	1A	2295	C	N3-C4-C5	6.39	124.46	121.90
32	1a	603	U	O5'-P-OP2	6.39	118.37	110.70
1	2A	1328	G	C5-C6-O6	-6.39	124.76	128.60
1	1A	1633	A	C2-N3-C4	6.39	113.80	110.60
1	2A	1073	A	N1-C2-N3	6.39	132.50	129.30
2	2B	1	U	N1-C2-O2	6.39	127.27	122.80
32	2a	251	G	N3-C4-N9	6.39	129.84	126.00
1	2A	1983	C	N3-C4-N4	6.39	122.47	118.00
1	1A	572	A	N3-C4-C5	-6.39	122.33	126.80
1	1A	2053	A	C6-N1-C2	6.39	122.43	118.60
32	1a	813	U	OP1-P-OP2	-6.39	110.02	119.60
1	1A	617	U	C5-C6-N1	-6.39	119.51	122.70
1	1A	835	A	C4-C5-C6	6.39	120.19	117.00
1	2A	2850	A	N7-C8-N9	6.39	116.99	113.80
1	1A	1820	A	C8-N9-C4	6.39	108.36	105.80
1	2A	1091	G	C8-N9-C4	-6.39	103.84	106.40
1	2A	2145	C	C2-N3-C4	6.39	123.09	119.90
1	2A	2416	C	C6-N1-C2	-6.39	117.75	120.30
1	1A	1520	G	N3-C2-N2	6.38	124.37	119.90
1	1A	2072	C	OP2-P-O3'	6.38	119.25	105.20
2	1B	42	C	O5'-P-OP1	-6.38	99.95	105.70
1	2A	1354	A	O5'-P-OP2	-6.38	99.95	105.70
1	2A	1924	C	C6-N1-C2	-6.38	117.75	120.30
32	2a	458	C	N3-C2-O2	-6.38	117.43	121.90
32	1a	781	A	C4-C5-C6	-6.38	113.81	117.00
32	2a	442	C	C2-N1-C1'	6.38	125.82	118.80
32	1a	1370	G	C6-C5-N7	-6.38	126.57	130.40
32	2a	397	A	C8-N9-C4	-6.38	103.25	105.80
1	1A	751	G	C6-N1-C2	-6.38	121.27	125.10
1	1A	1725	G	N7-C8-N9	6.38	116.29	113.10
1	1A	2862	G	OP2-P-O3'	6.38	119.23	105.20
32	1a	1406	U	C2-N3-C4	-6.38	123.17	127.00
1	1A	1291	G	N9-C4-C5	6.38	107.95	105.40
1	1A	1823	G	N1-C6-O6	-6.38	116.07	119.90
1	1A	1856	A	C2-N3-C4	6.38	113.79	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2033	U	N3-C4-C5	-6.38	110.78	114.60
32	1a	901	A	N1-C6-N6	6.38	122.42	118.60
1	1A	354	A	N9-C1'-C2'	-6.38	104.99	112.00
1	1A	673	G	C5-C6-O6	6.37	132.42	128.60
1	1A	2260	C	N1-C2-O2	-6.37	115.08	118.90
2	1B	80	U	N3-C4-O4	-6.37	114.94	119.40
1	2A	2039	C	C6-N1-C2	-6.37	117.75	120.30
1	1A	1478	C	N1-C2-O2	-6.37	115.08	118.90
1	1A	2448	G	C5-C6-O6	6.37	132.42	128.60
32	1a	670	G	C4-C5-N7	-6.37	108.25	110.80
32	1a	1026	G	N7-C8-N9	6.37	116.28	113.10
1	2A	1617	C	C6-N1-C2	-6.37	117.75	120.30
1	2A	2475	C	C6-N1-C2	-6.37	117.75	120.30
1	2A	2896	C	C6-N1-C2	-6.37	117.75	120.30
1	1A	990	A	O5'-P-OP2	-6.37	99.97	105.70
1	1A	1024	G	N1-C6-O6	-6.37	116.08	119.90
1	1A	2092	G	C5-C6-O6	6.37	132.42	128.60
1	2A	652(T)	C	C5-C6-N1	6.37	124.19	121.00
1	2A	1606	G	OP1-P-O3'	6.37	119.22	105.20
1	1A	425	G	C2-N3-C4	-6.37	108.72	111.90
1	1A	441	C	O5'-P-OP2	-6.37	99.97	105.70
1	1A	874	U	N3-C4-C5	6.37	118.42	114.60
1	1A	2525	G	C6-N1-C2	6.37	128.92	125.10
1	2A	226	G	O4'-C1'-N9	6.37	113.30	108.20
32	1a	174	C	C5-C6-N1	6.37	124.18	121.00
1	2A	1913	A	N7-C8-N9	6.37	116.98	113.80
1	1A	196	A	C4-C5-N7	6.37	113.88	110.70
1	1A	369	A	C5-C6-N1	6.37	120.88	117.70
1	1A	843	C	N1-C2-N3	6.37	123.66	119.20
1	1A	1148	C	C5-C6-N1	6.37	124.18	121.00
1	1A	1316	C	N3-C4-N4	-6.37	113.54	118.00
32	1a	841	U	N1-C2-O2	6.37	127.26	122.80
1	2A	1586	A	O5'-P-OP2	6.37	118.34	110.70
1	2A	2783	G	C4-C5-N7	-6.37	108.25	110.80
1	1A	800	C	C5-C4-N4	6.36	124.65	120.20
1	1A	1739	U	C5-C6-N1	-6.36	119.52	122.70
1	1A	2419	G	C8-N9-C1'	-6.36	118.73	127.00
1	1A	2678	C	C6-N1-C2	-6.36	117.75	120.30
1	2A	675	A	C2-N3-C4	-6.36	107.42	110.60
1	2A	1373	A	N7-C8-N9	-6.36	110.62	113.80
32	2a	1406	U	O5'-P-OP1	6.36	118.33	110.70
1	1A	850	U	C5-C6-N1	-6.36	119.52	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1229	G	C5-C6-O6	6.36	132.42	128.60
1	1A	2102	G	C8-N9-C4	6.36	108.94	106.40
1	1A	2627	U	N1-C2-O2	6.36	127.25	122.80
32	1a	326	G	C5-C6-O6	6.36	132.42	128.60
1	2A	2689	U	N3-C2-O2	-6.36	117.75	122.20
1	1A	330	U	C2-N3-C4	6.36	130.82	127.00
1	2A	1032	A	O5'-P-OP2	-6.36	99.98	105.70
1	1A	836	A	OP1-P-OP2	-6.36	110.06	119.60
1	2A	2132	U	C5-C4-O4	6.36	129.72	125.90
1	1A	631	A	N1-C6-N6	-6.36	114.79	118.60
1	1A	1425	A	C4-C5-N7	6.36	113.88	110.70
1	1A	1653	C	N3-C4-N4	6.36	122.45	118.00
1	1A	1747	A	C8-N9-C4	6.36	108.34	105.80
1	1A	1861	C	N3-C4-C5	6.36	124.44	121.90
1	1A	1950	A	O5'-P-OP1	-6.36	99.98	105.70
1	1A	2207	C	N1-C2-O2	6.36	122.71	118.90
1	1A	2445	A	C2-N3-C4	6.36	113.78	110.60
1	1A	2790	G	C5-C6-N1	6.36	114.68	111.50
32	1a	576	G	C8-N9-C1'	-6.36	118.73	127.00
1	1A	497	A	N9-C4-C5	6.36	108.34	105.80
1	1A	762	G	N3-C4-N9	6.35	129.81	126.00
1	1A	1863	C	N1-C2-N3	6.35	123.65	119.20
32	2a	404	U	O5'-P-OP2	-6.35	99.98	105.70
1	1A	1668	G	OP1-P-OP2	6.35	129.13	119.60
32	1a	1035	A	C8-N9-C4	-6.35	103.26	105.80
1	1A	1573	G	C4-C5-N7	-6.35	108.26	110.80
1	1A	1993	A	C2-N3-C4	-6.35	107.42	110.60
1	1A	2457	G	N1-C6-O6	-6.35	116.09	119.90
1	1A	2565	G	N3-C4-N9	6.35	129.81	126.00
1	2A	100	G	C8-N9-C4	6.35	108.94	106.40
1	2A	958	U	N1-C2-N3	6.35	118.71	114.90
32	2a	533	A	O5'-P-OP2	6.35	118.32	110.70
32	1a	603	U	O5'-P-OP1	-6.35	99.99	105.70
1	2A	1497	U	N3-C4-O4	-6.35	114.96	119.40
1	1A	1965	U	N1-C2-N3	6.35	118.71	114.90
1	1A	2638	C	C6-N1-C2	6.35	122.84	120.30
32	1a	1097	C	N3-C2-O2	-6.35	117.46	121.90
1	2A	2058	A	C4-C5-C6	6.35	120.17	117.00
1	1A	87	G	N3-C2-N2	-6.34	115.46	119.90
1	1A	700	A	C5-C6-N6	-6.34	118.62	123.70
1	1A	700	A	N1-C6-N6	6.34	122.41	118.60
1	1A	2204	G	N3-C4-N9	-6.34	122.19	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	821	G	C6-C5-N7	-6.34	126.59	130.40
32	1a	1292	U	O5'-P-OP2	-6.34	99.99	105.70
1	1A	616	G	C4-C5-N7	-6.34	108.26	110.80
1	1A	2118	U	OP2-P-O3'	6.34	119.15	105.20
32	1a	773	G	N3-C4-N9	-6.34	122.19	126.00
1	2A	308	G	C5-C6-O6	-6.34	124.79	128.60
1	2A	2893	G	N3-C2-N2	6.34	124.34	119.90
1	1A	556	C	OP1-P-OP2	-6.34	110.09	119.60
1	1A	1312	G	C5-C6-O6	-6.34	124.80	128.60
1	2A	2336	A	O5'-P-OP2	-6.34	99.99	105.70
1	1A	1714	G	N1-C6-O6	-6.34	116.10	119.90
1	1A	1902	C	C6-N1-C2	-6.34	117.76	120.30
32	1a	68	G	O5'-P-OP2	-6.34	100.00	105.70
1	2A	1071	G	N1-C6-O6	6.34	123.70	119.90
1	2A	1362	C	O5'-P-OP1	-6.34	100.00	105.70
1	2A	2273	A	O5'-P-OP2	-6.34	99.99	105.70
1	1A	451	G	N1-C6-O6	-6.34	116.10	119.90
1	2A	602	G	O5'-P-OP2	-6.34	100.00	105.70
1	2A	1807	G	O5'-P-OP2	-6.34	100.00	105.70
1	1A	1756	U	N1-C2-O2	-6.34	118.36	122.80
32	2a	1030(D)	A	C8-N9-C4	-6.34	103.27	105.80
1	1A	1725	G	C6-N1-C2	-6.33	121.30	125.10
1	1A	677	C	C2-N3-C4	-6.33	116.73	119.90
1	1A	1293	A	N7-C8-N9	6.33	116.97	113.80
1	1A	2636	G	N3-C2-N2	6.33	124.33	119.90
32	1a	1150	U	C5-C6-N1	6.33	125.87	122.70
1	1A	733	G	N3-C2-N2	6.33	124.33	119.90
1	1A	1221	G	C8-N9-C1'	6.33	135.23	127.00
1	1A	2044	U	O5'-P-OP2	6.33	118.30	110.70
32	1a	625	G	O5'-P-OP1	-6.33	100.00	105.70
32	1a	1505	G	C4-C5-N7	-6.33	108.27	110.80
1	1A	255	G	C4-C5-N7	6.33	113.33	110.80
1	1A	330	U	C5-C4-O4	6.33	129.70	125.90
1	1A	364	A	O5'-P-OP1	-6.33	100.00	105.70
1	1A	1507	A	O4'-C1'-N9	6.33	113.26	108.20
1	1A	1977	U	C5-C6-N1	-6.33	119.54	122.70
1	1A	2283	G	N3-C2-N2	6.33	124.33	119.90
1	1A	1115	A	C8-N9-C4	6.33	108.33	105.80
1	2A	1670	C	OP1-P-O3'	6.33	119.11	105.20
32	2a	777	A	O5'-P-OP2	-6.33	100.01	105.70
32	2a	1375	A	C8-N9-C4	-6.33	103.27	105.80
1	1A	1340	U	C4-C5-C6	6.32	123.49	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2511	C	N3-C4-N4	6.32	122.43	118.00
32	1a	902	G	OP2-P-O3'	6.32	119.11	105.20
32	1a	1125	U	O5'-P-OP1	-6.32	100.01	105.70
1	2A	746	A	O5'-P-OP1	-6.32	100.01	105.70
1	2A	1062	G	O4'-C1'-N9	6.32	113.26	108.20
1	2A	1261	C	C2-N1-C1'	-6.32	111.84	118.80
1	1A	2523	U	C2-N3-C4	-6.32	123.21	127.00
1	1A	2582	G	C4-C5-N7	-6.32	108.27	110.80
1	2A	1992	G	C5-C6-O6	-6.32	124.81	128.60
1	1A	1635	C	N3-C4-C5	6.32	124.43	121.90
1	1A	1814	A	C6-C5-N7	6.32	136.72	132.30
1	1A	226	C	C2-N3-C4	-6.32	116.74	119.90
1	1A	486	A	C5-C6-N6	6.32	128.75	123.70
32	1a	1184	G	N1-C6-O6	6.32	123.69	119.90
1	2A	602	G	N3-C4-N9	6.32	129.79	126.00
1	1A	2828	G	C5-C6-O6	6.32	132.39	128.60
1	1A	2881	C	N3-C2-O2	6.32	126.32	121.90
1	1A	747	G	N1-C2-N2	-6.31	110.52	116.20
1	1A	1142	A	O4'-C1'-N9	6.31	113.25	108.20
1	1A	837	C	N3-C2-O2	6.31	126.32	121.90
1	1A	877	G	N1-C6-O6	-6.31	116.11	119.90
1	1A	1154	U	N3-C4-O4	6.31	123.82	119.40
1	1A	1662	A	O5'-P-OP1	-6.31	100.02	105.70
1	2A	1062	G	N7-C8-N9	6.31	116.26	113.10
1	1A	816	G	OP2-P-O3'	6.31	119.08	105.20
1	1A	906	G	C8-N9-C4	6.31	108.92	106.40
1	1A	2551	C	C6-N1-C2	6.31	122.82	120.30
4	1E	119	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	1A	740	C	N3-C2-O2	-6.31	117.48	121.90
1	1A	2091	G	C6-N1-C2	-6.31	121.31	125.10
1	1A	335	A	O5'-P-OP1	6.30	118.27	110.70
1	1A	640	A	OP1-P-OP2	6.30	129.06	119.60
1	1A	1383	G	C4-C5-N7	-6.30	108.28	110.80
1	1A	1833	A	O5'-P-OP2	6.30	118.27	110.70
1	1A	2023	A	C4-C5-N7	-6.30	107.55	110.70
1	1A	2201	C	C5-C6-N1	6.30	124.15	121.00
32	1a	1441	G	C5-C6-O6	6.30	132.38	128.60
1	2A	272(E)	G	C8-N9-C4	6.30	108.92	106.40
1	1A	365	G	N9-C4-C5	6.30	107.92	105.40
1	2A	395	U	N1-C2-O2	6.30	127.21	122.80
1	1A	578	U	O4'-C1'-N1	6.30	113.24	108.20
1	1A	1072	U	N3-C2-O2	-6.30	117.79	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1451	U	C5-C4-O4	6.30	129.68	125.90
1	1A	2227	G	N3-C4-C5	6.30	131.75	128.60
32	1a	663	A	O5'-P-OP1	-6.30	100.03	105.70
32	2a	1475	G	N7-C8-N9	6.30	116.25	113.10
1	1A	906	G	C4-N9-C1'	-6.30	118.31	126.50
1	2A	1323	U	N1-C2-O2	-6.30	118.39	122.80
1	1A	980	C	C4-C5-C6	6.30	120.55	117.40
1	1A	1814	A	C4-C5-C6	-6.30	113.85	117.00
32	2a	802	A	N7-C8-N9	6.30	116.95	113.80
1	1A	744	C	N3-C4-N4	-6.30	113.59	118.00
1	1A	2277	U	N3-C4-C5	-6.30	110.82	114.60
1	1A	2308	U	N3-C4-O4	6.30	123.81	119.40
1	1A	2400	A	C8-N9-C4	-6.30	103.28	105.80
1	1A	2475	C	C2-N3-C4	-6.30	116.75	119.90
1	1A	2879	G	C8-N9-C4	-6.30	103.88	106.40
1	1A	821	A	N1-C6-N6	-6.29	114.82	118.60
1	2A	366	C	N1-C2-O2	-6.29	115.12	118.90
1	2A	1427	A	C6-N1-C2	-6.29	114.82	118.60
1	1A	505	A	C5-C6-N6	6.29	128.74	123.70
1	1A	1845	G	C5-C6-O6	-6.29	124.82	128.60
1	1A	2072	C	N1-C2-O2	-6.29	115.12	118.90
1	1A	2411	G	O5'-P-OP2	-6.29	100.03	105.70
32	1a	814	A	O5'-P-OP2	6.29	118.25	110.70
1	2A	1595	G	O5'-P-OP1	-6.29	100.03	105.70
1	1A	480	A	N9-C4-C5	6.29	108.32	105.80
1	1A	722	A	C4-C5-N7	6.29	113.84	110.70
1	1A	1031	C	O5'-P-OP2	-6.29	100.04	105.70
1	1A	2079	A	C5-N7-C8	6.29	107.05	103.90
32	1a	768	A	N9-C4-C5	-6.29	103.28	105.80
1	2A	33	U	N1-C2-O2	6.29	127.20	122.80
1	2A	1283	G	C8-N9-C4	6.29	108.92	106.40
1	2A	2074	U	C5-C6-N1	6.29	125.85	122.70
1	1A	2272	C	C5-C4-N4	6.29	124.60	120.20
1	1A	8	A	O5'-P-OP2	6.29	118.25	110.70
1	1A	500	G	N1-C6-O6	-6.29	116.13	119.90
1	1A	1410	G	N1-C6-O6	-6.29	116.13	119.90
32	1a	1521	G	OP1-P-OP2	6.29	129.03	119.60
1	2A	1187	G	O5'-P-OP1	6.29	118.25	110.70
1	1A	594	A	C2-N3-C4	6.29	113.74	110.60
1	1A	666	C	C5-C6-N1	6.29	124.14	121.00
1	1A	799	A	N9-C4-C5	-6.29	103.29	105.80
1	1A	850	U	N3-C2-O2	-6.29	117.80	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2137	G	N3-C4-C5	-6.29	125.46	128.60
11	1P	39	LYS	CD-CE-NZ	-6.29	97.25	111.70
1	2A	988	A	C4-C5-N7	6.29	113.84	110.70
1	2A	1445(A)	C	O5'-P-OP1	-6.29	100.04	105.70
32	2a	1482	G	N1-C6-O6	-6.29	116.13	119.90
1	1A	214	A	O5'-P-OP1	6.28	118.24	110.70
1	1A	1833	A	N7-C8-N9	-6.28	110.66	113.80
19	1X	73	ARG	NE-CZ-NH1	-6.28	117.16	120.30
32	1a	1411	C	C6-N1-C2	6.28	122.81	120.30
1	1A	194	G	N1-C2-N2	-6.28	110.55	116.20
1	1A	476	G	N9-C4-C5	-6.28	102.89	105.40
1	1A	477	C	C2-N3-C4	-6.28	116.76	119.90
1	1A	786	G	C5-C6-O6	-6.28	124.83	128.60
1	2A	1256	G	N9-C4-C5	-6.28	102.89	105.40
1	2A	1662	C	C2-N3-C4	-6.28	116.76	119.90
32	2a	1452	C	N1-C2-O2	6.28	122.67	118.90
1	2A	35	G	N1-C2-N2	-6.28	110.55	116.20
32	2a	798	G	C8-N9-C4	-6.28	103.89	106.40
1	1A	292	G	N3-C4-C5	6.28	131.74	128.60
1	1A	1709	C	C6-N1-C2	6.28	122.81	120.30
1	1A	1958	A	N9-C4-C5	-6.28	103.29	105.80
32	1a	1513	A	N1-C2-N3	-6.28	126.16	129.30
1	2A	1450(A)	C	C6-N1-C2	-6.28	117.79	120.30
1	1A	573	G	C8-N9-C4	-6.28	103.89	106.40
1	1A	2029	C	C5-C4-N4	6.28	124.59	120.20
1	1A	2619	G	C5-C6-O6	6.28	132.37	128.60
1	2A	226	G	C5-C6-O6	-6.28	124.83	128.60
32	2a	1037	C	C6-N1-C2	-6.27	117.79	120.30
2	1B	102	A	N1-C2-N3	6.27	132.44	129.30
32	1a	449	C	N1-C2-O2	6.27	122.66	118.90
1	1A	553	A	N3-C4-N9	6.27	132.41	127.40
32	1a	163	C	C6-N1-C2	-6.27	117.79	120.30
32	1a	284	G	C8-N9-C4	6.27	108.91	106.40
1	2A	1838	C	C4-C5-C6	6.27	120.53	117.40
1	2A	2372	G	N1-C6-O6	6.27	123.66	119.90
1	1A	1921	G	C5-C6-N1	6.27	114.63	111.50
32	1a	1436	U	C5-C4-O4	-6.27	122.14	125.90
1	1A	2802	C	C6-N1-C1'	6.27	128.32	120.80
32	1a	1466	C	C6-N1-C2	-6.27	117.79	120.30
1	1A	1104	G	C5-C6-O6	-6.26	124.84	128.60
1	1A	1221	G	C6-C5-N7	6.26	134.16	130.40
1	1A	1256	U	O5'-P-OP2	6.26	118.22	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2273	C	C6-N1-C2	-6.26	117.79	120.30
1	2A	2162	G	C4-N9-C1'	6.26	134.64	126.50
1	2A	2238	G	C5-C6-O6	-6.26	124.84	128.60
32	1a	187	C	C5-C6-N1	6.26	124.13	121.00
1	2A	1518	U	C5-C4-O4	6.26	129.66	125.90
1	1A	734	C	C2-N3-C4	-6.26	116.77	119.90
1	1A	960	C	O5'-P-OP2	-6.26	100.06	105.70
1	1A	1391	C	N1-C2-O2	6.26	122.66	118.90
2	2B	33	G	N1-C6-O6	6.26	123.66	119.90
1	1A	498	A	O5'-P-OP2	-6.26	100.07	105.70
32	1a	1514	C	C6-N1-C2	-6.26	117.80	120.30
32	1a	670	G	C5-C6-O6	6.26	132.35	128.60
1	1A	2279	A	OP1-P-OP2	6.26	128.99	119.60
32	1a	780	A	N1-C2-N3	-6.26	126.17	129.30
32	1a	1062	U	N3-C2-O2	-6.26	117.82	122.20
1	1A	1522	G	N9-C4-C5	6.25	107.90	105.40
1	2A	391	G	C5-C6-N1	6.25	114.63	111.50
1	1A	2591	C	C5-C6-N1	-6.25	117.87	121.00
1	1A	2858	G	N7-C8-N9	-6.25	109.97	113.10
32	1a	404	U	C2-N1-C1'	6.25	125.20	117.70
1	2A	1437	C	N1-C2-O2	6.25	122.65	118.90
32	2a	295	C	C5-C6-N1	-6.25	117.87	121.00
1	2A	806	C	N1-C2-O2	-6.25	115.15	118.90
1	1A	234	G	OP1-P-O3'	6.25	118.95	105.20
1	1A	820	U	C6-N1-C2	6.25	124.75	121.00
1	1A	1690	G	C4-C5-N7	-6.25	108.30	110.80
1	2A	1791	A	N7-C8-N9	6.25	116.92	113.80
1	2A	1826	G	N1-C6-O6	-6.25	116.15	119.90
1	1A	413	G	N7-C8-N9	6.25	116.22	113.10
1	1A	515	G	N1-C6-O6	6.25	123.65	119.90
1	1A	1130	A	C4-C5-N7	-6.25	107.58	110.70
1	1A	2610	A	N1-C6-N6	-6.25	114.85	118.60
32	1a	1019	C	C6-N1-C2	-6.25	117.80	120.30
1	1A	1437	U	C2-N3-C4	-6.25	123.25	127.00
1	1A	1533	G	OP1-P-O3'	6.25	118.94	105.20
1	2A	2603	G	O5'-P-OP1	6.25	118.19	110.70
1	1A	2324	U	O5'-P-OP2	6.24	118.19	110.70
1	2A	2744	G	O5'-P-OP2	-6.24	100.08	105.70
1	1A	2802	C	N3-C4-N4	-6.24	113.63	118.00
32	1a	1529	G	O4'-C1'-N9	6.24	113.19	108.20
1	2A	57	C	C6-N1-C2	-6.24	117.80	120.30
1	2A	2177	C	C2-N1-C1'	6.24	125.67	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1495	U	C2-N3-C4	6.24	130.75	127.00
1	1A	492	A	C5-C6-N1	6.24	120.82	117.70
1	1A	802	C	N3-C4-C5	-6.24	119.40	121.90
32	1a	874	G	N7-C8-N9	-6.24	109.98	113.10
32	1a	919	A	N1-C6-N6	-6.24	114.86	118.60
32	1a	1243	C	N1-C2-O2	-6.24	115.16	118.90
1	2A	645	C	C2-N3-C4	6.24	123.02	119.90
1	2A	655	A	N7-C8-N9	6.24	116.92	113.80
1	1A	1024	G	C4-C5-N7	-6.24	108.31	110.80
32	1a	687	A	P-O3'-C3'	6.24	127.19	119.70
32	1a	1053	G	C8-N9-C4	6.24	108.89	106.40
1	2A	1091	G	N3-C4-C5	-6.24	125.48	128.60
1	2A	2613	U	N3-C2-O2	-6.24	117.83	122.20
2	2B	1	U	C5-C6-N1	6.24	125.82	122.70
1	1A	1411	A	C5-C6-N6	-6.24	118.71	123.70
32	1a	93	G	C2-N3-C4	6.24	115.02	111.90
1	2A	408	G	O5'-P-OP2	-6.24	100.09	105.70
1	1A	89	U	C5-C6-N1	-6.23	119.58	122.70
1	1A	2634	C	N3-C4-C5	6.23	124.39	121.90
32	1a	781	A	C4-C5-N7	6.23	113.82	110.70
1	2A	2422	A	C2-N3-C4	-6.23	107.48	110.60
1	1A	1340	U	C5-C6-N1	-6.23	119.58	122.70
1	1A	2568	C	C2-N3-C4	-6.23	116.78	119.90
1	2A	483	A	OP1-P-OP2	6.23	128.95	119.60
1	1A	1953	U	N3-C4-C5	6.23	118.34	114.60
1	2A	988	A	N7-C8-N9	6.23	116.92	113.80
1	2A	2426	A	N9-C4-C5	-6.23	103.31	105.80
32	2a	1500	A	C6-N1-C2	6.23	122.34	118.60
1	2A	1477	A	O5'-P-OP2	-6.23	100.09	105.70
1	2A	2804	C	C6-N1-C2	-6.23	117.81	120.30
1	1A	82	G	C5-C6-O6	-6.23	124.86	128.60
1	1A	791	G	C5-C6-O6	6.23	132.34	128.60
1	1A	2234	G	N3-C4-C5	6.23	131.71	128.60
1	1A	2245	U	N3-C2-O2	-6.23	117.84	122.20
1	2A	1340	U	C2-N3-C4	-6.23	123.26	127.00
1	2A	1689	A	C5-C6-N6	-6.23	118.72	123.70
1	1A	201	G	O5'-P-OP1	6.23	118.17	110.70
1	1A	1091	A	N1-C6-N6	-6.23	114.86	118.60
32	1a	1054	C	N3-C4-N4	-6.23	113.64	118.00
1	1A	1228	G	N1-C6-O6	-6.22	116.17	119.90
2	2B	54	G	C8-N9-C4	-6.22	103.91	106.40
32	2a	848	C	C6-N1-C2	-6.22	117.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	171	A	O5'-P-OP2	6.22	118.17	110.70
1	1A	1573	G	N3-C2-N2	-6.22	115.54	119.90
1	2A	572	A	N9-C4-C5	6.22	108.29	105.80
1	2A	587	C	O4'-C1'-N1	-6.22	103.22	108.20
1	1A	1690	G	C2-N3-C4	6.22	115.01	111.90
1	1A	1851	U	N1-C2-N3	6.22	118.63	114.90
32	1a	191	G	C4-C5-N7	-6.22	108.31	110.80
32	1a	1348	U	O5'-P-OP2	-6.22	100.10	105.70
1	1A	641	G	N1-C2-N2	-6.22	110.60	116.20
1	2A	1652	A	N3-C4-C5	6.22	131.15	126.80
1	2A	2505	G	C8-N9-C4	-6.22	103.91	106.40
1	1A	594	A	O5'-P-OP1	-6.22	100.10	105.70
1	2A	614	U	N3-C2-O2	-6.22	117.85	122.20
1	2A	2142	C	O4'-C1'-N1	6.22	113.17	108.20
1	1A	821	A	C2-N3-C4	6.22	113.71	110.60
1	1A	2858	G	N9-C4-C5	6.22	107.89	105.40
1	2A	192	C	N3-C4-N4	6.22	122.35	118.00
1	1A	546	G	N1-C6-O6	-6.21	116.17	119.90
32	2a	810	C	N3-C4-C5	6.21	124.39	121.90
1	2A	250	G	N1-C6-O6	-6.21	116.17	119.90
32	2a	560	U	C5-C6-N1	6.21	125.81	122.70
1	1A	1183	G	C4-C5-N7	-6.21	108.31	110.80
1	1A	1995	G	OP1-P-OP2	6.21	128.92	119.60
1	1A	2703	C	N3-C4-C5	6.21	124.38	121.90
1	2A	964	C	O5'-P-OP2	-6.21	100.11	105.70
1	2A	2425	A	N7-C8-N9	6.21	116.91	113.80
32	2a	1085	U	O5'-P-OP1	-6.21	100.11	105.70
1	1A	1766	G	N3-C2-N2	6.21	124.25	119.90
1	1A	2455	C	N1-C2-O2	-6.21	115.17	118.90
1	1A	2460	A	C2-N3-C4	6.21	113.70	110.60
1	2A	1394	U	O5'-P-OP2	6.21	118.15	110.70
1	1A	217	A	C4-N9-C1'	-6.21	115.13	126.30
1	1A	1989	C	O5'-P-OP2	-6.21	100.11	105.70
1	2A	1610	A	N1-C6-N6	6.21	122.32	118.60
32	2a	883	C	C4-C5-C6	6.21	120.50	117.40
1	1A	1455	C	C5-C6-N1	-6.21	117.90	121.00
1	1A	387	G	N3-C4-N9	-6.20	122.28	126.00
1	1A	1006	C	OP1-P-OP2	6.20	128.91	119.60
1	2A	415	A	O5'-P-OP1	6.20	118.14	110.70
32	2a	189(J)	G	C8-N9-C4	6.20	108.88	106.40
1	1A	1430	A	N9-C4-C5	6.20	108.28	105.80
1	1A	1736	A	C8-N9-C4	-6.20	103.32	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	251	A	C4-C5-C6	6.20	120.10	117.00
1	2A	1121	C	O5'-P-OP2	-6.20	100.12	105.70
1	2A	1992	G	N3-C4-N9	6.20	129.72	126.00
1	2A	2113	U	C5-C6-N1	6.20	125.80	122.70
1	2A	2334	G	C5-C6-O6	-6.20	124.88	128.60
32	2a	534	U	O5'-P-OP2	-6.20	100.12	105.70
32	2a	1528	U	C6-N1-C2	6.20	124.72	121.00
1	1A	61	C	OP1-P-OP2	6.20	128.90	119.60
1	1A	554	A	C5-N7-C8	-6.20	100.80	103.90
1	1A	1250	U	C5-C4-O4	-6.20	122.18	125.90
1	1A	1391	C	N3-C2-O2	-6.20	117.56	121.90
1	1A	2283	G	N3-C4-N9	6.20	129.72	126.00
1	1A	2776	G	OP2-P-O3'	6.20	118.83	105.20
32	1a	353	A	C4-C5-N7	6.20	113.80	110.70
32	2a	792	A	O4'-C1'-N9	6.20	113.16	108.20
1	1A	406	G	N7-C8-N9	-6.20	110.00	113.10
1	1A	2101	U	N1-C2-O2	-6.20	118.46	122.80
1	2A	12	U	C6-N1-C2	-6.20	117.28	121.00
32	2a	45	U	C6-N1-C2	6.20	124.72	121.00
32	2a	93	G	O4'-C1'-N9	6.20	113.16	108.20
32	2a	1182	G	N3-C4-C5	6.20	131.70	128.60
1	1A	1371	G	C4-C5-N7	-6.20	108.32	110.80
1	1A	1556	A	N1-C6-N6	6.20	122.32	118.60
1	1A	2429	C	N3-C4-C5	-6.20	119.42	121.90
1	1A	2639	G	N1-C6-O6	6.20	123.62	119.90
32	1a	901	A	N1-C2-N3	6.20	132.40	129.30
32	2a	1391	U	C5-C4-O4	6.20	129.62	125.90
32	2a	1501	C	N1-C2-O2	-6.20	115.18	118.90
1	1A	2368	C	N3-C2-O2	6.19	126.24	121.90
32	1a	487	A	C8-N9-C4	6.19	108.28	105.80
32	2a	1465	C	N3-C4-N4	6.19	122.33	118.00
1	1A	992	G	N9-C4-C5	6.19	107.88	105.40
1	1A	2134	G	C2-N3-C4	6.19	115.00	111.90
1	1A	2546	A	N1-C6-N6	6.19	122.31	118.60
32	1a	545	C	O5'-P-OP1	-6.19	100.13	105.70
32	1a	1258	G	C2-N3-C4	6.19	115.00	111.90
1	2A	1047	G	C2-N3-C4	6.19	115.00	111.90
1	2A	2207	G	C5-N7-C8	-6.19	101.20	104.30
1	1A	1050	C	C5-C6-N1	-6.19	117.90	121.00
1	1A	2048	C	N3-C4-N4	6.19	122.33	118.00
1	1A	2449	U	C5-C6-N1	-6.19	119.61	122.70
1	1A	2579	G	N1-C6-O6	-6.19	116.19	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	895	G	C5-C6-O6	6.19	132.31	128.60
1	2A	1700	A	O5'-P-OP2	6.19	118.13	110.70
1	2A	2206	G	C8-N9-C4	6.19	108.88	106.40
1	2A	2268	A	O5'-P-OP1	-6.19	100.13	105.70
1	1A	1696	G	C8-N9-C4	-6.19	103.92	106.40
1	2A	584	C	N1-C2-O2	-6.19	115.19	118.90
1	2A	1336	A	N1-C6-N6	-6.19	114.89	118.60
32	2a	1030	C	C6-N1-C2	-6.19	117.83	120.30
32	2a	1062	U	N3-C2-O2	-6.19	117.87	122.20
32	1a	971	G	C5-C6-N1	-6.19	108.41	111.50
1	1A	1440	U	O5'-P-OP2	6.18	118.12	110.70
1	1A	2050	U	C5-C4-O4	6.18	129.61	125.90
1	1A	2654	G	C8-N9-C4	-6.18	103.93	106.40
1	2A	80	G	N1-C6-O6	-6.18	116.19	119.90
1	1A	215	G	N3-C4-N9	-6.18	122.29	126.00
32	1a	1046	A	C5-C6-N6	-6.18	118.75	123.70
1	2A	1813	G	C8-N9-C4	6.18	108.87	106.40
1	1A	1283	A	N9-C4-C5	6.18	108.27	105.80
1	1A	2082	A	C5-C6-N6	6.18	128.64	123.70
32	1a	1436	U	N1-C2-N3	6.18	118.61	114.90
1	2A	1170	G	C5-C6-N1	-6.18	108.41	111.50
1	2A	2140	C	C2-N3-C4	6.18	122.99	119.90
1	1A	2249	G	N1-C2-N2	-6.18	110.64	116.20
1	1A	2691	A	C2-N3-C4	6.18	113.69	110.60
30	18	42	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	2A	678	C	C2-N3-C4	-6.18	116.81	119.90
1	2A	704	G	O4'-C1'-N9	6.18	113.14	108.20
1	2A	741	G	N3-C4-N9	-6.18	122.29	126.00
32	2a	1510	U	C5-C4-O4	-6.18	122.19	125.90
1	1A	909	G	OP2-P-O3'	6.18	118.79	105.20
32	1a	157	G	C4-C5-N7	-6.18	108.33	110.80
1	1A	1151	U	C6-N1-C2	6.18	124.70	121.00
1	1A	2092	G	O5'-P-OP2	-6.18	100.14	105.70
1	2A	791	C	C5-C6-N1	-6.18	117.91	121.00
1	2A	1670	C	N3-C4-C5	-6.18	119.43	121.90
1	1A	1298	G	C2-N3-C4	-6.17	108.81	111.90
1	2A	2017	U	O5'-P-OP1	-6.17	100.14	105.70
32	2a	301	G	O5'-P-OP1	6.17	118.11	110.70
1	1A	555	G	C4-C5-N7	6.17	113.27	110.80
1	1A	1567	G	N7-C8-N9	6.17	116.19	113.10
1	2A	271(Y)	U	O4'-C1'-N1	6.17	113.14	108.20
1	1A	1343	C	N1-C2-O2	-6.17	115.20	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	647	C	C6-N1-C2	-6.17	117.83	120.30
32	1a	452	A	O4'-C1'-N9	6.17	113.13	108.20
32	1a	718	G	O5'-P-OP2	6.17	118.10	110.70
32	1a	1151	A	OP1-P-OP2	6.17	128.85	119.60
1	2A	1838	C	N1-C2-N3	6.17	123.52	119.20
1	2A	2263	C	N3-C2-O2	6.17	126.22	121.90
1	2A	2346	A	O5'-P-OP1	-6.17	100.15	105.70
1	2A	2592	G	N1-C6-O6	-6.17	116.20	119.90
1	1A	12	U	C6-N1-C2	-6.17	117.30	121.00
1	1A	842	C	N3-C4-N4	-6.17	113.68	118.00
1	1A	1375	U	N3-C4-O4	-6.17	115.08	119.40
1	1A	1543	U	O4'-C1'-N1	6.17	113.13	108.20
1	2A	2392	A	O5'-P-OP1	-6.17	100.15	105.70
32	1a	174	C	N3-C2-O2	-6.17	117.58	121.90
1	2A	44	G	O5'-P-OP2	-6.17	100.15	105.70
32	2a	1063	C	C6-N1-C2	-6.17	117.83	120.30
1	1A	504	A	N7-C8-N9	6.16	116.88	113.80
1	2A	915	C	N1-C2-O2	6.16	122.60	118.90
1	2A	1837	C	O5'-P-OP1	-6.16	100.15	105.70
1	1A	448	U	N1-C2-O2	-6.16	118.49	122.80
1	2A	1231	G	C5-C6-N1	-6.16	108.42	111.50
32	2a	768	A	N1-C2-N3	6.16	132.38	129.30
1	1A	860	U	N3-C4-O4	-6.16	115.09	119.40
1	1A	1669	G	C4-C5-N7	-6.16	108.33	110.80
1	1A	1911	A	OP1-P-OP2	6.16	128.84	119.60
1	1A	2091	G	O5'-P-OP1	6.16	118.09	110.70
32	1a	754	C	N3-C2-O2	-6.16	117.59	121.90
1	2A	50	U	C6-N1-C2	6.16	124.70	121.00
1	2A	1320	C	C2-N3-C4	-6.16	116.82	119.90
1	2A	1320	C	C6-N1-C2	6.16	122.76	120.30
1	2A	1997	G	OP2-P-O3'	6.16	118.75	105.20
32	2a	876	G	C6-C5-N7	6.16	134.10	130.40
1	1A	372	G	O5'-P-OP2	-6.16	100.16	105.70
1	1A	2590	G	N1-C6-O6	-6.16	116.20	119.90
1	2A	1005	C	O5'-P-OP1	-6.16	100.16	105.70
1	1A	2782	C	N1-C2-O2	-6.16	115.21	118.90
1	1A	2835	C	C6-N1-C2	6.16	122.76	120.30
32	1a	1252	A	N1-C6-N6	-6.16	114.91	118.60
1	2A	2508	G	C5-C6-N1	6.16	114.58	111.50
32	2a	820	U	N1-C2-O2	-6.16	118.49	122.80
32	1a	1134	G	C8-N9-C4	-6.16	103.94	106.40
1	1A	31	C	N1-C2-O2	-6.15	115.21	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1054	C	N3-C4-C5	-6.15	119.44	121.90
1	2A	2786	U	C5-C6-N1	6.15	125.78	122.70
1	1A	826	U	N1-C2-O2	-6.15	118.49	122.80
1	1A	2106	C	N3-C4-C5	6.15	124.36	121.90
1	1A	2257	U	C5-C6-N1	-6.15	119.62	122.70
1	1A	2682	A	O4'-C1'-N9	-6.15	103.28	108.20
1	1A	1965	U	C5-C6-N1	-6.15	119.63	122.70
1	1A	8	A	OP1-P-OP2	-6.14	110.38	119.60
1	1A	86	C	N3-C4-C5	6.14	124.36	121.90
1	1A	481	C	N1-C2-O2	-6.14	115.21	118.90
1	1A	562	C	C5-C6-N1	-6.14	117.93	121.00
1	1A	751	G	N1-C6-O6	6.14	123.59	119.90
1	1A	863	C	N3-C2-O2	-6.14	117.60	121.90
1	1A	1383	G	C6-N1-C2	-6.14	121.41	125.10
1	1A	1804	A	C8-N9-C4	6.14	108.26	105.80
32	2a	517	G	C8-N9-C4	-6.14	103.94	106.40
1	1A	99	G	C8-N9-C4	6.14	108.86	106.40
1	1A	476	G	C5-C6-O6	-6.14	124.91	128.60
1	1A	782	A	C5-C6-N6	6.14	128.61	123.70
1	1A	1556	A	O4'-C1'-N9	6.14	113.11	108.20
1	1A	2368	C	N3-C4-C5	6.14	124.36	121.90
1	2A	1365	A	C6-N1-C2	-6.14	114.92	118.60
1	2A	2129	C	C5-C6-N1	6.14	124.07	121.00
1	1A	24	G	C5-N7-C8	6.14	107.37	104.30
1	1A	417	A	N9-C4-C5	-6.14	103.34	105.80
1	1A	649	C	C5-C6-N1	-6.14	117.93	121.00
1	1A	1279	C	C2-N3-C4	-6.14	116.83	119.90
1	1A	1369	U	N1-C2-N3	6.14	118.58	114.90
1	1A	2088	C	C4-C5-C6	6.14	120.47	117.40
1	2A	1246	A	C8-N9-C4	6.14	108.26	105.80
1	1A	34	C	OP1-P-OP2	6.14	128.81	119.60
1	1A	2713	C	C2-N3-C4	-6.14	116.83	119.90
32	2a	1028	C	C2-N1-C1'	6.14	125.55	118.80
1	1A	1397	C	OP1-P-O3'	6.14	118.70	105.20
2	1B	93	G	C8-N9-C4	-6.14	103.94	106.40
32	1a	139	G	OP1-P-OP2	-6.14	110.39	119.60
1	2A	1696	G	C5-C6-O6	-6.14	124.92	128.60
1	2A	1928	A	O5'-P-OP1	-6.14	100.18	105.70
1	1A	1110	C	N1-C2-O2	6.13	122.58	118.90
1	1A	1204	C	C5-C6-N1	-6.13	117.93	121.00
1	1A	1458	A	O5'-P-OP1	6.13	118.06	110.70
1	1A	2004	C	N3-C4-N4	-6.13	113.71	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1246	A	C2-N3-C4	-6.13	107.53	110.60
1	1A	1626	A	O5'-P-OP2	-6.13	100.18	105.70
1	1A	349	G	N1-C6-O6	6.13	123.58	119.90
1	2A	90	U	N3-C4-O4	-6.13	115.11	119.40
1	2A	417	C	O5'-P-OP1	-6.13	100.18	105.70
1	2A	529	A	O4'-C1'-N9	6.13	113.10	108.20
1	2A	2058	A	C5-C6-N6	-6.13	118.80	123.70
1	1A	1314	A	C4-C5-C6	6.13	120.06	117.00
1	2A	1682	G	N1-C6-O6	-6.13	116.22	119.90
1	1A	529	U	O5'-P-OP1	-6.13	100.18	105.70
1	1A	2258	G	C5-N7-C8	6.13	107.36	104.30
32	1a	880	C	O5'-P-OP2	-6.13	100.18	105.70
32	2a	1331	G	O4'-C1'-N9	6.13	113.10	108.20
32	1a	863	U	C6-N1-C1'	6.13	129.78	121.20
1	2A	562	U	N1-C2-N3	6.13	118.58	114.90
1	2A	958	U	N3-C2-O2	-6.13	117.91	122.20
1	1A	2443	U	N3-C4-O4	-6.12	115.11	119.40
1	1A	1658	C	C4-C5-C6	6.12	120.46	117.40
1	1A	1831	C	C4-C5-C6	6.12	120.46	117.40
1	1A	2428	C	N3-C4-C5	6.12	124.35	121.90
1	1A	2607	G	C4-C5-N7	-6.12	108.35	110.80
1	1A	45	C	C2-N1-C1'	-6.12	112.07	118.80
1	1A	1234	A	O5'-P-OP2	-6.12	100.19	105.70
1	1A	2654	G	C5-C6-O6	6.12	132.27	128.60
1	2A	464	U	OP1-P-OP2	-6.12	110.42	119.60
1	2A	1359	A	C2-N3-C4	6.12	113.66	110.60
1	2A	975	C	C6-N1-C2	-6.12	117.85	120.30
1	2A	1405	U	O5'-P-OP2	-6.12	100.19	105.70
2	2B	24	G	N3-C4-N9	6.12	129.67	126.00
32	2a	918	A	N1-C6-N6	-6.12	114.93	118.60
1	1A	660	C	N1-C2-N3	6.12	123.48	119.20
1	1A	2590	G	C4-C5-N7	-6.12	108.35	110.80
32	1a	866	C	OP1-P-OP2	6.12	128.78	119.60
1	1A	1039	G	C5-C6-O6	6.12	132.27	128.60
1	2A	251	A	C6-N1-C2	-6.12	114.93	118.60
1	2A	1108	U	C6-N1-C2	-6.12	117.33	121.00
1	1A	1097	G	C5-C6-N1	-6.11	108.44	111.50
1	1A	2562	G	C8-N9-C4	-6.11	103.95	106.40
32	1a	261	U	N1-C2-O2	-6.11	118.52	122.80
1	2A	118	A	O5'-P-OP1	-6.11	100.20	105.70
1	2A	575	A	O5'-P-OP2	6.11	118.04	110.70
1	1A	1097	G	O5'-P-OP2	6.11	118.03	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1742	G	N7-C8-N9	6.11	116.16	113.10
1	2A	349	G	C5-C6-O6	6.11	132.27	128.60
1	1A	191	U	C5-C6-N1	-6.11	119.64	122.70
1	1A	326	C	N3-C2-O2	-6.11	117.62	121.90
1	1A	1211	U	C4-C5-C6	6.11	123.37	119.70
1	2A	216	A	C2-N3-C4	-6.11	107.54	110.60
1	2A	1657	C	OP2-P-O3'	6.11	118.64	105.20
1	2A	125	G	C8-N9-C4	-6.11	103.96	106.40
1	1A	23	G	N3-C2-N2	-6.11	115.62	119.90
1	1A	251	A	N1-C6-N6	6.11	122.26	118.60
1	1A	2187	G	C2-N3-C4	6.11	114.95	111.90
1	2A	1656	C	O5'-P-OP2	-6.11	100.20	105.70
1	2A	2296	U	N3-C2-O2	-6.11	117.93	122.20
23	21	21	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	1A	96	C	N1-C2-N3	6.10	123.47	119.20
1	1A	1848	G	O5'-P-OP2	-6.10	100.21	105.70
1	1A	1884	A	C8-N9-C4	6.10	108.24	105.80
1	2A	989	G	OP2-P-O3'	6.10	118.63	105.20
1	1A	2061	C	O5'-P-OP2	-6.10	100.21	105.70
1	1A	2767	U	N3-C2-O2	-6.10	117.93	122.20
1	2A	1775	U	N1-C2-N3	6.10	118.56	114.90
2	1B	50	G	C6-C5-N7	6.10	134.06	130.40
32	2a	664	G	N9-C4-C5	6.10	107.84	105.40
1	1A	495	G	C5-N7-C8	6.10	107.35	104.30
1	1A	1816	A	N1-C6-N6	6.10	122.26	118.60
1	1A	2600	G	N1-C6-O6	-6.10	116.24	119.90
32	1a	644	G	C6-C5-N7	6.10	134.06	130.40
1	2A	529	A	N3-C4-C5	6.10	131.07	126.80
1	1A	1262	C	C2-N3-C4	-6.10	116.85	119.90
1	1A	1361	C	O5'-P-OP2	-6.10	100.21	105.70
1	1A	1823	G	N7-C8-N9	-6.10	110.05	113.10
32	2a	454	C	N3-C2-O2	-6.10	117.63	121.90
1	1A	726	C	C5-C6-N1	-6.10	117.95	121.00
1	2A	761	A	C5-N7-C8	6.10	106.95	103.90
1	1A	724	A	N1-C6-N6	-6.09	114.94	118.60
1	1A	1956	C	O5'-P-OP2	-6.09	100.22	105.70
1	2A	62	C	C5-C6-N1	-6.09	117.95	121.00
1	2A	1040	C	C6-N1-C2	6.09	122.74	120.30
1	2A	2005	A	N1-C2-N3	-6.09	126.25	129.30
1	2A	2013	A	C2-N3-C4	-6.09	107.55	110.60
32	2a	266	G	C2'-C3'-O3'	6.09	123.45	113.70
1	2A	532	A	N7-C8-N9	6.09	116.85	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2473	U	N3-C2-O2	-6.09	117.94	122.20
1	1A	1567	G	O5'-P-OP1	6.09	118.01	110.70
1	1A	2511	C	N1-C2-O2	-6.09	115.25	118.90
1	1A	2735	G	N3-C4-N9	6.09	129.66	126.00
1	2A	1092	C	C2-N3-C4	6.09	122.95	119.90
1	2A	1499	C	OP2-P-O3'	6.09	118.60	105.20
1	1A	1598	C	C4-C5-C6	6.09	120.44	117.40
1	1A	2597	U	N1-C2-N3	6.09	118.55	114.90
2	2B	64	C	C6-N1-C2	6.09	122.74	120.30
1	1A	320	C	N1-C2-O2	-6.09	115.25	118.90
1	2A	97	C	C5-C6-N1	-6.09	117.96	121.00
32	2a	810	C	C6-N1-C2	6.09	122.73	120.30
1	1A	1548	C	C6-N1-C2	-6.09	117.86	120.30
1	1A	2448	G	N9-C4-C5	6.09	107.83	105.40
32	1a	481	G	N3-C4-N9	6.09	129.65	126.00
32	1a	1495	U	C5-C6-N1	6.09	125.74	122.70
1	2A	331	A	N1-C6-N6	-6.09	114.95	118.60
1	2A	1247	A	C2-N3-C4	-6.09	107.56	110.60
1	2A	1466	G	C8-N9-C4	6.09	108.83	106.40
1	2A	2062	A	C6-N1-C2	-6.09	114.95	118.60
1	2A	2763	G	N3-C4-N9	6.09	129.65	126.00
32	2a	1253	G	O5'-P-OP2	-6.09	100.22	105.70
1	1A	1254	G	N3-C2-N2	-6.08	115.64	119.90
1	1A	1482	G	OP1-P-OP2	-6.08	110.47	119.60
1	2A	1073	A	O5'-P-OP2	-6.08	100.23	105.70
1	1A	243	G	C4-C5-N7	-6.08	108.37	110.80
32	1a	781	A	C8-N9-C4	6.08	108.23	105.80
32	2a	1203	C	C6-N1-C2	6.08	122.73	120.30
1	1A	1661	C	C6-N1-C2	-6.08	117.87	120.30
1	1A	618	C	C4-C5-C6	-6.08	114.36	117.40
1	1A	2323	A	N1-C6-N6	-6.08	114.95	118.60
1	2A	2319	G	C2-N3-C4	-6.08	108.86	111.90
1	1A	395	C	C6-N1-C2	6.08	122.73	120.30
1	1A	583	C	C5-C4-N4	6.08	124.45	120.20
1	1A	1068	G	C6-N1-C2	6.08	128.75	125.10
1	2A	1807	G	N7-C8-N9	-6.08	110.06	113.10
1	1A	203	G	O5'-P-OP2	-6.07	100.23	105.70
1	1A	1117	G	N3-C4-C5	-6.07	125.56	128.60
32	1a	135	C	OP1-P-OP2	-6.07	110.49	119.60
1	2A	988	A	C5-C6-N6	-6.07	118.84	123.70
1	1A	902	G	N9-C4-C5	-6.07	102.97	105.40
1	1A	1354	A	C8-N9-C4	-6.07	103.37	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1203	G	N9-C4-C5	-6.07	102.97	105.40
1	1A	1646	C	C2-N3-C4	-6.07	116.86	119.90
1	1A	1811	A	O5'-P-OP2	-6.07	100.24	105.70
1	2A	2834	G	C5-C6-O6	6.07	132.24	128.60
1	1A	1403	U	N3-C2-O2	-6.07	117.95	122.20
1	1A	1600	A	OP2-P-O3'	6.07	118.55	105.20
1	1A	1843	A	N1-C6-N6	-6.07	114.96	118.60
1	2A	507	A	C5-N7-C8	-6.07	100.86	103.90
1	1A	167	G	N9-C4-C5	6.07	107.83	105.40
1	1A	586	G	N3-C2-N2	-6.07	115.65	119.90
1	1A	697	C	C2-N1-C1'	6.07	125.47	118.80
1	1A	1291	G	C4-C5-N7	-6.07	108.37	110.80
1	1A	1802	C	C2-N3-C4	-6.07	116.87	119.90
32	2a	548	G	N1-C6-O6	6.07	123.54	119.90
32	1a	78	G	O4'-C1'-N9	6.07	113.05	108.20
1	1A	748	G	C8-N9-C4	6.06	108.83	106.40
1	1A	1392	G	N1-C6-O6	-6.06	116.26	119.90
10	1O	104	ARG	NE-CZ-NH1	6.06	123.33	120.30
32	1a	624	C	C6-N1-C2	-6.06	117.88	120.30
32	1a	1210	C	C6-N1-C2	6.06	122.72	120.30
1	2A	44	G	OP1-P-OP2	6.06	128.69	119.60
1	2A	734	A	C2-N3-C4	-6.06	107.57	110.60
32	2a	1086	U	N1-C2-O2	6.06	127.04	122.80
1	1A	274	U	N1-C2-N3	-6.06	111.26	114.90
2	1B	59	A	C6-N1-C2	-6.06	114.96	118.60
32	1a	1052	U	N3-C2-O2	-6.06	117.96	122.20
1	2A	1087	G	N3-C4-C5	6.06	131.63	128.60
1	1A	843	C	N1-C2-O2	-6.06	115.27	118.90
1	1A	2419	G	C4-N9-C1'	6.06	134.38	126.50
1	1A	2623	U	N3-C4-O4	6.06	123.64	119.40
1	1A	516	G	N9-C4-C5	6.06	107.82	105.40
32	1a	105	G	N9-C4-C5	-6.06	102.98	105.40
32	1a	1406	U	O5'-P-OP2	-6.06	100.25	105.70
1	2A	2207	G	C8-N9-C4	-6.06	103.98	106.40
1	1A	174	U	O5'-P-OP2	-6.06	100.25	105.70
1	1A	1537	G	N7-C8-N9	-6.06	110.07	113.10
1	2A	878	A	C8-N9-C4	-6.06	103.38	105.80
1	1A	725	C	C4-C5-C6	6.05	120.43	117.40
1	1A	1851	U	C5-C4-O4	6.05	129.53	125.90
2	1B	13	A	C8-N9-C4	6.05	108.22	105.80
1	2A	1501	C	N3-C4-C5	-6.05	119.48	121.90
1	2A	2827	C	C2-N3-C4	-6.05	116.87	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	269	C	C2-N1-C1'	-6.05	112.14	118.80
1	1A	1640	G	C8-N9-C4	-6.05	103.98	106.40
1	1A	1918	G	C5-C6-O6	6.05	132.23	128.60
1	2A	798	G	C5-C6-O6	6.05	132.23	128.60
1	2A	1865	G	N9-C4-C5	6.05	107.82	105.40
1	1A	722	A	C6-C5-N7	-6.05	128.06	132.30
1	1A	779	C	N1-C2-N3	6.05	123.43	119.20
1	1A	979	G	C5-N7-C8	6.05	107.33	104.30
1	1A	1138	C	O4'-C1'-N1	6.05	113.04	108.20
1	1A	2839	C	OP2-P-O3'	6.05	118.51	105.20
32	1a	174	C	OP1-P-O3'	6.05	118.51	105.20
1	2A	935	C	O5'-P-OP2	-6.05	100.26	105.70
1	2A	1091	G	C2-N3-C4	6.05	114.92	111.90
1	2A	2751	G	N3-C4-C5	6.05	131.62	128.60
1	1A	20	C	N3-C4-N4	-6.05	113.77	118.00
1	1A	274	U	C5-C6-N1	6.05	125.72	122.70
1	1A	2287	C	C4-C5-C6	6.05	120.42	117.40
1	2A	2302	G	N9-C4-C5	6.05	107.82	105.40
1	1A	271	U	N3-C4-O4	-6.05	115.17	119.40
1	1A	780	G	N7-C8-N9	-6.05	110.08	113.10
1	1A	2250	G	OP1-P-OP2	6.05	128.67	119.60
1	1A	2476	C	N3-C4-C5	6.05	124.32	121.90
1	1A	107	G	C5-N7-C8	6.04	107.32	104.30
1	1A	2804	C	N3-C4-N4	6.04	122.23	118.00
1	1A	2891	C	OP1-P-OP2	6.04	128.67	119.60
32	1a	309	G	OP1-P-O3'	6.04	118.50	105.20
1	2A	1420	U	P-O3'-C3'	6.04	126.95	119.70
1	1A	952	G	C8-N9-C1'	6.04	134.85	127.00
1	1A	2047	C	O5'-P-OP2	-6.04	100.26	105.70
32	1a	622	A	N1-C6-N6	-6.04	114.97	118.60
32	1a	889	A	O5'-P-OP1	-6.04	100.26	105.70
1	1A	1536	A	N1-C6-N6	-6.04	114.97	118.60
32	1a	1523	G	OP1-P-OP2	6.04	128.66	119.60
1	2A	1646	C	OP1-P-O3'	6.04	118.49	105.20
32	2a	351	G	C2-N3-C4	-6.04	108.88	111.90
1	1A	354	A	C5-C6-N1	-6.04	114.68	117.70
1	1A	1512	G	O5'-P-OP2	-6.04	100.26	105.70
1	1A	2356	U	O4'-C1'-N1	-6.04	103.37	108.20
1	2A	50	U	O5'-P-OP1	-6.04	100.26	105.70
1	2A	2513	G	C2-N3-C4	6.04	114.92	111.90
1	1A	1137	G	N1-C6-O6	-6.04	116.28	119.90
1	1A	1742	G	N1-C6-O6	6.04	123.52	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1838	G	N9-C1'-C2'	-6.04	105.36	112.00
1	2A	1031	G	N1-C6-O6	6.04	123.52	119.90
1	2A	1235	G	C8-N9-C4	-6.04	103.98	106.40
32	2a	883	C	O5'-P-OP1	-6.04	100.27	105.70
1	1A	2165	C	C2-N3-C4	6.04	122.92	119.90
1	2A	1082	U	N3-C2-O2	-6.04	117.97	122.20
1	2A	1250	G	O5'-P-OP2	-6.04	100.27	105.70
1	1A	2239	A	N1-C2-N3	-6.04	126.28	129.30
2	1B	108	U	C5-C4-O4	6.04	129.52	125.90
32	1a	1300	G	C8-N9-C4	6.04	108.81	106.40
1	2A	2302	G	C4-C5-N7	-6.04	108.39	110.80
1	1A	164	G	N3-C2-N2	6.03	124.12	119.90
1	1A	1833	A	C5-C6-N6	-6.03	118.87	123.70
1	1A	1884	A	O5'-P-OP1	-6.03	100.27	105.70
1	1A	1958	A	N7-C8-N9	6.03	116.82	113.80
1	2A	2036	C	O5'-P-OP1	-6.03	100.27	105.70
1	1A	196	A	C5-C6-N6	-6.03	118.88	123.70
1	1A	1221	G	N1-C2-N2	6.03	121.63	116.20
1	1A	2802	C	N3-C4-C5	6.03	124.31	121.90
32	2a	1115	C	N3-C4-C5	-6.03	119.49	121.90
1	1A	1369	U	C2-N3-C4	-6.03	123.38	127.00
1	1A	1414	G	N1-C6-O6	-6.03	116.28	119.90
1	2A	2879	C	N3-C4-N4	6.03	122.22	118.00
1	1A	1133	G	C2-N3-C4	6.03	114.91	111.90
32	1a	226	G	N7-C8-N9	-6.03	110.09	113.10
1	2A	1251	C	C5-C6-N1	6.03	124.01	121.00
1	1A	852	G	C2-N3-C4	6.03	114.91	111.90
1	1A	1548	C	OP2-P-O3'	6.03	118.45	105.20
1	1A	2007	G	C5-N7-C8	6.03	107.31	104.30
1	2A	143	G	C4-C5-N7	-6.03	108.39	110.80
1	2A	694	U	N3-C2-O2	6.02	126.42	122.20
1	2A	2668	G	N1-C6-O6	-6.02	116.29	119.90
1	1A	50	G	C6-N1-C2	-6.02	121.49	125.10
1	1A	2065	C	OP2-P-O3'	6.02	118.45	105.20
1	2A	1233	C	O5'-P-OP1	-6.02	100.28	105.70
1	1A	179	A	C6-N1-C2	6.02	122.21	118.60
1	1A	594	A	N1-C6-N6	-6.02	114.99	118.60
1	1A	1128	U	C6-N1-C2	-6.02	117.39	121.00
1	1A	2551	C	C2-N3-C4	-6.02	116.89	119.90
32	1a	811	C	C6-N1-C2	6.02	122.71	120.30
32	1a	1475	G	N1-C6-O6	6.02	123.51	119.90
1	2A	753	C	O5'-P-OP2	6.02	117.92	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1537	G	N3-C4-C5	-6.02	125.59	128.60
1	1A	758	G	C6-C5-N7	-6.02	126.79	130.40
1	2A	1687	G	C5-C6-O6	6.02	132.21	128.60
1	1A	68	C	O5'-P-OP1	-6.01	100.29	105.70
1	1A	1909	C	O5'-P-OP2	6.01	117.92	110.70
1	2A	1618	A	C5-C6-N6	6.01	128.51	123.70
1	2A	2893	G	C5-C6-N1	6.01	114.51	111.50
32	2a	1221	G	C8-N9-C4	6.01	108.81	106.40
1	1A	579	G	C8-N9-C4	-6.01	104.00	106.40
1	1A	1132	A	C2-N3-C4	6.01	113.61	110.60
1	1A	2579	G	C8-N9-C4	6.01	108.81	106.40
1	1A	1014	U	N1-C2-N3	-6.01	111.29	114.90
1	1A	1711	A	C8-N9-C4	-6.01	103.40	105.80
32	1a	353	A	OP2-P-O3'	6.01	118.42	105.20
1	2A	9	U	N3-C4-C5	-6.01	110.99	114.60
32	2a	383	A	C8-N9-C4	6.01	108.20	105.80
32	2a	1189	C	C6-N1-C2	6.01	122.70	120.30
1	1A	1921	G	C5-N7-C8	-6.01	101.30	104.30
1	1A	2624	C	C2-N3-C4	6.01	122.91	119.90
1	2A	1054	A	O4'-C1'-N9	6.01	113.01	108.20
2	2B	115	G	N1-C6-O6	6.01	123.51	119.90
1	2A	527	C	C6-N1-C1'	6.01	128.01	120.80
1	1A	82	G	N1-C6-O6	6.01	123.50	119.90
1	1A	760	G	C8-N9-C4	6.01	108.80	106.40
1	1A	954	C	C6-N1-C2	6.01	122.70	120.30
1	2A	743	G	N1-C6-O6	-6.01	116.30	119.90
1	2A	1170	G	N7-C8-N9	6.01	116.10	113.10
1	1A	1807	G	N1-C2-N2	-6.00	110.80	116.20
1	1A	74	G	C8-N9-C4	6.00	108.80	106.40
1	1A	986	A	N7-C8-N9	6.00	116.80	113.80
1	1A	1853	G	C5-C6-O6	6.00	132.20	128.60
1	1A	1986	G	N3-C4-N9	6.00	129.60	126.00
1	1A	2122	G	C8-N9-C4	6.00	108.80	106.40
1	1A	2514	G	C2-N3-C4	-6.00	108.90	111.90
1	1A	2514	G	N3-C2-N2	6.00	124.10	119.90
1	2A	250	G	C6-C5-N7	6.00	134.00	130.40
1	2A	2105	C	C2-N3-C4	6.00	122.90	119.90
32	2a	1486	G	OP2-P-O3'	6.00	118.40	105.20
1	1A	1042	A	N7-C8-N9	-6.00	110.80	113.80
1	2A	177	G	O4'-C1'-N9	6.00	113.00	108.20
1	2A	679	C	N3-C2-O2	6.00	126.10	121.90
1	2A	792	G	N1-C2-N3	-6.00	120.30	123.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1343	G	N1-C6-O6	-6.00	116.30	119.90
1	1A	1439	A	N9-C4-C5	6.00	108.20	105.80
1	1A	2726	A	N1-C6-N6	-6.00	115.00	118.60
32	1a	394	G	O5'-P-OP1	-6.00	100.30	105.70
1	2A	906	G	C5-C6-N1	-6.00	108.50	111.50
32	2a	1100	C	C2-N1-C1'	-6.00	112.20	118.80
32	2a	1477	C	OP2-P-O3'	6.00	118.39	105.20
1	2A	2858	C	C6-N1-C2	6.00	122.70	120.30
1	2A	911	A	OP1-P-O3'	5.99	118.39	105.20
32	2a	686	U	N3-C2-O2	-5.99	118.00	122.20
32	2a	704	A	C2-N3-C4	5.99	113.60	110.60
1	1A	476	G	C5-C6-N1	5.99	114.50	111.50
1	1A	1573	G	N9-C4-C5	5.99	107.80	105.40
32	1a	226	G	N9-C4-C5	-5.99	103.00	105.40
1	2A	2385	C	OP1-P-OP2	5.99	128.59	119.60
1	2A	2895	U	C6-N1-C2	-5.99	117.41	121.00
1	1A	479	C	O5'-P-OP1	-5.99	100.31	105.70
1	1A	1001	G	C6-N1-C2	5.99	128.69	125.10
1	1A	2245	U	N3-C4-O4	-5.99	115.21	119.40
32	1a	78	G	N1-C2-N2	5.99	121.59	116.20
1	1A	533	G	N3-C2-N2	-5.99	115.71	119.90
1	1A	722	A	N9-C4-C5	-5.99	103.41	105.80
1	1A	791	G	C4-C5-N7	-5.99	108.40	110.80
1	1A	2025	G	C5-C6-O6	5.99	132.19	128.60
1	1A	2448	G	C4-C5-N7	-5.99	108.41	110.80
32	1a	325	A	C8-N9-C4	5.99	108.19	105.80
1	2A	983	A	C8-N9-C4	5.99	108.19	105.80
1	2A	1770	G	C5-C6-N1	5.99	114.49	111.50
44	2l	29	GLY	N-CA-C	-5.99	98.13	113.10
1	1A	716	G	N7-C8-N9	-5.99	110.11	113.10
1	1A	2902	G	N9-C4-C5	-5.99	103.00	105.40
32	1a	1151	A	O5'-P-OP2	-5.99	100.31	105.70
1	2A	655	A	C4-C5-C6	5.99	119.99	117.00
1	2A	1420	U	C2-N1-C1'	-5.99	110.52	117.70
32	1a	114	U	OP1-P-OP2	5.99	128.58	119.60
32	1a	332	G	O5'-P-OP1	-5.99	100.31	105.70
1	2A	416	C	O5'-P-OP2	-5.99	100.31	105.70
1	2A	474	G	OP2-P-O3'	5.99	118.37	105.20
2	2B	8	U	N3-C2-O2	5.99	126.39	122.20
32	2a	404	U	C5-C6-N1	5.99	125.69	122.70
1	1A	1264	G	N9-C4-C5	-5.98	103.01	105.40
1	1A	2031	G	N1-C2-N2	5.98	121.59	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	166	G	N1-C6-O6	-5.98	116.31	119.90
1	1A	505	A	N1-C6-N6	-5.98	115.01	118.60
1	1A	1861	C	C5-C4-N4	-5.98	116.01	120.20
1	1A	2574	U	N1-C2-O2	5.98	126.99	122.80
1	2A	1804	C	C5-C6-N1	5.98	123.99	121.00
32	2a	343	U	C4-C5-C6	-5.98	116.11	119.70
1	1A	2194	U	C4-C5-C6	5.98	123.29	119.70
32	1a	115	G	C8-N9-C4	-5.98	104.01	106.40
32	1a	971	G	O5'-P-OP2	-5.98	100.32	105.70
32	1a	1094	G	O5'-P-OP1	-5.98	100.32	105.70
1	2A	2822	G	C8-N9-C4	5.98	108.79	106.40
32	2a	776	G	C6-C5-N7	-5.98	126.81	130.40
1	1A	124	A	OP2-P-O3'	5.98	118.35	105.20
1	2A	445	C	N3-C2-O2	5.98	126.08	121.90
1	1A	840	A	O5'-P-OP2	-5.98	100.32	105.70
1	2A	2010	G	OP1-P-OP2	-5.98	110.64	119.60
32	2a	1108	G	C8-N9-C1'	-5.98	119.23	127.00
1	1A	1807	G	C6-C5-N7	-5.98	126.81	130.40
32	2a	1511	G	OP2-P-O3'	5.98	118.35	105.20
1	1A	183	G	O5'-P-OP2	-5.97	100.32	105.70
32	1a	189(A)	C	O5'-P-OP1	5.97	117.87	110.70
1	2A	2723	C	C6-N1-C2	-5.97	117.91	120.30
32	2a	1100	C	N1-C2-O2	-5.97	115.31	118.90
1	1A	647	G	C5-C6-O6	5.97	132.18	128.60
1	1A	1256	U	OP1-P-OP2	-5.97	110.64	119.60
1	1A	2095	C	C2-N3-C4	-5.97	116.91	119.90
1	1A	2698	G	C4-C5-N7	5.97	113.19	110.80
32	1a	1493	A	C2-N3-C4	5.97	113.59	110.60
32	2a	618	C	C2-N3-C4	5.97	122.89	119.90
1	1A	1550	C	O5'-P-OP2	-5.97	100.33	105.70
1	2A	11	G	C5-N7-C8	-5.97	101.31	104.30
32	2a	1362	C	C6-N1-C2	-5.97	117.91	120.30
1	1A	776	G	C5-N7-C8	-5.97	101.31	104.30
1	1A	933	C	N1-C2-O2	5.97	122.48	118.90
1	1A	1355	G	N3-C2-N2	-5.97	115.72	119.90
1	1A	1709	C	N3-C4-C5	5.97	124.29	121.90
1	1A	1806	U	N1-C2-O2	-5.97	118.62	122.80
1	1A	697	C	C5-C6-N1	5.97	123.98	121.00
1	1A	508	A	N1-C2-N3	5.97	132.28	129.30
1	1A	537	G	N7-C8-N9	-5.97	110.12	113.10
1	2A	674	G	N1-C6-O6	-5.97	116.32	119.90
1	1A	781	A	N1-C6-N6	5.96	122.18	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	878	G	N1-C2-N3	5.96	127.48	123.90
1	1A	1492	C	C6-N1-C2	-5.96	117.91	120.30
1	1A	2238	C	C5-C6-N1	-5.96	118.02	121.00
2	2B	13	A	O5'-P-OP2	-5.96	100.33	105.70
32	2a	701	C	O5'-P-OP2	-5.96	100.33	105.70
1	1A	1192	C	N1-C2-O2	-5.96	115.32	118.90
1	1A	2155	G	O4'-C1'-N9	5.96	112.97	108.20
32	1a	1382	C	N1-C2-O2	5.96	122.48	118.90
1	2A	911	A	OP1-P-OP2	5.96	128.54	119.60
1	1A	281	G	C5-C6-O6	5.96	132.18	128.60
1	1A	1692	G	N1-C2-N3	-5.96	120.32	123.90
1	1A	2764	G	O4'-C1'-N9	5.96	112.97	108.20
1	2A	2829	C	C6-N1-C2	5.96	122.69	120.30
32	1a	607	A	N1-C6-N6	5.96	122.18	118.60
1	1A	1059	C	N3-C4-N4	-5.96	113.83	118.00
1	1A	2006	G	N3-C4-N9	-5.96	122.42	126.00
1	1A	2527	C	C5-C4-N4	-5.96	116.03	120.20
32	1a	899	C	C6-N1-C2	5.96	122.68	120.30
1	2A	2599	G	C4-C5-N7	-5.96	108.42	110.80
32	2a	993	G	C4-N9-C1'	5.96	134.25	126.50
46	2n	44	LEU	CA-CB-CG	5.96	129.00	115.30
1	1A	1184	G	N9-C4-C5	5.96	107.78	105.40
1	1A	1853	G	N1-C2-N2	-5.96	110.84	116.20
1	1A	2640	C	C5-C4-N4	-5.96	116.03	120.20
32	1a	521	G	OP1-P-OP2	5.96	128.53	119.60
1	1A	255	G	C5-C6-N1	5.96	114.48	111.50
1	1A	1248	G	C5-C6-O6	-5.96	125.03	128.60
1	1A	1299	A	C4-C5-N7	-5.96	107.72	110.70
1	1A	2512	U	N1-C2-O2	5.96	126.97	122.80
1	1A	968	U	C2-N3-C4	-5.95	123.43	127.00
32	1a	681	C	N1-C2-O2	-5.95	115.33	118.90
1	2A	1883	G	C5-N7-C8	5.95	107.28	104.30
1	1A	987	G	N3-C2-N2	5.95	124.06	119.90
1	1A	1539	C	C2-N3-C4	-5.95	116.92	119.90
1	1A	2368	C	N1-C2-O2	-5.95	115.33	118.90
1	1A	2394	G	C8-N9-C4	-5.95	104.02	106.40
32	1a	57	G	N1-C6-O6	-5.95	116.33	119.90
1	2A	1657	C	OP1-P-O3'	-5.95	92.11	105.20
1	1A	308	U	C5-C4-O4	-5.95	122.33	125.90
1	1A	1080	G	N3-C2-N2	-5.95	115.74	119.90
1	1A	1148	C	N3-C2-O2	-5.95	117.74	121.90
1	1A	1611	C	O5'-P-OP2	-5.95	100.35	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1821	C	OP1-P-O3'	5.95	118.29	105.20
1	1A	2537	G	OP2-P-O3'	5.95	118.29	105.20
32	2a	134	A	N9-C4-C5	-5.95	103.42	105.80
1	1A	557	A	C5-C6-N6	5.95	128.46	123.70
1	1A	114	C	C5-C4-N4	5.95	124.36	120.20
1	1A	246	A	O5'-P-OP1	5.95	117.83	110.70
1	1A	821	A	N9-C4-C5	5.95	108.18	105.80
1	1A	1006	C	O5'-P-OP1	5.95	117.83	110.70
32	1a	73	G	N1-C6-O6	-5.95	116.33	119.90
32	1a	926	G	N9-C4-C5	5.95	107.78	105.40
1	1A	1727	U	N3-C4-C5	5.94	118.17	114.60
1	1A	1804	A	N9-C1'-C2'	-5.94	105.46	112.00
1	1A	2165	C	C6-N1-C2	-5.94	117.92	120.30
32	1a	1181	G	C6-N1-C2	5.94	128.67	125.10
32	1a	1486	G	N3-C4-C5	5.94	131.57	128.60
1	2A	193	U	N3-C2-O2	5.94	126.36	122.20
1	2A	1076	C	N1-C1'-C2'	5.94	121.73	114.00
32	2a	46	G	N1-C6-O6	5.94	123.47	119.90
1	1A	35	G	C4-C5-N7	-5.94	108.42	110.80
1	1A	794	U	N3-C4-C5	-5.94	111.03	114.60
1	1A	847	A	O5'-P-OP1	-5.94	100.35	105.70
1	1A	2068	G	N7-C8-N9	-5.94	110.13	113.10
32	1a	189(L)	G	N3-C4-C5	-5.94	125.63	128.60
32	1a	363	A	O5'-P-OP2	-5.94	100.35	105.70
1	2A	1690	A	N9-C4-C5	-5.94	103.42	105.80
1	1A	96	C	N3-C2-O2	-5.94	117.74	121.90
1	1A	461	U	C2-N3-C4	-5.94	123.44	127.00
1	1A	1769	G	C6-C5-N7	5.94	133.96	130.40
1	1A	2714	U	N3-C2-O2	5.94	126.36	122.20
1	2A	1089	G	O4'-C1'-N9	5.94	112.95	108.20
1	2A	1815	A	N9-C4-C5	5.94	108.18	105.80
1	2A	2475	C	N3-C4-C5	-5.94	119.52	121.90
32	2a	122	G	C6-N1-C2	-5.94	121.53	125.10
1	1A	696	C	C5-C6-N1	5.94	123.97	121.00
1	2A	1092	C	C6-N1-C2	-5.94	117.92	120.30
1	2A	2248	C	O5'-P-OP2	-5.94	100.36	105.70
32	2a	876	G	N1-C6-O6	-5.94	116.34	119.90
1	1A	164	G	N1-C2-N2	-5.94	110.86	116.20
1	1A	815	G	C8-N9-C4	-5.94	104.03	106.40
1	1A	1085	G	C8-N9-C4	5.94	108.78	106.40
1	2A	803	U	N3-C2-O2	-5.94	118.04	122.20
32	2a	909	A	C5-C6-N6	-5.94	118.95	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1840	A	N1-C6-N6	-5.94	115.04	118.60
1	1A	2020	G	N9-C4-C5	5.94	107.77	105.40
1	2A	421	U	O5'-P-OP2	-5.94	100.36	105.70
1	1A	595	A	C5-N7-C8	5.93	106.87	103.90
1	1A	748	G	N1-C6-O6	-5.93	116.34	119.90
1	1A	860	U	C2-N3-C4	-5.93	123.44	127.00
1	1A	1762	G	N3-C4-N9	-5.93	122.44	126.00
1	1A	2863	C	O5'-P-OP2	-5.93	100.36	105.70
32	2a	1472	U	O5'-P-OP2	-5.93	100.36	105.70
1	1A	515	G	N1-C2-N2	5.93	121.54	116.20
1	1A	1747	A	O4'-C1'-N9	-5.93	103.45	108.20
1	1A	2047	C	N3-C2-O2	5.93	126.05	121.90
1	1A	2720	G	C8-N9-C4	5.93	108.77	106.40
1	1A	360	C	C5-C4-N4	5.93	124.35	120.20
1	1A	533	G	OP1-P-OP2	5.93	128.50	119.60
1	1A	600	G	C4-C5-N7	-5.93	108.43	110.80
1	1A	1532	A	O5'-P-OP2	-5.93	100.36	105.70
1	1A	1692	G	C4-C5-N7	-5.93	108.43	110.80
1	2A	204	A	O5'-P-OP2	-5.93	100.36	105.70
1	1A	854	U	C6-N1-C2	-5.93	117.44	121.00
1	1A	1304	C	N3-C2-O2	-5.93	117.75	121.90
1	1A	2335	G	N3-C2-N2	5.93	124.05	119.90
32	1a	536	C	C6-N1-C2	-5.93	117.93	120.30
32	1a	1063	C	N1-C2-O2	5.93	122.46	118.90
32	1a	1457	G	C8-N9-C4	5.93	108.77	106.40
32	2a	574	A	O5'-P-OP1	5.93	117.82	110.70
1	1A	2480	G	C5-C6-O6	-5.93	125.04	128.60
1	2A	271(W)	G	C5-C6-N1	-5.93	108.54	111.50
1	2A	602	G	N3-C4-C5	-5.93	125.64	128.60
1	1A	407	U	C2-N3-C4	-5.93	123.44	127.00
1	1A	2084	A	C8-N9-C4	5.93	108.17	105.80
32	1a	802	A	C5-C6-N6	-5.93	118.96	123.70
1	2A	1834	U	N1-C2-O2	5.93	126.95	122.80
1	1A	1666	G	N3-C2-N2	5.92	124.05	119.90
1	1A	1862	G	OP2-P-O3'	5.92	118.23	105.20
32	1a	1273	G	C8-N9-C4	5.92	108.77	106.40
1	2A	193	U	C5-C6-N1	-5.92	119.74	122.70
1	2A	2123	G	N3-C4-N9	5.92	129.55	126.00
1	1A	1816	A	C4-C5-N7	5.92	113.66	110.70
32	1a	825	G	C5-C6-N1	5.92	114.46	111.50
1	2A	365	C	C4-C5-C6	5.92	120.36	117.40
1	1A	122	G	N1-C2-N2	-5.92	110.87	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	180	A	OP1-P-O3'	-5.92	92.17	105.20
1	1A	1843	A	C8-N9-C4	-5.92	103.43	105.80
32	1a	649	G	O5'-P-OP2	-5.92	100.37	105.70
32	1a	1442	G	C8-N9-C4	-5.92	104.03	106.40
1	1A	808	A	C2-N3-C4	5.92	113.56	110.60
1	1A	1245	C	C5-C6-N1	-5.92	118.04	121.00
1	1A	2297	C	N3-C2-O2	-5.92	117.76	121.90
1	1A	2506	G	C5-C6-O6	5.92	132.15	128.60
1	1A	713	G	N7-C8-N9	-5.92	110.14	113.10
1	1A	1482	G	C8-N9-C4	-5.92	104.03	106.40
1	2A	2036	C	OP1-P-OP2	5.92	128.48	119.60
1	2A	2339	G	O5'-P-OP2	-5.92	100.37	105.70
1	1A	877	G	C4-C5-N7	-5.92	108.43	110.80
1	1A	2040	G	O5'-P-OP1	-5.92	100.38	105.70
32	1a	552	U	C5-C6-N1	-5.92	119.74	122.70
1	2A	1378	A	O5'-P-OP1	-5.92	100.38	105.70
1	1A	1171	G	N3-C2-N2	-5.92	115.76	119.90
1	1A	1702	A	C5-C6-N6	5.92	128.43	123.70
1	1A	2776	G	C4-C5-N7	5.92	113.17	110.80
32	1a	1065	U	P-O3'-C3'	5.92	126.80	119.70
1	1A	716	G	O4'-C1'-N9	-5.91	103.47	108.20
1	1A	1320	A	N1-C6-N6	5.91	122.15	118.60
1	1A	1708	G	C5-N7-C8	5.91	107.26	104.30
1	1A	2291	G	N1-C6-O6	5.91	123.45	119.90
1	2A	1935	G	C5-C6-O6	-5.91	125.05	128.60
1	1A	1359	U	O4'-C1'-N1	5.91	112.93	108.20
1	1A	2138	G	C8-N9-C4	-5.91	104.04	106.40
1	1A	2640	C	C2-N3-C4	-5.91	116.94	119.90
13	1R	67	LEU	CB-CG-CD2	-5.91	100.95	111.00
32	1a	542	G	C8-N9-C4	-5.91	104.04	106.40
32	1a	834	C	O5'-P-OP2	-5.91	100.38	105.70
1	2A	1899	G	C8-N9-C4	-5.91	104.04	106.40
1	1A	1820	A	N3-C4-C5	5.91	130.94	126.80
1	1A	1850	A	C4-C5-C6	5.91	119.95	117.00
32	1a	533	A	C6-N1-C2	-5.91	115.06	118.60
1	2A	1883	G	N3-C4-N9	5.91	129.54	126.00
1	1A	2283	G	OP2-P-O3'	5.91	118.19	105.20
1	1A	2638	C	N3-C2-O2	5.91	126.03	121.90
32	1a	719	C	C4-C5-C6	5.91	120.35	117.40
1	2A	250	G	N9-C4-C5	5.91	107.76	105.40
1	2A	417	C	N3-C4-N4	5.91	122.13	118.00
1	2A	866	A	N9-C4-C5	-5.91	103.44	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	280	C	C6-N1-C2	5.91	122.66	120.30
32	2a	1287	A	N1-C6-N6	-5.91	115.06	118.60
1	1A	2220	A	C5-N7-C8	5.90	106.85	103.90
2	1B	89	G	N1-C6-O6	5.90	123.44	119.90
1	2A	234	C	C6-N1-C2	-5.90	117.94	120.30
1	2A	780	G	O5'-P-OP2	-5.90	100.39	105.70
32	2a	22	G	C8-N9-C4	-5.90	104.04	106.40
1	1A	844	C	C6-N1-C2	5.90	122.66	120.30
1	1A	1119	A	O4'-C1'-N9	5.90	112.92	108.20
1	1A	1309	U	OP2-P-O3'	5.90	118.19	105.20
1	1A	1725	G	C5-N7-C8	-5.90	101.35	104.30
1	1A	2046	G	N7-C8-N9	-5.90	110.15	113.10
1	1A	2597	U	N3-C4-O4	-5.90	115.27	119.40
1	1A	2728	C	C6-N1-C2	5.90	122.66	120.30
1	1A	2745	G	C4-C5-N7	-5.90	108.44	110.80
32	1a	1087	G	N3-C4-C5	-5.90	125.65	128.60
1	2A	116	C	N1-C2-O2	-5.90	115.36	118.90
1	2A	1650	G	N9-C4-C5	5.90	107.76	105.40
1	2A	2318	G	C4-N9-C1'	5.90	134.17	126.50
32	2a	687	A	P-O3'-C3'	5.90	126.78	119.70
1	1A	1171	G	N1-C2-N3	5.90	127.44	123.90
1	1A	1455	C	C2-N3-C4	-5.90	116.95	119.90
1	1A	2023	A	C5-N7-C8	5.90	106.85	103.90
1	1A	2657	G	N7-C8-N9	5.90	116.05	113.10
1	2A	1536	C	C6-N1-C2	-5.90	117.94	120.30
32	2a	438	G	N3-C2-N2	5.90	124.03	119.90
32	2a	647	C	C5-C6-N1	5.90	123.95	121.00
1	1A	2698	G	N3-C2-N2	5.90	124.03	119.90
2	1B	55	U	OP1-P-OP2	5.90	128.45	119.60
32	1a	33	A	O5'-P-OP2	-5.90	100.39	105.70
1	1A	164	G	C5-C6-N1	5.90	114.45	111.50
1	1A	947	A	N1-C6-N6	5.90	122.14	118.60
1	1A	1346	U	N3-C2-O2	-5.90	118.07	122.20
1	1A	1627	A	C4-C5-N7	5.90	113.65	110.70
1	1A	1640	G	N9-C4-C5	5.90	107.76	105.40
1	1A	2602	A	OP2-P-O3'	5.90	118.17	105.20
1	2A	780	G	N1-C6-O6	5.90	123.44	119.90
1	2A	2476	A	C8-N9-C4	-5.90	103.44	105.80
1	2A	2611	U	OP2-P-O3'	5.90	118.17	105.20
32	2a	721	G	N1-C6-O6	5.90	123.44	119.90
1	2A	1602	U	N3-C4-C5	5.90	118.14	114.60
1	2A	2307	G	C5-C6-O6	-5.90	125.06	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1790	A	N1-C2-N3	5.89	132.25	129.30
1	1A	1821	C	C2-N3-C4	-5.89	116.95	119.90
1	1A	1951	G	C5-C6-O6	5.89	132.14	128.60
32	1a	674	G	OP1-P-O3'	5.89	118.17	105.20
1	2A	2167	U	C5-C4-O4	5.89	129.44	125.90
1	2A	2185	C	N3-C2-O2	-5.89	117.77	121.90
32	2a	1373	G	C8-N9-C4	-5.89	104.04	106.40
1	1A	542	C	C2-N3-C4	-5.89	116.95	119.90
1	1A	1867	C	C6-N1-C2	-5.89	117.94	120.30
2	1B	90	A	N1-C2-N3	-5.89	126.35	129.30
32	1a	848	C	C5-C6-N1	5.89	123.95	121.00
1	2A	2810	A	N1-C6-N6	5.89	122.14	118.60
32	2a	531	U	N1-C2-O2	5.89	126.92	122.80
1	1A	1051	C	C5-C4-N4	5.89	124.32	120.20
1	2A	31	C	O5'-P-OP1	-5.89	100.40	105.70
1	2A	2852	G	C8-N9-C4	5.89	108.76	106.40
1	1A	2240	G	N9-C4-C5	5.89	107.76	105.40
32	1a	486	U	N3-C2-O2	-5.89	118.08	122.20
1	1A	1132	A	C8-N9-C4	-5.89	103.44	105.80
1	1A	2588	G	N1-C6-O6	-5.89	116.37	119.90
1	1A	2697	G	OP2-P-O3'	5.89	118.15	105.20
1	2A	920	G	C8-N9-C4	-5.89	104.05	106.40
1	2A	2223	G	O5'-P-OP2	-5.89	100.40	105.70
1	1A	1637	G	C5-C6-O6	5.89	132.13	128.60
1	1A	1862	G	C8-N9-C4	-5.89	104.05	106.40
32	1a	343	U	N3-C2-O2	-5.89	118.08	122.20
1	1A	2831	A	N1-C2-N3	5.88	132.24	129.30
1	1A	870	G	N9-C4-C5	5.88	107.75	105.40
1	1A	2636	G	C5-C6-N1	5.88	114.44	111.50
1	2A	645	C	N1-C2-O2	5.88	122.43	118.90
32	2a	372	C	N1-C2-O2	5.88	122.43	118.90
32	2a	709	G	N7-C8-N9	5.88	116.04	113.10
1	1A	847	A	C5-C6-N6	5.88	128.40	123.70
1	1A	1062	G	OP1-P-OP2	-5.88	110.78	119.60
1	1A	1692	G	C2-N3-C4	5.88	114.84	111.90
32	1a	984	C	C6-N1-C2	5.88	122.65	120.30
1	1A	2458	G	C2-N3-C4	5.88	114.84	111.90
1	1A	2529	C	C5-C4-N4	-5.88	116.09	120.20
1	2A	2162	G	C8-N9-C1'	-5.88	119.36	127.00
1	2A	2615	U	N3-C4-C5	5.88	118.13	114.60
32	2a	1274	G	C8-N9-C4	-5.88	104.05	106.40
1	1A	1924	C	O5'-P-OP1	-5.88	100.41	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	700	G	O5'-P-OP2	-5.88	100.41	105.70
32	1a	1170	A	C8-N9-C4	-5.88	103.45	105.80
32	2a	1103	C	C6-N1-C2	-5.88	117.95	120.30
1	1A	2314	G	O5'-P-OP2	-5.87	100.41	105.70
1	2A	214	G	C2-N3-C4	5.87	114.84	111.90
1	2A	2429	G	O5'-P-OP2	-5.87	100.41	105.70
1	1A	102	U	N1-C2-O2	-5.87	118.69	122.80
1	1A	2439	C	C2-N1-C1'	-5.87	112.34	118.80
32	1a	340	U	C6-N1-C2	5.87	124.52	121.00
32	1a	900	A	N1-C2-N3	-5.87	126.36	129.30
1	2A	2420	C	C6-N1-C2	5.87	122.65	120.30
1	1A	869	U	N1-C2-N3	5.87	118.42	114.90
1	1A	2007	G	N7-C8-N9	-5.87	110.17	113.10
1	1A	2024	G	C5-C6-O6	5.87	132.12	128.60
2	1B	117	G	O5'-P-OP1	5.87	117.74	110.70
1	2A	1115	G	C8-N9-C4	5.87	108.75	106.40
1	1A	34	C	N3-C4-C5	-5.87	119.55	121.90
1	1A	2245	U	OP1-P-OP2	5.87	128.40	119.60
1	1A	2802	C	C5-C6-N1	-5.87	118.07	121.00
32	1a	1035	A	N7-C8-N9	5.87	116.73	113.80
1	2A	27	G	OP1-P-OP2	-5.87	110.80	119.60
1	2A	212	G	OP2-P-O3'	5.87	118.11	105.20
1	2A	1063	G	C4-N9-C1'	5.87	134.13	126.50
1	2A	1076	C	C2-N3-C4	5.87	122.83	119.90
1	2A	2817	G	N1-C6-O6	-5.87	116.38	119.90
32	2a	656	C	C6-N1-C2	-5.87	117.95	120.30
1	1A	1221	G	OP1-P-O3'	5.87	118.11	105.20
1	2A	2148	G	N3-C4-N9	5.87	129.52	126.00
1	1A	24	G	C4-C5-N7	-5.87	108.45	110.80
1	1A	966	G	N1-C2-N2	-5.87	110.92	116.20
1	1A	1980	C	N1-C2-O2	-5.87	115.38	118.90
1	1A	2618	C	C5-C6-N1	-5.87	118.07	121.00
1	1A	2775	G	C8-N9-C4	5.87	108.75	106.40
1	2A	2299	G	N1-C6-O6	5.87	123.42	119.90
1	2A	2316	C	C6-N1-C2	-5.87	117.95	120.30
32	2a	1023	G	N7-C8-N9	5.87	116.03	113.10
1	1A	35	G	C5-C6-O6	5.86	132.12	128.60
1	1A	565	C	C2-N3-C4	-5.86	116.97	119.90
1	1A	1701	A	O5'-P-OP2	5.86	117.74	110.70
1	1A	2606	C	C6-N1-C2	5.86	122.64	120.30
2	1B	75	G	N1-C2-N3	5.86	127.42	123.90
1	2A	1650	G	C5-C6-O6	5.86	132.12	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	25	19	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	1A	1319	U	OP1-P-OP2	5.86	128.39	119.60
1	1A	1922	A	C2-N3-C4	5.86	113.53	110.60
1	1A	1981	G	C5-N7-C8	5.86	107.23	104.30
32	1a	227	G	N3-C2-N2	5.86	124.00	119.90
1	2A	2596	U	N1-C2-N3	5.86	118.42	114.90
32	2a	575	G	O4'-C1'-N9	-5.86	103.51	108.20
32	2a	698	G	C5-C6-O6	-5.86	125.08	128.60
32	2a	904	C	N3-C2-O2	5.86	126.00	121.90
1	1A	101	A	C6-C5-N7	-5.86	128.20	132.30
2	1B	109	C	OP1-P-OP2	5.86	128.39	119.60
32	1a	1037	C	C4-C5-C6	5.86	120.33	117.40
1	2A	2275	C	O4'-C1'-N1	-5.86	103.51	108.20
1	2A	2296	U	N1-C2-O2	5.86	126.90	122.80
2	2B	26	A	O5'-P-OP2	5.86	117.73	110.70
1	1A	249	G	O5'-P-OP1	-5.86	100.43	105.70
32	1a	49	U	N1-C2-O2	5.86	126.90	122.80
1	1A	1011	G	C5-C6-O6	5.86	132.12	128.60
32	2a	396	G	N1-C6-O6	5.86	123.42	119.90
1	1A	1528	U	N1-C2-O2	-5.86	118.70	122.80
1	1A	2016	C	N1-C2-O2	-5.86	115.39	118.90
1	1A	2569	G	C4-C5-N7	-5.86	108.46	110.80
1	1A	2619	G	C8-N9-C4	-5.86	104.06	106.40
1	1A	2714	U	C6-N1-C2	5.86	124.51	121.00
2	1B	106	G	C8-N9-C4	5.86	108.74	106.40
32	1a	1003	G	C8-N9-C4	-5.86	104.06	106.40
1	1A	115	G	N1-C2-N3	5.85	127.41	123.90
1	1A	2354	C	OP1-P-OP2	-5.85	110.82	119.60
1	1A	803	C	C5-C6-N1	-5.85	118.07	121.00
1	1A	1694	G	C6-N1-C2	-5.85	121.59	125.10
1	1A	2179	G	N1-C6-O6	-5.85	116.39	119.90
32	1a	767	A	N1-C2-N3	5.85	132.23	129.30
1	2A	513	A	N7-C8-N9	5.85	116.73	113.80
1	2A	691	C	C6-N1-C2	-5.85	117.96	120.30
32	2a	115	G	P-O3'-C3'	5.85	126.72	119.70
32	2a	398	C	C5-C4-N4	5.85	124.30	120.20
1	1A	499	G	OP2-P-O3'	5.85	118.07	105.20
1	1A	1054	C	C2-N1-C1'	5.85	125.24	118.80
1	1A	1360	C	C2-N3-C4	-5.85	116.97	119.90
1	1A	2171	G	C8-N9-C1'	5.85	134.61	127.00
1	1A	194	G	N3-C4-N9	5.85	129.51	126.00
1	1A	1690	G	N7-C8-N9	-5.85	110.17	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1994	A	N7-C8-N9	5.85	116.72	113.80
1	1A	2260	C	OP2-P-O3'	5.85	118.07	105.20
32	1a	621	A	N1-C6-N6	-5.85	115.09	118.60
32	1a	1480	G	C5-C6-O6	5.85	132.11	128.60
1	2A	1247	A	O5'-P-OP2	5.85	117.72	110.70
1	2A	1899	G	N7-C8-N9	5.85	116.03	113.10
32	2a	266	G	N3-C4-N9	5.85	129.51	126.00
1	1A	2485	U	C6-N1-C1'	-5.85	113.01	121.20
2	1B	99	G	N7-C8-N9	-5.85	110.18	113.10
1	2A	226	G	N1-C2-N2	5.85	121.46	116.20
1	2A	1662	C	N3-C4-N4	-5.85	113.91	118.00
32	2a	865	A	N7-C8-N9	5.85	116.72	113.80
32	1a	1345	U	O4'-C1'-N1	5.84	112.88	108.20
32	1a	1403	C	C6-N1-C2	-5.84	117.96	120.30
1	2A	639	U	C5-C6-N1	-5.84	119.78	122.70
1	2A	1017	G	O5'-P-OP1	-5.84	100.44	105.70
1	2A	1681	G	C5-N7-C8	-5.84	101.38	104.30
1	2A	2596	U	C5-C6-N1	-5.84	119.78	122.70
32	1a	1415	G	OP1-P-O3'	5.84	118.05	105.20
1	2A	1859	A	O5'-P-OP2	-5.84	100.44	105.70
1	1A	2006	G	N9-C4-C5	5.84	107.74	105.40
1	1A	2224	C	N1-C2-O2	-5.84	115.39	118.90
1	1A	2653	G	O4'-C1'-N9	-5.84	103.53	108.20
32	1a	509	A	C8-N9-C4	-5.84	103.46	105.80
32	1a	821	G	C5-C6-O6	-5.84	125.09	128.60
1	2A	190	A	O5'-P-OP2	-5.84	100.44	105.70
1	2A	1309	G	N1-C6-O6	5.84	123.41	119.90
1	2A	2207	G	C5-C6-N1	-5.84	108.58	111.50
1	2A	2255	G	C8-N9-C4	-5.84	104.06	106.40
1	1A	193	A	OP1-P-O3'	5.84	118.05	105.20
1	1A	2467	G	N3-C4-C5	-5.84	125.68	128.60
32	1a	346	G	C2-N3-C4	5.84	114.82	111.90
32	1a	1112	C	OP2-P-O3'	5.84	118.05	105.20
1	1A	1083	G	C5-C6-O6	-5.84	125.10	128.60
1	1A	1681	A	C5-C6-N6	5.84	128.37	123.70
32	2a	530	G	N3-C2-N2	5.84	123.99	119.90
1	1A	1690	G	C5-N7-C8	5.84	107.22	104.30
1	1A	1006	C	N1-C2-O2	-5.83	115.40	118.90
32	2a	1370	G	N3-C4-N9	5.83	129.50	126.00
1	1A	724	A	C5-N7-C8	5.83	106.82	103.90
1	1A	733	G	O5'-P-OP1	-5.83	100.45	105.70
1	1A	1183	G	C5-N7-C8	5.83	107.22	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1354	A	C5-C6-N1	-5.83	114.78	117.70
1	1A	1681	A	N1-C6-N6	-5.83	115.10	118.60
32	1a	1515	C	OP1-P-OP2	5.83	128.35	119.60
32	2a	266	G	C4-C5-C6	5.83	122.30	118.80
32	2a	343	U	C5-C6-N1	-5.83	119.78	122.70
1	1A	1317	G	C5-C6-O6	-5.83	125.10	128.60
32	1a	260	G	C5-C6-N1	-5.83	108.58	111.50
1	2A	808	G	C5-C6-N1	5.83	114.42	111.50
1	2A	1616	A	C8-N9-C4	-5.83	103.47	105.80
1	1A	2274	U	OP1-P-OP2	-5.83	110.86	119.60
1	1A	2475	C	N3-C4-N4	-5.83	113.92	118.00
1	2A	2137	C	N1-C2-O2	5.83	122.40	118.90
1	1A	731	G	N3-C4-C5	-5.83	125.69	128.60
1	1A	1620	G	OP2-P-O3'	5.83	118.02	105.20
1	1A	2519	C	C6-N1-C2	-5.83	117.97	120.30
1	1A	2826	C	OP2-P-O3'	5.83	118.02	105.20
1	1A	2880	C	C6-N1-C2	-5.83	117.97	120.30
1	1A	2900	G	C5-C6-O6	-5.83	125.10	128.60
2	1B	79	C	C2-N3-C4	-5.83	116.99	119.90
2	1B	115	G	C2-N3-C4	-5.83	108.99	111.90
1	2A	445	C	OP1-P-O3'	5.83	118.02	105.20
1	2A	900	A	P-O3'-C3'	5.83	126.69	119.70
1	2A	1497	U	C5-C4-O4	5.83	129.40	125.90
1	1A	360	C	N3-C4-C5	-5.83	119.57	121.90
1	1A	1838	G	C2-N3-C4	-5.83	108.99	111.90
1	2A	745	G	OP1-P-OP2	-5.83	110.86	119.60
1	2A	2182	G	N3-C4-N9	-5.83	122.50	126.00
1	1A	460	C	N3-C2-O2	-5.83	117.82	121.90
1	1A	2479	C	O5'-P-OP2	-5.83	100.46	105.70
1	1A	2621	U	C6-N1-C2	5.83	124.50	121.00
32	1a	297	G	C8-N9-C4	5.83	108.73	106.40
32	2a	266	G	C6-C5-N7	-5.83	126.91	130.40
1	1A	20	C	C4-C5-C6	5.82	120.31	117.40
1	1A	1449	C	C2-N3-C4	-5.82	116.99	119.90
1	1A	1456	G	N3-C4-N9	-5.82	122.51	126.00
1	1A	1728	G	N3-C4-N9	-5.82	122.51	126.00
1	1A	2125	C	C2-N3-C4	5.82	122.81	119.90
32	1a	1442	G	N1-C6-O6	-5.82	116.41	119.90
1	2A	1632	A	N7-C8-N9	-5.82	110.89	113.80
1	1A	2611	G	N3-C4-N9	-5.82	122.51	126.00
32	2a	901	A	N1-C2-N3	5.82	132.21	129.30
1	1A	2537	G	N3-C2-N2	5.82	123.97	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1006	C	N1-C2-O2	5.82	122.39	118.90
1	2A	1466	G	N7-C8-N9	-5.82	110.19	113.10
1	2A	2549	G	OP1-P-OP2	5.82	128.33	119.60
1	2A	2852	G	N9-C4-C5	-5.82	103.07	105.40
32	2a	122	G	N3-C4-C5	-5.82	125.69	128.60
1	1A	1714	G	C4-C5-N7	-5.82	108.47	110.80
1	1A	115	G	C6-N1-C2	-5.82	121.61	125.10
1	1A	213	G	O5'-P-OP2	-5.82	100.46	105.70
1	1A	731	G	N1-C2-N3	-5.82	120.41	123.90
1	1A	906	G	N3-C4-C5	5.82	131.51	128.60
1	1A	2280	A	C8-N9-C4	-5.82	103.47	105.80
23	11	61	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	2A	576	U	N1-C2-N3	5.82	118.39	114.90
1	2A	1332	G	N1-C6-O6	5.82	123.39	119.90
1	1A	2074	G	C8-N9-C4	-5.82	104.07	106.40
1	1A	2239	A	C2-N3-C4	5.82	113.51	110.60
32	1a	1437	C	O5'-P-OP1	-5.82	100.47	105.70
1	1A	2641	A	C5-N7-C8	-5.81	100.99	103.90
1	1A	2056	U	C5-C4-O4	5.81	129.39	125.90
32	2a	1134	G	N3-C4-C5	-5.81	125.69	128.60
1	1A	174	U	C2-N3-C4	-5.81	123.51	127.00
1	1A	209	G	C5-C6-O6	-5.81	125.11	128.60
1	1A	1151	U	C4-C5-C6	-5.81	116.21	119.70
1	1A	2370	G	N1-C6-O6	-5.81	116.41	119.90
1	2A	1954	G	OP1-P-OP2	5.81	128.32	119.60
1	1A	2560	G	N9-C4-C5	5.81	107.72	105.40
1	1A	2651	A	C8-N9-C4	5.81	108.12	105.80
32	1a	794	A	C5-C6-N1	-5.81	114.80	117.70
32	1a	1030(C)	G	C8-N9-C4	-5.81	104.08	106.40
1	2A	417	C	C6-N1-C2	-5.81	117.98	120.30
1	2A	2462	U	O5'-P-OP2	-5.81	100.47	105.70
1	2A	2807	G	N3-C4-N9	-5.81	122.51	126.00
1	1A	2403	G	OP1-P-OP2	5.81	128.31	119.60
1	1A	566	C	OP1-P-OP2	5.80	128.31	119.60
1	1A	1375	U	O5'-P-OP1	5.80	117.67	110.70
1	1A	2083	G	C2-N3-C4	5.80	114.80	111.90
1	2A	2085	C	C6-N1-C2	5.80	122.62	120.30
1	2A	2175	C	C2-N1-C1'	-5.80	112.42	118.80
32	2a	860	A	O5'-P-OP2	5.80	117.67	110.70
1	1A	1232	G	C4-C5-N7	5.80	113.12	110.80
1	1A	588	C	C6-N1-C2	-5.80	117.98	120.30
1	1A	2759	U	C5-C6-N1	-5.80	119.80	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1037	C	N3-C4-C5	-5.80	119.58	121.90
32	1a	1527	C	N3-C4-N4	5.80	122.06	118.00
1	1A	1178	A	OP1-P-OP2	5.80	128.30	119.60
1	2A	1264	G	OP1-P-OP2	5.80	128.30	119.60
32	2a	1152	A	C8-N9-C4	-5.80	103.48	105.80
1	1A	201	G	N3-C4-C5	5.80	131.50	128.60
2	1B	56	G	O5'-P-OP1	5.80	117.66	110.70
32	1a	158	G	C4-C5-N7	-5.80	108.48	110.80
32	1a	454	C	O5'-P-OP2	-5.80	100.48	105.70
32	1a	575	G	O4'-C1'-N9	-5.80	103.56	108.20
32	1a	732	C	N3-C4-N4	-5.80	113.94	118.00
1	2A	774	A	C8-N9-C4	-5.80	103.48	105.80
32	2a	351	G	N3-C4-C5	5.80	131.50	128.60
32	2a	1108	G	N3-C4-C5	-5.80	125.70	128.60
1	1A	596	G	C6-N1-C2	-5.79	121.62	125.10
1	1A	795	G	C5-C6-N1	5.79	114.40	111.50
1	1A	473	A	N1-C2-N3	5.79	132.20	129.30
1	1A	1823	G	C4-C5-N7	-5.79	108.48	110.80
1	1A	2245	U	C5-C4-O4	5.79	129.38	125.90
1	1A	2620	G	N9-C1'-C2'	-5.79	105.63	112.00
1	2A	1775	U	N1-C2-O2	-5.79	118.75	122.80
1	2A	2057	A	O5'-P-OP1	5.79	117.65	110.70
1	2A	2208	A	O4'-C1'-N9	5.79	112.83	108.20
1	2A	846	C	C6-N1-C2	5.79	122.62	120.30
1	2A	2318	G	N7-C8-N9	5.79	116.00	113.10
1	2A	2559	C	C6-N1-C2	5.79	122.62	120.30
32	2a	1139	G	C5-N7-C8	5.79	107.20	104.30
1	1A	563	G	C8-N9-C4	-5.79	104.08	106.40
32	1a	1299	A	C8-N9-C4	-5.79	103.48	105.80
1	2A	1244	G	N9-C4-C5	-5.79	103.08	105.40
1	2A	2009	G	N3-C4-N9	-5.79	122.53	126.00
1	1A	1653	C	C5-C4-N4	-5.79	116.15	120.20
1	1A	1869	C	O5'-P-OP2	-5.79	100.49	105.70
1	1A	2319	G	C5-C6-O6	-5.79	125.13	128.60
1	1A	2352	G	O5'-P-OP2	-5.79	100.49	105.70
1	1A	2358	A	C2-N3-C4	-5.79	107.70	110.60
1	1A	2434	A	N7-C8-N9	5.79	116.69	113.80
1	2A	455	C	N1-C2-O2	5.79	122.37	118.90
1	2A	942	G	C8-N9-C4	5.79	108.72	106.40
1	2A	1085	A	C8-N9-C4	5.79	108.11	105.80
1	1A	849	A	C8-N9-C4	-5.79	103.48	105.80
1	1A	1728	G	C5-N7-C8	-5.79	101.41	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2063	U	OP2-P-O3'	5.79	117.93	105.20
1	1A	2552	C	N3-C4-N4	-5.79	113.95	118.00
1	2A	203	C	C6-N1-C2	5.79	122.61	120.30
1	2A	1997	G	C5'-C4'-O4'	5.79	116.04	109.10
1	2A	2783	G	N9-C4-C5	5.79	107.71	105.40
1	1A	435	G	C5-N7-C8	5.78	107.19	104.30
1	1A	859	C	N3-C2-O2	5.78	125.95	121.90
1	1A	1472	G	C4-C5-N7	5.78	113.11	110.80
1	2A	1652	A	OP1-P-OP2	5.78	128.28	119.60
1	2A	1769	G	C4-C5-N7	5.78	113.11	110.80
1	2A	2197	U	N1-C2-O2	5.78	126.85	122.80
1	2A	2780	G	O4'-C1'-N9	-5.78	103.57	108.20
32	2a	768	A	C2-N3-C4	-5.78	107.71	110.60
1	1A	819	C	C2-N3-C4	-5.78	117.01	119.90
1	1A	2783	G	C5-C6-O6	-5.78	125.13	128.60
1	1A	1427	G	C4-C5-N7	-5.78	108.49	110.80
2	1B	117	G	O5'-P-OP2	-5.78	100.50	105.70
1	2A	232	G	C8-N9-C4	5.78	108.71	106.40
1	2A	867	C	C6-N1-C2	5.78	122.61	120.30
1	2A	1863	G	C8-N9-C4	5.78	108.71	106.40
1	1A	1303	C	C5-C6-N1	-5.78	118.11	121.00
1	1A	2239	A	C8-N9-C4	-5.78	103.49	105.80
1	2A	2416	C	N3-C4-C5	-5.78	119.59	121.90
1	1A	1433	C	N3-C2-O2	-5.78	117.86	121.90
1	1A	2674	A	N7-C8-N9	5.78	116.69	113.80
1	2A	248	G	N9-C4-C5	5.78	107.71	105.40
1	2A	784	A	C8-N9-C4	5.78	108.11	105.80
1	2A	2508	G	O5'-P-OP2	5.78	117.63	110.70
1	1A	1068	G	N3-C4-C5	5.78	131.49	128.60
1	1A	1316	C	C2-N1-C1'	-5.78	112.45	118.80
1	1A	1648	U	C5-C6-N1	-5.78	119.81	122.70
1	1A	2452	C	OP1-P-OP2	5.78	128.26	119.60
1	2A	698	C	OP1-P-OP2	5.78	128.26	119.60
1	2A	788	A	C6-C5-N7	-5.78	128.26	132.30
1	2A	1655	A	N7-C8-N9	-5.78	110.91	113.80
1	2A	2836	U	N3-C2-O2	-5.78	118.16	122.20
1	2A	2506	U	O4'-C1'-N1	5.77	112.82	108.20
1	1A	2029	C	N3-C4-C5	5.77	124.21	121.90
1	1A	2620	G	N3-C2-N2	-5.77	115.86	119.90
1	1A	2654	G	N3-C2-N2	5.77	123.94	119.90
32	1a	776	G	N9-C4-C5	-5.77	103.09	105.40
1	2A	145	G	C8-N9-C4	5.77	108.71	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1047	G	N3-C4-N9	5.77	129.46	126.00
1	1A	2514	G	C5-N7-C8	-5.77	101.42	104.30
1	2A	1208	C	N1-C2-O2	-5.77	115.44	118.90
1	2A	2467	C	N3-C2-O2	-5.77	117.86	121.90
2	2B	1	U	C2-N1-C1'	5.77	124.62	117.70
1	1A	1947	C	O5'-P-OP1	-5.77	100.51	105.70
1	1A	2572	C	N1-C2-N3	5.77	123.24	119.20
29	17	10	ARG	NE-CZ-NH2	-5.77	117.42	120.30
32	1a	142	G	C4-N9-C1'	-5.77	119.00	126.50
32	1a	1385	G	O5'-P-OP2	-5.77	100.51	105.70
1	2A	738	G	N1-C6-O6	-5.77	116.44	119.90
1	2A	2858	C	N3-C4-C5	5.77	124.21	121.90
32	2a	189(A)	C	C6-N1-C2	5.77	122.61	120.30
32	2a	833	U	N3-C2-O2	-5.77	118.16	122.20
1	1A	475	A	N7-C8-N9	-5.77	110.92	113.80
1	1A	703	G	C2-N3-C4	-5.77	109.02	111.90
1	1A	770	G	N3-C4-N9	5.77	129.46	126.00
1	1A	1306	G	C2-N3-C4	-5.77	109.02	111.90
1	1A	2514	G	N1-C2-N2	-5.77	111.01	116.20
1	1A	2789	A	C5-C6-N6	5.77	128.31	123.70
32	1a	1391	U	N3-C2-O2	-5.77	118.16	122.20
1	2A	481	G	O5'-P-OP1	5.77	117.62	110.70
1	2A	2599	G	C5-N7-C8	5.77	107.18	104.30
1	1A	35	G	OP2-P-O3'	5.77	117.89	105.20
32	1a	696	A	C5-C6-N6	-5.77	119.09	123.70
1	1A	1022	C	OP2-P-O3'	5.76	117.88	105.20
1	1A	2384	G	C5-C6-O6	-5.76	125.14	128.60
1	2A	878	A	N7-C8-N9	5.76	116.68	113.80
1	2A	1076	C	C5-C6-N1	5.76	123.88	121.00
32	2a	662	G	C5-C6-O6	-5.76	125.14	128.60
1	2A	1251	C	OP1-P-OP2	5.76	128.24	119.60
32	2a	623	C	C5-C4-N4	-5.76	116.17	120.20
1	1A	651	U	C6-N1-C2	-5.76	117.54	121.00
1	1A	1870	G	O5'-P-OP2	-5.76	100.52	105.70
1	2A	8	A	O5'-P-OP2	5.76	117.61	110.70
1	2A	2893	G	N9-C4-C5	-5.76	103.10	105.40
1	1A	1640	G	N3-C4-N9	-5.76	122.54	126.00
1	1A	1867	C	N1-C2-O2	5.76	122.36	118.90
1	1A	2134	G	N3-C4-N9	5.76	129.46	126.00
1	1A	2416	C	OP2-P-O3'	5.76	117.87	105.20
1	2A	94(A)	G	C6-N1-C2	-5.76	121.64	125.10
1	2A	97	C	C6-N1-C2	5.76	122.60	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	192	C	N3-C4-C5	5.76	124.20	121.90
2	1B	81	G	C5-C6-O6	5.76	132.06	128.60
1	2A	349	G	C4-C5-N7	-5.76	108.50	110.80
1	2A	2805	G	N3-C2-N2	5.76	123.93	119.90
1	1A	436	C	C2-N3-C4	-5.76	117.02	119.90
1	1A	572	A	C2-N3-C4	5.76	113.48	110.60
1	1A	2291	G	C5-C6-O6	-5.76	125.15	128.60
32	1a	339	C	C5-C6-N1	-5.76	118.12	121.00
32	1a	971	G	N3-C4-N9	-5.76	122.55	126.00
32	2a	1290	G	C8-N9-C4	-5.76	104.10	106.40
1	1A	35	G	N7-C8-N9	-5.75	110.22	113.10
1	1A	500	G	C5-C6-O6	5.75	132.05	128.60
1	1A	2418	U	C5-C6-N1	-5.75	119.82	122.70
1	1A	2513	C	C2-N1-C1'	-5.75	112.47	118.80
1	2A	515	A	O5'-P-OP1	-5.75	100.52	105.70
1	1A	533	G	O5'-P-OP1	-5.75	100.52	105.70
1	1A	1646	C	C5-C6-N1	-5.75	118.12	121.00
1	1A	2409	G	C5-C6-O6	-5.75	125.15	128.60
32	1a	1181	G	N3-C4-C5	5.75	131.48	128.60
1	2A	460	A	N1-C6-N6	5.75	122.05	118.60
32	2a	47	C	OP1-P-O3'	5.75	117.86	105.20
32	2a	872	A	C8-N9-C4	-5.75	103.50	105.80
1	1A	782	A	O5'-P-OP1	-5.75	100.52	105.70
1	1A	877	G	C5-C6-O6	5.75	132.05	128.60
1	1A	1278	G	C2-N3-C4	5.75	114.78	111.90
1	1A	1978	U	N1-C2-N3	5.75	118.35	114.90
2	1B	27	C	C6-N1-C2	5.75	122.60	120.30
32	1a	299	G	N9-C4-C5	-5.75	103.10	105.40
1	2A	464	U	C2-N3-C4	-5.75	123.55	127.00
1	2A	570	G	C5-C6-N1	5.75	114.38	111.50
2	2B	2	C	N1-C2-O2	5.75	122.35	118.90
1	1A	1700	G	C2'-C3'-O3'	5.75	122.90	113.70
1	1A	418	G	N1-C2-N3	5.75	127.35	123.90
1	1A	2179	G	C4-C5-N7	-5.75	108.50	110.80
2	1B	101	G	N1-C6-O6	5.75	123.35	119.90
32	1a	795	C	N3-C2-O2	5.75	125.92	121.90
1	2A	2032	G	C6-N1-C2	-5.75	121.65	125.10
32	2a	630	G	N7-C8-N9	5.75	115.97	113.10
1	1A	30	G	C5-N7-C8	5.75	107.17	104.30
1	1A	733	G	N7-C8-N9	-5.75	110.23	113.10
1	1A	1056	A	C2-N3-C4	-5.75	107.73	110.60
1	1A	1306	G	C5-C6-O6	5.75	132.05	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1798	U	OP2-P-O3'	5.75	117.84	105.20
1	2A	2540	C	O5'-P-OP2	-5.75	100.53	105.70
32	1a	1067	A	N9-C4-C5	5.75	108.10	105.80
1	2A	1178	C	C6-N1-C2	5.75	122.60	120.30
1	2A	1445(A)	C	C6-N1-C2	-5.75	118.00	120.30
1	1A	462	C	N1-C2-O2	-5.74	115.45	118.90
1	1A	837	C	C5-C4-N4	-5.74	116.18	120.20
1	1A	1076	G	N7-C8-N9	-5.74	110.23	113.10
1	1A	1102	G	C4-C5-N7	5.74	113.10	110.80
1	1A	1336	C	N3-C4-C5	-5.74	119.60	121.90
32	1a	162	A	N1-C6-N6	5.74	122.05	118.60
32	1a	428	G	O5'-P-OP2	-5.74	100.53	105.70
32	2a	281	G	C6-C5-N7	-5.74	126.95	130.40
1	1A	2194	U	N1-C2-N3	5.74	118.34	114.90
32	1a	1495	U	C6-N1-C2	-5.74	117.56	121.00
1	2A	2641	G	OP2-P-O3'	5.74	117.83	105.20
1	1A	2080	A	N7-C8-N9	-5.74	110.93	113.80
2	1B	69	G	OP2-P-O3'	5.74	117.83	105.20
32	1a	794	A	C6-N1-C2	5.74	122.04	118.60
1	2A	195	A	P-O3'-C3'	5.74	126.59	119.70
1	2A	666	G	N1-C6-O6	5.74	123.34	119.90
32	2a	1065	U	P-O3'-C3'	5.74	126.59	119.70
1	1A	468	G	C5-C6-O6	-5.74	125.16	128.60
1	1A	1155	C	C6-N1-C2	-5.74	118.00	120.30
1	1A	1253	C	C2-N3-C4	-5.74	117.03	119.90
1	1A	1959	A	OP1-P-OP2	5.74	128.21	119.60
1	1A	2302	G	N1-C6-O6	-5.74	116.46	119.90
1	1A	2464	C	C2-N3-C4	-5.74	117.03	119.90
1	1A	2623	U	C4-C5-C6	5.74	123.14	119.70
1	1A	2692	C	C6-N1-C2	-5.74	118.00	120.30
2	2B	22	U	C6-N1-C2	-5.74	117.56	121.00
1	1A	1240	G	C8-N9-C4	-5.74	104.11	106.40
1	1A	2779	G	C5-C6-O6	5.74	132.04	128.60
1	1A	2640	C	O5'-P-OP2	-5.74	100.54	105.70
32	1a	141	A	O5'-P-OP2	-5.74	100.54	105.70
1	2A	1632	A	C5-N7-C8	5.74	106.77	103.90
1	1A	981	C	N1-C2-O2	-5.73	115.46	118.90
1	1A	1191	C	C6-N1-C2	5.73	122.59	120.30
1	2A	864	G	OP1-P-OP2	-5.73	111.00	119.60
1	1A	974	G	OP1-P-OP2	-5.73	111.00	119.60
1	1A	1007	G	N3-C2-N2	-5.73	115.89	119.90
1	1A	1370	G	N1-C2-N2	-5.73	111.04	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1650	C	O5'-P-OP1	-5.73	100.54	105.70
1	1A	1696	G	OP2-P-O3'	5.73	117.81	105.20
32	1a	1082	G	N9-C4-C5	-5.73	103.11	105.40
1	1A	1299	A	C6-N1-C2	-5.73	115.16	118.60
1	1A	1675	U	N3-C2-O2	-5.73	118.19	122.20
1	1A	2055	A	OP1-P-OP2	-5.73	111.00	119.60
1	2A	207	A	N1-C2-N3	5.73	132.16	129.30
1	2A	1926	U	C6-N1-C1'	5.73	129.22	121.20
2	2B	5	C	C5-C6-N1	-5.73	118.14	121.00
32	1a	169	C	C5-C6-N1	-5.73	118.14	121.00
1	1A	1816	A	C8-N9-C4	-5.73	103.51	105.80
1	1A	2025	G	C5-N7-C8	5.73	107.16	104.30
32	1a	607	A	C4-C5-C6	5.73	119.86	117.00
32	1a	1524	C	C5-C6-N1	-5.73	118.14	121.00
1	2A	906	G	C6-N1-C2	5.73	128.54	125.10
1	2A	1427	A	C5-C6-N1	5.73	120.56	117.70
32	2a	1014	A	N7-C8-N9	5.73	116.66	113.80
1	1A	952	G	C6-C5-N7	5.73	133.84	130.40
1	1A	177	G	C5-C6-O6	5.72	132.03	128.60
1	1A	765	A	C6-C5-N7	-5.72	128.29	132.30
1	1A	852	G	N3-C4-C5	-5.72	125.74	128.60
1	1A	2602	A	C8-N9-C4	5.72	108.09	105.80
32	1a	1033	G	N3-C2-N2	5.72	123.91	119.90
32	1a	1532	U	C6-N1-C2	-5.72	117.56	121.00
1	2A	1124	C	O5'-P-OP1	-5.72	100.55	105.70
1	2A	1577	C	O5'-P-OP2	-5.72	100.55	105.70
32	2a	795	C	N3-C2-O2	-5.72	117.89	121.90
1	1A	657	A	O5'-P-OP2	5.72	117.57	110.70
1	1A	902	G	C4-C5-N7	5.72	113.09	110.80
1	1A	989	G	C4-N9-C1'	5.72	133.94	126.50
1	1A	1966	U	N3-C4-C5	5.72	118.03	114.60
1	1A	2402	U	C4-C5-C6	5.72	123.13	119.70
1	1A	2442	A	O5'-P-OP2	-5.72	100.55	105.70
1	1A	2902	G	C6-N1-C2	5.72	128.53	125.10
2	1B	71	C	C4-C5-C6	5.72	120.26	117.40
1	2A	363(E)	U	C5-C4-O4	-5.72	122.47	125.90
1	2A	1806	C	C2-N1-C1'	-5.72	112.50	118.80
1	2A	2588	G	N1-C6-O6	5.72	123.33	119.90
32	2a	115	G	N1-C6-O6	-5.72	116.47	119.90
32	2a	458	C	N1-C2-O2	5.72	122.33	118.90
1	1A	1358	U	N3-C4-O4	-5.72	115.39	119.40
32	1a	446	G	C5-C6-O6	-5.72	125.17	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	883	G	C6-C5-N7	5.72	133.83	130.40
1	1A	476	G	OP1-P-OP2	5.72	128.18	119.60
1	1A	569	G	N7-C8-N9	5.72	115.96	113.10
1	1A	1870	G	OP1-P-OP2	5.72	128.18	119.60
1	1A	2053	A	C5-C6-N1	-5.72	114.84	117.70
1	1A	2633	A	N1-C2-N3	-5.72	126.44	129.30
32	1a	699	C	N3-C2-O2	-5.72	117.90	121.90
1	2A	1082	U	N1-C2-O2	5.72	126.80	122.80
32	2a	518	C	C6-N1-C2	-5.72	118.01	120.30
32	1a	647	C	N3-C4-C5	-5.72	119.61	121.90
1	2A	2532	G	C5-C6-O6	-5.72	125.17	128.60
32	2a	500	G	C5-C6-O6	-5.72	125.17	128.60
1	1A	491	G	C5-C6-O6	-5.72	125.17	128.60
1	1A	1480	A	N1-C2-N3	5.72	132.16	129.30
1	2A	956	G	C2-N3-C4	-5.72	109.04	111.90
1	1A	283	G	N3-C2-N2	-5.71	115.90	119.90
1	1A	1200	G	N1-C2-N3	5.71	127.33	123.90
1	1A	2596	U	C6-N1-C1'	5.71	129.20	121.20
1	1A	2814	C	C6-N1-C2	-5.71	118.01	120.30
32	1a	1054	C	C5-C4-N4	5.71	124.20	120.20
1	2A	647	G	C8-N9-C4	-5.71	104.11	106.40
1	2A	759	G	O5'-P-OP1	-5.71	100.56	105.70
1	2A	2250	G	N1-C6-O6	-5.71	116.47	119.90
32	2a	1495	U	C6-N1-C2	-5.71	117.57	121.00
32	1a	1513	A	C5-C6-N1	5.71	120.56	117.70
32	2a	1452	C	N3-C2-O2	-5.71	117.90	121.90
1	1A	2713	C	N1-C2-N3	5.71	123.20	119.20
32	1a	482	A	OP1-P-O3'	5.71	117.77	105.20
32	2a	1152	A	N7-C8-N9	5.71	116.66	113.80
1	1A	1104	G	C8-N9-C4	5.71	108.68	106.40
1	1A	2138	G	C8-N9-C1'	-5.71	119.58	127.00
32	2a	230	G	N3-C2-N2	-5.71	115.90	119.90
1	1A	838	C	N3-C4-C5	5.71	124.18	121.90
1	1A	932	C	O5'-P-OP1	5.71	117.55	110.70
1	1A	1749	G	OP2-P-O3'	5.71	117.76	105.20
1	1A	2298	A	C4-C5-C6	5.71	119.85	117.00
1	1A	2612	A	N1-C2-N3	5.71	132.15	129.30
1	2A	330	A	O4'-C1'-N9	5.71	112.77	108.20
1	2A	960	A	N1-C6-N6	5.71	122.03	118.60
1	2A	1332	G	C6-C5-N7	-5.71	126.97	130.40
2	2B	30	C	N3-C4-C5	-5.71	119.62	121.90
2	1B	4	C	N1-C2-O2	-5.71	115.48	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	123	G	C8-N9-C4	5.71	108.68	106.40
1	2A	2372	G	C5-C6-O6	-5.71	125.18	128.60
32	2a	354	G	O5'-P-OP2	-5.71	100.56	105.70
1	1A	976	G	O5'-P-OP2	-5.70	100.57	105.70
1	1A	2346	G	OP2-P-O3'	5.70	117.75	105.20
2	1B	55	U	N1-C2-O2	-5.70	118.81	122.80
5	1F	53	THR	N-CA-CB	-5.70	99.47	110.30
1	2A	421	U	OP1-P-O3'	5.70	117.75	105.20
1	2A	756	C	C6-N1-C2	-5.70	118.02	120.30
1	2A	1379	A	N1-C6-N6	5.70	122.02	118.60
1	2A	1847	A	O5'-P-OP1	5.70	117.54	110.70
1	2A	1959	G	OP2-P-O3'	5.70	117.75	105.20
1	2A	2432	A	N9-C4-C5	-5.70	103.52	105.80
2	2B	27	C	N1-C2-O2	5.70	122.32	118.90
1	1A	2902	G	C4-C5-C6	-5.70	115.38	118.80
32	1a	820	U	N1-C2-N3	5.70	118.32	114.90
1	2A	531	C	C5-C6-N1	-5.70	118.15	121.00
1	2A	2138	C	N3-C4-C5	-5.70	119.62	121.90
1	1A	2745	G	N9-C4-C5	5.70	107.68	105.40
1	2A	2168	G	C8-N9-C4	-5.70	104.12	106.40
1	1A	451	G	C6-C5-N7	5.70	133.82	130.40
1	1A	1262	C	N1-C2-N3	5.70	123.19	119.20
1	1A	1358	U	C5-C6-N1	-5.70	119.85	122.70
1	1A	1994	A	C2-N3-C4	-5.70	107.75	110.60
1	1A	2134	G	N1-C6-O6	-5.70	116.48	119.90
1	1A	882	A	C2-N3-C4	5.70	113.45	110.60
1	1A	2092	G	N1-C6-O6	-5.70	116.48	119.90
1	1A	2116	G	N1-C6-O6	-5.70	116.48	119.90
13	1R	67	LEU	CA-CB-CG	5.70	128.40	115.30
32	1a	266	G	C4-N9-C1'	5.70	133.91	126.50
32	1a	1283	G	C8-N9-C4	-5.70	104.12	106.40
1	2A	508	G	N1-C6-O6	5.70	123.32	119.90
1	1A	308	U	N3-C4-O4	5.70	123.39	119.40
1	2A	1071	G	C5-C6-N1	-5.70	108.65	111.50
1	2A	2319	G	C4-C5-N7	5.70	113.08	110.80
1	2A	2517	C	O5'-P-OP2	-5.70	100.57	105.70
32	2a	1222	G	C5-C6-O6	-5.70	125.18	128.60
1	2A	2804	C	C5-C6-N1	5.69	123.85	121.00
32	2a	576	G	C8-N9-C4	5.69	108.68	106.40
1	1A	369	A	C6-N1-C2	-5.69	115.18	118.60
1	1A	1138	C	N3-C4-C5	5.69	124.18	121.90
1	1A	1775	C	C6-N1-C2	-5.69	118.02	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1884	A	N7-C8-N9	-5.69	110.95	113.80
1	2A	2238	G	N3-C2-N2	-5.69	115.92	119.90
32	2a	278	G	N1-C6-O6	-5.69	116.48	119.90
32	2a	485	G	N3-C4-N9	5.69	129.42	126.00
32	2a	1401	G	C8-N9-C4	5.69	108.68	106.40
1	1A	610	C	OP1-P-O3'	5.69	117.72	105.20
1	1A	1487	G	O5'-P-OP2	-5.69	100.58	105.70
1	1A	2550	C	C2-N3-C4	-5.69	117.06	119.90
1	1A	2622	C	N3-C4-N4	5.69	121.98	118.00
32	1a	394	G	C8-N9-C4	-5.69	104.12	106.40
32	1a	507	C	N1-C2-O2	5.69	122.31	118.90
32	2a	1487	G	N3-C2-N2	-5.69	115.92	119.90
1	1A	60	G	N3-C4-N9	-5.69	122.59	126.00
1	1A	2191	A	C4-C5-C6	-5.69	114.16	117.00
1	1A	121	G	OP1-P-OP2	5.69	128.13	119.60
1	1A	645	G	C2-N3-C4	5.69	114.74	111.90
1	1A	1126	C	C2-N3-C4	5.69	122.74	119.90
1	1A	1700	G	OP2-P-O3'	-5.69	92.69	105.20
1	1A	2511	C	C5-C6-N1	5.69	123.84	121.00
32	1a	613	C	O5'-P-OP2	-5.69	100.58	105.70
32	1a	938	A	O5'-P-OP1	-5.69	100.58	105.70
32	1a	1406	U	N3-C4-O4	-5.69	115.42	119.40
1	2A	1271	G	N9-C4-C5	-5.69	103.12	105.40
1	2A	1618	A	N9-C4-C5	5.69	108.08	105.80
32	2a	796	C	C6-N1-C2	5.69	122.58	120.30
1	1A	42	G	C4-C5-N7	5.69	113.07	110.80
1	1A	1210	G	N7-C8-N9	-5.69	110.26	113.10
1	1A	1788	U	N3-C2-O2	5.69	126.18	122.20
1	1A	1854	G	OP2-P-O3'	5.69	117.71	105.20
1	1A	2580	C	N3-C4-N4	5.69	121.98	118.00
1	1A	747	G	C5-C6-O6	5.68	132.01	128.60
1	1A	2250	G	C5'-C4'-O4'	-5.68	102.28	109.10
1	1A	2580	C	OP2-P-O3'	5.68	117.70	105.20
32	1a	821	G	N1-C6-O6	5.68	123.31	119.90
1	2A	1630	G	C4-C5-N7	-5.68	108.53	110.80
1	2A	2538	C	O5'-P-OP1	-5.68	100.58	105.70
1	1A	96	C	N3-C4-C5	-5.68	119.63	121.90
1	1A	579	G	C5-C6-O6	5.68	132.01	128.60
1	1A	2273	C	N3-C2-O2	-5.68	117.92	121.90
1	1A	2569	G	C5-N7-C8	5.68	107.14	104.30
32	1a	576	G	N1-C2-N2	-5.68	111.09	116.20
1	2A	493	G	O5'-P-OP1	-5.68	100.59	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1269	A	C2-N3-C4	-5.68	107.76	110.60
32	2a	52	G	C4-C5-N7	5.68	113.07	110.80
1	1A	992	G	C4-C5-N7	-5.68	108.53	110.80
1	1A	2423	A	C5-N7-C8	-5.68	101.06	103.90
32	1a	1182	G	N1-C6-O6	-5.68	116.49	119.90
32	2a	352	C	OP2-P-O3'	5.68	117.70	105.20
1	1A	495	G	N1-C2-N2	5.68	121.31	116.20
1	1A	641	G	OP2-P-O3'	5.68	117.69	105.20
1	1A	807	G	N1-C2-N2	-5.68	111.09	116.20
1	1A	2088	C	N3-C4-C5	-5.68	119.63	121.90
1	1A	2738	A	C5-N7-C8	-5.68	101.06	103.90
1	2A	2233	U	N1-C2-O2	-5.68	118.83	122.80
1	2A	2838	G	N3-C2-N2	-5.68	115.92	119.90
32	2a	686	U	C2-N3-C4	-5.68	123.59	127.00
1	1A	2007	G	N1-C6-O6	-5.68	116.49	119.90
32	1a	220	G	N3-C4-C5	-5.68	125.76	128.60
1	1A	1168	G	C5-C6-N1	5.68	114.34	111.50
1	1A	1184	G	C4-C5-N7	-5.68	108.53	110.80
1	2A	2046	G	N9-C4-C5	-5.68	103.13	105.40
1	2A	2275	C	C5'-C4'-O4'	-5.68	102.29	109.10
32	2a	411	A	C8-N9-C4	-5.68	103.53	105.80
32	2a	1484	C	N3-C4-C5	5.68	124.17	121.90
1	1A	1201	A	C5-C6-N6	-5.67	119.16	123.70
32	1a	595	G	C8-N9-C1'	-5.67	119.62	127.00
1	2A	1572	A	O5'-P-OP2	-5.67	100.59	105.70
32	2a	52	G	N9-C4-C5	-5.67	103.13	105.40
32	2a	509	A	C8-N9-C4	-5.67	103.53	105.80
32	1a	1030	C	C2-N3-C4	5.67	122.74	119.90
32	1a	1062	U	O5'-P-OP2	-5.67	100.59	105.70
1	1A	199	C	OP2-P-O3'	5.67	117.68	105.20
1	1A	1845	G	C6-C5-N7	-5.67	127.00	130.40
1	1A	2023	A	N1-C6-N6	-5.67	115.20	118.60
1	1A	2283	G	N1-C2-N2	-5.67	111.10	116.20
1	1A	2406	C	N1-C2-N3	5.67	123.17	119.20
2	1B	111	G	N1-C6-O6	-5.67	116.50	119.90
32	1a	133	U	N3-C2-O2	5.67	126.17	122.20
32	1a	831	U	C6-N1-C2	-5.67	117.60	121.00
1	1A	1314	A	N1-C2-N3	5.67	132.13	129.30
32	1a	596	C	N3-C2-O2	-5.67	117.93	121.90
1	2A	1763	G	C4-C5-N7	-5.67	108.53	110.80
1	1A	353	G	O4'-C1'-N9	-5.67	103.67	108.20
1	1A	1279	C	N3-C4-C5	5.67	124.17	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	490	G	O5'-P-OP2	-5.67	100.60	105.70
1	2A	1056	G	N1-C6-O6	5.67	123.30	119.90
1	2A	1104	C	C2-N1-C1'	-5.67	112.56	118.80
1	2A	1863	G	N9-C4-C5	-5.67	103.13	105.40
1	2A	2162	G	N3-C4-N9	5.67	129.40	126.00
1	1A	213	G	N1-C6-O6	-5.67	116.50	119.90
1	1A	1474	C	N1-C2-O2	-5.67	115.50	118.90
1	1A	1649	A	N1-C2-N3	-5.67	126.47	129.30
1	1A	1684	A	OP2-P-O3'	5.67	117.67	105.20
1	1A	2054	G	C5-C6-N1	-5.67	108.67	111.50
1	1A	2740	G	C8-N9-C4	-5.67	104.13	106.40
1	2A	260	G	C4-C5-N7	-5.67	108.53	110.80
1	2A	669	G	OP1-P-OP2	-5.67	111.10	119.60
32	2a	93	G	C4-N9-C1'	-5.67	119.13	126.50
32	2a	1442	G	N3-C4-C5	-5.67	125.77	128.60
32	1a	329	A	N1-C6-N6	5.67	122.00	118.60
1	1A	12	U	N3-C2-O2	-5.66	118.23	122.20
1	1A	2158	C	C2-N1-C1'	5.66	125.03	118.80
1	1A	2516	U	N3-C4-O4	-5.66	115.44	119.40
1	1A	2697	G	O5'-P-OP2	-5.66	100.60	105.70
1	2A	2378	A	N3-C4-N9	5.66	131.93	127.40
1	2A	2725	A	C2-N3-C4	-5.66	107.77	110.60
32	2a	833	U	OP2-P-O3'	5.66	117.66	105.20
1	1A	283	G	C4-C5-N7	-5.66	108.53	110.80
1	1A	702	A	O4'-C1'-N9	5.66	112.73	108.20
1	1A	1655	A	N1-C2-N3	-5.66	126.47	129.30
32	2a	902	G	C4-C5-N7	-5.66	108.53	110.80
1	1A	31	C	C6-N1-C2	-5.66	118.04	120.30
1	1A	1447	G	N3-C4-N9	-5.66	122.60	126.00
1	1A	1829	U	C2-N3-C4	-5.66	123.60	127.00
1	2A	227	A	N1-C2-N3	5.66	132.13	129.30
32	2a	1445	C	C6-N1-C2	5.66	122.56	120.30
1	1A	648	G	C5-C6-N1	5.66	114.33	111.50
1	1A	770	G	N3-C2-N2	5.66	123.86	119.90
1	1A	1630	A	C4-C5-C6	-5.66	114.17	117.00
1	1A	2193	A	N9-C4-C5	-5.66	103.54	105.80
1	1A	2737	C	OP2-P-O3'	5.66	117.65	105.20
1	2A	228	A	N3-C4-N9	-5.66	122.87	127.40
1	2A	630	G	N1-C6-O6	-5.66	116.50	119.90
1	2A	690	G	C5-N7-C8	5.66	107.13	104.30
1	2A	1416	G	C4-N9-C1'	-5.66	119.14	126.50
1	2A	1992	G	O4'-C1'-N9	-5.66	103.67	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	142	G	N1-C2-N2	-5.66	111.11	116.20
1	1A	1590	C	N3-C2-O2	5.66	125.86	121.90
1	1A	2262	G	N1-C6-O6	-5.66	116.51	119.90
1	2A	2681	C	N3-C2-O2	-5.66	117.94	121.90
1	1A	46	C	C6-N1-C2	-5.66	118.04	120.30
1	1A	1802	C	C4-C5-C6	5.66	120.23	117.40
1	2A	2707	G	N1-C6-O6	5.66	123.29	119.90
32	2a	64	G	N1-C6-O6	5.66	123.29	119.90
32	2a	892	A	C6-N1-C2	-5.66	115.21	118.60
32	2a	1015	A	N7-C8-N9	5.66	116.63	113.80
1	1A	1834	A	N7-C8-N9	-5.65	110.97	113.80
1	1A	2080	A	C5-N7-C8	5.65	106.73	103.90
18	1W	23	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	2A	217	G	N1-C6-O6	-5.65	116.51	119.90
1	1A	1341	C	N1-C2-O2	5.65	122.29	118.90
32	1a	899	C	N1-C2-O2	-5.65	115.51	118.90
32	2a	884	U	OP1-P-OP2	5.65	128.08	119.60
1	1A	1465	A	N1-C2-N3	-5.65	126.47	129.30
32	1a	734	G	OP2-P-O3'	5.65	117.63	105.20
1	2A	221	A	C5'-C4'-C3'	-5.65	106.96	116.00
1	2A	1296	G	O5'-P-OP2	-5.65	100.61	105.70
1	2A	1651	G	N1-C6-O6	-5.65	116.51	119.90
1	1A	130	G	N7-C8-N9	-5.65	110.28	113.10
1	1A	2188	G	C6-C5-N7	5.65	133.79	130.40
1	2A	2353	G	N1-C6-O6	5.65	123.29	119.90
32	2a	1098	C	O5'-P-OP1	-5.65	100.62	105.70
1	1A	1455	C	OP1-P-O3'	-5.65	92.77	105.20
1	1A	2015	U	C5-C6-N1	-5.65	119.88	122.70
1	1A	2620	G	C6-N1-C2	-5.65	121.71	125.10
9	1N	138	LEU	CB-CG-CD1	-5.65	101.40	111.00
32	1a	1419	G	C6-N1-C2	5.65	128.49	125.10
1	2A	2895	U	C5-C6-N1	5.65	125.52	122.70
1	1A	175	G	C5-C6-O6	5.65	131.99	128.60
1	1A	553	A	C2-N3-C4	5.65	113.42	110.60
1	1A	1472	G	C6-C5-N7	-5.65	127.01	130.40
1	1A	2525	G	C5-C6-O6	5.65	131.99	128.60
1	1A	2530	A	C4-C5-C6	5.65	119.82	117.00
1	2A	1313	U	OP1-P-OP2	-5.65	111.13	119.60
1	1A	61	C	O5'-P-OP2	-5.64	100.62	105.70
1	2A	2074	U	C6-N1-C2	-5.64	117.61	121.00
1	2A	2501	C	C6-N1-C2	5.64	122.56	120.30
32	2a	1442(A)	G	N1-C6-O6	5.64	123.29	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2843	G	N3-C4-C5	-5.64	125.78	128.60
1	2A	752	A	N7-C8-N9	5.64	116.62	113.80
1	2A	1236	G	N1-C6-O6	-5.64	116.51	119.90
32	2a	1274	G	N7-C8-N9	5.64	115.92	113.10
1	1A	1009	C	O5'-P-OP2	-5.64	100.62	105.70
1	1A	1307	C	N3-C4-C5	5.64	124.16	121.90
1	1A	2099	A	O5'-P-OP2	5.64	117.47	110.70
1	2A	1616	A	N7-C8-N9	5.64	116.62	113.80
1	1A	1622	C	C6-N1-C2	-5.64	118.04	120.30
1	1A	1833	A	C8-N9-C4	5.64	108.06	105.80
1	1A	2131	U	N1-C2-N3	5.64	118.28	114.90
32	1a	1197	G	N3-C4-N9	5.64	129.38	126.00
1	2A	2891	G	N1-C6-O6	5.64	123.28	119.90
1	1A	479	C	O5'-P-OP2	5.64	117.47	110.70
1	1A	2466	G	OP1-P-OP2	5.64	128.06	119.60
32	1a	266	G	P-O3'-C3'	5.64	126.47	119.70
1	2A	676	A	OP2-P-O3'	5.64	117.60	105.20
1	2A	2331	G	C8-N9-C4	5.64	108.66	106.40
32	2a	771	G	N3-C4-C5	5.64	131.42	128.60
1	1A	729	G	N1-C6-O6	-5.64	116.52	119.90
1	1A	1252	C	N3-C2-O2	-5.64	117.95	121.90
1	1A	2650	G	N3-C4-C5	-5.64	125.78	128.60
3	1D	260	ARG	NE-CZ-NH2	-5.64	117.48	120.30
32	1a	148	G	N3-C4-N9	5.64	129.38	126.00
32	1a	754	C	N3-C4-N4	-5.64	114.06	118.00
1	2A	482	A	C4-C5-C6	5.64	119.82	117.00
1	1A	757	G	C8-N9-C4	5.63	108.65	106.40
3	1D	60	ARG	NE-CZ-NH1	-5.63	117.48	120.30
32	1a	312	C	C6-N1-C2	5.63	122.55	120.30
1	2A	2144	U	C6-N1-C2	-5.63	117.62	121.00
1	2A	2821	A	N9-C4-C5	-5.63	103.55	105.80
32	2a	397	A	C4-C5-C6	5.63	119.82	117.00
1	1A	1627	A	N9-C4-C5	-5.63	103.55	105.80
1	1A	2405	A	OP1-P-OP2	5.63	128.05	119.60
1	1A	2561	G	C2-N3-C4	5.63	114.72	111.90
32	2a	897	C	C4-C5-C6	5.63	120.22	117.40
1	1A	109	A	C5-C6-N1	5.63	120.52	117.70
1	1A	1821	C	C6-N1-C2	5.63	122.55	120.30
1	1A	2179	G	C5-C6-O6	5.63	131.98	128.60
32	1a	800	G	O5'-P-OP2	-5.63	100.63	105.70
1	2A	2040	C	O5'-P-OP1	-5.63	100.63	105.70
1	2A	2505	G	N7-C8-N9	5.63	115.92	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2282	G	C6-N1-C2	-5.63	121.72	125.10
32	1a	831	U	N3-C4-O4	5.63	123.34	119.40
1	2A	271(S)	G	N1-C6-O6	5.63	123.28	119.90
1	2A	297	C	O5'-P-OP2	-5.63	100.63	105.70
1	1A	627	G	C5'-C4'-O4'	5.63	115.86	109.10
1	1A	768	C	C2-N3-C4	-5.63	117.09	119.90
1	1A	2842	U	O5'-P-OP2	-5.63	100.64	105.70
16	1U	50	ARG	CB-CA-C	5.63	121.66	110.40
1	2A	831	G	O5'-P-OP1	-5.63	100.63	105.70
1	1A	1350	C	OP1-P-OP2	-5.63	111.16	119.60
1	1A	1833	A	N1-C6-N6	5.63	121.98	118.60
32	1a	105	G	C5-C6-O6	-5.63	125.22	128.60
1	2A	80	G	C4-C5-N7	-5.63	108.55	110.80
1	2A	2136	C	C6-N1-C2	-5.63	118.05	120.30
32	2a	388	G	C8-N9-C4	5.63	108.65	106.40
1	1A	1102	G	C8-N9-C4	5.62	108.65	106.40
1	2A	1046	A	N3-C4-C5	-5.62	122.86	126.80
32	2a	1014	A	C8-N9-C4	-5.62	103.55	105.80
1	1A	52	A	N7-C8-N9	5.62	116.61	113.80
1	1A	107	G	C4-C5-N7	-5.62	108.55	110.80
1	1A	2001	C	N1-C2-O2	-5.62	115.53	118.90
1	1A	2576	A	C4-C5-N7	5.62	113.51	110.70
32	1a	322	C	C6-N1-C2	5.62	122.55	120.30
1	2A	740	U	OP1-P-O3'	5.62	117.57	105.20
1	2A	2139	C	C6-N1-C2	-5.62	118.05	120.30
1	2A	2206	G	N7-C8-N9	-5.62	110.29	113.10
32	2a	802	A	C5-C6-N6	-5.62	119.20	123.70
1	1A	285	U	C5-C4-O4	-5.62	122.53	125.90
1	1A	833	C	N3-C4-N4	-5.62	114.07	118.00
1	1A	1861	C	C6-N1-C2	5.62	122.55	120.30
32	1a	498	U	N3-C4-O4	-5.62	115.47	119.40
1	2A	1982	C	C5-C6-N1	-5.62	118.19	121.00
32	2a	60	A	P-O3'-C3'	5.62	126.45	119.70
1	1A	1594	C	O5'-P-OP2	-5.62	100.64	105.70
1	1A	1972	G	N9-C4-C5	-5.62	103.15	105.40
1	1A	2056	U	C5-C6-N1	-5.62	119.89	122.70
1	2A	74	A	O5'-P-OP1	5.62	117.44	110.70
1	2A	2056	G	C8-N9-C1'	-5.62	119.69	127.00
2	2B	41	U	OP1-P-O3'	5.62	117.56	105.20
32	2a	1282	C	C5-C6-N1	5.62	123.81	121.00
1	1A	1091	A	O4'-C1'-N9	5.62	112.69	108.20
2	1B	55	U	N1-C2-N3	5.62	118.27	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	98	G	OP1-P-OP2	5.62	128.03	119.60
32	1a	1033	G	N9-C4-C5	-5.62	103.15	105.40
1	2A	1320	C	N3-C4-C5	5.62	124.15	121.90
32	2a	19	C	N1-C2-O2	-5.62	115.53	118.90
32	2a	414	A	OP1-P-O3'	5.62	117.56	105.20
1	1A	1608	G	C8-N9-C4	-5.62	104.15	106.40
32	1a	1497	G	C5-C6-O6	-5.62	125.23	128.60
1	2A	1148	A	N9-C4-C5	5.62	108.05	105.80
1	2A	1825	A	O5'-P-OP1	-5.62	100.64	105.70
32	2a	832	C	C6-N1-C2	-5.62	118.05	120.30
1	1A	96	C	C5-C4-N4	5.62	124.13	120.20
1	1A	1052	C	C6-N1-C2	5.62	122.55	120.30
1	1A	1211	U	C5-C4-O4	5.62	129.27	125.90
32	1a	502	G	OP1-P-OP2	-5.62	111.18	119.60
1	2A	2733	A	C8-N9-C4	-5.62	103.55	105.80
32	2a	1530	G	N7-C8-N9	-5.62	110.29	113.10
1	1A	61	C	C2-N1-C1'	-5.61	112.62	118.80
1	1A	397	G	C5-C6-N1	5.61	114.31	111.50
1	1A	598	A	C2-N3-C4	-5.61	107.79	110.60
1	2A	1970	A	O4'-C1'-N9	-5.61	103.71	108.20
1	2A	2373	G	C8-N9-C4	5.61	108.64	106.40
1	1A	2285	A	OP2-P-O3'	5.61	117.55	105.20
1	1A	2805	G	C8-N9-C4	-5.61	104.16	106.40
9	1N	25	ARG	NE-CZ-NH1	-5.61	117.49	120.30
32	1a	996	A	N7-C8-N9	5.61	116.61	113.80
32	1a	1276	G	N3-C4-C5	-5.61	125.79	128.60
1	2A	2629	A	C2-N3-C4	-5.61	107.79	110.60
1	1A	274	U	N3-C4-O4	5.61	123.33	119.40
1	1A	705	C	OP1-P-OP2	5.61	128.02	119.60
1	1A	731	G	N3-C4-N9	5.61	129.37	126.00
1	1A	740	C	N1-C2-O2	5.61	122.27	118.90
32	1a	872	A	O4'-C1'-N9	5.61	112.69	108.20
1	2A	2167	U	N1-C2-O2	5.61	126.73	122.80
1	2A	2443	C	C6-N1-C2	-5.61	118.06	120.30
1	1A	1003	U	N1-C2-N3	5.61	118.27	114.90
1	1A	1269	G	N3-C2-N2	5.61	123.83	119.90
1	1A	1427	G	C5-N7-C8	5.61	107.10	104.30
1	1A	2584	A	C2-N3-C4	5.61	113.40	110.60
1	1A	1577	C	OP2-P-O3'	5.61	117.54	105.20
1	1A	2265	G	N1-C2-N2	5.61	121.25	116.20
32	1a	253	U	OP2-P-O3'	5.61	117.54	105.20
1	1A	452	G	C5-C6-O6	-5.61	125.24	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	766	C	C2-N3-C4	-5.61	117.10	119.90
1	1A	2510	C	C5-C6-N1	-5.61	118.20	121.00
32	1a	774	G	C5-C6-N1	-5.61	108.70	111.50
32	1a	1532	U	C5-C6-N1	5.61	125.50	122.70
1	2A	2886	G	N9-C4-C5	5.61	107.64	105.40
1	1A	2792	U	C2-N3-C4	-5.60	123.64	127.00
1	2A	2444	G	C5-C6-O6	5.60	131.96	128.60
1	2A	2463	C	C6-N1-C2	5.60	122.54	120.30
1	1A	596	G	O5'-P-OP1	5.60	117.42	110.70
1	1A	659	C	O5'-P-OP2	-5.60	100.66	105.70
1	1A	907	U	O5'-P-OP1	5.60	117.42	110.70
1	1A	1314	A	C5-C6-N6	5.60	128.18	123.70
1	1A	1958	A	C6-C5-N7	-5.60	128.38	132.30
1	1A	2440	G	N7-C8-N9	5.60	115.90	113.10
1	1A	2512	U	N3-C4-O4	-5.60	115.48	119.40
1	1A	2654	G	N1-C6-O6	-5.60	116.54	119.90
32	1a	353	A	N1-C6-N6	5.60	121.96	118.60
32	1a	1209	C	N3-C4-C5	-5.60	119.66	121.90
1	2A	612	C	N1-C2-O2	-5.60	115.54	118.90
1	2A	2307	G	N1-C6-O6	5.60	123.26	119.90
1	2A	2870	C	C6-N1-C2	-5.60	118.06	120.30
32	2a	1023	G	C8-N9-C4	-5.60	104.16	106.40
32	1a	189(G)	G	N1-C6-O6	5.60	123.26	119.90
32	1a	1299	A	N9-C4-C5	5.60	108.04	105.80
1	2A	718	A	C4-C5-C6	5.60	119.80	117.00
1	1A	238	C	OP1-P-O3'	5.60	117.52	105.20
1	1A	731	G	N3-C2-N2	5.60	123.82	119.90
1	1A	1182	G	N1-C6-O6	5.60	123.26	119.90
1	1A	1274	G	N1-C6-O6	-5.60	116.54	119.90
32	1a	620	C	C6-N1-C2	5.60	122.54	120.30
32	1a	1024	G	C2-N3-C4	5.60	114.70	111.90
1	2A	1462	C	C6-N1-C2	-5.60	118.06	120.30
1	1A	73	A	C5-C6-N1	5.60	120.50	117.70
1	1A	108	G	C4-C5-N7	-5.60	108.56	110.80
1	1A	476	G	N3-C4-N9	5.60	129.36	126.00
1	1A	1122	C	O4'-C1'-N1	5.60	112.68	108.20
1	1A	1595	C	C6-N1-C2	-5.60	118.06	120.30
1	1A	1822	A	C5-C6-N6	5.60	128.18	123.70
1	1A	2006	G	OP2-P-O3'	5.60	117.52	105.20
1	1A	2876	U	N3-C2-O2	-5.60	118.28	122.20
1	1A	860	U	N1-C2-N3	5.60	118.26	114.90
1	1A	2649	U	N1-C2-N3	5.60	118.26	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2718	G	N1-C6-O6	-5.60	116.54	119.90
1	1A	2898	C	N3-C2-O2	-5.60	117.98	121.90
32	1a	200	G	C8-N9-C4	5.60	108.64	106.40
1	2A	854	G	C5-C6-O6	5.60	131.96	128.60
1	2A	1133	U	N1-C2-O2	-5.60	118.88	122.80
32	2a	711	G	OP1-P-O3'	5.60	117.51	105.20
32	1a	1134	G	N3-C4-C5	-5.59	125.80	128.60
1	2A	1688	U	O5'-P-OP2	-5.59	100.67	105.70
1	2A	2234	G	N1-C2-N2	-5.59	111.17	116.20
1	2A	2805	G	C2-N3-C4	5.59	114.70	111.90
2	2B	50	G	O5'-P-OP2	-5.59	100.66	105.70
32	2a	111	G	C5-C6-N1	-5.59	108.70	111.50
1	1A	106	U	C2-N3-C4	-5.59	123.64	127.00
1	1A	339	G	O5'-P-OP2	-5.59	100.67	105.70
1	1A	1448	C	C6-N1-C2	5.59	122.54	120.30
1	1A	2115	G	N7-C8-N9	-5.59	110.30	113.10
1	1A	2386	C	C5-C6-N1	-5.59	118.20	121.00
1	1A	2626	A	C2-N3-C4	5.59	113.40	110.60
32	1a	345	C	N1-C2-O2	5.59	122.26	118.90
32	1a	670	G	N9-C4-C5	5.59	107.64	105.40
1	2A	1690	A	C4-C5-N7	5.59	113.50	110.70
1	2A	2609	U	O5'-P-OP2	-5.59	100.67	105.70
32	2a	1134	G	C2-N3-C4	5.59	114.70	111.90
1	1A	102	U	N3-C2-O2	5.59	126.11	122.20
1	1A	167	G	C4-C5-N7	-5.59	108.56	110.80
1	1A	1050	C	C4-C5-C6	5.59	120.20	117.40
1	1A	2235	G	C8-N9-C4	5.59	108.64	106.40
1	1A	2762	A	C2-N3-C4	5.59	113.40	110.60
1	2A	2154	G	N1-C6-O6	5.59	123.25	119.90
1	1A	124	A	C6-N1-C2	5.59	121.95	118.60
1	1A	355	A	C5-C6-N6	-5.59	119.23	123.70
1	1A	1215	G	OP2-P-O3'	5.59	117.50	105.20
1	1A	1976	G	C8-N9-C4	-5.59	104.16	106.40
1	1A	2051	G	N1-C2-N2	5.59	121.23	116.20
1	1A	2233	G	O5'-P-OP1	-5.59	100.67	105.70
1	1A	2551	C	N3-C4-N4	-5.59	114.09	118.00
1	1A	2569	G	C5-C6-N1	-5.59	108.71	111.50
1	2A	463	G	C4-C5-N7	-5.59	108.56	110.80
1	2A	763	G	O4'-C1'-N9	-5.59	103.73	108.20
32	2a	1279	A	N7-C8-N9	5.59	116.59	113.80
32	2a	1412	C	O5'-P-OP1	-5.59	100.67	105.70
1	1A	828	A	N7-C8-N9	-5.59	111.01	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1268	C	C6-N1-C2	5.59	122.53	120.30
32	1a	584	G	C8-N9-C1'	-5.59	119.73	127.00
32	1a	1325	C	O5'-P-OP2	-5.59	100.67	105.70
32	1a	1382	C	C6-N1-C2	-5.59	118.06	120.30
1	2A	1909	C	N3-C2-O2	-5.59	117.99	121.90
32	2a	1057	G	C8-N9-C4	5.59	108.64	106.40
1	1A	294	C	O5'-P-OP1	5.59	117.40	110.70
1	1A	1199	C	C2-N3-C4	-5.59	117.11	119.90
1	1A	1341	C	C5-C6-N1	-5.59	118.21	121.00
1	1A	2441	G	C8-N9-C4	-5.59	104.17	106.40
1	2A	1835	G	OP2-P-O3'	5.59	117.49	105.20
1	2A	2061	G	O4'-C1'-N9	5.59	112.67	108.20
1	2A	2553	G	C5-C6-O6	-5.59	125.25	128.60
1	2A	2822	G	N7-C8-N9	-5.59	110.31	113.10
1	1A	2522	C	C6-N1-C2	-5.58	118.07	120.30
1	1A	355	A	N9-C4-C5	-5.58	103.57	105.80
1	1A	1676	G	N9-C4-C5	5.58	107.63	105.40
1	1A	1692	G	C5-C6-O6	5.58	131.95	128.60
32	1a	728	A	O5'-P-OP1	-5.58	100.67	105.70
32	1a	1504	G	C8-N9-C4	5.58	108.63	106.40
1	1A	886	U	N3-C4-O4	-5.58	115.49	119.40
1	1A	1043	G	C5-C6-O6	5.58	131.95	128.60
1	1A	2111	U	C5-C6-N1	-5.58	119.91	122.70
1	1A	2221	A	OP1-P-OP2	-5.58	111.23	119.60
1	1A	2430	A	N1-C2-N3	-5.58	126.51	129.30
1	1A	2698	G	C5-N7-C8	-5.58	101.51	104.30
32	1a	762	C	N3-C2-O2	-5.58	117.99	121.90
1	1A	2566	U	N1-C2-O2	-5.58	118.89	122.80
1	2A	673	C	C4-C5-C6	5.58	120.19	117.40
32	2a	1111	A	C8-N9-C4	-5.58	103.57	105.80
1	1A	542	C	N3-C4-C5	5.58	124.13	121.90
1	1A	616	G	O5'-P-OP2	-5.58	100.68	105.70
1	1A	665	C	N1-C2-O2	-5.58	115.55	118.90
1	1A	724	A	C4-C5-N7	-5.58	107.91	110.70
1	1A	1159	U	N3-C2-O2	5.58	126.11	122.20
1	2A	1421	G	C5-C6-N1	-5.58	108.71	111.50
32	2a	5	U	N3-C4-O4	5.58	123.31	119.40
32	2a	1530	G	C4-N9-C1'	-5.58	119.25	126.50
1	1A	173	C	N3-C2-O2	-5.58	118.00	121.90
1	1A	606	G	C5-C6-N1	5.58	114.29	111.50
1	1A	1452	U	C2-N3-C4	-5.58	123.65	127.00
1	1A	2407	C	C6-N1-C2	5.58	122.53	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	142	G	C8-N9-C1'	5.58	134.25	127.00
32	1a	878	G	C2-N3-C4	-5.58	109.11	111.90
32	1a	1062	U	C6-N1-C2	-5.58	117.65	121.00
1	1A	1001	G	C8-N9-C4	5.58	108.63	106.40
1	1A	1588	G	N1-C6-O6	-5.58	116.56	119.90
1	1A	1691	C	C2-N3-C4	-5.58	117.11	119.90
1	1A	1739	U	C6-N1-C2	5.58	124.34	121.00
1	1A	2250	G	C8-N9-C4	5.58	108.63	106.40
1	2A	2449	U	OP2-P-O3'	5.58	117.47	105.20
1	1A	76	C	N1-C2-O2	5.57	122.24	118.90
1	1A	2427	G	O5'-P-OP1	5.57	117.39	110.70
32	1a	78	G	C8-N9-C1'	5.57	134.25	127.00
32	1a	490	G	N1-C6-O6	-5.57	116.56	119.90
32	1a	584	G	N3-C4-N9	5.57	129.34	126.00
32	1a	1082	G	C4-C5-N7	5.57	113.03	110.80
1	2A	1045	A	N7-C8-N9	5.57	116.59	113.80
1	2A	2332	U	C5-C4-O4	5.57	129.24	125.90
32	2a	248	C	O5'-P-OP2	-5.57	100.69	105.70
1	1A	1715	A	C5-C6-N1	-5.57	114.91	117.70
32	1a	1224	G	C4-C5-N7	-5.57	108.57	110.80
1	1A	556	C	C5-C6-N1	-5.57	118.22	121.00
1	1A	1186	U	O4'-C1'-N1	5.57	112.66	108.20
1	1A	1697	G	C8-N9-C4	-5.57	104.17	106.40
1	1A	2251	G	C5-C6-O6	5.57	131.94	128.60
1	1A	2566	U	C2-N3-C4	-5.57	123.66	127.00
2	1B	9	G	OP2-P-O3'	5.57	117.46	105.20
32	1a	1030(D)	A	N7-C8-N9	5.57	116.59	113.80
1	2A	2056	G	C4-N9-C1'	5.57	133.74	126.50
1	2A	2598	A	OP2-P-O3'	5.57	117.45	105.20
32	2a	740	U	O5'-P-OP2	-5.57	100.69	105.70
49	2q	63	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	1A	1144	A	C8-N9-C4	-5.57	103.57	105.80
1	1A	1720	U	C2-N3-C4	-5.57	123.66	127.00
1	2A	2815	C	N1-C2-O2	-5.57	115.56	118.90
32	2a	649	G	C4-N9-C1'	-5.57	119.26	126.50
1	1A	1678	A	OP1-P-O3'	5.57	117.44	105.20
1	1A	2278	A	N1-C6-N6	5.57	121.94	118.60
1	1A	2877	G	C5-C6-O6	-5.57	125.26	128.60
32	1a	774	G	OP2-P-O3'	5.57	117.44	105.20
1	2A	2514	U	N1-C2-N3	-5.57	111.56	114.90
1	2A	2635	C	N3-C4-N4	5.57	121.89	118.00
1	2A	76	C	C6-N1-C2	-5.56	118.08	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1020	U	C2-N1-C1'	5.56	124.38	117.70
1	1A	645	G	OP1-P-O3'	5.56	117.44	105.20
1	1A	654	G	C5-C6-O6	5.56	131.94	128.60
1	1A	855	G	C5-N7-C8	5.56	107.08	104.30
1	1A	1234	A	C5-C6-N6	-5.56	119.25	123.70
1	1A	1334	U	C5-C6-N1	-5.56	119.92	122.70
1	1A	2200	C	N3-C4-C5	-5.56	119.67	121.90
2	1B	112	U	N3-C4-C5	-5.56	111.26	114.60
1	2A	2049	G	N9-C4-C5	5.56	107.62	105.40
2	2B	11	C	C6-N1-C2	-5.56	118.08	120.30
1	1A	716	G	C6-C5-N7	5.56	133.74	130.40
1	1A	1216	G	C5-N7-C8	-5.56	101.52	104.30
1	1A	2209	G	N1-C6-O6	5.56	123.23	119.90
1	1A	2348	A	O4'-C1'-N9	-5.56	103.75	108.20
1	1A	2597	U	P-O3'-C3'	5.56	126.37	119.70
1	2A	1073	A	OP1-P-OP2	5.56	127.94	119.60
1	2A	2425	A	OP1-P-OP2	-5.56	111.26	119.60
1	1A	308	U	N1-C2-O2	-5.56	118.91	122.80
1	1A	479	C	N3-C4-N4	-5.56	114.11	118.00
1	1A	893	C	N3-C4-C5	5.56	124.12	121.90
1	2A	310	A	OP1-P-O3'	5.56	117.43	105.20
1	2A	1256	G	C8-N9-C4	5.56	108.62	106.40
32	2a	1515	C	C6-N1-C2	5.56	122.52	120.30
1	2A	2331	G	C5-C6-O6	-5.56	125.27	128.60
1	2A	2439	A	O5'-P-OP2	-5.56	100.70	105.70
1	1A	616	G	OP1-P-OP2	5.55	127.93	119.60
1	1A	1628	G	OP2-P-O3'	5.55	117.42	105.20
1	1A	1882	U	O5'-P-OP1	-5.55	100.70	105.70
1	1A	2401	G	OP1-P-O3'	5.55	117.42	105.20
1	1A	2467	G	N3-C2-N2	5.55	123.79	119.90
1	1A	2596	U	O4'-C1'-N1	5.55	112.64	108.20
32	1a	427	U	OP2-P-O3'	5.55	117.42	105.20
1	2A	661	C	C2-N3-C4	-5.55	117.12	119.90
32	2a	375	U	O5'-P-OP2	5.55	117.37	110.70
32	2a	649	G	N3-C4-N9	-5.55	122.67	126.00
32	2a	700	G	OP2-P-O3'	5.55	117.42	105.20
1	1A	2453	C	N3-C4-N4	-5.55	114.11	118.00
1	1A	2512	U	OP1-P-OP2	-5.55	111.27	119.60
32	1a	625	G	C8-N9-C4	-5.55	104.18	106.40
32	1a	1192	C	O5'-P-OP2	5.55	117.36	110.70
32	1a	1316	G	C8-N9-C4	5.55	108.62	106.40
1	2A	2349	G	C5-C6-N1	5.55	114.28	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2521	C	N3-C4-C5	-5.55	119.68	121.90
1	1A	130	G	N9-C4-C5	5.55	107.62	105.40
1	1A	494	G	N7-C8-N9	-5.55	110.32	113.10
1	1A	1353	A	N9-C4-C5	-5.55	103.58	105.80
1	1A	2265	G	C4-C5-N7	-5.55	108.58	110.80
32	1a	372	C	C4-C5-C6	-5.55	114.62	117.40
1	2A	2252	G	N3-C2-N2	5.55	123.79	119.90
32	2a	860	A	C8-N9-C4	-5.55	103.58	105.80
1	1A	200	A	C2-N3-C4	5.55	113.38	110.60
1	1A	730	C	N3-C4-C5	5.55	124.12	121.90
1	1A	2255	U	C5-C6-N1	5.55	125.47	122.70
1	1A	2291	G	C5-N7-C8	-5.55	101.53	104.30
1	1A	2611	G	C6-C5-N7	5.55	133.73	130.40
32	1a	781	A	OP2-P-O3'	5.55	117.41	105.20
1	2A	250	G	C5-C6-N1	5.55	114.28	111.50
1	2A	1649	G	N3-C2-N2	5.55	123.78	119.90
1	1A	659	C	OP2-P-O3'	5.55	117.41	105.20
1	1A	2272	C	N3-C4-N4	-5.55	114.12	118.00
32	1a	730	G	C8-N9-C4	5.55	108.62	106.40
1	2A	779	U	N1-C2-O2	-5.55	118.92	122.80
32	2a	455	C	C5-C6-N1	5.55	123.77	121.00
32	2a	569	C	C4-C5-C6	5.55	120.17	117.40
32	2a	1286	A	C8-N9-C4	-5.55	103.58	105.80
1	1A	303	C	O5'-P-OP2	-5.55	100.71	105.70
1	1A	367	C	C4-C5-C6	5.55	120.17	117.40
32	1a	185	A	C8-N9-C4	-5.55	103.58	105.80
1	2A	2481	G	O5'-P-OP2	-5.55	100.71	105.70
32	2a	43	C	N1-C2-O2	-5.55	115.57	118.90
1	1A	2049	G	N1-C6-O6	-5.54	116.57	119.90
32	1a	190	U	C6-N1-C2	-5.54	117.67	121.00
32	1a	266	G	C6-C5-N7	-5.54	127.07	130.40
1	2A	453	C	O5'-P-OP2	5.54	117.35	110.70
1	2A	2049	G	N3-C4-N9	-5.54	122.67	126.00
1	1A	858	U	N1-C2-N3	5.54	118.23	114.90
1	1A	975	U	C2-N3-C4	-5.54	123.67	127.00
1	2A	249	C	N3-C2-O2	5.54	125.78	121.90
1	2A	950	G	C8-N9-C4	-5.54	104.18	106.40
1	2A	1261	C	C6-N1-C1'	5.54	127.45	120.80
32	2a	220	G	C6-C5-N7	-5.54	127.07	130.40
1	1A	167	G	N1-C2-N3	5.54	127.22	123.90
1	1A	274	U	C6-N1-C1'	-5.54	113.44	121.20
1	1A	1092	A	N7-C8-N9	5.54	116.57	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1666	G	C5-N7-C8	5.54	107.07	104.30
1	1A	1823	G	OP2-P-O3'	5.54	117.39	105.20
1	1A	2187	G	N1-C6-O6	-5.54	116.58	119.90
5	1F	195	ASP	CB-CA-C	-5.54	99.32	110.40
1	2A	1973	G	C5-C6-O6	5.54	131.93	128.60
1	1A	554	A	N7-C8-N9	5.54	116.57	113.80
1	1A	901	G	C4-C5-N7	-5.54	108.58	110.80
32	1a	777	A	C6-N1-C2	5.54	121.92	118.60
32	2a	869	G	O5'-P-OP1	-5.54	100.71	105.70
1	1A	1858	C	C5-C4-N4	5.54	124.08	120.20
8	1I	43	ASN	N-CA-CB	5.54	120.57	110.60
32	2a	505	G	OP1-P-O3'	5.54	117.38	105.20
32	2a	724	G	C5-C6-O6	-5.54	125.28	128.60
1	1A	329	U	O5'-P-OP1	-5.54	100.72	105.70
1	2A	2467	C	C5-C6-N1	5.54	123.77	121.00
32	2a	145	G	N3-C2-N2	-5.54	116.02	119.90
1	1A	2093	A	C6-N1-C2	-5.54	115.28	118.60
1	2A	2078	C	N1-C2-O2	-5.54	115.58	118.90
32	2a	404	U	C2-N3-C4	5.54	130.32	127.00
32	2a	945	G	N1-C6-O6	5.54	123.22	119.90
1	1A	2193	A	C6-C5-N7	-5.53	128.43	132.30
32	1a	23	C	OP1-P-OP2	-5.53	111.30	119.60
1	2A	47	C	N3-C4-C5	5.53	124.11	121.90
1	2A	702	G	O5'-P-OP2	-5.53	100.72	105.70
1	2A	1663	C	N3-C4-N4	-5.53	114.13	118.00
1	1A	1169	C	OP1-P-OP2	5.53	127.90	119.60
1	1A	1453	C	C4-C5-C6	5.53	120.17	117.40
32	1a	405	U	O5'-P-OP2	5.53	117.34	110.70
32	1a	899	C	C5-C6-N1	-5.53	118.23	121.00
1	1A	40	C	C4-C5-C6	5.53	120.17	117.40
1	1A	138	G	C4-C5-N7	-5.53	108.59	110.80
1	1A	801	C	C2-N3-C4	-5.53	117.14	119.90
1	1A	852	G	N3-C4-N9	5.53	129.32	126.00
1	1A	2086	C	N3-C4-C5	-5.53	119.69	121.90
32	1a	588	G	OP2-P-O3'	5.53	117.37	105.20
1	2A	353	G	C6-C5-N7	-5.53	127.08	130.40
1	2A	726	G	O5'-P-OP1	-5.53	100.72	105.70
1	2A	2133	G	N3-C4-C5	5.53	131.37	128.60
1	2A	2858	C	C5-C4-N4	-5.53	116.33	120.20
32	2a	900	A	O5'-P-OP2	5.53	117.34	110.70
1	1A	1331	G	N1-C2-N2	-5.53	111.22	116.20
1	1A	1804	A	N7-C8-N9	-5.53	111.04	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	940	G	N1-C6-O6	-5.53	116.58	119.90
1	1A	367	C	OP2-P-O3'	5.53	117.36	105.20
1	1A	765	A	C2-N3-C4	-5.53	107.84	110.60
1	1A	2464	C	N3-C2-O2	5.53	125.77	121.90
32	1a	1031	G	O4'-C1'-N9	5.53	112.62	108.20
32	2a	675	A	OP1-P-O3'	5.53	117.36	105.20
32	2a	918	A	C8-N9-C4	-5.53	103.59	105.80
1	1A	590	A	C4-C5-C6	-5.53	114.24	117.00
1	1A	1418	U	C2-N1-C1'	5.53	124.33	117.70
1	1A	1515	C	N1-C2-O2	-5.53	115.58	118.90
1	1A	1642	A	N1-C2-N3	5.53	132.06	129.30
1	1A	2603	C	C6-N1-C2	-5.53	118.09	120.30
32	1a	334	C	OP2-P-O3'	5.53	117.36	105.20
1	2A	2559	C	O5'-P-OP2	-5.53	100.73	105.70
2	2B	30	C	C6-N1-C2	-5.53	118.09	120.30
32	2a	577	G	OP2-P-O3'	5.53	117.36	105.20
1	1A	250	G	N1-C6-O6	5.52	123.22	119.90
1	1A	618	C	N3-C4-C5	5.52	124.11	121.90
1	1A	1708	G	C8-N9-C4	5.52	108.61	106.40
1	1A	1892	G	C4-N9-C1'	-5.52	119.32	126.50
32	2a	38	G	N3-C4-C5	5.52	131.36	128.60
32	2a	574	A	C5-C6-N6	-5.52	119.28	123.70
32	2a	811	C	N3-C2-O2	5.52	125.77	121.90
1	1A	288	U	O5'-P-OP2	-5.52	100.73	105.70
1	1A	1104	G	N1-C6-O6	5.52	123.21	119.90
1	1A	1293	A	C5-N7-C8	-5.52	101.14	103.90
32	1a	965	A	N3-C4-C5	5.52	130.67	126.80
1	2A	1913	A	N9-C4-C5	5.52	108.01	105.80
1	2A	2030	A	C4-C5-C6	-5.52	114.24	117.00
32	2a	564	C	OP2-P-O3'	5.52	117.35	105.20
1	1A	581	G	N3-C2-N2	5.52	123.77	119.90
32	1a	878	G	N1-C2-N2	-5.52	111.23	116.20
1	2A	1903	G	C8-N9-C4	-5.52	104.19	106.40
1	2A	2433	A	N9-C4-C5	-5.52	103.59	105.80
1	1A	562	C	OP1-P-OP2	-5.52	111.32	119.60
1	1A	1461	U	C5-C4-O4	5.52	129.21	125.90
1	1A	1702	A	N7-C8-N9	-5.52	111.04	113.80
1	1A	1752	G	C5-C6-O6	5.52	131.91	128.60
1	1A	2117	C	OP2-P-O3'	5.52	117.34	105.20
1	1A	2569	G	C5-C6-O6	5.52	131.91	128.60
1	1A	2807	C	C6-N1-C2	-5.52	118.09	120.30
32	1a	1406	U	C5-C6-N1	-5.52	119.94	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1071	G	C5-N7-C8	-5.52	101.54	104.30
32	2a	1030	C	C6-N1-C1'	-5.52	114.18	120.80
1	1A	198	C	N3-C2-O2	-5.52	118.04	121.90
1	1A	322	G	N3-C4-C5	-5.52	125.84	128.60
1	1A	1701	A	OP1-P-OP2	-5.52	111.32	119.60
1	1A	1952	G	N1-C6-O6	-5.52	116.59	119.90
2	1B	75	G	C5-C6-N1	5.52	114.26	111.50
32	1a	559	A	C8-N9-C4	-5.52	103.59	105.80
32	1a	885	G	C8-N9-C4	5.52	108.61	106.40
32	1a	1054	C	N1-C2-O2	5.52	122.21	118.90
32	1a	1075	C	C6-N1-C2	5.52	122.51	120.30
32	1a	1131	G	N1-C6-O6	5.52	123.21	119.90
1	1A	1317	G	N9-C4-C5	-5.52	103.19	105.40
1	1A	1934	A	O5'-P-OP2	-5.52	100.74	105.70
1	1A	1041	C	C6-N1-C2	-5.51	118.09	120.30
1	1A	1065	U	C2-N3-C4	-5.51	123.69	127.00
1	1A	1274	G	N3-C4-N9	-5.51	122.69	126.00
1	1A	1659	G	O5'-P-OP1	5.51	117.32	110.70
1	1A	1724	A	N1-C6-N6	5.51	121.91	118.60
1	1A	1813	C	N1-C2-O2	-5.51	115.59	118.90
1	1A	1870	G	C8-N9-C4	5.51	108.61	106.40
1	1A	2229	A	C6-C5-N7	-5.51	128.44	132.30
1	2A	301	G	N3-C4-N9	-5.51	122.69	126.00
1	2A	1094	U	O4'-C1'-N1	5.51	112.61	108.20
2	1B	27	C	C5-C6-N1	-5.51	118.24	121.00
2	1B	113	G	O5'-P-OP2	-5.51	100.74	105.70
1	1A	1201	A	N1-C2-N3	-5.51	126.55	129.30
1	1A	2010	C	C4-C5-C6	5.51	120.16	117.40
1	1A	2622	C	C6-N1-C2	-5.51	118.10	120.30
1	2A	602	G	N3-C2-N2	5.51	123.76	119.90
1	2A	2827	C	N3-C4-C5	5.51	124.10	121.90
1	1A	45	C	C4-C5-C6	-5.51	114.64	117.40
1	1A	201	G	C4-C5-N7	5.51	113.00	110.80
1	1A	790	G	C8-N9-C4	-5.51	104.20	106.40
1	1A	843	C	C5-C6-N1	-5.51	118.25	121.00
1	2A	1071	G	N9-C1'-C2'	-5.51	105.94	112.00
1	2A	1351	C	C6-N1-C2	-5.51	118.10	120.30
1	2A	1658	C	C2-N1-C1'	5.51	124.86	118.80
1	1A	762	G	C6-C5-N7	-5.51	127.09	130.40
15	1T	118	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	2A	231	C	C6-N1-C2	-5.51	118.10	120.30
1	2A	594	U	C5-C6-N1	-5.51	119.95	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1482	G	O5'-P-OP2	-5.51	100.74	105.70
1	2A	2447	G	OP2-P-O3'	5.51	117.32	105.20
32	2a	1421	G	O5'-P-OP2	-5.51	100.74	105.70
1	1A	824	A	N1-C2-N3	5.51	132.05	129.30
32	1a	622	A	N9-C4-C5	5.51	108.00	105.80
32	1a	965	A	C2-N3-C4	-5.51	107.85	110.60
32	1a	1162	C	C5-C6-N1	5.51	123.75	121.00
1	2A	1086	A	C2-N3-C4	5.51	113.35	110.60
1	2A	1536	C	C2-N3-C4	5.51	122.65	119.90
1	2A	2105	C	C2-N1-C1'	5.51	124.86	118.80
32	2a	424	G	OP1-P-O3'	5.51	117.31	105.20
32	2a	1132	C	N3-C4-C5	-5.51	119.70	121.90
1	1A	596	G	C5-C6-N1	5.50	114.25	111.50
1	1A	765	A	C5-C6-N1	-5.50	114.95	117.70
32	1a	890	G	O4'-C1'-N9	5.50	112.60	108.20
1	2A	271(M)	G	P-O3'-C3'	5.50	126.31	119.70
32	2a	900	A	O5'-P-OP1	-5.50	100.75	105.70
1	1A	34	C	C6-N1-C2	-5.50	118.10	120.30
1	1A	114	C	N3-C4-N4	-5.50	114.15	118.00
1	1A	713	G	O5'-P-OP2	-5.50	100.75	105.70
1	1A	1285	G	C8-N9-C4	-5.50	104.20	106.40
1	1A	1560	U	N1-C2-O2	-5.50	118.95	122.80
1	2A	214	G	C8-N9-C4	-5.50	104.20	106.40
1	2A	494	G	C4-C5-N7	-5.50	108.60	110.80
1	2A	1203	G	C5-C6-O6	-5.50	125.30	128.60
32	2a	1112	C	O5'-P-OP1	5.50	117.30	110.70
1	1A	143	C	O5'-P-OP1	-5.50	100.75	105.70
1	1A	1259	A	C4-C5-N7	-5.50	107.95	110.70
1	1A	1451	U	N3-C2-O2	-5.50	118.35	122.20
1	1A	2134	G	N7-C8-N9	5.50	115.85	113.10
1	1A	2608	U	C2-N3-C4	-5.50	123.70	127.00
1	1A	2663	C	O5'-P-OP1	5.50	117.30	110.70
32	1a	549	C	O5'-P-OP2	5.50	117.30	110.70
32	1a	799	G	C4-C5-N7	-5.50	108.60	110.80
1	2A	529	A	N7-C8-N9	5.50	116.55	113.80
1	2A	2058	A	C6-N1-C2	-5.50	115.30	118.60
1	1A	2862	G	C8-N9-C4	5.50	108.60	106.40
32	1a	1465	C	N1-C2-N3	5.50	123.05	119.20
32	2a	93	G	C8-N9-C1'	5.50	134.15	127.00
1	1A	973	G	OP1-P-O3'	5.50	117.30	105.20
1	1A	1837	C	C2-N3-C4	-5.50	117.15	119.90
1	1A	2019	G	C5'-C4'-O4'	5.50	115.70	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1091	G	O3'-P-O5'	5.50	114.45	104.00
32	2a	1394	A	C6-N1-C2	5.50	121.90	118.60
1	1A	89	U	N3-C2-O2	-5.50	118.35	122.20
1	1A	577	U	C2-N3-C4	-5.50	123.70	127.00
1	1A	839	G	O4'-C1'-N9	-5.50	103.80	108.20
1	1A	1155	C	N3-C4-C5	-5.50	119.70	121.90
1	1A	1383	G	C5-C6-N1	5.50	114.25	111.50
1	1A	2636	G	N1-C2-N2	-5.50	111.25	116.20
32	1a	1137	C	C2-N3-C4	5.50	122.65	119.90
32	1a	1495	U	N3-C4-C5	-5.50	111.30	114.60
1	2A	1275	A	N7-C8-N9	-5.50	111.05	113.80
1	2A	2158	A	P-O3'-C3'	5.50	126.30	119.70
1	1A	2034	G	O5'-P-OP2	-5.50	100.75	105.70
1	2A	473	G	N3-C2-N2	-5.50	116.05	119.90
1	2A	2137	C	C5-C6-N1	5.50	123.75	121.00
1	2A	2138	C	C2-N3-C4	5.50	122.65	119.90
1	1A	36	G	C5-C6-O6	5.49	131.90	128.60
1	1A	502	G	C8-N9-C4	5.49	108.60	106.40
1	1A	2016	C	O5'-P-OP1	5.49	117.29	110.70
32	1a	888	G	C5-N7-C8	-5.49	101.55	104.30
1	2A	789	A	C5-C6-N6	-5.49	119.31	123.70
1	2A	1810	A	N1-C6-N6	5.49	121.90	118.60
1	2A	2207	G	C8-N9-C1'	-5.49	119.86	127.00
32	2a	1034	G	N1-C6-O6	5.49	123.20	119.90
1	1A	1522	G	N3-C4-N9	-5.49	122.70	126.00
32	1a	119	A	OP1-P-O3'	5.49	117.28	105.20
1	1A	115	G	O5'-P-OP1	5.49	117.29	110.70
1	1A	633	G	N1-C6-O6	-5.49	116.61	119.90
1	1A	2358	A	OP1-P-OP2	-5.49	111.36	119.60
1	1A	2449	U	C4-C5-C6	5.49	123.00	119.70
1	2A	228	A	C4-C5-C6	-5.49	114.25	117.00
1	1A	119	G	N9-C4-C5	-5.49	103.20	105.40
1	1A	857	U	C5-C4-O4	-5.49	122.61	125.90
1	1A	905	U	N3-C2-O2	-5.49	118.36	122.20
1	1A	1305	G	C5-C6-O6	5.49	131.89	128.60
1	1A	1371	G	O4'-C1'-N9	5.49	112.59	108.20
1	1A	1391	C	N3-C4-N4	-5.49	114.16	118.00
1	1A	1981	G	OP2-P-O3'	5.49	117.27	105.20
1	1A	2006	G	C4-C5-N7	-5.49	108.61	110.80
1	1A	2234	G	N7-C8-N9	-5.49	110.36	113.10
1	1A	2390	A	C6-C5-N7	-5.49	128.46	132.30
1	2A	473	G	O5'-P-OP2	-5.49	100.76	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2382	G	C8-N9-C4	5.49	108.60	106.40
1	2A	2643	G	O5'-P-OP1	-5.49	100.76	105.70
32	2a	518	C	N3-C2-O2	-5.49	118.06	121.90
1	1A	826	U	C5-C4-O4	-5.49	122.61	125.90
1	1A	1207	C	OP2-P-O3'	5.49	117.27	105.20
32	1a	1355	G	C8-N9-C4	-5.49	104.20	106.40
1	1A	715	G	OP2-P-O3'	5.49	117.27	105.20
1	1A	1033	G	C4-C5-N7	-5.49	108.61	110.80
32	1a	911	U	N1-C2-O2	-5.49	118.96	122.80
1	2A	2504	U	OP1-P-O3'	5.49	117.27	105.20
1	2A	2507	C	C2-N3-C4	5.49	122.64	119.90
1	2A	2553	G	N9-C4-C5	-5.49	103.21	105.40
1	1A	844	C	N3-C4-C5	5.48	124.09	121.90
1	1A	1033	G	O5'-P-OP2	5.48	117.28	110.70
1	1A	1630	A	C8-N9-C4	5.48	107.99	105.80
1	1A	1674	G	N3-C4-C5	-5.48	125.86	128.60
1	1A	2802	C	C6-N1-C2	5.48	122.49	120.30
1	2A	236	C	C6-N1-C2	5.48	122.49	120.30
32	2a	323	U	N3-C2-O2	-5.48	118.36	122.20
32	2a	869	G	C2-N3-C4	-5.48	109.16	111.90
32	2a	930	C	C2-N1-C1'	-5.48	112.77	118.80
1	1A	2454	C	C6-N1-C2	5.48	122.49	120.30
1	1A	2651	A	N9-C4-C5	-5.48	103.61	105.80
32	1a	1480	G	O5'-P-OP1	-5.48	100.77	105.70
1	2A	1806	C	N1-C2-O2	-5.48	115.61	118.90
1	2A	271(X)	G	C5-C6-O6	5.48	131.89	128.60
32	2a	266	G	C8-N9-C1'	-5.48	119.88	127.00
32	2a	1217	C	C5-C6-N1	-5.48	118.26	121.00
1	1A	1027	A	C6-N1-C2	-5.48	115.31	118.60
1	1A	1383	G	C2-N3-C4	5.48	114.64	111.90
1	1A	2414	C	O5'-P-OP2	-5.48	100.77	105.70
2	1B	41	U	N1-C2-N3	5.48	118.19	114.90
32	1a	757	U	C5-C6-N1	-5.48	119.96	122.70
1	2A	205	G	OP1-P-OP2	5.48	127.82	119.60
1	1A	1956	C	OP1-P-OP2	5.48	127.81	119.60
32	1a	188	C	N1-C2-O2	5.48	122.19	118.90
1	2A	2447	G	OP1-P-O3'	-5.48	93.15	105.20
1	2A	2457	U	N3-C2-O2	-5.48	118.37	122.20
1	1A	533	G	OP1-P-O3'	5.47	117.24	105.20
1	1A	609	A	N1-C2-N3	5.47	132.04	129.30
1	1A	1832	G	O4'-C1'-N9	5.47	112.58	108.20
32	1a	948	C	C6-N1-C2	5.47	122.49	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1081	G	C8-N9-C4	5.47	108.59	106.40
1	2A	1689	A	C5-N7-C8	-5.47	101.16	103.90
1	2A	2616	C	N3-C2-O2	-5.47	118.07	121.90
1	2A	2738	A	O5'-P-OP1	-5.47	100.77	105.70
32	2a	557	G	O5'-P-OP2	-5.47	100.77	105.70
32	2a	664	G	C4-C5-N7	-5.47	108.61	110.80
32	2a	1072	G	C5-C6-O6	5.47	131.88	128.60
1	1A	649	C	C6-N1-C2	5.47	122.49	120.30
1	1A	2286	A	C2-N3-C4	-5.47	107.86	110.60
1	1A	2329	C	C4-C5-C6	5.47	120.14	117.40
1	1A	2361	G	OP1-P-OP2	5.47	127.81	119.60
32	1a	189(G)	G	N3-C2-N2	-5.47	116.07	119.90
32	1a	821	G	C4-C5-C6	5.47	122.08	118.80
32	1a	1331	G	O4'-C1'-N9	5.47	112.58	108.20
1	2A	271(X)	G	C2-N3-C4	-5.47	109.16	111.90
1	2A	1311	G	OP1-P-O3'	5.47	117.24	105.20
1	2A	1933	G	OP1-P-OP2	5.47	127.81	119.60
1	2A	2030	A	N3-C4-C5	5.47	130.63	126.80
1	2A	2300	G	N9-C4-C5	5.47	107.59	105.40
32	2a	438	G	N3-C4-N9	5.47	129.28	126.00
32	2a	800	G	N1-C6-O6	5.47	123.18	119.90
1	1A	1645	C	N3-C4-N4	-5.47	114.17	118.00
1	1A	1665	G	N7-C8-N9	-5.47	110.36	113.10
32	1a	1343	G	OP2-P-O3'	5.47	117.24	105.20
32	1a	1499	A	O5'-P-OP2	-5.47	100.78	105.70
32	2a	125	U	O5'-P-OP2	-5.47	100.78	105.70
1	1A	722	A	C5-N7-C8	-5.47	101.17	103.90
1	1A	1222	A	O4'-C1'-N9	5.47	112.58	108.20
1	1A	2137	G	N7-C8-N9	5.47	115.83	113.10
1	1A	2614	A	OP2-P-O3'	5.47	117.23	105.20
1	1A	2826	C	OP1-P-OP2	5.47	127.80	119.60
1	2A	2312	U	C6-N1-C2	-5.47	117.72	121.00
1	2A	2855	C	C5-C6-N1	5.47	123.73	121.00
1	2A	1846	G	C2-N3-C4	-5.47	109.17	111.90
1	1A	248	G	O5'-P-OP2	-5.47	100.78	105.70
1	1A	489	G	N1-C6-O6	-5.47	116.62	119.90
1	1A	1434	G	OP1-P-OP2	5.47	127.80	119.60
1	1A	2407	C	N3-C4-C5	5.47	124.09	121.90
1	1A	2853	G	C5-C6-O6	5.47	131.88	128.60
2	1B	1	U	C6-N1-C1'	-5.47	113.55	121.20
2	1B	24	G	C6-N1-C2	-5.47	121.82	125.10
32	1a	823	G	O5'-P-OP2	5.47	117.26	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1049	U	C5-C4-O4	-5.47	122.62	125.90
1	1A	831	A	O4'-C1'-N9	5.46	112.57	108.20
1	1A	1196	C	OP1-P-OP2	-5.46	111.40	119.60
1	1A	1371	G	C8-N9-C4	-5.46	104.21	106.40
1	1A	1455	C	C6-N1-C2	5.46	122.49	120.30
1	1A	2606	C	C2-N3-C4	-5.46	117.17	119.90
4	1E	154	LYS	CD-CE-NZ	-5.46	99.13	111.70
32	1a	104	G	O5'-P-OP1	-5.46	100.78	105.70
32	1a	906	G	OP1-P-OP2	5.46	127.80	119.60
1	2A	701	G	C6-N1-C2	5.46	128.38	125.10
1	2A	2400	G	N1-C6-O6	5.46	123.18	119.90
1	2A	2894	G	C6-C5-N7	5.46	133.68	130.40
32	2a	64	G	C2-N3-C4	-5.46	109.17	111.90
1	1A	702	A	N3-C4-C5	5.46	130.62	126.80
1	1A	1264	G	C4-C5-N7	5.46	112.98	110.80
32	1a	398	C	C6-N1-C2	5.46	122.48	120.30
32	1a	528	C	C5-C6-N1	5.46	123.73	121.00
32	1a	671	G	O5'-P-OP1	-5.46	100.78	105.70
1	2A	2377	A	C8-N9-C4	5.46	107.98	105.80
1	2A	2645	G	N9-C4-C5	5.46	107.58	105.40
1	1A	1766	G	C5-C6-O6	-5.46	125.32	128.60
1	1A	1815	A	C8-N9-C4	5.46	107.98	105.80
1	1A	2489	C	O5'-P-OP2	-5.46	100.78	105.70
32	1a	1113	C	C6-N1-C2	-5.46	118.11	120.30
32	1a	1140	C	C6-N1-C2	-5.46	118.12	120.30
32	1a	1441	G	N1-C6-O6	-5.46	116.62	119.90
1	1A	1558	G	OP1-P-O3'	5.46	117.21	105.20
1	1A	84	G	N7-C8-N9	-5.46	110.37	113.10
1	1A	188	A	C4-C5-N7	-5.46	107.97	110.70
1	1A	332	G	N3-C2-N2	-5.46	116.08	119.90
1	1A	905	U	C5-C6-N1	-5.46	119.97	122.70
1	1A	1001	G	N3-C4-C5	5.46	131.33	128.60
1	1A	1550	C	C6-N1-C2	-5.46	118.12	120.30
2	1B	51	G	O5'-P-OP1	5.46	117.25	110.70
2	1B	80	U	C5-C4-O4	5.46	129.18	125.90
10	2O	23	ARG	CB-CG-CD	5.46	125.79	111.60
1	1A	694	G	N1-C6-O6	5.46	123.17	119.90
1	1A	1196	C	N3-C4-C5	5.46	124.08	121.90
32	1a	194	C	C5-C6-N1	5.46	123.73	121.00
2	2B	101	G	N9-C4-C5	-5.46	103.22	105.40
32	2a	655	A	O5'-P-OP2	-5.46	100.79	105.70
1	1A	2275	C	N1-C2-O2	-5.46	115.63	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1B	24	G	C5-C6-N1	5.46	114.23	111.50
1	2A	551	G	N1-C6-O6	-5.46	116.63	119.90
1	2A	1935	G	C4-C5-N7	5.46	112.98	110.80
1	1A	643	C	C5-C6-N1	-5.45	118.27	121.00
1	1A	737	G	C2-N3-C4	5.45	114.63	111.90
1	1A	1050	C	N1-C2-N3	5.45	123.02	119.20
1	1A	1414	G	C5-C6-O6	5.45	131.87	128.60
1	1A	2207	C	C2-N3-C4	5.45	122.63	119.90
1	1A	2481	A	OP1-P-OP2	5.45	127.78	119.60
32	1a	1000	U	O4'-C1'-N1	5.45	112.56	108.20
1	2A	417	C	C5-C6-N1	5.45	123.73	121.00
1	2A	940	G	C5-C6-O6	5.45	131.87	128.60
1	1A	514	G	N1-C2-N3	5.45	127.17	123.90
32	1a	1022	G	N3-C2-N2	5.45	123.72	119.90
1	1A	315	C	N3-C2-O2	5.45	125.72	121.90
1	1A	350	G	C8-N9-C4	5.45	108.58	106.40
1	1A	395	C	C5-C6-N1	-5.45	118.28	121.00
1	1A	795	G	N1-C6-O6	-5.45	116.63	119.90
1	1A	1168	G	C2-N3-C4	5.45	114.62	111.90
1	1A	1204	C	N3-C4-C5	5.45	124.08	121.90
1	1A	1328	U	N1-C2-N3	5.45	118.17	114.90
1	1A	1857	G	C5-C6-O6	5.45	131.87	128.60
1	1A	2068	G	N1-C6-O6	-5.45	116.63	119.90
1	1A	2467	G	N3-C4-N9	5.45	129.27	126.00
1	1A	2691	A	O5'-P-OP2	-5.45	100.80	105.70
1	1A	2735	G	C5-N7-C8	5.45	107.03	104.30
1	2A	363(E)	U	N3-C4-O4	5.45	123.22	119.40
1	2A	1666	G	N3-C2-N2	5.45	123.72	119.90
1	2A	2886	G	C4-C5-N7	-5.45	108.62	110.80
1	1A	1837	C	N3-C4-C5	5.45	124.08	121.90
1	1A	2297	C	OP2-P-O3'	5.45	117.19	105.20
1	1A	2548	G	N1-C2-N3	5.45	127.17	123.90
1	2A	97	C	N3-C4-N4	-5.45	114.19	118.00
1	2A	220	G	N3-C2-N2	-5.45	116.09	119.90
1	2A	551	G	N3-C4-C5	-5.45	125.88	128.60
1	2A	1076	C	C6-N1-C1'	-5.45	114.26	120.80
1	2A	1969	A	C8-N9-C4	-5.45	103.62	105.80
1	1A	935	C	P-O3'-C3'	5.45	126.24	119.70
1	1A	1742	G	C8-N9-C4	-5.45	104.22	106.40
1	1A	2534	U	N3-C2-O2	5.45	126.01	122.20
1	2A	17	G	OP1-P-OP2	-5.45	111.43	119.60
1	2A	2699	C	C2-N3-C4	-5.45	117.18	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2B	30	C	C4-C5-C6	5.45	120.12	117.40
32	2a	572	A	C8-N9-C1'	5.45	137.50	127.70
1	1A	315	C	N1-C2-O2	-5.45	115.63	118.90
1	1A	579	G	C4-C5-N7	-5.45	108.62	110.80
1	1A	2620	G	C5-C6-N1	5.45	114.22	111.50
1	1A	2702	C	O5'-P-OP2	5.45	117.23	110.70
1	1A	2776	G	N9-C4-C5	-5.45	103.22	105.40
32	1a	1276	G	C4-N9-C1'	5.45	133.58	126.50
1	2A	575	A	O5'-P-OP1	-5.45	100.80	105.70
1	2A	1120	G	O5'-P-OP2	-5.45	100.80	105.70
1	1A	724	A	C4-C5-C6	5.44	119.72	117.00
1	1A	1037	C	O5'-P-OP1	-5.44	100.80	105.70
1	1A	1922	A	N3-C4-C5	-5.44	122.99	126.80
32	1a	1144	G	C2-N3-C4	5.44	114.62	111.90
1	2A	145	G	N1-C6-O6	5.44	123.17	119.90
1	2A	365	C	C2-N3-C4	-5.44	117.18	119.90
1	2A	1954	G	N3-C4-N9	-5.44	122.73	126.00
1	1A	1106	U	N3-C2-O2	5.44	126.01	122.20
1	1A	2250	G	N1-C2-N3	-5.44	120.63	123.90
1	1A	2289	G	C4-C5-N7	-5.44	108.62	110.80
32	1a	354	G	C4-N9-C1'	5.44	133.57	126.50
1	2A	538	G	OP2-P-O3'	5.44	117.17	105.20
1	2A	1718	G	C4-C5-N7	-5.44	108.62	110.80
1	2A	1835	G	C5'-C4'-C3'	-5.44	107.29	116.00
1	2A	1883	G	C8-N9-C4	5.44	108.58	106.40
1	2A	2718	G	C8-N9-C4	-5.44	104.22	106.40
32	2a	33	A	N1-C6-N6	-5.44	115.33	118.60
1	1A	834	U	N1-C2-N3	5.44	118.16	114.90
13	1R	114	VAL	CB-CA-C	-5.44	101.06	111.40
32	1a	173	U	O5'-P-OP1	-5.44	100.80	105.70
32	1a	825	G	C6-C5-N7	5.44	133.66	130.40
32	1a	1531	A	C4-C5-C6	-5.44	114.28	117.00
1	2A	214	G	N1-C6-O6	-5.44	116.64	119.90
1	2A	571	A	N1-C6-N6	-5.44	115.34	118.60
1	2A	2196	C	OP1-P-O3'	5.44	117.17	105.20
1	2A	2473	U	N1-C2-O2	5.44	126.61	122.80
1	2A	2789	C	N1-C2-O2	-5.44	115.64	118.90
1	1A	455	A	C5'-C4'-C3'	-5.44	107.30	116.00
1	2A	2137	C	C6-N1-C2	-5.44	118.12	120.30
1	1A	1711	A	C4-C5-C6	5.44	119.72	117.00
1	1A	1803	G	C4-C5-N7	-5.44	108.62	110.80
1	1A	2080	A	C2-N3-C4	-5.44	107.88	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2387	G	O5'-P-OP2	-5.44	100.81	105.70
1	1A	2804	C	C5-C6-N1	5.44	123.72	121.00
32	1a	533	A	C8-N9-C1'	-5.44	117.91	127.70
32	1a	1341	U	C2-N1-C1'	-5.44	111.18	117.70
1	2A	329	G	OP1-P-OP2	5.44	127.76	119.60
1	2A	1773	A	N9-C1'-C2'	-5.44	106.02	112.00
32	2a	619	U	C5-C6-N1	-5.44	119.98	122.70
32	2a	632	A	C8-N9-C4	-5.44	103.62	105.80
1	1A	252	C	N3-C4-C5	-5.44	119.73	121.90
1	1A	1316	C	OP2-P-O3'	5.44	117.16	105.20
1	1A	1921	G	C4-C5-N7	5.44	112.97	110.80
32	1a	1076	C	N1-C2-O2	-5.44	115.64	118.90
1	2A	285	C	OP2-P-O3'	5.44	117.16	105.20
1	2A	725	G	N3-C2-N2	-5.44	116.09	119.90
1	2A	1638	C	C5-C6-N1	-5.44	118.28	121.00
32	2a	1093	A	N1-C6-N6	5.44	121.86	118.60
1	1A	1959	A	C4-C5-N7	-5.43	107.98	110.70
32	1a	1105	A	C8-N9-C4	-5.43	103.63	105.80
32	1a	1417	G	N1-C6-O6	-5.43	116.64	119.90
1	2A	189	G	N3-C2-N2	-5.43	116.10	119.90
1	2A	2629	A	C5-C6-N1	-5.43	114.98	117.70
1	1A	452	G	C5-C6-N1	5.43	114.22	111.50
1	1A	1015	C	C4-C5-C6	5.43	120.12	117.40
1	1A	2401	G	C5-C6-O6	5.43	131.86	128.60
1	1A	2443	U	C4-C5-C6	5.43	122.96	119.70
1	1A	2697	G	C6-C5-N7	5.43	133.66	130.40
32	1a	779	C	OP1-P-OP2	-5.43	111.45	119.60
1	2A	1758	G	C8-N9-C4	5.43	108.57	106.40
32	2a	886	G	N1-C6-O6	5.43	123.16	119.90
1	1A	344	A	N7-C8-N9	5.43	116.52	113.80
1	1A	1925	G	OP2-P-O3'	5.43	117.15	105.20
32	1a	754	C	C5-C4-N4	5.43	124.00	120.20
1	2A	778	G	N3-C4-C5	5.43	131.31	128.60
1	1A	409	G	N3-C2-N2	5.43	123.70	119.90
1	1A	2883	A	O4'-C1'-N9	5.43	112.54	108.20
32	1a	220	G	C8-N9-C4	-5.43	104.23	106.40
32	1a	1526	G	C5-C6-N1	5.43	114.21	111.50
1	2A	103	A	C5-C6-N6	-5.43	119.36	123.70
1	2A	271(J)	C	N1-C2-N3	-5.43	115.40	119.20
1	2A	1075	C	N3-C2-O2	-5.43	118.10	121.90
1	2A	1649	G	N1-C2-N2	-5.43	111.31	116.20
1	2A	1984	G	C5-N7-C8	-5.43	101.59	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	816	A	O5'-P-OP2	-5.43	100.81	105.70
1	1A	1065	U	N1-C2-O2	-5.43	119.00	122.80
1	1A	2139	A	C2-N3-C4	5.43	113.31	110.60
1	2A	303	U	N3-C4-O4	-5.43	115.60	119.40
32	2a	1058	G	O5'-P-OP1	5.43	117.21	110.70
1	1A	614	C	C2-N3-C4	-5.42	117.19	119.90
1	1A	961	C	N3-C4-C5	5.42	124.07	121.90
1	1A	1539	C	N1-C2-O2	5.42	122.16	118.90
1	1A	1980	C	N3-C4-N4	5.42	121.80	118.00
32	1a	194	C	C2-N1-C1'	5.42	124.77	118.80
32	1a	573	A	O5'-P-OP1	5.42	117.21	110.70
32	1a	1108	G	N3-C4-C5	-5.42	125.89	128.60
1	1A	981	C	N3-C4-N4	5.42	121.80	118.00
1	1A	1220	U	P-O3'-C3'	5.42	126.21	119.70
1	1A	1494	G	N9-C4-C5	5.42	107.57	105.40
1	1A	2442	A	C5-C6-N1	5.42	120.41	117.70
1	1A	2463	A	C6-N1-C2	-5.42	115.35	118.60
32	1a	266	G	O4'-C1'-N9	-5.42	103.86	108.20
34	1b	231	GLU	C-N-CD	5.42	139.79	128.40
1	2A	1333	C	C6-N1-C2	-5.42	118.13	120.30
1	1A	692	C	N1-C2-O2	5.42	122.15	118.90
2	1B	116	G	C5-C6-O6	-5.42	125.35	128.60
32	1a	423	G	C4-C5-N7	5.42	112.97	110.80
1	2A	271(J)	C	C6-N1-C2	5.42	122.47	120.30
1	2A	461	C	N3-C4-N4	5.42	121.80	118.00
1	2A	2177	C	C2-N3-C4	5.42	122.61	119.90
1	2A	2230	G	O5'-P-OP1	-5.42	100.82	105.70
32	2a	115	G	N3-C2-N2	5.42	123.69	119.90
1	1A	10	G	C2-N3-C4	5.42	114.61	111.90
1	1A	1135	G	N9-C1'-C2'	5.42	121.05	114.00
1	1A	2102	G	O5'-P-OP1	5.42	117.20	110.70
32	1a	67	C	C5-C4-N4	5.42	123.99	120.20
1	2A	1444	G	N1-C6-O6	-5.42	116.65	119.90
1	2A	1663	C	N3-C4-C5	5.42	124.07	121.90
1	2A	2446	G	N1-C2-N2	-5.42	111.32	116.20
1	1A	2088	C	C5-C4-N4	5.42	123.99	120.20
32	1a	141	A	O4'-C1'-N9	5.42	112.53	108.20
32	1a	1471	G	OP2-P-O3'	5.42	117.12	105.20
1	2A	195	A	C8-N9-C4	-5.42	103.63	105.80
32	2a	1048	G	N9-C1'-C2'	-5.42	106.04	112.00
32	2a	1158	C	C5-C6-N1	5.42	123.71	121.00
1	1A	1346	U	C2-N3-C4	-5.42	123.75	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	467	G	N9-C1'-C2'	-5.42	106.04	112.00
1	2A	1349	A	O5'-P-OP1	-5.42	100.83	105.70
1	2A	1502	C	OP2-P-O3'	5.42	117.12	105.20
1	2A	1982	C	C2-N3-C4	-5.42	117.19	119.90
1	2A	2043	C	N3-C4-C5	5.42	124.07	121.90
32	2a	220	G	N3-C4-N9	5.42	129.25	126.00
32	2a	572	A	N3-C4-N9	-5.42	123.07	127.40
1	2A	1632	A	C8-N9-C4	5.42	107.97	105.80
32	2a	1505	G	O5'-P-OP1	5.42	117.20	110.70
1	1A	635	C	C5-C6-N1	-5.41	118.29	121.00
1	1A	824	A	OP1-P-OP2	5.41	127.72	119.60
1	1A	1383	G	N3-C4-C5	-5.41	125.89	128.60
1	1A	1578	C	C6-N1-C2	-5.41	118.13	120.30
1	1A	1826	C	C6-N1-C2	5.41	122.47	120.30
1	1A	2021	C	OP2-P-O3'	5.41	117.11	105.20
1	1A	2286	A	C4-C5-N7	-5.41	107.99	110.70
1	1A	2353	G	N7-C8-N9	5.41	115.81	113.10
1	1A	2387	G	N1-C6-O6	5.41	123.15	119.90
1	1A	2903	G	C8-N9-C1'	5.41	134.04	127.00
2	1B	1	U	N3-C4-O4	5.41	123.19	119.40
16	1U	55	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	2A	2694	G	N1-C6-O6	-5.41	116.65	119.90
2	2B	92	C	OP2-P-O3'	5.41	117.11	105.20
32	2a	1303	C	N1-C2-O2	5.41	122.15	118.90
1	1A	1175	A	O5'-P-OP2	-5.41	100.83	105.70
1	1A	1911	A	C5-C6-N1	-5.41	114.99	117.70
32	1a	895	G	N1-C6-O6	-5.41	116.65	119.90
1	1A	500	G	OP2-P-O3'	5.41	117.10	105.20
1	1A	1664	A	N7-C8-N9	-5.41	111.09	113.80
1	1A	1991	A	O5'-P-OP2	5.41	117.19	110.70
1	1A	2220	A	N7-C8-N9	-5.41	111.09	113.80
32	1a	129	U	C6-N1-C2	-5.41	117.75	121.00
32	1a	509	A	C4-C5-C6	5.41	119.71	117.00
32	2a	704	A	C8-N9-C4	-5.41	103.64	105.80
1	1A	389	G	C4-C5-N7	5.41	112.96	110.80
1	1A	1714	G	N9-C4-C5	5.41	107.56	105.40
1	1A	2092	G	N1-C2-N2	-5.41	111.33	116.20
1	1A	2559	U	C5-C6-N1	-5.41	120.00	122.70
1	2A	1046	A	N1-C6-N6	-5.41	115.36	118.60
1	2A	1320	C	C5-C6-N1	-5.41	118.30	121.00
2	2B	25	A	O5'-P-OP1	-5.41	100.83	105.70
32	2a	91	C	C6-N1-C2	5.41	122.46	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	530	G	C2-N3-C4	5.41	114.60	111.90
32	2a	1466	C	N1-C2-O2	-5.41	115.65	118.90
1	1A	150	C	N3-C2-O2	-5.41	118.11	121.90
1	1A	2347	A	O5'-P-OP1	-5.41	100.83	105.70
1	1A	2777	A	C5-C6-N1	-5.41	115.00	117.70
1	1A	2902	G	C8-N9-C4	5.41	108.56	106.40
1	2A	1170	G	C8-N9-C4	-5.41	104.24	106.40
32	2a	560	U	C2-N1-C1'	5.41	124.19	117.70
1	1A	1035	G	C6-N1-C2	-5.41	121.86	125.10
1	1A	1852	A	N9-C4-C5	5.41	107.96	105.80
1	1A	1875	C	N3-C4-C5	5.41	124.06	121.90
1	1A	2057	G	O4'-C1'-N9	5.41	112.52	108.20
1	1A	2193	A	C4-C5-N7	5.41	113.40	110.70
1	1A	2612	A	C4-C5-N7	-5.41	108.00	110.70
1	2A	204	A	C5-C6-N6	-5.41	119.38	123.70
1	2A	753	C	C2-N3-C4	-5.41	117.20	119.90
1	2A	1913	A	C5-C6-N1	-5.41	115.00	117.70
2	2B	54	G	N9-C4-C5	5.41	107.56	105.40
2	2B	109	C	OP1-P-OP2	5.41	127.71	119.60
1	1A	124	A	N1-C2-N3	-5.40	126.60	129.30
1	1A	1700	G	C4-N9-C1'	5.40	133.53	126.50
1	1A	1716	A	C8-N9-C4	-5.40	103.64	105.80
5	1F	176	LEU	CB-CG-CD1	-5.40	101.82	111.00
32	1a	262	A	OP1-P-O3'	5.40	117.08	105.20
32	1a	859	A	OP1-P-O3'	5.40	117.08	105.20
32	1a	892	A	OP2-P-O3'	5.40	117.09	105.20
1	2A	595	C	N3-C2-O2	5.40	125.68	121.90
1	2A	752	A	C8-N9-C4	-5.40	103.64	105.80
1	2A	1271	G	N7-C8-N9	-5.40	110.40	113.10
32	2a	830	G	C4-C5-N7	5.40	112.96	110.80
32	2a	1001	A	C4-C5-N7	-5.40	108.00	110.70
1	1A	841	G	N7-C8-N9	-5.40	110.40	113.10
1	1A	1242	G	C6-C5-N7	5.40	133.64	130.40
1	1A	2873	C	O5'-P-OP2	-5.40	100.84	105.70
32	1a	1514	C	OP2-P-O3'	5.40	117.08	105.20
1	2A	752	A	OP1-P-O3'	-5.40	93.32	105.20
1	2A	2055	C	N1-C2-O2	-5.40	115.66	118.90
1	2A	2479	G	C8-N9-C4	-5.40	104.24	106.40
1	1A	909	G	OP1-P-O3'	-5.40	93.32	105.20
1	1A	1411	A	N3-C4-N9	5.40	131.72	127.40
1	1A	2385	G	C2-N3-C4	-5.40	109.20	111.90
1	1A	2402	U	N3-C4-C5	-5.40	111.36	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2761	A	OP2-P-O3'	5.40	117.08	105.20
1	2A	90	U	N3-C2-O2	-5.40	118.42	122.20
1	2A	828	U	OP2-P-O3'	5.40	117.08	105.20
1	2A	2476	A	N1-C6-N6	-5.40	115.36	118.60
2	2B	52	A	N1-C6-N6	5.40	121.84	118.60
32	2a	760	G	O5'-P-OP2	-5.40	100.84	105.70
32	2a	1226	C	C6-N1-C2	-5.40	118.14	120.30
1	1A	480	A	C8-N9-C4	-5.40	103.64	105.80
1	1A	1149	A	O4'-C1'-N9	5.40	112.52	108.20
1	1A	2712	C	N1-C2-O2	-5.40	115.66	118.90
32	1a	474	G	O5'-P-OP1	5.40	117.18	110.70
1	2A	2366	A	O5'-P-OP2	-5.40	100.84	105.70
1	1A	722	A	C5-C6-N6	-5.40	119.38	123.70
1	1A	1309	U	C5-C6-N1	-5.40	120.00	122.70
1	1A	1769	G	N9-C4-C5	5.40	107.56	105.40
32	1a	1024	G	N3-C4-C5	-5.40	125.90	128.60
1	2A	2397	G	OP2-P-O3'	5.40	117.07	105.20
1	1A	2491	G	C5-N7-C8	5.39	107.00	104.30
1	2A	311	A	OP1-P-OP2	-5.39	111.51	119.60
32	2a	885	G	N3-C4-C5	-5.39	125.90	128.60
1	1A	2227	G	C2-N3-C4	-5.39	109.20	111.90
1	1A	2700	U	N3-C4-C5	-5.39	111.36	114.60
32	1a	181	G	N9-C4-C5	5.39	107.56	105.40
1	2A	1721	G	N3-C4-C5	-5.39	125.90	128.60
1	1A	188	A	C5-C6-N6	5.39	128.01	123.70
1	1A	1966	U	C5-C4-O4	-5.39	122.67	125.90
1	1A	2251	G	N7-C8-N9	-5.39	110.40	113.10
1	1A	608	G	OP1-P-OP2	-5.39	111.52	119.60
1	1A	1152	G	N1-C2-N3	-5.39	120.67	123.90
1	1A	1303	C	N1-C2-N3	5.39	122.97	119.20
1	1A	2874	G	C5-C6-O6	5.39	131.83	128.60
1	1A	2897	U	O5'-P-OP1	-5.39	100.85	105.70
1	2A	2832	U	C6-N1-C2	5.39	124.23	121.00
32	2a	140	A	C8-N9-C4	-5.39	103.64	105.80
32	2a	649	G	C8-N9-C4	5.39	108.56	106.40
1	1A	587	C	N1-C2-O2	-5.39	115.67	118.90
1	1A	1392	G	C4-C5-N7	-5.39	108.64	110.80
1	1A	2633	A	O5'-P-OP1	-5.39	100.85	105.70
1	2A	271(Y)	U	N3-C2-O2	-5.39	118.43	122.20
1	1A	476	G	C6-N1-C2	-5.39	121.87	125.10
1	1A	1088	G	C4-N9-C1'	5.39	133.50	126.50
1	1A	2260	C	C2-N3-C4	-5.39	117.21	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	588	G	C8-N9-C4	-5.39	104.25	106.40
32	1a	1046	A	C6-N1-C2	-5.39	115.37	118.60
1	2A	113	G	N3-C4-C5	5.39	131.29	128.60
1	2A	1696	G	C5-C6-N1	5.39	114.19	111.50
32	2a	1217	C	C4-C5-C6	5.39	120.09	117.40
1	1A	75	C	N3-C4-N4	5.38	121.77	118.00
1	1A	119	G	C5-C6-O6	-5.38	125.37	128.60
1	1A	150	C	OP2-P-O3'	5.38	117.04	105.20
1	1A	582	G	C4-C5-N7	5.38	112.95	110.80
1	1A	1486	G	N7-C8-N9	-5.38	110.41	113.10
1	1A	1649	A	N1-C6-N6	-5.38	115.37	118.60
1	1A	2426	G	O5'-P-OP1	5.38	117.16	110.70
15	1T	96	ARG	CA-CB-CG	5.38	125.25	113.40
1	2A	247	G	O5'-P-OP2	-5.38	100.85	105.70
1	1A	554	A	C4-C5-N7	5.38	113.39	110.70
30	18	57	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	2A	1678	G	N7-C8-N9	5.38	115.79	113.10
32	2a	230	G	N9-C4-C5	5.38	107.55	105.40
1	1A	654	G	N7-C8-N9	-5.38	110.41	113.10
1	1A	1523	C	N1-C2-O2	-5.38	115.67	118.90
27	15	13	LYS	CD-CE-NZ	5.38	124.08	111.70
1	2A	527	C	N3-C2-O2	5.38	125.67	121.90
1	2A	1179	C	C6-N1-C2	5.38	122.45	120.30
32	2a	1129	C	C5-C6-N1	5.38	123.69	121.00
1	1A	2702	C	N3-C2-O2	5.38	125.67	121.90
1	2A	1411	C	OP2-P-O3'	5.38	117.03	105.20
32	2a	1140	C	C6-N1-C2	-5.38	118.15	120.30
1	1A	1143	U	C6-N1-C2	-5.38	117.77	121.00
1	1A	2525	G	C5-C6-N1	-5.38	108.81	111.50
32	1a	125	U	OP2-P-O3'	5.38	117.03	105.20
32	1a	301	G	N3-C4-C5	-5.38	125.91	128.60
32	1a	728	A	O5'-P-OP2	-5.38	100.86	105.70
1	2A	1236	G	O5'-P-OP2	5.38	117.16	110.70
32	2a	360	A	C6-N1-C2	-5.38	115.37	118.60
1	1A	86	C	O5'-P-OP2	-5.38	100.86	105.70
1	1A	317	U	O5'-P-OP2	-5.38	100.86	105.70
1	2A	1751	C	OP2-P-O3'	5.38	117.03	105.20
1	2A	1964	G	N3-C2-N2	5.38	123.66	119.90
1	2A	2419	U	OP1-P-O3'	5.38	117.03	105.20
1	2A	2465	C	C6-N1-C2	-5.38	118.15	120.30
32	2a	673	G	N3-C2-N2	5.38	123.66	119.90
32	2a	977	A	C8-N9-C4	-5.38	103.65	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	722	A	C2-N3-C4	-5.38	107.91	110.60
1	2A	2406	U	O4'-C1'-N1	-5.38	103.90	108.20
1	1A	857	U	N3-C4-O4	5.37	123.16	119.40
1	1A	1105	G	N9-C1'-C2'	-5.37	106.09	112.00
1	1A	1281	G	C2-N3-C4	-5.37	109.21	111.90
1	1A	1423	G	N1-C2-N2	-5.37	111.36	116.20
1	1A	2077	C	N3-C2-O2	5.37	125.66	121.90
16	1U	19	LYS	CD-CE-NZ	-5.37	99.34	111.70
1	2A	236	C	C2-N3-C4	-5.37	117.21	119.90
1	2A	1882	C	O5'-P-OP1	-5.37	100.86	105.70
1	2A	2166	G	C8-N9-C4	-5.37	104.25	106.40
32	2a	616	G	C8-N9-C4	-5.37	104.25	106.40
32	2a	1461	G	N1-C6-O6	5.37	123.12	119.90
32	2a	1495	U	C5-C6-N1	5.37	125.39	122.70
1	1A	642	G	OP2-P-O3'	5.37	117.02	105.20
1	1A	1670	G	OP1-P-OP2	-5.37	111.54	119.60
1	1A	2521	G	N3-C2-N2	5.37	123.66	119.90
32	1a	1211	U	C2-N3-C4	-5.37	123.78	127.00
1	2A	2146	C	C2-N1-C1'	5.37	124.71	118.80
1	2A	2358	G	N3-C4-C5	5.37	131.29	128.60
32	2a	390	C	C5-C6-N1	-5.37	118.31	121.00
32	2a	818	G	O4'-C1'-N9	5.37	112.50	108.20
32	2a	993	G	C8-N9-C1'	-5.37	120.02	127.00
1	1A	1696	G	N9-C4-C5	5.37	107.55	105.40
32	1a	1145	C	C6-N1-C2	-5.37	118.15	120.30
1	2A	1779	U	O4'-C1'-N1	5.37	112.50	108.20
2	1B	1	U	N1-C2-N3	-5.37	111.68	114.90
32	1a	23	C	C6-N1-C2	-5.37	118.15	120.30
32	1a	635	G	C5-C6-O6	-5.37	125.38	128.60
1	2A	474	G	N7-C8-N9	5.37	115.78	113.10
32	2a	791	G	N1-C6-O6	5.37	123.12	119.90
1	1A	25	U	C2-N1-C1'	5.37	124.14	117.70
1	1A	1042	A	C5-N7-C8	5.37	106.58	103.90
1	1A	1494	G	O4'-C1'-N9	5.37	112.49	108.20
1	2A	2042	A	N3-C4-C5	5.37	130.56	126.80
32	2a	186	C	C6-N1-C2	-5.37	118.15	120.30
32	2a	1060	C	C6-N1-C2	-5.37	118.15	120.30
1	1A	162	G	C8-N9-C4	-5.37	104.25	106.40
1	1A	706	C	C4-C5-C6	-5.37	114.72	117.40
1	1A	2250	G	N9-C4-C5	-5.37	103.25	105.40
32	1a	308	C	N3-C2-O2	-5.37	118.14	121.90
32	1a	1175	G	N1-C6-O6	5.37	123.12	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1197	G	N9-C4-C5	-5.37	103.25	105.40
1	2A	214	G	N9-C4-C5	5.37	107.55	105.40
32	2a	345	C	N1-C2-O2	-5.37	115.68	118.90
1	1A	702	A	C8-N9-C1'	5.36	137.35	127.70
1	1A	1282	G	N3-C4-C5	5.36	131.28	128.60
1	1A	1354	A	C5-C6-N6	5.36	127.99	123.70
1	1A	1924	C	N1-C2-O2	-5.36	115.68	118.90
32	1a	346	G	C6-N1-C2	-5.36	121.88	125.10
32	1a	427	U	C5-C6-N1	5.36	125.38	122.70
1	2A	767	U	N3-C4-O4	-5.36	115.65	119.40
1	2A	1054	A	C8-N9-C4	-5.36	103.65	105.80
1	2A	2571	C	O5'-P-OP1	-5.36	100.87	105.70
1	2A	2836	U	N1-C2-O2	5.36	126.56	122.80
1	2A	2896	C	N1-C2-O2	5.36	122.12	118.90
32	2a	490	G	N1-C6-O6	-5.36	116.68	119.90
1	1A	20	C	N1-C2-N3	5.36	122.95	119.20
1	1A	149	A	C2-N3-C4	-5.36	107.92	110.60
1	1A	920	G	OP2-P-O3'	5.36	117.00	105.20
1	1A	1985	U	C2-N1-C1'	5.36	124.14	117.70
1	1A	2129	C	C5-C6-N1	5.36	123.68	121.00
27	15	15	ARG	NE-CZ-NH1	-5.36	117.62	120.30
32	1a	322	C	N3-C4-C5	5.36	124.05	121.90
32	1a	1010	G	N3-C4-C5	5.36	131.28	128.60
1	2A	1122	G	O5'-P-OP2	-5.36	100.87	105.70
1	1A	1475	G	C2-N3-C4	5.36	114.58	111.90
1	1A	1700	G	N1-C2-N2	-5.36	111.38	116.20
1	1A	1809	U	C5-C6-N1	-5.36	120.02	122.70
1	1A	2441	G	C5-C6-N1	-5.36	108.82	111.50
32	1a	28	G	N3-C2-N2	-5.36	116.15	119.90
32	1a	668	G	OP2-P-O3'	5.36	116.99	105.20
1	2A	260	G	N9-C4-C5	5.36	107.54	105.40
1	2A	602	G	N1-C2-N2	-5.36	111.38	116.20
1	1A	652	A	O5'-P-OP1	5.36	117.13	110.70
1	1A	1527	G	N3-C4-C5	5.36	131.28	128.60
1	2A	353	G	C5-C6-O6	-5.36	125.39	128.60
1	1A	1184	G	C6-N1-C2	-5.36	121.89	125.10
1	1A	1482	G	N1-C6-O6	-5.36	116.69	119.90
1	1A	2784	C	O5'-P-OP2	5.36	117.13	110.70
2	1B	82	G	N1-C6-O6	-5.36	116.69	119.90
1	1A	1613	A	C4-C5-C6	-5.36	114.32	117.00
1	1A	2387	G	C8-N9-C4	5.36	108.54	106.40
1	1A	2484	G	C6-N1-C2	-5.36	121.89	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1024	G	C8-N9-C4	-5.36	104.26	106.40
32	1a	1504	G	C5-C6-O6	-5.36	125.39	128.60
1	2A	271(M)	G	C8-N9-C4	-5.36	104.26	106.40
1	1A	1178	A	O5'-P-OP1	-5.35	100.88	105.70
1	1A	2171	G	C6-C5-N7	5.35	133.61	130.40
1	1A	1739	U	C2-N3-C4	-5.35	123.79	127.00
1	2A	227	A	C6-N1-C2	-5.35	115.39	118.60
1	2A	1602	U	C6-N1-C2	5.35	124.21	121.00
1	2A	2106	G	N3-C4-C5	-5.35	125.92	128.60
1	2A	2695	C	C6-N1-C2	5.35	122.44	120.30
2	2B	24	G	N9-C4-C5	-5.35	103.26	105.40
15	2T	53	ARG	CB-CA-C	-5.35	99.69	110.40
1	1A	2007	G	C4-C5-N7	-5.35	108.66	110.80
1	2A	871	U	C5-C4-O4	-5.35	122.69	125.90
1	2A	1858	G	O4'-C1'-N9	5.35	112.48	108.20
32	2a	795	C	N1-C2-O2	5.35	122.11	118.90
1	1A	1441	A	C8-N9-C4	5.35	107.94	105.80
1	1A	2041	A	C2-N3-C4	-5.35	107.92	110.60
1	2A	531	C	N1-C2-O2	5.35	122.11	118.90
32	2a	9	G	C5-C6-O6	-5.35	125.39	128.60
32	2a	1163	C	N1-C2-O2	5.35	122.11	118.90
32	2a	1184	G	O5'-P-OP1	-5.35	100.89	105.70
51	2s	30	LEU	CA-CB-CG	5.35	127.60	115.30
1	1A	150	C	C2-N3-C4	-5.35	117.23	119.90
1	1A	194	G	P-O3'-C3'	5.35	126.12	119.70
1	1A	201	G	C5-N7-C8	-5.35	101.63	104.30
1	1A	1273	G	C5-N7-C8	5.35	106.97	104.30
1	1A	1729	G	N1-C6-O6	-5.35	116.69	119.90
1	1A	1845	G	N1-C2-N3	5.35	127.11	123.90
32	1a	455	C	N1-C2-O2	5.35	122.11	118.90
32	2a	830	G	C6-C5-N7	-5.35	127.19	130.40
1	1A	474	U	N3-C4-O4	-5.35	115.66	119.40
1	1A	2552	C	N3-C4-C5	5.35	124.04	121.90
1	2A	655	A	C6-C5-N7	-5.35	128.56	132.30
1	2A	1533	G	N7-C8-N9	5.35	115.77	113.10
1	2A	1899	G	OP1-P-O3'	5.35	116.96	105.20
1	1A	520	G	N9-C4-C5	5.34	107.54	105.40
1	1A	1615	G	N1-C2-N2	-5.34	111.39	116.20
34	1b	178	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	1A	41	C	O5'-P-OP1	5.34	117.11	110.70
1	1A	179	A	C5-C6-N1	-5.34	115.03	117.70
1	1A	1345	G	N1-C6-O6	5.34	123.11	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1874	C	C6-N1-C2	5.34	122.44	120.30
1	1A	2633	A	OP2-P-O3'	5.34	116.95	105.20
1	1A	2788	A	C5-N7-C8	5.34	106.57	103.90
32	1a	183	G	C4-N9-C1'	5.34	133.44	126.50
1	2A	2747	G	N3-C2-N2	-5.34	116.16	119.90
1	1A	1630	A	N1-C6-N6	-5.34	115.39	118.60
1	1A	2641	A	O4'-C1'-N9	5.34	112.47	108.20
2	1B	48	A	C8-N9-C4	5.34	107.94	105.80
32	1a	1217	C	C2-N1-C1'	-5.34	112.92	118.80
1	2A	1256	G	OP1-P-OP2	5.34	127.61	119.60
1	2A	2499	C	N3-C2-O2	5.34	125.64	121.90
32	2a	184	G	C8-N9-C4	-5.34	104.26	106.40
1	1A	162	G	OP1-P-O3'	5.34	116.95	105.20
1	1A	1959	A	C6-N1-C2	-5.34	115.40	118.60
1	1A	2255	U	N1-C2-O2	-5.34	119.06	122.80
1	1A	2335	G	N7-C8-N9	5.34	115.77	113.10
32	1a	820	U	N3-C2-O2	-5.34	118.46	122.20
1	2A	502	A	N1-C2-N3	5.34	131.97	129.30
32	1a	134	A	N9-C4-C5	-5.34	103.67	105.80
32	1a	819	A	C6-C5-N7	-5.34	128.56	132.30
1	2A	1251	C	C5-C4-N4	-5.34	116.46	120.20
1	2A	2514	U	N3-C4-O4	5.34	123.14	119.40
32	2a	917	G	N1-C6-O6	5.34	123.10	119.90
1	1A	217	A	N3-C4-N9	-5.34	123.13	127.40
1	1A	2193	A	N3-C4-N9	5.34	131.67	127.40
1	1A	2292	G	C6-C5-N7	5.34	133.60	130.40
32	1a	884	U	OP1-P-OP2	5.34	127.60	119.60
32	1a	1026	G	N3-C4-N9	5.34	129.20	126.00
1	2A	789	A	C4-C5-N7	5.34	113.37	110.70
1	2A	1032	A	C2-N3-C4	-5.34	107.93	110.60
1	2A	1838	C	C2-N3-C4	-5.34	117.23	119.90
1	2A	2231	C	O5'-P-OP2	-5.34	100.90	105.70
32	2a	304	U	OP1-P-OP2	5.34	127.61	119.60
32	2a	549	C	N3-C4-C5	5.34	124.03	121.90
32	2a	733	A	C8-N9-C4	5.34	107.93	105.80
32	2a	1161	C	N1-C2-O2	5.34	122.10	118.90
1	1A	50	G	N1-C2-N3	5.33	127.10	123.90
1	1A	2887	G	C8-N9-C4	5.33	108.53	106.40
1	2A	2483	C	C5-C6-N1	5.33	123.67	121.00
1	1A	2024	G	C8-N9-C4	5.33	108.53	106.40
1	1A	2436	C	C2-N1-C1'	-5.33	112.93	118.80
1	1A	2792	U	N1-C2-N3	5.33	118.10	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	30	U	N3-C2-O2	-5.33	118.47	122.20
32	1a	858	G	N7-C8-N9	5.33	115.77	113.10
1	2A	746	A	O4'-C1'-N9	5.33	112.47	108.20
1	2A	2853	C	N1-C2-O2	-5.33	115.70	118.90
32	2a	1259	C	C5-C6-N1	5.33	123.67	121.00
32	2a	1510	U	N3-C4-O4	5.33	123.13	119.40
1	1A	483	A	N1-C2-N3	-5.33	126.63	129.30
1	1A	577	U	OP2-P-O3'	5.33	116.93	105.20
1	1A	1453	C	N1-C2-N3	5.33	122.93	119.20
1	1A	2065	C	C6-N1-C2	-5.33	118.17	120.30
32	1a	807	A	N9-C4-C5	5.33	107.93	105.80
1	2A	303	U	N1-C2-O2	5.33	126.53	122.80
1	2A	1919	A	N7-C8-N9	5.33	116.47	113.80
32	2a	136	C	C6-N1-C2	-5.33	118.17	120.30
32	2a	281	G	N1-C6-O6	5.33	123.10	119.90
32	2a	1279	A	C2-N3-C4	5.33	113.27	110.60
1	1A	815	G	N3-C2-N2	-5.33	116.17	119.90
1	1A	1426	G	C5-C6-O6	-5.33	125.40	128.60
1	1A	1666	G	N7-C8-N9	-5.33	110.44	113.10
1	1A	2574	U	C5-C4-O4	5.33	129.10	125.90
21	1Z	77	ASP	CB-CG-OD1	5.33	123.10	118.30
1	2A	1394	U	O5'-P-OP1	-5.33	100.90	105.70
1	2A	2433	A	C5-C6-N6	-5.33	119.44	123.70
1	2A	2827	C	C5-C6-N1	-5.33	118.33	121.00
32	2a	851	G	N7-C8-N9	5.33	115.77	113.10
1	1A	60	G	N1-C6-O6	5.33	123.10	119.90
1	1A	218	A	C8-N9-C4	-5.33	103.67	105.80
1	1A	731	G	OP1-P-OP2	5.33	127.59	119.60
1	1A	877	G	N3-C4-C5	-5.33	125.94	128.60
1	1A	1178	A	N9-C4-C5	5.33	107.93	105.80
1	1A	1524	A	O5'-P-OP2	-5.33	100.90	105.70
1	1A	1784	G	C5-N7-C8	-5.33	101.64	104.30
1	1A	2142	G	C8-N9-C4	-5.33	104.27	106.40
2	1B	38	C	N1-C2-O2	5.33	122.10	118.90
1	2A	281	G	N1-C6-O6	5.33	123.10	119.90
32	2a	644	G	N7-C8-N9	-5.33	110.44	113.10
32	2a	912	C	O5'-P-OP2	-5.33	100.91	105.70
32	2a	1081	G	C8-N9-C4	5.33	108.53	106.40
1	1A	1280	U	C5-C6-N1	-5.33	120.04	122.70
1	1A	2693	C	N1-C2-O2	-5.33	115.70	118.90
32	1a	821	G	N3-C4-N9	5.33	129.20	126.00
32	2a	1005	A	P-O3'-C3'	5.33	126.09	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	987	G	C5-C6-N1	5.33	114.16	111.50
1	1A	1398	U	O5'-P-OP1	-5.33	100.91	105.70
2	1B	90	A	C8-N9-C4	5.33	107.93	105.80
1	1A	614	C	N3-C2-O2	-5.32	118.17	121.90
1	1A	822	G	O4'-C1'-N9	5.32	112.46	108.20
1	1A	883	G	C5-N7-C8	-5.32	101.64	104.30
1	1A	2501	G	N3-C4-N9	5.32	129.19	126.00
1	2A	116	C	C6-N1-C2	-5.32	118.17	120.30
32	2a	1059	C	OP1-P-O3'	5.32	116.91	105.20
32	2a	1363	C	C6-N1-C1'	5.32	127.19	120.80
1	1A	2099	A	C8-N9-C4	5.32	107.93	105.80
1	1A	2245	U	C2-N3-C4	-5.32	123.81	127.00
32	1a	1397	C	C6-N1-C2	-5.32	118.17	120.30
32	2a	918	A	OP2-P-O3'	5.32	116.91	105.20
32	2a	1511	G	C4-C5-N7	-5.32	108.67	110.80
1	1A	500	G	N3-C2-N2	5.32	123.62	119.90
1	1A	500	G	O5'-P-OP2	-5.32	100.91	105.70
1	1A	845	G	C4-C5-N7	-5.32	108.67	110.80
1	1A	1093	G	C8-N9-C1'	-5.32	120.08	127.00
1	1A	1386	U	N1-C2-N3	5.32	118.09	114.90
1	1A	2100	C	O5'-P-OP1	-5.32	100.91	105.70
1	1A	2429	C	O5'-P-OP2	-5.32	100.91	105.70
3	1D	222	ARG	NE-CZ-NH1	-5.32	117.64	120.30
32	1a	189(D)	C	C6-N1-C1'	-5.32	114.41	120.80
32	1a	857	C	N3-C4-C5	-5.32	119.77	121.90
1	2A	858	U	N1-C2-O2	5.32	126.52	122.80
32	2a	232	G	C5-C6-O6	-5.32	125.41	128.60
32	1a	1175	G	C5-C6-O6	-5.32	125.41	128.60
32	2a	19	C	OP1-P-OP2	5.32	127.58	119.60
1	1A	36	G	N1-C6-O6	-5.32	116.71	119.90
1	1A	762	G	N3-C4-C5	-5.32	125.94	128.60
1	1A	1175	A	N1-C6-N6	-5.32	115.41	118.60
1	1A	1508	G	O5'-P-OP1	-5.32	100.91	105.70
1	1A	1946	C	O5'-P-OP2	5.32	117.08	110.70
2	1B	104	U	C6-N1-C2	5.32	124.19	121.00
18	1W	83	LYS	CD-CE-NZ	-5.32	99.47	111.70
32	1a	353	A	C5-C6-N6	-5.32	119.45	123.70
32	1a	550	G	OP1-P-OP2	5.32	127.58	119.60
1	2A	1717	G	C4-C5-N7	-5.32	108.67	110.80
1	2A	1789	A	N7-C8-N9	-5.32	111.14	113.80
1	1A	818	G	N3-C2-N2	5.32	123.62	119.90
1	1A	1392	G	C5-N7-C8	5.32	106.96	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2073	A	C4-C5-N7	-5.32	108.04	110.70
1	1A	2138	G	N7-C8-N9	5.32	115.76	113.10
1	1A	2637	G	N9-C4-C5	5.32	107.53	105.40
1	1A	2722	C	OP1-P-O3'	5.32	116.89	105.20
32	1a	487	A	N1-C6-N6	5.32	121.79	118.60
1	2A	826	U	N1-C2-N3	5.32	118.09	114.90
1	2A	1020	A	O5'-P-OP1	-5.32	100.92	105.70
1	2A	1052	C	C5-C6-N1	5.32	123.66	121.00
1	2A	2155	G	N1-C2-N2	5.32	120.98	116.20
1	1A	841	G	C8-N9-C4	5.31	108.53	106.40
1	1A	1067	A	C4-C5-C6	5.31	119.66	117.00
1	2A	614(C)	A	O5'-P-OP2	-5.31	100.92	105.70
1	2A	1791	A	C5'-C4'-C3'	-5.31	107.50	116.00
1	1A	765	A	C4-C5-C6	5.31	119.66	117.00
1	1A	1344	C	N3-C4-N4	-5.31	114.28	118.00
1	1A	1422	C	C5-C4-N4	5.31	123.92	120.20
1	1A	1812	C	C6-N1-C1'	-5.31	114.42	120.80
1	1A	2030	C	C5-C6-N1	-5.31	118.34	121.00
1	1A	2215	G	C8-N9-C4	5.31	108.53	106.40
1	1A	2360	U	C5-C4-O4	5.31	129.09	125.90
1	1A	2587	C	C6-N1-C2	5.31	122.42	120.30
18	1W	107	LEU	CA-CB-CG	5.31	127.52	115.30
32	1a	227	G	C8-N9-C4	5.31	108.53	106.40
32	1a	776	G	N1-C6-O6	5.31	123.09	119.90
1	2A	1883	G	C8-N9-C1'	-5.31	120.09	127.00
1	2A	2886	G	N3-C2-N2	-5.31	116.18	119.90
1	1A	202	A	O5'-P-OP1	5.31	117.07	110.70
1	1A	815	G	N1-C2-N3	5.31	127.09	123.90
1	1A	1107	U	N1-C2-O2	5.31	126.52	122.80
1	1A	1236	G	N7-C8-N9	-5.31	110.44	113.10
32	1a	1181	G	N1-C6-O6	5.31	123.09	119.90
1	2A	587	C	N3-C2-O2	-5.31	118.18	121.90
1	2A	1986	A	C2-N3-C4	-5.31	107.94	110.60
1	2A	2877	G	O5'-P-OP1	5.31	117.07	110.70
1	1A	17	G	C6-N1-C2	-5.31	121.92	125.10
1	1A	612	C	C5-C6-N1	-5.31	118.34	121.00
1	1A	1178	A	C8-N9-C4	-5.31	103.68	105.80
1	1A	1985	U	OP1-P-O3'	5.31	116.88	105.20
1	1A	2399	U	N1-C2-O2	-5.31	119.08	122.80
1	1A	2568	C	C5-C6-N1	-5.31	118.34	121.00
32	1a	155	C	C6-N1-C2	-5.31	118.18	120.30
32	1a	563	A	C5-N7-C8	-5.31	101.25	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2632	A	N1-C6-N6	5.31	121.78	118.60
32	2a	574	A	C4-C5-N7	5.31	113.35	110.70
1	1A	1207	C	C5-C4-N4	-5.31	116.48	120.20
1	1A	2395	G	N1-C6-O6	-5.31	116.72	119.90
1	1A	2738	A	N1-C2-N3	5.31	131.95	129.30
1	2A	1231	G	OP1-P-OP2	-5.31	111.64	119.60
1	2A	1536	C	N3-C4-N4	5.31	121.72	118.00
1	2A	1776	G	N3-C4-N9	5.31	129.18	126.00
21	2Z	155	LEU	CA-CB-CG	5.31	127.51	115.30
32	1a	1003	G	C4-N9-C1'	5.31	133.40	126.50
1	2A	1997	G	C5-C6-N1	5.31	114.15	111.50
32	2a	1486	G	C8-N9-C4	5.31	108.52	106.40
1	1A	1842	G	C8-N9-C4	-5.30	104.28	106.40
1	1A	2034	G	N9-C4-C5	5.30	107.52	105.40
1	1A	2516	U	C2-N3-C4	-5.30	123.82	127.00
1	2A	411	G	O5'-P-OP1	-5.30	100.93	105.70
1	2A	1016	G	N3-C4-C5	5.30	131.25	128.60
1	2A	1610	A	N9-C4-C5	-5.30	103.68	105.80
1	1A	1694	G	N3-C2-N2	-5.30	116.19	119.90
1	1A	1771	G	N1-C6-O6	5.30	123.08	119.90
1	1A	2265	G	O4'-C1'-N9	-5.30	103.96	108.20
32	1a	345	C	C6-N1-C1'	-5.30	114.44	120.80
32	1a	696	A	N1-C6-N6	5.30	121.78	118.60
1	2A	494	G	N9-C4-C5	5.30	107.52	105.40
1	2A	1690	A	C6-C5-N7	-5.30	128.59	132.30
1	2A	2035	G	C4-N9-C1'	-5.30	119.61	126.50
1	2A	2232	U	N3-C4-C5	5.30	117.78	114.60
1	2A	2353	G	C5-C6-O6	-5.30	125.42	128.60
1	1A	215	G	C8-N9-C1'	5.30	133.89	127.00
1	1A	555	G	C5-C6-N1	5.30	114.15	111.50
1	1A	1383	G	C5-N7-C8	5.30	106.95	104.30
1	1A	2250	G	C2-N3-C4	5.30	114.55	111.90
32	1a	176	C	C6-N1-C2	-5.30	118.18	120.30
32	1a	1022	G	N3-C4-N9	5.30	129.18	126.00
32	1a	1529	G	C8-N9-C4	-5.30	104.28	106.40
1	2A	944	G	C5-C6-O6	5.30	131.78	128.60
1	2A	2140	C	C6-N1-C2	-5.30	118.18	120.30
32	2a	906	G	C5-C6-O6	-5.30	125.42	128.60
1	1A	41	C	OP2-P-O3'	5.30	116.86	105.20
1	1A	454	U	C4-C5-C6	-5.30	116.52	119.70
1	1A	616	G	C5-N7-C8	5.30	106.95	104.30
1	1A	1110	C	C6-N1-C2	-5.30	118.18	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1255	A	C5-N7-C8	-5.30	101.25	103.90
1	1A	2329	C	C6-N1-C2	-5.30	118.18	120.30
1	1A	2561	G	OP2-P-O3'	5.30	116.86	105.20
32	1a	149	A	C5-C6-N1	-5.30	115.05	117.70
32	1a	644	G	N1-C6-O6	-5.30	116.72	119.90
1	2A	1264	G	C5-C6-O6	5.30	131.78	128.60
1	2A	2307	G	N3-C4-N9	5.30	129.18	126.00
1	2A	2378	A	C8-N9-C1'	-5.30	118.16	127.70
1	2A	2446	G	N3-C2-N2	5.30	123.61	119.90
32	2a	498	U	N3-C4-O4	-5.30	115.69	119.40
1	1A	10	G	O4'-C1'-N9	5.30	112.44	108.20
1	1A	387	G	N3-C4-C5	5.30	131.25	128.60
1	1A	1269	G	C5-C6-O6	5.30	131.78	128.60
1	1A	2024	G	C4-C5-N7	-5.30	108.68	110.80
1	1A	2238	C	N1-C2-O2	-5.30	115.72	118.90
32	1a	266	G	N7-C8-N9	5.30	115.75	113.10
32	1a	324	G	OP2-P-O3'	5.30	116.86	105.20
1	2A	1180	C	N1-C2-O2	5.30	122.08	118.90
1	2A	2763	G	N3-C4-C5	-5.30	125.95	128.60
32	2a	1349	A	C8-N9-C4	5.30	107.92	105.80
1	1A	1828	C	N1-C2-O2	-5.30	115.72	118.90
1	1A	2008	A	OP2-P-O3'	5.30	116.85	105.20
1	1A	2351	G	O5'-P-OP2	-5.30	100.93	105.70
1	1A	2561	G	C5'-C4'-O4'	5.30	115.45	109.10
1	1A	2653	G	C5'-C4'-C3'	-5.30	107.53	116.00
32	1a	189(D)	C	C6-N1-C2	-5.30	118.18	120.30
1	2A	1369	G	C5-C6-N1	5.30	114.15	111.50
1	2A	1933	G	N9-C4-C5	5.30	107.52	105.40
32	2a	1043	C	C5-C4-N4	5.30	123.91	120.20
1	1A	839	G	N3-C4-N9	5.29	129.18	126.00
1	1A	1179	U	OP2-P-O3'	5.29	116.85	105.20
32	1a	569	C	O5'-P-OP2	-5.29	100.94	105.70
32	1a	1066	C	C6-N1-C2	5.29	122.42	120.30
1	2A	937	U	N1-C2-O2	-5.29	119.09	122.80
1	2A	2125	G	N3-C2-N2	5.29	123.61	119.90
1	2A	2583	G	OP2-P-O3'	5.29	116.84	105.20
32	2a	302	G	OP2-P-O3'	5.29	116.85	105.20
1	1A	827	G	N3-C2-N2	-5.29	116.20	119.90
1	1A	1143	U	C5-C6-N1	5.29	125.35	122.70
1	1A	2403	G	O4'-C1'-N9	5.29	112.43	108.20
32	1a	618	C	O5'-P-OP1	-5.29	100.94	105.70
1	2A	80	G	C5-C6-O6	5.29	131.78	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	300	A	N1-C6-N6	5.29	121.78	118.60
1	2A	2083	G	O5'-P-OP1	-5.29	100.94	105.70
1	2A	2817	G	C5-C6-O6	5.29	131.78	128.60
2	2B	33	G	C2-N3-C4	-5.29	109.25	111.90
1	1A	1012	C	C2-N3-C4	-5.29	117.25	119.90
32	1a	187	C	C2-N1-C1'	5.29	124.62	118.80
32	1a	250	A	N3-C4-C5	-5.29	123.10	126.80
1	2A	2262	U	OP1-P-OP2	-5.29	111.67	119.60
1	1A	846	G	OP1-P-OP2	5.29	127.53	119.60
1	1A	2440	G	C5-C6-N1	5.29	114.14	111.50
1	1A	2616	U	N3-C2-O2	-5.29	118.50	122.20
1	1A	2619	G	N1-C6-O6	-5.29	116.73	119.90
1	1A	2668	U	N3-C2-O2	-5.29	118.50	122.20
32	1a	68	G	C4-N9-C1'	-5.29	119.62	126.50
1	2A	1473	G	N9-C4-C5	-5.29	103.28	105.40
1	2A	1574	C	C2-N3-C4	5.29	122.55	119.90
1	2A	1702	G	N1-C6-O6	-5.29	116.73	119.90
1	2A	1747(A)	G	N1-C6-O6	5.29	123.07	119.90
32	2a	316	G	C8-N9-C4	-5.29	104.28	106.40
32	2a	563	A	O4'-C1'-N9	5.29	112.43	108.20
32	2a	1287	A	C6-N1-C2	5.29	121.77	118.60
1	1A	2376	C	N3-C4-C5	5.29	124.02	121.90
1	1A	2725	A	C6-N1-C2	5.29	121.77	118.60
1	2A	718	A	C5-C6-N1	-5.29	115.06	117.70
1	1A	170	A	C5-C6-N1	5.29	120.34	117.70
1	1A	716	G	C6-N1-C2	5.29	128.27	125.10
1	1A	791	G	O5'-P-OP1	-5.29	100.94	105.70
1	1A	1026	A	C4-C5-N7	5.29	113.34	110.70
1	1A	1533	G	C8-N9-C4	-5.29	104.29	106.40
1	1A	2562	G	N3-C4-C5	-5.29	125.96	128.60
1	1A	2779	G	N1-C6-O6	-5.29	116.73	119.90
1	2A	103	A	N1-C6-N6	5.29	121.77	118.60
1	2A	189	G	C5-N7-C8	5.29	106.94	104.30
1	2A	2852	G	N3-C2-N2	5.29	123.60	119.90
32	2a	509	A	N7-C8-N9	5.29	116.44	113.80
1	1A	658	A	N7-C8-N9	5.28	116.44	113.80
1	1A	2724	U	C2-N3-C4	-5.28	123.83	127.00
4	1E	77	ILE	CG1-CB-CG2	-5.28	99.78	111.40
32	1a	451	A	OP1-P-OP2	5.28	127.53	119.60
32	1a	479	C	C2-N3-C4	5.28	122.54	119.90
1	2A	271(H)	G	O5'-P-OP2	-5.28	100.95	105.70
1	2A	1180	C	C6-N1-C2	5.28	122.41	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1551	C	OP2-P-O3'	5.28	116.83	105.20
15	2T	96	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	1A	2278	A	C6-N1-C2	5.28	121.77	118.60
32	1a	541	G	C8-N9-C4	5.28	108.51	106.40
1	2A	386	G	C6-N1-C2	-5.28	121.93	125.10
32	2a	671	G	OP2-P-O3'	5.28	116.82	105.20
1	1A	96	C	OP1-P-OP2	5.28	127.52	119.60
1	1A	127	C	N3-C2-O2	5.28	125.60	121.90
1	1A	781	A	C4-C5-C6	5.28	119.64	117.00
1	1A	1212	C	OP2-P-O3'	5.28	116.81	105.20
1	1A	1652	G	N1-C2-N3	5.28	127.07	123.90
13	1R	64	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	2A	531	C	C6-N1-C2	5.28	122.41	120.30
32	2a	794	A	N7-C8-N9	5.28	116.44	113.80
1	2A	1997	G	OP1-P-OP2	-5.28	111.68	119.60
32	2a	991	U	P-O3'-C3'	5.28	126.03	119.70
1	1A	415	G	N3-C2-N2	5.28	123.59	119.90
1	1A	533	G	N1-C2-N2	5.28	120.95	116.20
1	1A	854	U	OP2-P-O3'	5.28	116.81	105.20
1	1A	1230	C	OP2-P-O3'	-5.28	93.59	105.20
1	1A	1611	C	N3-C4-N4	-5.28	114.31	118.00
1	1A	2078	G	O4'-C1'-N9	-5.28	103.98	108.20
32	1a	156	G	N7-C8-N9	5.28	115.74	113.10
1	2A	94(A)	G	N3-C4-C5	-5.28	125.96	128.60
1	1A	72	A	N1-C2-N3	5.28	131.94	129.30
1	1A	835	A	N7-C8-N9	-5.28	111.16	113.80
1	1A	2632	C	C2-N1-C1'	-5.28	113.00	118.80
11	1P	41	ARG	NE-CZ-NH1	5.28	122.94	120.30
32	1a	57	G	N3-C4-C5	-5.28	125.96	128.60
1	2A	61	G	C4-C5-N7	5.28	112.91	110.80
1	2A	1649	G	C8-N9-C4	5.28	108.51	106.40
1	2A	2278	A	N1-C6-N6	-5.28	115.43	118.60
32	2a	190	U	N1-C2-N3	5.28	118.06	114.90
32	2a	1530	G	N9-C4-C5	-5.28	103.29	105.40
1	1A	255	G	N1-C6-O6	5.27	123.06	119.90
1	1A	827	G	C4-C5-C6	5.27	121.97	118.80
32	1a	142	G	O4'-C1'-N9	5.27	112.42	108.20
32	1a	736	C	C6-N1-C2	-5.27	118.19	120.30
1	2A	2629	A	C5'-C4'-O4'	5.27	115.43	109.10
1	1A	1529	G	N1-C6-O6	-5.27	116.74	119.90
32	1a	15	G	C6-C5-N7	-5.27	127.24	130.40
32	1a	427	U	C6-N1-C2	-5.27	117.84	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	902	G	O5'-P-OP1	5.27	117.03	110.70
32	1a	1287	A	C5-C6-N6	5.27	127.92	123.70
1	2A	551	G	C5-C6-O6	5.27	131.76	128.60
1	2A	2814	C	N1-C2-O2	-5.27	115.74	118.90
32	2a	295	C	N3-C4-C5	5.27	124.01	121.90
1	1A	645	G	O5'-P-OP1	-5.27	100.96	105.70
1	2A	206	U	N3-C2-O2	-5.27	118.51	122.20
32	2a	953	G	O5'-P-OP2	-5.27	100.96	105.70
1	1A	729	G	O5'-P-OP2	5.27	117.02	110.70
1	1A	1104	G	N3-C4-N9	5.27	129.16	126.00
1	1A	1377	A	N1-C2-N3	5.27	131.94	129.30
1	1A	1814	A	N7-C8-N9	-5.27	111.17	113.80
1	1A	2207	C	C2-N1-C1'	5.27	124.60	118.80
1	1A	2578	A	C5-C6-N1	-5.27	115.07	117.70
1	2A	975(A)	G	OP1-P-O3'	5.27	116.80	105.20
32	2a	938	A	C8-N9-C4	-5.27	103.69	105.80
32	1a	1505	G	O5'-P-OP1	5.27	117.02	110.70
1	2A	1807	G	N9-C1'-C2'	-5.27	106.21	112.00
32	2a	1373	G	O4'-C1'-N9	5.27	112.41	108.20
1	1A	1028	C	C5-C4-N4	-5.27	116.51	120.20
1	1A	1652	G	C5-C6-O6	-5.27	125.44	128.60
1	2A	1670	C	C4-C5-C6	5.27	120.03	117.40
32	2a	923	A	O5'-P-OP1	-5.27	100.96	105.70
1	1A	246	A	C8-N9-C4	-5.26	103.69	105.80
1	1A	559	U	C5-C6-N1	-5.26	120.07	122.70
1	1A	723	A	O5'-P-OP2	-5.26	100.96	105.70
1	1A	1245	C	C2-N1-C1'	-5.26	113.01	118.80
1	1A	1715	A	C2-N3-C4	-5.26	107.97	110.60
1	1A	1911	A	C8-N9-C4	5.26	107.91	105.80
1	1A	2623	U	OP1-P-O3'	5.26	116.78	105.20
1	1A	2646	G	C8-N9-C4	-5.26	104.29	106.40
1	1A	2659	U	N3-C2-O2	-5.26	118.51	122.20
32	1a	557	G	N3-C2-N2	5.26	123.58	119.90
1	2A	1005	C	OP1-P-OP2	5.26	127.50	119.60
32	2a	625	G	N9-C4-C5	5.26	107.51	105.40
32	2a	1011	G	C5-C6-O6	5.26	131.76	128.60
32	2a	1394	A	N9-C4-C5	-5.26	103.69	105.80
32	1a	576	G	N3-C2-N2	5.26	123.58	119.90
32	1a	936	C	C6-N1-C2	5.26	122.41	120.30
1	2A	2817	G	C4-C5-N7	-5.26	108.69	110.80
1	1A	200	A	OP2-P-O3'	5.26	116.78	105.20
1	1A	964	A	OP2-P-O3'	5.26	116.77	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	78	G	C4-N9-C1'	-5.26	119.66	126.50
1	2A	37	C	C2-N3-C4	-5.26	117.27	119.90
1	2A	98	G	N3-C2-N2	5.26	123.58	119.90
1	2A	465	G	C2-N3-C4	5.26	114.53	111.90
1	2A	1126	A	OP1-P-OP2	5.26	127.49	119.60
1	2A	1313	U	O4'-C1'-N1	5.26	112.41	108.20
1	2A	1903	G	N9-C4-C5	5.26	107.50	105.40
32	2a	1416	G	N1-C6-O6	5.26	123.06	119.90
1	1A	407	U	N3-C2-O2	-5.26	118.52	122.20
1	1A	618	C	C5-C6-N1	5.26	123.63	121.00
1	1A	1126	C	N1-C2-O2	5.26	122.06	118.90
1	1A	2712	C	N3-C2-O2	5.26	125.58	121.90
1	2A	666	G	C5-C6-O6	-5.26	125.44	128.60
1	2A	1740	G	C5-C6-N1	5.26	114.13	111.50
1	2A	2519	U	C5-C4-O4	-5.26	122.74	125.90
32	2a	517	G	N3-C4-C5	-5.26	125.97	128.60
32	2a	1395	C	N3-C4-C5	-5.26	119.80	121.90
2	1B	68	C	OP2-P-O3'	5.26	116.77	105.20
15	1T	53	ARG	CB-CA-C	-5.26	99.88	110.40
1	2A	2434	A	OP2-P-O3'	5.26	116.77	105.20
1	2A	2678	C	OP2-P-O3'	5.26	116.77	105.20
32	2a	1151	A	O5'-P-OP2	-5.26	100.97	105.70
1	1A	620	U	N1-C2-N3	5.26	118.05	114.90
1	1A	1646	C	O5'-P-OP2	-5.26	100.97	105.70
32	1a	356	A	N1-C2-N3	-5.26	126.67	129.30
1	2A	107	C	OP2-P-O3'	5.26	116.77	105.20
1	2A	1087	G	N9-C4-C5	5.26	107.50	105.40
32	2a	35	G	N9-C4-C5	5.26	107.50	105.40
32	2a	1391	U	N3-C2-O2	-5.26	118.52	122.20
1	1A	2596	U	N3-C2-O2	-5.25	118.52	122.20
1	1A	2700	U	C5-C4-O4	-5.25	122.75	125.90
2	1B	36	C	C6-N1-C2	5.25	122.40	120.30
1	1A	106	U	N3-C4-O4	-5.25	115.72	119.40
1	1A	773	G	OP1-P-O3'	5.25	116.76	105.20
1	1A	788	G	C4-C5-N7	-5.25	108.70	110.80
1	1A	1026	A	N1-C2-N3	-5.25	126.67	129.30
1	1A	2083	G	O4'-C1'-N9	5.25	112.40	108.20
1	1A	2548	G	C5-C6-N1	-5.25	108.87	111.50
1	1A	2635	G	N3-C4-C5	-5.25	125.97	128.60
32	1a	189(L)	G	C2-N3-C4	5.25	114.53	111.90
32	1a	560	U	P-O3'-C3'	5.25	126.00	119.70
32	1a	722	A	C5-N7-C8	-5.25	101.27	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	55	G	C8-N9-C4	-5.25	104.30	106.40
1	2A	662	G	O5'-P-OP1	-5.25	100.97	105.70
32	2a	1001	A	C5-N7-C8	5.25	106.53	103.90
1	1A	24	G	N7-C8-N9	-5.25	110.47	113.10
27	15	16	ARG	CG-CD-NE	5.25	122.83	111.80
1	2A	212	G	O5'-P-OP2	-5.25	100.97	105.70
1	1A	1869	C	N3-C2-O2	-5.25	118.22	121.90
1	1A	2902	G	N3-C2-N2	5.25	123.58	119.90
1	1A	661	G	C5-C6-N1	-5.25	108.88	111.50
1	1A	980	C	C5-C6-N1	-5.25	118.38	121.00
1	1A	1301	U	N1-C2-N3	5.25	118.05	114.90
1	1A	1425	A	O4'-C1'-N9	-5.25	104.00	108.20
1	1A	1701	A	C5-N7-C8	5.25	106.52	103.90
1	2A	741	G	N1-C6-O6	-5.25	116.75	119.90
1	2A	2237	G	C4-C5-N7	-5.25	108.70	110.80
1	2A	2788	C	OP2-P-O3'	5.25	116.75	105.20
1	1A	697	C	N1-C2-O2	5.25	122.05	118.90
1	1A	1726	U	OP1-P-OP2	5.25	127.47	119.60
1	1A	1807	G	N3-C4-C5	-5.25	125.98	128.60
1	1A	2099	A	N9-C4-C5	-5.25	103.70	105.80
1	1A	2534	U	C5-C4-O4	-5.25	122.75	125.90
1	1A	2621	U	C5-C4-O4	-5.25	122.75	125.90
18	1W	92	ARG	NE-CZ-NH1	-5.25	117.68	120.30
32	1a	186	C	OP1-P-O3'	5.25	116.74	105.20
32	2a	1125	U	C6-N1-C1'	-5.25	113.85	121.20
32	2a	1351	U	O5'-P-OP1	-5.25	100.98	105.70
1	2A	1973	G	O5'-P-OP2	-5.25	100.98	105.70
1	2A	1982	C	N3-C4-C5	5.25	124.00	121.90
32	2a	525	C	C5-C6-N1	5.25	123.62	121.00
1	1A	702	A	N9-C4-C5	5.24	107.90	105.80
1	1A	1148	C	C6-N1-C2	-5.24	118.20	120.30
1	1A	2858	G	N3-C4-N9	-5.24	122.85	126.00
1	2A	2182	G	C8-N9-C1'	5.24	133.82	127.00
1	2A	2234	G	C5-C6-O6	5.24	131.75	128.60
32	2a	230	G	C5-C6-N1	-5.24	108.88	111.50
32	2a	266	G	N1-C2-N2	-5.24	111.48	116.20
32	2a	533	A	N1-C2-N3	5.24	131.92	129.30
1	1A	2086	C	O5'-P-OP2	-5.24	100.98	105.70
1	1A	2637	G	C4-C5-N7	-5.24	108.70	110.80
32	1a	732	C	N3-C4-C5	5.24	124.00	121.90
32	1a	784	C	C5-C6-N1	-5.24	118.38	121.00
1	2A	1666	G	N1-C6-O6	-5.24	116.76	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2003	G	OP2-P-O3'	5.24	116.73	105.20
1	2A	2154	G	N9-C4-C5	-5.24	103.30	105.40
1	2A	2783	G	C6-C5-N7	5.24	133.54	130.40
1	1A	1080	G	N1-C2-N2	5.24	120.92	116.20
1	1A	1757	C	C2-N1-C1'	-5.24	113.04	118.80
1	1A	1921	G	C6-N1-C2	-5.24	121.96	125.10
1	1A	1925	G	C8-N9-C4	-5.24	104.30	106.40
1	1A	2460	A	C5-N7-C8	5.24	106.52	103.90
2	1B	104	U	OP2-P-O3'	5.24	116.72	105.20
32	1a	722	A	C5-C6-N1	-5.24	115.08	117.70
1	2A	819	A	C8-N9-C4	-5.24	103.70	105.80
1	2A	2505	G	N1-C6-O6	-5.24	116.76	119.90
1	2A	1092	C	C2-N1-C1'	5.24	124.56	118.80
32	2a	572	A	N3-C4-C5	5.24	130.47	126.80
1	1A	120	G	OP2-P-O3'	5.24	116.72	105.20
1	1A	252	C	C5-C4-N4	5.24	123.86	120.20
1	1A	422	U	C2-N1-C1'	5.24	123.98	117.70
1	1A	1106	U	N3-C4-O4	5.24	123.06	119.40
1	1A	1220	U	C2-N1-C1'	-5.24	111.42	117.70
1	1A	1361	C	N3-C4-C5	5.24	123.99	121.90
1	1A	1884	A	C5-N7-C8	5.24	106.52	103.90
1	1A	2523	U	N1-C2-O2	-5.24	119.14	122.80
32	1a	1068	G	O5'-P-OP2	-5.24	100.99	105.70
32	1a	1208	C	C6-N1-C2	-5.24	118.21	120.30
32	2a	931	C	OP2-P-O3'	5.24	116.72	105.20
1	1A	199	C	C5-C6-N1	-5.23	118.38	121.00
1	1A	1031	C	N3-C4-C5	5.23	123.99	121.90
1	1A	1342	G	N7-C8-N9	-5.23	110.48	113.10
32	1a	338	A	O5'-P-OP1	-5.23	100.99	105.70
1	2A	1102	C	C2-N3-C4	5.23	122.52	119.90
1	1A	12	U	C2-N1-C1'	5.23	123.98	117.70
1	1A	621	G	C5-C6-O6	5.23	131.74	128.60
1	1A	2072	C	N3-C2-O2	5.23	125.56	121.90
1	1A	2185	C	N1-C2-O2	5.23	122.04	118.90
1	2A	1084	A	N9-C4-C5	-5.23	103.71	105.80
1	2A	2033	A	O4'-C1'-N9	5.23	112.39	108.20
1	2A	2306	C	N3-C2-O2	-5.23	118.24	121.90
2	2B	101	G	C8-N9-C4	5.23	108.49	106.40
32	2a	1276	G	C8-N9-C4	-5.23	104.31	106.40
1	1A	807	G	C8-N9-C4	5.23	108.49	106.40
1	1A	2238	C	N3-C2-O2	5.23	125.56	121.90
1	1A	2442	A	OP1-P-OP2	5.23	127.44	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	163	C	C6-N1-C1'	5.23	127.08	120.80
1	2A	1531	C	C2-N1-C1'	5.23	124.55	118.80
1	2A	2388	A	OP1-P-OP2	-5.23	111.75	119.60
1	2A	2585	U	OP1-P-O3'	5.23	116.70	105.20
32	2a	777	A	C8-N9-C4	-5.23	103.71	105.80
1	1A	252	C	N3-C2-O2	-5.23	118.24	121.90
1	1A	385	G	C5-C6-O6	-5.23	125.46	128.60
1	1A	1208	G	C8-N9-C1'	5.23	133.80	127.00
1	1A	1718	U	C2-N3-C4	-5.23	123.86	127.00
32	1a	792	A	N1-C6-N6	-5.23	115.46	118.60
32	2a	134	A	C5-C6-N6	-5.23	119.52	123.70
32	2a	404	U	C6-N1-C2	-5.23	117.86	121.00
32	2a	633	G	O5'-P-OP2	-5.23	100.99	105.70
1	1A	367	C	C5-C6-N1	-5.23	118.39	121.00
1	1A	369	A	N3-C4-N9	5.23	131.58	127.40
1	1A	2200	C	O4'-C1'-N1	5.23	112.38	108.20
32	1a	1228	C	C5-C6-N1	5.23	123.61	121.00
1	2A	955	C	N1-C2-O2	-5.23	115.76	118.90
1	2A	1471	A	C6-C5-N7	-5.23	128.64	132.30
1	2A	2678	C	N3-C4-N4	-5.23	114.34	118.00
32	2a	814	A	OP2-P-O3'	5.23	116.70	105.20
2	1B	116	G	C4-N9-C1'	5.23	133.29	126.50
32	1a	732	C	O5'-P-OP1	-5.23	101.00	105.70
32	1a	824	C	OP2-P-O3'	5.23	116.70	105.20
1	2A	1660	C	O5'-P-OP2	-5.23	101.00	105.70
1	1A	744	C	C5-C4-N4	5.22	123.86	120.20
1	1A	791	G	OP1-P-OP2	5.22	127.44	119.60
1	1A	855	G	C5-C6-N1	5.22	114.11	111.50
1	1A	872	C	C5-C6-N1	-5.22	118.39	121.00
1	1A	1183	G	N1-C6-O6	-5.22	116.77	119.90
1	1A	1721	G	O4'-C1'-N9	-5.22	104.02	108.20
1	1A	2349	G	C5-C6-O6	-5.22	125.47	128.60
1	2A	1239	G	N1-C6-O6	5.22	123.03	119.90
1	2A	2579	C	C5-C4-N4	-5.22	116.54	120.20
32	2a	770	C	N1-C2-O2	-5.22	115.77	118.90
1	1A	191	U	N3-C4-O4	-5.22	115.74	119.40
1	1A	225	C	C2-N3-C4	-5.22	117.29	119.90
1	1A	251	A	N1-C2-N3	5.22	131.91	129.30
1	1A	594	A	N7-C8-N9	-5.22	111.19	113.80
32	1a	73	G	C6-C5-N7	5.22	133.53	130.40
32	1a	544	G	C5-C6-N1	5.22	114.11	111.50
32	1a	572	A	O5'-P-OP2	-5.22	101.00	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	801	U	C5-C6-N1	-5.22	120.09	122.70
32	1a	1174	G	C8-N9-C1'	5.22	133.79	127.00
32	1a	1441	G	O5'-P-OP2	-5.22	101.00	105.70
1	2A	856	C	N3-C4-C5	-5.22	119.81	121.90
1	2A	982	C	N3-C2-O2	5.22	125.56	121.90
1	2A	2012	G	O5'-P-OP2	-5.22	101.00	105.70
1	1A	622	G	C8-N9-C4	5.22	108.49	106.40
1	1A	1213	U	C5-C4-O4	-5.22	122.77	125.90
2	1B	50	G	C4-C5-C6	-5.22	115.67	118.80
32	1a	768	A	N1-C2-N3	-5.22	126.69	129.30
1	2A	2351	G	C5-C6-O6	-5.22	125.47	128.60
1	1A	746	A	OP2-P-O3'	5.22	116.68	105.20
1	1A	1747	A	P-O3'-C3'	5.22	125.96	119.70
1	1A	1859	G	OP2-P-O3'	5.22	116.68	105.20
1	1A	2185	C	C6-N1-C2	-5.22	118.21	120.30
32	1a	113	G	C5-C6-O6	5.22	131.73	128.60
32	1a	624	C	N3-C4-C5	-5.22	119.81	121.90
32	2a	271	C	C6-N1-C2	-5.22	118.21	120.30
32	2a	1265	G	O5'-P-OP1	-5.22	101.00	105.70
1	1A	82	G	N3-C4-N9	5.22	129.13	126.00
1	1A	1801	G	OP1-P-OP2	5.22	127.43	119.60
1	1A	2204	G	N9-C4-C5	5.22	107.49	105.40
1	1A	2697	G	N3-C2-N2	5.22	123.55	119.90
1	1A	674	G	C5-C6-O6	5.22	131.73	128.60
1	1A	949	C	C2-N3-C4	-5.22	117.29	119.90
1	1A	1093	G	N7-C8-N9	5.22	115.71	113.10
1	1A	1097	G	C6-N1-C2	5.22	128.23	125.10
1	1A	1981	G	N7-C8-N9	-5.22	110.49	113.10
1	1A	2049	G	C6-C5-N7	5.22	133.53	130.40
1	1A	2668	U	C2-N1-C1'	5.22	123.96	117.70
1	2A	807	U	N3-C4-O4	5.22	123.05	119.40
1	1A	1347	A	O5'-P-OP1	5.21	116.96	110.70
1	1A	2804	C	C2-N3-C4	5.21	122.51	119.90
32	1a	446	G	N1-C6-O6	5.21	123.03	119.90
32	1a	1169	A	N7-C8-N9	5.21	116.41	113.80
1	2A	136	G	O5'-P-OP1	-5.21	101.01	105.70
1	2A	502	A	C2-N3-C4	-5.21	107.99	110.60
1	2A	1385	G	O4'-C1'-N9	5.21	112.37	108.20
1	2A	2330	G	C4-C5-N7	-5.21	108.71	110.80
32	2a	297	G	C8-N9-C4	5.21	108.49	106.40
32	2a	665	A	OP1-P-OP2	5.21	127.42	119.60
32	2a	1412	C	O5'-P-OP2	5.21	116.96	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2l	88	GLY	N-CA-C	5.21	126.14	113.10
1	1A	722	A	O5'-P-OP1	-5.21	101.01	105.70
1	1A	859	C	C2-N3-C4	-5.21	117.29	119.90
1	1A	1062	G	OP2-P-O3'	5.21	116.67	105.20
1	1A	1506	G	C5-C6-O6	5.21	131.73	128.60
1	1A	2061	C	O5'-P-OP1	5.21	116.95	110.70
1	1A	2654	G	N1-C2-N2	-5.21	111.51	116.20
1	2A	787	U	C6-N1-C2	-5.21	117.87	121.00
1	2A	2287	A	O5'-P-OP2	-5.21	101.01	105.70
32	1a	563	A	C8-N9-C4	-5.21	103.72	105.80
32	1a	1003	G	N7-C8-N9	5.21	115.70	113.10
32	1a	1370	G	C4-C5-N7	5.21	112.88	110.80
1	2A	1564	C	C6-N1-C2	-5.21	118.22	120.30
1	2A	2755	C	C5-C6-N1	5.21	123.61	121.00
32	2a	22	G	C2-N3-C4	5.21	114.50	111.90
1	1A	1221	G	N3-C4-N9	-5.21	122.88	126.00
1	1A	1685	C	OP2-P-O3'	5.21	116.66	105.20
1	1A	2615	G	N1-C6-O6	5.21	123.03	119.90
1	1A	2615	G	N9-C4-C5	-5.21	103.32	105.40
1	2A	2089	U	C4-C5-C6	5.21	122.83	119.70
32	2a	709	G	N9-C4-C5	5.21	107.48	105.40
32	2a	1491	G	N9-C1'-C2'	-5.21	106.27	112.00
1	1A	195	U	C4-C5-C6	5.21	122.82	119.70
1	1A	367	C	C2-N3-C4	-5.21	117.30	119.90
1	1A	836	A	O4'-C1'-N9	-5.21	104.03	108.20
1	1A	2065	C	N3-C2-O2	5.21	125.54	121.90
1	1A	2396	G	C5-C6-O6	5.21	131.72	128.60
1	1A	2513	C	N1-C2-O2	-5.21	115.78	118.90
1	1A	2595	G	C5-N7-C8	5.21	106.90	104.30
32	1a	525	C	C5-C4-N4	-5.21	116.56	120.20
32	1a	1370	G	N9-C4-C5	-5.21	103.32	105.40
1	2A	1276	A	N9-C4-C5	-5.21	103.72	105.80
1	2A	2426	A	C4-C5-N7	5.21	113.30	110.70
32	2a	668	G	O5'-P-OP2	5.21	116.95	110.70
32	2a	1183	A	OP1-P-O3'	5.21	116.65	105.20
1	2A	743	G	C4-C5-N7	-5.21	108.72	110.80
1	2A	2591	C	N1-C2-O2	-5.21	115.78	118.90
1	1A	396	C	N3-C4-C5	5.20	123.98	121.90
1	1A	529	U	OP1-P-OP2	5.20	127.41	119.60
1	1A	794	U	C5-C4-O4	5.20	129.02	125.90
1	1A	1117	G	C2-N3-C4	5.20	114.50	111.90
1	1A	1280	U	N3-C4-O4	-5.20	115.76	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1543	U	N3-C4-O4	-5.20	115.76	119.40
1	1A	1612	C	N3-C4-C5	5.20	123.98	121.90
1	1A	1623	U	OP2-P-O3'	5.20	116.65	105.20
1	1A	2060	G	C5-C6-N1	-5.20	108.90	111.50
1	1A	2256	U	N1-C2-N3	5.20	118.02	114.90
1	1A	2312	G	O5'-P-OP1	-5.20	101.02	105.70
1	1A	2713	C	OP2-P-O3'	5.20	116.65	105.20
32	1a	1409	C	N3-C2-O2	-5.20	118.26	121.90
1	2A	340	A	O5'-P-OP2	5.20	116.94	110.70
1	2A	1084	A	C6-N1-C2	5.20	121.72	118.60
2	2B	33	G	C5-C6-N1	-5.20	108.90	111.50
32	2a	685	G	N3-C4-C5	5.20	131.20	128.60
32	2a	753	A	N1-C2-N3	5.20	131.90	129.30
32	2a	1026	G	C5-N7-C8	-5.20	101.70	104.30
1	1A	514	G	N9-C4-C5	5.20	107.48	105.40
1	1A	736	A	C6-N1-C2	-5.20	115.48	118.60
32	1a	744	C	OP2-P-O3'	5.20	116.64	105.20
1	2A	630	G	C5-C6-O6	5.20	131.72	128.60
1	2A	1813	G	N9-C4-C5	-5.20	103.32	105.40
1	1A	452	G	C6-N1-C2	-5.20	121.98	125.10
1	1A	875	U	OP2-P-O3'	5.20	116.64	105.20
32	1a	569	C	N3-C4-N4	-5.20	114.36	118.00
1	2A	378	C	C6-N1-C2	-5.20	118.22	120.30
1	2A	700	G	C5-C6-N1	5.20	114.10	111.50
1	2A	753	C	O5'-P-OP1	-5.20	101.02	105.70
1	2A	989	G	C5-C6-O6	-5.20	125.48	128.60
32	2a	691	G	C5-C6-O6	-5.20	125.48	128.60
1	1A	274	U	C2-N1-C1'	5.20	123.94	117.70
1	1A	1665	G	O4'-C1'-N9	-5.20	104.04	108.20
1	2A	453	C	N3-C4-C5	5.20	123.98	121.90
1	2A	553	G	N9-C4-C5	5.20	107.48	105.40
1	2A	871	U	N3-C4-O4	5.20	123.04	119.40
1	2A	2302	G	C8-N9-C4	-5.20	104.32	106.40
1	2A	2807	G	C5-C6-O6	5.20	131.72	128.60
32	2a	435	C	C5-C6-N1	5.20	123.60	121.00
1	1A	872	C	OP2-P-O3'	5.20	116.63	105.20
1	1A	1080	G	C5-C6-O6	-5.20	125.48	128.60
1	1A	1135	G	N3-C4-N9	5.20	129.12	126.00
1	2A	2091	U	C5-C4-O4	-5.20	122.78	125.90
32	2a	299	G	O5'-P-OP2	5.20	116.94	110.70
32	2a	910	C	C6-N1-C2	5.20	122.38	120.30
1	1A	801	C	C5-C4-N4	-5.20	116.56	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	889	G	OP2-P-O3'	5.20	116.63	105.20
1	1A	1674	G	C8-N9-C4	-5.20	104.32	106.40
1	1A	2339	A	C2-N3-C4	5.20	113.20	110.60
2	1B	38	C	N3-C2-O2	-5.20	118.26	121.90
32	1a	1247	U	C5-C4-O4	-5.20	122.78	125.90
1	2A	2673	G	N3-C4-N9	5.20	129.12	126.00
1	2A	2707	G	C2-N3-C4	-5.20	109.30	111.90
1	1A	1093	G	C8-N9-C4	-5.19	104.32	106.40
1	1A	2286	A	OP2-P-O3'	5.19	116.63	105.20
1	1A	2903	G	C4-N9-C1'	-5.19	119.75	126.50
2	1B	79	C	N1-C2-N3	5.19	122.83	119.20
32	1a	533	A	N1-C2-N3	5.19	131.90	129.30
1	2A	1655	A	OP2-P-O3'	5.19	116.63	105.20
32	2a	1003	G	N9-C4-C5	5.19	107.48	105.40
1	1A	209	G	C8-N9-C4	5.19	108.48	106.40
1	1A	1153	G	O5'-P-OP1	-5.19	101.03	105.70
1	1A	1602	G	C5-C6-N1	-5.19	108.90	111.50
32	1a	34	C	C6-N1-C2	5.19	122.38	120.30
32	1a	182	U	N3-C2-O2	-5.19	118.57	122.20
32	1a	226	G	N3-C2-N2	5.19	123.53	119.90
1	2A	213	A	C5-C6-N1	5.19	120.30	117.70
1	2A	2126	A	P-O3'-C3'	5.19	125.93	119.70
32	2a	556	C	OP1-P-OP2	5.19	127.39	119.60
32	2a	999	C	C2-N1-C1'	5.19	124.51	118.80
1	1A	747	G	O5'-P-OP2	-5.19	101.03	105.70
1	1A	837	C	N1-C2-O2	-5.19	115.79	118.90
1	1A	1031	C	C4-C5-C6	-5.19	114.81	117.40
1	1A	1052	C	N1-C2-O2	-5.19	115.79	118.90
1	1A	2250	G	OP2-P-O3'	5.19	116.62	105.20
1	1A	2251	G	C5-N7-C8	5.19	106.89	104.30
1	1A	2326	C	O5'-P-OP1	5.19	116.93	110.70
1	1A	2409	G	N3-C2-N2	-5.19	116.27	119.90
32	1a	43	C	C6-N1-C2	5.19	122.38	120.30
32	1a	816	A	O5'-P-OP2	-5.19	101.03	105.70
1	2A	701	G	N3-C4-N9	-5.19	122.89	126.00
1	2A	798	G	N1-C6-O6	-5.19	116.79	119.90
1	2A	1587	A	N3-C4-C5	-5.19	123.17	126.80
1	2A	2078	C	C4-C5-C6	5.19	120.00	117.40
1	1A	807	G	N9-C4-C5	-5.19	103.32	105.40
32	1a	888	G	N1-C2-N2	-5.19	111.53	116.20
32	1a	1525	G	C4-N9-C1'	-5.19	119.75	126.50
1	2A	1960	A	O5'-P-OP2	-5.19	101.03	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	873	U	C2-N3-C4	-5.19	123.89	127.00
1	1A	876	A	O5'-P-OP2	-5.19	101.03	105.70
1	1A	1342	G	C5-N7-C8	5.19	106.89	104.30
1	1A	2286	A	C5-C6-N6	5.19	127.85	123.70
1	1A	2790	G	N1-C6-O6	-5.19	116.79	119.90
32	1a	381	C	C6-N1-C2	-5.19	118.22	120.30
1	2A	113	G	N3-C4-N9	-5.19	122.89	126.00
1	2A	620	G	N3-C2-N2	-5.19	116.27	119.90
1	2A	1082	U	C6-N1-C1'	-5.19	113.94	121.20
1	2A	1807	G	C5-N7-C8	5.19	106.89	104.30
1	2A	2008	C	C6-N1-C2	5.19	122.38	120.30
1	2A	2372	G	O5'-P-OP1	-5.19	101.03	105.70
1	2A	2805	G	N1-C2-N2	-5.19	111.53	116.20
1	1A	24	G	N1-C6-O6	-5.19	116.79	119.90
1	1A	255	G	N9-C4-C5	-5.19	103.33	105.40
1	1A	855	G	N1-C6-O6	-5.19	116.79	119.90
1	1A	1956	C	C5-C4-N4	5.19	123.83	120.20
2	1B	8	U	N3-C4-C5	5.19	117.71	114.60
32	2a	1127	G	C8-N9-C4	5.19	108.47	106.40
1	1A	1285	G	OP2-P-O3'	5.18	116.61	105.20
1	1A	2890	C	O5'-P-OP1	-5.18	101.03	105.70
1	2A	1299	G	N3-C4-N9	-5.18	122.89	126.00
32	2a	1074	G	O5'-P-OP1	-5.18	101.03	105.70
1	1A	1406	A	N1-C6-N6	5.18	121.71	118.60
1	1A	1696	G	C5-C6-O6	5.18	131.71	128.60
1	1A	2018	C	N3-C4-C5	5.18	123.97	121.90
32	1a	926	G	C8-N9-C4	-5.18	104.33	106.40
1	2A	2371	G	C5-C6-O6	-5.18	125.49	128.60
32	2a	1484	C	C6-N1-C2	5.18	122.37	120.30
32	1a	112	G	N1-C2-N2	5.18	120.86	116.20
32	2a	396	G	C5-C6-O6	-5.18	125.49	128.60
1	1A	104	C	N3-C4-N4	-5.18	114.37	118.00
1	1A	1135	G	C4-N9-C1'	5.18	133.23	126.50
1	1A	2042	A	C5-C6-N1	5.18	120.29	117.70
1	1A	2772	G	C4-C5-N7	-5.18	108.73	110.80
32	1a	901	A	C6-C5-N7	-5.18	128.67	132.30
1	2A	878	A	O4'-C1'-N9	5.18	112.34	108.20
1	2A	1902	C	N3-C4-C5	5.18	123.97	121.90
32	2a	774	G	OP2-P-O3'	5.18	116.59	105.20
32	2a	1505	G	C8-N9-C4	-5.18	104.33	106.40
1	1A	475	A	N9-C4-C5	-5.18	103.73	105.80
1	1A	670	C	C4-C5-C6	-5.18	114.81	117.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1889	G	N1-C6-O6	-5.18	116.79	119.90
1	1A	2607	G	O5'-P-OP2	-5.18	101.04	105.70
1	1A	2898	C	C6-N1-C2	-5.18	118.23	120.30
1	2A	181	A	OP2-P-O3'	5.18	116.59	105.20
1	2A	1386	C	O5'-P-OP1	-5.18	101.04	105.70
1	2A	2617	C	C6-N1-C2	5.18	122.37	120.30
1	1A	119	G	N7-C8-N9	-5.18	110.51	113.10
1	1A	2560	G	N1-C6-O6	-5.18	116.79	119.90
1	1A	2833	A	C2-N3-C4	-5.18	108.01	110.60
32	1a	120	A	O4'-C1'-N9	-5.18	104.06	108.20
32	1a	355	C	N3-C2-O2	-5.18	118.28	121.90
1	2A	34	C	C6-N1-C2	-5.18	118.23	120.30
1	2A	700	G	C2-N3-C4	5.18	114.49	111.90
1	2A	896	A	C5-C6-N6	5.18	127.84	123.70
1	2A	2728	U	OP2-P-O3'	5.18	116.59	105.20
1	1A	186	A	C5-C6-N1	-5.17	115.11	117.70
1	1A	1216	G	C6-C5-N7	-5.17	127.30	130.40
1	1A	1700	G	O5'-P-OP1	-5.17	101.04	105.70
1	1A	2078	G	C8-N9-C4	5.17	108.47	106.40
1	1A	2249	G	N3-C2-N2	5.17	123.52	119.90
1	1A	2642	G	C5-C6-N1	5.17	114.09	111.50
1	1A	2863	C	OP2-P-O3'	5.17	116.58	105.20
32	1a	204	U	N3-C2-O2	-5.17	118.58	122.20
32	1a	1200	C	OP1-P-O3'	5.17	116.58	105.20
1	2A	62	C	C2-N1-C1'	-5.17	113.11	118.80
1	2A	562	U	C2-N3-C4	-5.17	123.89	127.00
1	2A	1672	C	N3-C4-C5	-5.17	119.83	121.90
1	2A	2145	C	C2-N1-C1'	5.17	124.49	118.80
1	2A	2674	G	C5-C6-O6	5.17	131.71	128.60
1	1A	2034	G	C4-C5-N7	-5.17	108.73	110.80
1	1A	2095	C	OP2-P-O3'	5.17	116.58	105.20
1	2A	686	G	C8-N9-C4	-5.17	104.33	106.40
1	2A	1079	C	N3-C2-O2	-5.17	118.28	121.90
1	2A	1958	C	C2-N3-C4	-5.17	117.31	119.90
1	1A	673	G	C5-C6-N1	-5.17	108.92	111.50
1	1A	1414	G	N3-C2-N2	5.17	123.52	119.90
1	1A	1606	G	OP1-P-O3'	5.17	116.58	105.20
1	1A	1702	A	N9-C4-C5	5.17	107.87	105.80
1	1A	2106	C	C6-N1-C2	5.17	122.37	120.30
1	1A	2608	U	N3-C2-O2	5.17	125.82	122.20
32	1a	1052	U	N1-C2-O2	5.17	126.42	122.80
32	1a	1181	G	C8-N9-C4	5.17	108.47	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1278	U	C6-N1-C2	-5.17	117.90	121.00
1	2A	271	A	C2-N3-C4	5.17	113.19	110.60
1	2A	370	G	O5'-P-OP2	5.17	116.91	110.70
1	2A	630	G	O5'-P-OP2	-5.17	101.05	105.70
1	2A	2657	A	O5'-P-OP2	5.17	116.91	110.70
32	2a	732	C	OP1-P-OP2	-5.17	111.84	119.60
1	1A	451	G	C6-N1-C2	-5.17	122.00	125.10
1	1A	2511	C	C6-N1-C2	-5.17	118.23	120.30
1	1A	2813	G	N3-C2-N2	-5.17	116.28	119.90
32	1a	308	C	C6-N1-C2	-5.17	118.23	120.30
32	1a	617	G	N3-C4-C5	-5.17	126.02	128.60
1	2A	1255	U	N3-C2-O2	-5.17	118.58	122.20
1	2A	1814	G	N1-C6-O6	5.17	123.00	119.90
1	2A	2690	C	OP1-P-O3'	5.17	116.57	105.20
1	1A	918	U	C2-N3-C4	-5.17	123.90	127.00
1	1A	1575	A	OP2-P-O3'	5.17	116.57	105.20
1	1A	1595	C	N3-C2-O2	-5.17	118.28	121.90
1	1A	1683	C	OP1-P-O3'	5.17	116.57	105.20
1	1A	1746	G	C6-N1-C2	-5.17	122.00	125.10
1	1A	1988	A	N7-C8-N9	-5.17	111.22	113.80
1	1A	2073	A	C5-C6-N1	-5.17	115.11	117.70
1	1A	2700	U	N3-C2-O2	5.17	125.82	122.20
1	1A	2843	G	C6-C5-N7	-5.17	127.30	130.40
1	2A	363(C)	G	N7-C8-N9	-5.17	110.52	113.10
1	2A	1607	C	N1-C2-O2	5.17	122.00	118.90
1	2A	2260	C	O5'-P-OP2	-5.17	101.05	105.70
32	2a	728	A	C8-N9-C4	-5.17	103.73	105.80
32	2a	899	C	OP1-P-OP2	-5.17	111.85	119.60
32	2a	1011	G	N1-C6-O6	-5.17	116.80	119.90
32	2a	1137	C	C6-N1-C2	-5.17	118.23	120.30
1	1A	523	G	OP2-P-O3'	5.17	116.57	105.20
1	1A	962	G	N9-C4-C5	-5.17	103.33	105.40
1	1A	1718	U	C6-N1-C2	5.17	124.10	121.00
1	2A	1277	G	C2-N3-C4	-5.17	109.32	111.90
32	2a	1093	A	N9-C4-C5	-5.17	103.73	105.80
1	1A	652	A	C5-C6-N6	-5.17	119.57	123.70
1	2A	2358	G	C2-N3-C4	-5.17	109.32	111.90
1	1A	852	G	C6-N1-C2	-5.16	122.00	125.10
1	1A	1137	G	C4-C5-N7	-5.16	108.73	110.80
1	1A	1394	G	C5-C6-O6	5.16	131.70	128.60
1	1A	1755	C	C5-C6-N1	-5.16	118.42	121.00
1	1A	1837	C	C6-N1-C2	5.16	122.37	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2163	G	C2-N3-C4	5.16	114.48	111.90
2	1B	79	C	N3-C4-N4	-5.16	114.39	118.00
32	1a	906	G	O5'-P-OP1	-5.16	101.05	105.70
32	1a	1341	U	C5-C4-O4	5.16	129.00	125.90
1	2A	1309	G	C5-C6-O6	-5.16	125.50	128.60
1	2A	1326	U	O5'-P-OP2	5.16	116.90	110.70
1	2A	2133	G	C8-N9-C4	5.16	108.47	106.40
32	2a	13	U	N1-C2-N3	-5.16	111.80	114.90
32	2a	1103	C	C5-C6-N1	5.16	123.58	121.00
1	1A	1069	U	N1-C2-O2	-5.16	119.19	122.80
1	1A	1567	G	N9-C4-C5	5.16	107.47	105.40
1	2A	1381	G	C8-N9-C4	-5.16	104.33	106.40
1	2A	1937	A	C5-C6-N6	5.16	127.83	123.70
1	2A	2320	A	C2-N3-C4	5.16	113.18	110.60
32	2a	1286	A	N7-C8-N9	5.16	116.38	113.80
1	1A	116	A	N1-C6-N6	-5.16	115.50	118.60
1	1A	501	U	C4-C5-C6	5.16	122.80	119.70
1	1A	1155	C	C6-N1-C1'	-5.16	114.61	120.80
1	1A	1951	G	OP1-P-OP2	5.16	127.34	119.60
1	1A	2012	C	N3-C4-C5	5.16	123.96	121.90
1	1A	2054	G	C5-C6-O6	5.16	131.70	128.60
1	1A	2400	A	O4'-C1'-N9	5.16	112.33	108.20
1	1A	2597	U	C4-C5-C6	5.16	122.80	119.70
32	1a	286	G	C5-C6-O6	5.16	131.70	128.60
32	2a	798	G	N9-C4-C5	5.16	107.46	105.40
1	1A	556	C	N1-C2-O2	-5.16	115.81	118.90
1	1A	1522	G	C4-C5-N7	-5.16	108.74	110.80
1	1A	1807	G	C5-N7-C8	-5.16	101.72	104.30
1	1A	2117	C	OP1-P-O3'	-5.16	93.85	105.20
1	1A	2657	G	O5'-P-OP1	-5.16	101.06	105.70
2	1B	93	G	N7-C8-N9	5.16	115.68	113.10
32	1a	782	A	N1-C2-N3	5.16	131.88	129.30
32	1a	1528	U	O5'-P-OP1	5.16	116.89	110.70
1	2A	1079	C	N3-C4-C5	-5.16	119.84	121.90
1	2A	1270	C	C5-C4-N4	5.16	123.81	120.20
1	2A	1838	C	O4'-C1'-N1	5.16	112.33	108.20
1	2A	2447	G	N3-C2-N2	-5.16	116.29	119.90
1	2A	2520	C	C2-N3-C4	-5.16	117.32	119.90
2	2B	101	G	N1-C6-O6	5.16	123.00	119.90
1	1A	94	G	OP1-P-OP2	5.16	127.33	119.60
1	1A	181	C	OP1-P-OP2	5.16	127.33	119.60
1	1A	931	C	N1-C2-N3	-5.16	115.59	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	41	U	C4-C5-C6	5.16	122.79	119.70
2	1B	90	A	N9-C4-C5	-5.16	103.74	105.80
32	1a	1421	G	C8-N9-C4	-5.16	104.34	106.40
1	2A	2093	G	C5-C6-O6	-5.16	125.51	128.60
1	2A	2205	C	C6-N1-C2	-5.16	118.24	120.30
32	2a	299	G	C6-C5-N7	-5.16	127.31	130.40
32	2a	872	A	O4'-C1'-N9	5.16	112.33	108.20
1	1A	594	A	N1-C2-N3	-5.16	126.72	129.30
1	1A	742	G	C6-C5-N7	5.16	133.49	130.40
1	1A	975	U	C6-N1-C2	5.16	124.09	121.00
1	1A	1152	G	C8-N9-C4	5.16	108.46	106.40
1	1A	1234	A	O5'-P-OP1	5.16	116.89	110.70
1	1A	1281	G	OP2-P-O3'	5.16	116.54	105.20
1	1A	2278	A	C5-C6-N1	-5.16	115.12	117.70
1	1A	2528	G	N9-C4-C5	5.16	107.46	105.40
1	1A	2591	C	N3-C4-C5	5.16	123.96	121.90
1	1A	2780	C	N1-C2-O2	5.16	121.99	118.90
32	1a	643	C	C6-N1-C2	5.16	122.36	120.30
1	2A	1573	G	N9-C4-C5	5.16	107.46	105.40
1	1A	369	A	N1-C6-N6	5.15	121.69	118.60
1	1A	505	A	C4-C5-N7	-5.15	108.12	110.70
1	1A	1627	A	C5-C6-N6	-5.15	119.58	123.70
1	1A	2230	U	C2-N1-C1'	5.15	123.89	117.70
1	2A	469	G	N1-C6-O6	5.15	122.99	119.90
1	1A	199	C	C6-N1-C2	5.15	122.36	120.30
1	1A	795	G	OP1-P-O3'	5.15	116.54	105.20
1	1A	818	G	C5-C6-O6	5.15	131.69	128.60
1	1A	1056	A	N7-C8-N9	-5.15	111.22	113.80
1	1A	1691	C	C5-C6-N1	-5.15	118.42	121.00
32	1a	1181	G	C4-N9-C1'	-5.15	119.80	126.50
32	1a	1505	G	N3-C2-N2	-5.15	116.29	119.90
1	2A	948	G	O5'-P-OP2	5.15	116.88	110.70
32	2a	1502	A	O5'-P-OP2	-5.15	101.06	105.70
1	1A	2288	G	N1-C6-O6	-5.15	116.81	119.90
32	1a	552	U	O5'-P-OP1	5.15	116.88	110.70
32	1a	1077	G	N9-C1'-C2'	-5.15	106.33	112.00
32	1a	1137	C	N1-C2-O2	5.15	121.99	118.90
1	2A	2597	G	OP2-P-O3'	5.15	116.53	105.20
32	2a	261	U	C5-C4-O4	5.15	128.99	125.90
1	1A	1263	C	O5'-P-OP2	-5.15	101.07	105.70
1	1A	1361	C	N3-C2-O2	-5.15	118.30	121.90
1	1A	1928	G	C6-C5-N7	-5.15	127.31	130.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2093	A	O5'-P-OP1	-5.15	101.07	105.70
15	1T	96	ARG	N-CA-CB	-5.15	101.33	110.60
32	1a	486	U	C5-C4-O4	5.15	128.99	125.90
1	2A	752	A	C2'-C3'-O3'	5.15	121.94	113.70
1	2A	2511	U	C2-N3-C4	-5.15	123.91	127.00
32	2a	1011	G	N9-C4-C5	5.15	107.46	105.40
1	1A	554	A	OP1-P-O3'	5.15	116.53	105.20
1	1A	985	G	C6-N1-C2	-5.15	122.01	125.10
2	1B	32	C	OP2-P-O3'	5.15	116.53	105.20
32	1a	550	G	N9-C4-C5	5.15	107.46	105.40
32	1a	1130	A	O5'-P-OP1	5.15	116.88	110.70
1	2A	36	G	OP2-P-O3'	5.15	116.52	105.20
1	2A	228	A	C8-N9-C1'	5.15	136.96	127.70
4	2E	13	ARG	NE-CZ-NH1	-5.15	117.73	120.30
32	2a	820	U	N3-C2-O2	5.15	125.80	122.20
32	2a	968	A	N1-C6-N6	-5.15	115.51	118.60
1	1A	1449	C	C4-C5-C6	5.15	119.97	117.40
1	1A	1874	C	N3-C2-O2	5.15	125.50	121.90
20	1Y	50	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	1A	106	U	N3-C2-O2	-5.14	118.60	122.20
1	1A	893	C	OP1-P-OP2	5.14	127.31	119.60
1	1A	1301	U	C2-N3-C4	-5.14	123.91	127.00
1	1A	1513	G	OP2-P-O3'	5.14	116.52	105.20
1	1A	1521	C	N1-C2-O2	-5.14	115.81	118.90
32	1a	1341	U	C6-N1-C1'	5.14	128.40	121.20
1	2A	143	G	N9-C4-C5	5.14	107.46	105.40
1	2A	1822	G	C8-N9-C4	5.14	108.46	106.40
32	2a	245	C	O5'-P-OP2	5.14	116.87	110.70
32	2a	858	G	C6-C5-N7	-5.14	127.31	130.40
32	2a	1465	C	N1-C2-O2	-5.14	115.81	118.90
1	1A	546	G	OP2-P-O3'	5.14	116.51	105.20
1	1A	593	G	C6-N1-C2	-5.14	122.02	125.10
1	1A	733	G	N1-C2-N2	-5.14	111.57	116.20
1	1A	1427	G	N9-C4-C5	5.14	107.46	105.40
1	1A	2525	G	N3-C2-N2	5.14	123.50	119.90
2	1B	36	C	N3-C2-O2	5.14	125.50	121.90
32	1a	264	U	C5-C4-O4	5.14	128.99	125.90
1	2A	53	A	O5'-P-OP1	-5.14	101.07	105.70
1	2A	555	U	O4'-C1'-N1	5.14	112.31	108.20
1	2A	655	A	N1-C6-N6	5.14	121.69	118.60
1	2A	875	G	O5'-P-OP1	5.14	116.87	110.70
32	2a	1020	U	C5-C6-N1	5.14	125.27	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2222	C	C5-C6-N1	-5.14	118.43	121.00
1	1A	2639	G	N3-C4-N9	5.14	129.09	126.00
1	2A	2042	A	C2-N3-C4	-5.14	108.03	110.60
32	2a	1094	G	N9-C4-C5	-5.14	103.34	105.40
1	1A	1827	U	C2-N3-C4	-5.14	123.92	127.00
1	1A	2181	G	N3-C4-N9	5.14	129.08	126.00
1	1A	2331	G	N1-C2-N3	5.14	126.98	123.90
32	1a	503	C	O5'-P-OP1	-5.14	101.08	105.70
1	2A	100	G	N7-C8-N9	-5.14	110.53	113.10
1	1A	398	A	C5-C6-N6	-5.14	119.59	123.70
1	1A	436	C	C5-C6-N1	-5.14	118.43	121.00
1	1A	986	A	C8-N9-C4	-5.14	103.75	105.80
1	1A	2556	G	N9-C4-C5	5.14	107.45	105.40
1	2A	1696	G	N1-C2-N3	-5.14	120.82	123.90
2	2B	71	C	C6-N1-C2	5.14	122.36	120.30
1	1A	787	U	C5-C6-N1	-5.14	120.13	122.70
1	1A	1067	A	OP2-P-O3'	5.14	116.50	105.20
1	1A	2748	G	N1-C6-O6	-5.14	116.82	119.90
32	1a	607	A	C6-C5-N7	-5.14	128.71	132.30
1	2A	1052	C	N3-C4-C5	-5.14	119.85	121.90
1	2A	2686	G	O5'-P-OP2	-5.14	101.08	105.70
1	2A	2744	G	OP2-P-O3'	5.14	116.50	105.20
4	2E	51	PHE	N-CA-C	-5.14	97.13	111.00
32	2a	450	G	N1-C6-O6	5.14	122.98	119.90
1	1A	178	G	OP2-P-O3'	5.13	116.50	105.20
1	1A	1263	C	OP2-P-O3'	5.13	116.50	105.20
1	1A	2331	G	N9-C4-C5	5.13	107.45	105.40
1	1A	2419	G	O4'-C1'-N9	-5.13	104.09	108.20
14	1S	59	LYS	N-CA-C	5.13	124.86	111.00
32	1a	858	G	C4-N9-C1'	5.13	133.18	126.50
1	2A	1283	G	N3-C2-N2	5.13	123.49	119.90
1	2A	2177	C	N1-C2-O2	5.13	121.98	118.90
1	2A	2727	G	C8-N9-C4	-5.13	104.35	106.40
32	2a	1029	C	C5-C6-N1	5.13	123.57	121.00
1	1A	499	G	C5-C6-O6	5.13	131.68	128.60
1	1A	639	G	C4-N9-C1'	-5.13	119.83	126.50
1	1A	2045	G	O5'-P-OP2	5.13	116.86	110.70
1	1A	2684	G	OP2-P-O3'	5.13	116.49	105.20
32	1a	279	A	O5'-P-OP2	-5.13	101.08	105.70
32	1a	933	G	N1-C6-O6	5.13	122.98	119.90
1	2A	192	C	C6-N1-C2	-5.13	118.25	120.30
32	2a	1530	G	N1-C6-O6	5.13	122.98	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	176	G	C8-N9-C4	-5.13	104.35	106.40
1	1A	958	C	N1-C2-O2	5.13	121.98	118.90
1	1A	1375	U	C5-C4-O4	5.13	128.98	125.90
1	1A	1543	U	O5'-P-OP1	-5.13	101.08	105.70
1	1A	1707	C	C6-N1-C2	-5.13	118.25	120.30
1	1A	2265	G	N7-C8-N9	-5.13	110.53	113.10
1	2A	553	G	C8-N9-C4	-5.13	104.35	106.40
1	2A	1075	C	C2-N1-C1'	5.13	124.44	118.80
1	2A	2427	C	O5'-P-OP2	5.13	116.86	110.70
32	2a	603	U	N3-C4-O4	5.13	122.99	119.40
32	2a	852	G	N3-C4-N9	-5.13	122.92	126.00
1	1A	1106	U	C5-C4-O4	-5.13	122.82	125.90
32	1a	863	U	O4'-C1'-N1	5.13	112.30	108.20
1	2A	2885	C	OP2-P-O3'	5.13	116.49	105.20
32	2a	111	G	N1-C6-O6	5.13	122.98	119.90
32	2a	1030	C	N3-C2-O2	-5.13	118.31	121.90
1	1A	68	C	C5-C6-N1	-5.13	118.44	121.00
1	1A	366	G	C4-C5-N7	-5.13	108.75	110.80
1	1A	989	G	C8-N9-C1'	-5.13	120.33	127.00
1	1A	1166	G	C5-C6-O6	5.13	131.68	128.60
1	1A	2255	U	C5-C4-O4	-5.13	122.82	125.90
1	1A	2623	U	N3-C4-C5	-5.13	111.52	114.60
32	1a	1046	A	N1-C6-N6	5.13	121.68	118.60
32	1a	1153	C	O5'-P-OP2	-5.13	101.08	105.70
1	2A	383	U	O4'-C1'-N1	5.13	112.30	108.20
1	2A	787	U	C5-C4-O4	5.13	128.98	125.90
1	2A	1204	A	N7-C8-N9	-5.13	111.24	113.80
1	2A	1956	U	N3-C4-C5	5.13	117.68	114.60
1	2A	2296	U	O5'-P-OP1	-5.13	101.08	105.70
1	1A	333	G	O5'-P-OP1	-5.13	101.09	105.70
1	1A	462	C	OP1-P-OP2	5.13	127.29	119.60
1	1A	569	G	N3-C4-N9	-5.13	122.92	126.00
1	1A	994	C	O5'-P-OP2	-5.13	101.09	105.70
1	1A	1716	A	O4'-C1'-N9	5.13	112.30	108.20
1	1A	1789	G	C5-C6-O6	-5.13	125.52	128.60
1	1A	2294	G	O4'-C1'-N9	5.13	112.30	108.20
1	1A	2557	G	N7-C8-N9	-5.13	110.54	113.10
32	1a	96	U	C5-C4-O4	-5.13	122.82	125.90
32	1a	485	G	C8-N9-C4	5.13	108.45	106.40
32	1a	514	C	N3-C4-N4	5.13	121.59	118.00
1	2A	1687	G	OP2-P-O3'	5.13	116.48	105.20
1	2A	1900	A	C2-N3-C4	5.13	113.16	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	761	G	N3-C2-N2	-5.13	116.31	119.90
32	2a	1100	C	C6-N1-C1'	5.13	126.95	120.80
2	1B	88	C	O4'-C1'-N1	5.12	112.30	108.20
1	2A	1605	C	N3-C4-C5	-5.12	119.85	121.90
32	2a	1442	G	P-O3'-C3'	5.12	125.85	119.70
1	1A	150	C	C5-C6-N1	-5.12	118.44	121.00
1	1A	604	C	N1-C2-N3	5.12	122.79	119.20
1	1A	839	G	N3-C2-N2	5.12	123.49	119.90
1	1A	1186	U	OP1-P-OP2	-5.12	111.91	119.60
1	1A	2509	A	N1-C6-N6	-5.12	115.53	118.60
2	1B	93	G	C5-N7-C8	-5.12	101.74	104.30
1	2A	390	A	N9-C4-C5	-5.12	103.75	105.80
1	2A	581	C	O5'-P-OP1	5.12	116.85	110.70
1	2A	856	C	C2'-C3'-O3'	5.12	121.90	113.70
1	2A	1925	C	C2-N1-C1'	-5.12	113.16	118.80
32	2a	453	A	OP1-P-OP2	5.12	127.28	119.60
32	2a	1002	G	C8-N9-C4	-5.12	104.35	106.40
1	1A	117	A	OP1-P-O3'	5.12	116.47	105.20
1	1A	251	A	OP1-P-OP2	5.12	127.28	119.60
1	1A	276	C	OP2-P-O3'	5.12	116.47	105.20
1	1A	720	C	C5-C4-N4	-5.12	116.61	120.20
1	1A	874	U	N1-C2-N3	5.12	117.97	114.90
1	1A	1000	C	N3-C2-O2	-5.12	118.31	121.90
1	1A	1171	G	N1-C6-O6	5.12	122.97	119.90
1	1A	1518	A	N3-C4-C5	-5.12	123.22	126.80
1	1A	1801	G	C5-C6-N1	-5.12	108.94	111.50
1	1A	2579	G	C5-C6-O6	5.12	131.67	128.60
1	1A	2734	A	C6-N1-C2	5.12	121.67	118.60
1	2A	1835	G	N3-C4-N9	5.12	129.07	126.00
1	2A	2586	C	N3-C2-O2	5.12	125.48	121.90
32	2a	473	G	C5-C6-O6	5.12	131.67	128.60
32	2a	656	C	OP1-P-OP2	-5.12	111.92	119.60
43	2k	118	GLY	N-CA-C	5.12	125.90	113.10
1	2A	1586	A	O5'-P-OP1	-5.12	101.09	105.70
1	1A	522	A	N1-C2-N3	-5.12	126.74	129.30
1	1A	966	G	N1-C2-N3	5.12	126.97	123.90
1	1A	1071	G	C5-C6-N1	-5.12	108.94	111.50
1	1A	2005	C	C5-C6-N1	-5.12	118.44	121.00
2	1B	77	U	N1-C2-O2	-5.12	119.22	122.80
32	1a	73	G	C4-N9-C1'	-5.12	119.85	126.50
32	1a	355	C	N1-C2-N3	5.12	122.78	119.20
32	1a	804	U	C5-C6-N1	-5.12	120.14	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	271(L)	U	C5-C6-N1	5.12	125.26	122.70
1	2A	1573	G	N1-C2-N2	5.12	120.81	116.20
1	2A	2428	G	C5-C6-O6	5.12	131.67	128.60
1	2A	2721	A	C8-N9-C4	-5.12	103.75	105.80
32	2a	1259	C	C6-N1-C2	-5.12	118.25	120.30
1	1A	1117	G	C4-C5-N7	-5.12	108.75	110.80
1	1A	2139	A	N1-C6-N6	-5.12	115.53	118.60
1	1A	2450	U	N3-C4-C5	5.12	117.67	114.60
1	1A	1110	C	C2-N1-C1'	5.12	124.43	118.80
1	1A	1142	A	OP2-P-O3'	5.12	116.45	105.20
1	1A	1729	G	C6-N1-C2	-5.12	122.03	125.10
1	1A	2071	G	C2-N3-C4	5.12	114.46	111.90
1	1A	2446	A	OP2-P-O3'	5.12	116.45	105.20
1	1A	2577	A	N1-C6-N6	-5.12	115.53	118.60
32	1a	740	U	C5-C4-O4	5.12	128.97	125.90
32	1a	797	C	C6-N1-C2	-5.12	118.25	120.30
1	2A	928	G	C8-N9-C4	-5.12	104.35	106.40
1	2A	1213	A	N1-C6-N6	5.12	121.67	118.60
1	1A	499	G	N3-C2-N2	5.11	123.48	119.90
1	1A	618	C	OP1-P-OP2	5.11	127.27	119.60
1	1A	623	G	O5'-P-OP2	-5.11	101.10	105.70
1	1A	1210	G	C6-C5-N7	5.11	133.47	130.40
1	1A	1371	G	N3-C4-C5	-5.11	126.04	128.60
1	1A	1375	U	N1-C2-N3	5.11	117.97	114.90
1	1A	1847	G	C8-N9-C1'	5.11	133.65	127.00
1	2A	1935	G	O5'-P-OP1	5.11	116.84	110.70
1	2A	2474	C	C6-N1-C1'	-5.11	114.67	120.80
1	1A	1332	A	O5'-P-OP2	-5.11	101.10	105.70
1	1A	2843	G	N3-C4-N9	5.11	129.07	126.00
1	2A	1509(A)	A	C8-N9-C4	-5.11	103.75	105.80
8	2I	75	LEU	CA-CB-CG	5.11	127.06	115.30
32	2a	740	U	C5-C4-O4	5.11	128.97	125.90
1	1A	712	C	C6-N1-C2	5.11	122.34	120.30
32	1a	1326	C	N3-C4-N4	-5.11	114.42	118.00
1	2A	258	G	N1-C6-O6	-5.11	116.83	119.90
1	2A	670	A	N3-C4-C5	-5.11	123.22	126.80
1	2A	992	C	C5-C6-N1	5.11	123.56	121.00
1	2A	1060	U	N1-C2-O2	5.11	126.38	122.80
32	2a	1006	C	N3-C4-C5	-5.11	119.86	121.90
1	1A	1958	A	N1-C6-N6	5.11	121.67	118.60
1	1A	1978	U	N1-C2-O2	-5.11	119.22	122.80
1	1A	2026	G	C5-N7-C8	5.11	106.85	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2826	C	O5'-P-OP1	-5.11	101.10	105.70
32	1a	740	U	OP1-P-OP2	5.11	127.26	119.60
1	2A	380	U	C5-C6-N1	5.11	125.25	122.70
1	2A	855	G	C8-N9-C4	-5.11	104.36	106.40
1	2A	2794	C	C6-N1-C2	-5.11	118.26	120.30
1	1A	262	C	C2-N3-C4	-5.11	117.35	119.90
1	1A	514	G	C4-C5-N7	-5.11	108.76	110.80
1	1A	1259	A	C8-N9-C4	5.11	107.84	105.80
16	1U	10	ARG	NE-CZ-NH2	-5.11	117.75	120.30
32	1a	150	C	N3-C4-C5	-5.11	119.86	121.90
32	1a	444	C	C5-C6-N1	-5.11	118.45	121.00
1	2A	778	G	C5-C6-O6	5.11	131.66	128.60
1	2A	790	C	N1-C2-O2	-5.11	115.84	118.90
1	2A	1316	U	C4-C5-C6	5.11	122.76	119.70
1	2A	2633	G	C8-N9-C4	-5.11	104.36	106.40
1	1A	1035	G	N3-C4-C5	-5.11	126.05	128.60
1	1A	1094	A	N1-C6-N6	-5.11	115.54	118.60
1	1A	1345	G	O5'-P-OP1	-5.11	101.11	105.70
1	1A	1401	G	C5-C6-O6	5.11	131.66	128.60
1	1A	2605	U	C5-C6-N1	-5.11	120.15	122.70
1	1A	2750	G	N9-C4-C5	5.11	107.44	105.40
1	1A	2881	C	C6-N1-C2	5.11	122.34	120.30
32	1a	1152	A	N1-C6-N6	-5.11	115.54	118.60
1	2A	667	U	N1-C2-O2	-5.11	119.23	122.80
1	2A	2053	G	C4-C5-N7	-5.11	108.76	110.80
32	2a	60	A	O4'-C1'-N9	-5.11	104.11	108.20
32	2a	555	C	N3-C4-N4	5.11	121.57	118.00
32	2a	991	U	C2-N1-C1'	5.11	123.83	117.70
32	2a	1229	A	OP1-P-O3'	5.11	116.43	105.20
32	2a	1442	G	C2-N3-C4	5.11	114.45	111.90
1	1A	197	C	C5-C6-N1	-5.10	118.45	121.00
1	1A	1525	G	O5'-P-OP1	-5.10	101.11	105.70
32	2a	52	G	O5'-P-OP1	5.10	116.83	110.70
1	1A	411	U	N3-C2-O2	5.10	125.77	122.20
1	1A	1094	A	N9-C4-C5	5.10	107.84	105.80
1	1A	1110	C	N3-C2-O2	-5.10	118.33	121.90
1	1A	1802	C	O5'-P-OP2	-5.10	101.11	105.70
1	1A	1833	A	O4'-C1'-N9	-5.10	104.12	108.20
1	1A	1970	G	N1-C6-O6	-5.10	116.84	119.90
1	1A	2803	A	C2-N3-C4	5.10	113.15	110.60
1	1A	2855	G	N3-C4-C5	-5.10	126.05	128.60
32	1a	1026	G	C4-N9-C1'	5.10	133.13	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1790	C	OP1-P-O3'	5.10	116.42	105.20
2	2B	87	G	C5-C6-N1	5.10	114.05	111.50
1	1A	1453	C	O5'-P-OP2	-5.10	101.11	105.70
1	1A	1621	C	C2-N3-C4	-5.10	117.35	119.90
32	1a	781	A	OP1-P-O3'	-5.10	93.98	105.20
32	1a	869	G	C8-N9-C4	5.10	108.44	106.40
1	2A	390	A	C8-N9-C4	5.10	107.84	105.80
1	1A	1245	C	N1-C2-N3	5.10	122.77	119.20
1	1A	1270	C	OP1-P-O3'	5.10	116.42	105.20
1	1A	1447	G	C4-C5-N7	-5.10	108.76	110.80
1	1A	1474	C	C6-N1-C1'	5.10	126.92	120.80
1	1A	1614	A	N1-C6-N6	-5.10	115.54	118.60
32	1a	172	A	C5-N7-C8	-5.10	101.35	103.90
1	2A	975(A)	G	C8-N9-C4	-5.10	104.36	106.40
1	2A	1046	A	N9-C4-C5	5.10	107.84	105.80
1	2A	1844	C	C2-N3-C4	-5.10	117.35	119.90
18	2W	23	LEU	CA-CB-CG	5.10	127.03	115.30
32	2a	1093	A	C4-C5-N7	5.10	113.25	110.70
32	2a	1348	U	N3-C2-O2	-5.10	118.63	122.20
1	1A	1117	G	N9-C4-C5	5.10	107.44	105.40
1	1A	1842	G	OP2-P-O3'	5.10	116.42	105.20
1	1A	2187	G	N3-C4-C5	-5.10	126.05	128.60
1	1A	2556	G	N3-C4-N9	-5.10	122.94	126.00
16	1U	10	ARG	NE-CZ-NH1	5.10	122.85	120.30
31	19	27	CYS	CA-CB-SG	5.10	123.18	114.00
1	2A	482	A	O5'-P-OP1	5.10	116.82	110.70
1	2A	2056	G	C6-C5-N7	-5.10	127.34	130.40
32	2a	1499	A	N9-C4-C5	-5.10	103.76	105.80
1	1A	1131	A	O4'-C1'-N9	5.10	112.28	108.20
1	1A	1290	G	N1-C6-O6	-5.10	116.84	119.90
1	1A	1665	G	O5'-P-OP2	-5.10	101.11	105.70
1	1A	2066	C	C2-N3-C4	-5.10	117.35	119.90
1	1A	2900	G	N1-C6-O6	5.10	122.96	119.90
32	1a	1442	G	C3'-C2'-C1'	5.10	105.58	101.50
1	1A	85	C	C2-N3-C4	-5.09	117.35	119.90
1	1A	1112	U	C6-N1-C2	-5.09	117.94	121.00
1	1A	1264	G	N3-C4-C5	5.09	131.15	128.60
1	1A	1578	C	N3-C2-O2	-5.09	118.33	121.90
1	1A	2842	U	C5-C6-N1	-5.09	120.15	122.70
32	1a	810	C	O5'-P-OP2	-5.09	101.11	105.70
32	1a	838	G	O5'-P-OP1	5.09	116.81	110.70
1	2A	154	G	N9-C4-C5	-5.09	103.36	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1203	G	N3-C4-N9	5.09	129.06	126.00
32	2a	27	G	C5-N7-C8	-5.09	101.75	104.30
32	2a	1471	G	N1-C6-O6	-5.09	116.84	119.90
1	1A	954	C	OP2-P-O3'	5.09	116.40	105.20
1	1A	2107	C	N3-C4-C5	5.09	123.94	121.90
1	2A	114	U	O5'-P-OP1	5.09	116.81	110.70
1	2A	778	G	C2-N3-C4	-5.09	109.35	111.90
1	2A	1314	C	N1-C2-O2	5.09	121.96	118.90
32	2a	785	G	O5'-P-OP2	-5.09	101.12	105.70
1	1A	577	U	N1-C2-N3	5.09	117.95	114.90
1	1A	844	C	N3-C2-O2	5.09	125.47	121.90
1	1A	2093	A	C4-C5-C6	5.09	119.55	117.00
1	1A	2222	C	C6-N1-C2	5.09	122.34	120.30
1	1A	2724	U	N3-C4-O4	5.09	122.96	119.40
32	1a	280	C	C6-N1-C2	5.09	122.34	120.30
32	1a	436	C	O5'-P-OP1	-5.09	101.12	105.70
32	1a	669	U	OP2-P-O3'	5.09	116.40	105.20
32	1a	814	A	C2-N3-C4	-5.09	108.05	110.60
32	1a	1457	G	N7-C8-N9	-5.09	110.55	113.10
1	2A	217	G	C5-N7-C8	5.09	106.84	104.30
1	2A	448	U	O5'-P-OP1	-5.09	101.12	105.70
1	2A	554	U	N3-C2-O2	-5.09	118.64	122.20
1	2A	1218	C	C2-N1-C1'	-5.09	113.20	118.80
1	2A	1638	C	C6-N1-C2	5.09	122.34	120.30
1	2A	1798	U	O5'-P-OP2	-5.09	101.12	105.70
32	2a	114	U	C5-C6-N1	-5.09	120.16	122.70
1	1A	1109	G	C2-N3-C4	5.09	114.44	111.90
1	1A	1409	C	OP1-P-O3'	-5.09	94.00	105.20
1	1A	1473	A	N7-C8-N9	-5.09	111.25	113.80
1	1A	1474	C	C5-C6-N1	-5.09	118.46	121.00
1	1A	2065	C	N3-C4-N4	5.09	121.56	118.00
31	19	22	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	2A	2570	G	N1-C6-O6	-5.09	116.85	119.90
1	2A	2837	G	C8-N9-C4	5.09	108.44	106.40
19	2X	8	ILE	CB-CA-C	-5.09	101.42	111.60
32	2a	315	A	N7-C8-N9	5.09	116.34	113.80
32	2a	622	A	OP2-P-O3'	5.09	116.39	105.20
32	2a	1139	G	C5-C6-N1	-5.09	108.95	111.50
1	1A	86	C	C6-N1-C2	5.09	122.33	120.30
1	1A	696	C	C2-N3-C4	5.09	122.44	119.90
1	1A	780	G	C5-C6-O6	5.09	131.65	128.60
1	1A	1296	G	C5-C6-N1	5.09	114.04	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1485	A	C2-N3-C4	-5.09	108.06	110.60
2	1B	99	G	C8-N9-C4	5.09	108.44	106.40
1	2A	399	G	N3-C4-C5	5.09	131.14	128.60
1	2A	710	G	O5'-P-OP1	5.09	116.81	110.70
1	1A	513	C	C4-C5-C6	5.09	119.94	117.40
1	1A	954	C	C5-C6-N1	-5.09	118.46	121.00
1	1A	2459	G	O4'-C1'-N9	5.09	112.27	108.20
1	1A	2599	A	C5-C6-N1	-5.09	115.16	117.70
17	1V	82	ARG	NE-CZ-NH2	-5.09	117.76	120.30
32	1a	694	A	O5'-P-OP2	5.09	116.81	110.70
32	1a	1201	A	P-O3'-C3'	5.09	125.80	119.70
1	2A	1302	A	C2-N3-C4	-5.09	108.06	110.60
1	2A	2554	U	C2-N1-C1'	-5.09	111.60	117.70
32	2a	831	U	C6-N1-C2	-5.09	117.95	121.00
1	1A	1747	A	C4-C5-C6	-5.08	114.46	117.00
1	1A	1836	U	N1-C2-O2	-5.08	119.24	122.80
1	1A	2585	C	C5-C4-N4	-5.08	116.64	120.20
1	1A	2587	C	OP2-P-O3'	5.08	116.39	105.20
1	1A	2780	C	C2-N1-C1'	5.08	124.39	118.80
1	2A	261	G	N3-C2-N2	-5.08	116.34	119.90
1	2A	739	G	OP1-P-O3'	5.08	116.39	105.20
1	2A	1858	G	N1-C6-O6	-5.08	116.85	119.90
1	1A	198	C	N3-C4-N4	-5.08	114.44	118.00
1	1A	534	C	C6-N1-C2	5.08	122.33	120.30
1	1A	935	C	N1-C2-O2	5.08	121.95	118.90
1	1A	1014	U	N3-C4-C5	5.08	117.65	114.60
1	1A	2060	G	C5-C6-O6	5.08	131.65	128.60
1	1A	2082	A	C6-C5-N7	5.08	135.86	132.30
1	2A	951	C	OP1-P-OP2	-5.08	111.98	119.60
1	2A	1319	G	O5'-P-OP1	-5.08	101.12	105.70
1	2A	2286	A	N1-C6-N6	-5.08	115.55	118.60
1	1A	407	U	N3-C4-O4	-5.08	115.84	119.40
1	1A	1027	A	C8-N9-C4	5.08	107.83	105.80
1	1A	1599	G	O5'-P-OP2	-5.08	101.13	105.70
1	1A	1869	C	OP1-P-OP2	5.08	127.22	119.60
1	1A	2125	C	C5-C6-N1	5.08	123.54	121.00
32	1a	766	A	N1-C6-N6	5.08	121.65	118.60
1	2A	9	U	C6-N1-C2	-5.08	117.95	121.00
1	2A	41	C	O5'-P-OP2	-5.08	101.13	105.70
1	2A	526	A	N1-C6-N6	-5.08	115.55	118.60
1	2A	662	G	OP2-P-O3'	5.08	116.38	105.20
1	2A	1379	A	OP1-P-O3'	5.08	116.38	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	200	G	C8-N9-C4	5.08	108.43	106.40
1	1A	1660	A	C5-N7-C8	5.08	106.44	103.90
1	1A	2466	G	O5'-P-OP2	-5.08	101.13	105.70
1	1A	2588	G	N9-C4-C5	5.08	107.43	105.40
1	2A	1560	G	N7-C8-N9	-5.08	110.56	113.10
32	2a	761	G	OP2-P-O3'	5.08	116.38	105.20
1	1A	39	C	C5-C6-N1	-5.08	118.46	121.00
1	1A	964	A	C6-N1-C2	5.08	121.65	118.60
1	1A	1088	G	OP2-P-O3'	5.08	116.37	105.20
1	1A	1480	A	OP2-P-O3'	5.08	116.37	105.20
1	1A	1925	G	N7-C8-N9	5.08	115.64	113.10
1	1A	2750	G	C5-C6-O6	5.08	131.65	128.60
1	1A	2846	U	N3-C2-O2	-5.08	118.64	122.20
1	2A	847	U	N3-C2-O2	-5.08	118.64	122.20
1	2A	2140	C	N1-C2-O2	5.08	121.95	118.90
1	1A	1065	U	OP1-P-OP2	5.08	127.22	119.60
1	1A	2137	G	C2-N3-C4	5.08	114.44	111.90
1	1A	2421	G	N3-C4-N9	5.08	129.05	126.00
1	1A	2589	A	C5-C6-N6	5.08	127.76	123.70
1	1A	2718	G	C8-N9-C4	5.08	108.43	106.40
32	1a	38	G	N1-C6-O6	5.08	122.95	119.90
1	2A	2319	G	C8-N9-C4	-5.08	104.37	106.40
32	2a	145	G	OP1-P-OP2	-5.08	111.98	119.60
32	2a	1201	A	C6-N1-C2	-5.08	115.55	118.60
1	1A	41	C	C5-C4-N4	5.08	123.75	120.20
1	1A	218	A	N7-C8-N9	5.08	116.34	113.80
1	1A	498	A	OP2-P-O3'	5.08	116.37	105.20
1	1A	1046	A	N1-C2-N3	-5.08	126.76	129.30
1	1A	1353	A	C8-N9-C4	5.08	107.83	105.80
1	1A	1868	C	O5'-P-OP1	-5.08	101.13	105.70
1	1A	2380	C	N3-C2-O2	-5.08	118.35	121.90
1	1A	2878	A	N1-C6-N6	5.08	121.64	118.60
1	2A	178	G	O5'-P-OP2	-5.08	101.13	105.70
1	2A	455	C	C4-C5-C6	5.08	119.94	117.40
1	2A	907	U	C5-C6-N1	5.08	125.24	122.70
1	2A	2694	G	C5-C6-O6	5.08	131.65	128.60
1	2A	2807	G	N9-C4-C5	5.08	107.43	105.40
1	1A	1200	G	N1-C2-N2	-5.07	111.63	116.20
1	2A	1085	A	O5'-P-OP1	-5.07	101.14	105.70
1	2A	2127	G	O5'-P-OP2	5.07	116.79	110.70
1	2A	2182	G	C4-C5-N7	-5.07	108.77	110.80
1	2A	2344	U	OP1-P-O3'	5.07	116.36	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	122	G	C5-C6-N1	5.07	114.04	111.50
32	2a	390	C	N3-C4-N4	-5.07	114.45	118.00
32	2a	664	G	C8-N9-C4	-5.07	104.37	106.40
1	1A	1735	U	O5'-P-OP2	-5.07	101.14	105.70
1	2A	192	C	C5-C4-N4	-5.07	116.65	120.20
1	2A	655	A	O4'-C1'-N9	5.07	112.26	108.20
1	2A	799	G	N1-C6-O6	-5.07	116.86	119.90
1	2A	1373	A	C8-N9-C4	5.07	107.83	105.80
1	2A	2198	A	O4'-C1'-N9	5.07	112.26	108.20
32	2a	17	U	N3-C2-O2	-5.07	118.65	122.20
32	2a	851	G	C5-N7-C8	-5.07	101.76	104.30
1	1A	38	A	N7-C8-N9	-5.07	111.27	113.80
1	1A	152	G	N1-C6-O6	5.07	122.94	119.90
1	1A	553	A	O5'-P-OP2	-5.07	101.14	105.70
1	1A	1365	G	N1-C2-N3	5.07	126.94	123.90
1	1A	1441	A	N7-C8-N9	-5.07	111.27	113.80
1	1A	1606	G	C4-N9-C1'	-5.07	119.91	126.50
1	1A	2133	C	C2-N3-C4	5.07	122.44	119.90
1	1A	2346	G	C6-C5-N7	-5.07	127.36	130.40
1	1A	2383	G	C8-N9-C4	5.07	108.43	106.40
1	1A	2893	A	C2-N3-C4	5.07	113.14	110.60
32	1a	148	G	C2-N3-C4	5.07	114.44	111.90
32	1a	615	C	C5-C6-N1	5.07	123.53	121.00
1	2A	2640	G	C4-C5-N7	-5.07	108.77	110.80
1	2A	2764	A	C2-N3-C4	-5.07	108.06	110.60
32	2a	353	A	OP2-P-O3'	5.07	116.36	105.20
1	1A	2429	C	C5-C4-N4	5.07	123.75	120.20
1	2A	1638	C	C2-N3-C4	-5.07	117.37	119.90
1	2A	2768	C	O5'-P-OP2	-5.07	101.14	105.70
32	2a	644	G	C8-N9-C4	5.07	108.43	106.40
32	2a	1301	U	C6-N1-C2	5.07	124.04	121.00
1	1A	176	G	N1-C2-N3	5.07	126.94	123.90
1	1A	582	G	C6-C5-N7	-5.07	127.36	130.40
1	1A	716	G	OP1-P-OP2	-5.07	112.00	119.60
1	1A	779	C	N3-C2-O2	-5.07	118.35	121.90
1	1A	1988	A	O4'-C1'-N9	-5.07	104.15	108.20
1	1A	2573	A	N9-C4-C5	5.07	107.83	105.80
46	1n	3	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	2A	763	G	C5-C6-O6	5.07	131.64	128.60
1	2A	840	C	N3-C4-C5	-5.07	119.87	121.90
1	2A	1410	G	OP2-P-O3'	5.07	116.35	105.20
1	2A	1904	G	N1-C6-O6	-5.07	116.86	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	446	G	N1-C2-N2	5.07	120.76	116.20
32	2a	678	U	N1-C2-O2	-5.07	119.25	122.80
32	2a	1243	C	C2-N3-C4	5.07	122.43	119.90
1	1A	931	C	C5-C6-N1	5.07	123.53	121.00
1	1A	2155	G	C8-N9-C1'	5.07	133.59	127.00
1	1A	2528	G	C4-C5-N7	-5.07	108.77	110.80
32	1a	1273	G	N9-C4-C5	-5.07	103.37	105.40
25	23	28	LEU	CA-CB-CG	-5.07	103.65	115.30
32	2a	500	G	C6-C5-N7	-5.07	127.36	130.40
32	2a	999	C	C5-C6-N1	5.07	123.53	121.00
1	1A	1664	A	C8-N9-C4	5.06	107.83	105.80
1	1A	2443	U	C6-N1-C2	5.06	124.04	121.00
1	1A	2619	G	N9-C4-C5	5.06	107.43	105.40
32	1a	644	G	C5-C6-O6	5.06	131.64	128.60
32	1a	1367	C	C6-N1-C2	-5.06	118.27	120.30
1	2A	9	U	P-O3'-C3'	5.06	125.78	119.70
1	2A	695	G	N1-C6-O6	-5.06	116.86	119.90
32	2a	9	G	O5'-P-OP2	-5.06	101.14	105.70
32	2a	1432	G	C5-C6-O6	5.06	131.64	128.60
1	1A	925	A	C2-N3-C4	-5.06	108.07	110.60
1	1A	938	G	C8-N9-C4	5.06	108.42	106.40
1	1A	1233	U	N3-C4-C5	5.06	117.64	114.60
1	1A	1457	C	N3-C4-C5	5.06	123.92	121.90
1	1A	2341	G	N1-C6-O6	5.06	122.94	119.90
1	1A	2381	A	O5'-P-OP2	-5.06	101.14	105.70
32	1a	613	C	O5'-P-OP1	5.06	116.78	110.70
32	2a	1054	C	N1-C2-O2	5.06	121.94	118.90
1	1A	748	G	OP1-P-OP2	5.06	127.19	119.60
32	1a	1233	G	N3-C2-N2	5.06	123.44	119.90
1	2A	2755	C	C2-N3-C4	5.06	122.43	119.90
32	2a	898	G	N9-C4-C5	-5.06	103.38	105.40
32	2a	912	C	N3-C2-O2	5.06	125.44	121.90
32	2a	1154	G	N9-C4-C5	-5.06	103.38	105.40
1	1A	1233	U	N3-C4-O4	-5.06	115.86	119.40
1	1A	1347	A	OP1-P-OP2	-5.06	112.01	119.60
1	1A	1630	A	N7-C8-N9	-5.06	111.27	113.80
1	1A	1986	G	N7-C8-N9	-5.06	110.57	113.10
1	1A	2080	A	C4-C5-C6	5.06	119.53	117.00
1	1A	2242	G	N1-C2-N2	5.06	120.75	116.20
1	1A	2769	U	OP1-P-O3'	5.06	116.33	105.20
2	1B	41	U	N3-C4-O4	-5.06	115.86	119.40
2	1B	48	A	C6-N1-C2	5.06	121.64	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	423	G	C5-C6-O6	-5.06	125.56	128.60
32	1a	509	A	N7-C8-N9	5.06	116.33	113.80
1	2A	190	A	OP1-P-OP2	5.06	127.19	119.60
1	2A	1077	A	O5'-P-OP1	-5.06	101.15	105.70
1	2A	1580	A	OP2-P-O3'	5.06	116.33	105.20
1	2A	2143	C	C6-N1-C2	-5.06	118.28	120.30
1	2A	2825	C	N1-C1'-C2'	-5.06	106.44	112.00
1	1A	385	G	N1-C6-O6	5.06	122.94	119.90
1	1A	1505	C	C6-N1-C2	-5.06	118.28	120.30
1	1A	1862	G	C6-N1-C2	5.06	128.13	125.10
1	1A	2088	C	N1-C2-N3	5.06	122.74	119.20
1	1A	2896	G	N3-C2-N2	-5.06	116.36	119.90
1	2A	960	A	N9-C4-C5	-5.06	103.78	105.80
1	2A	1635	G	N7-C8-N9	-5.06	110.57	113.10
1	2A	2516	G	C8-N9-C4	-5.06	104.38	106.40
32	2a	64	G	N3-C4-C5	5.06	131.13	128.60
32	2a	663	A	C2-N3-C4	-5.06	108.07	110.60
32	2a	860	A	N9-C4-C5	5.06	107.82	105.80
1	1A	541	C	N1-C2-O2	-5.06	115.87	118.90
1	1A	2176	G	N3-C4-N9	-5.06	122.97	126.00
32	1a	136	C	O5'-P-OP2	-5.06	101.15	105.70
32	1a	895	G	N9-C4-C5	5.06	107.42	105.40
1	2A	1108	U	C5-C6-N1	5.06	125.23	122.70
1	2A	1776	G	N1-C2-N2	-5.06	111.65	116.20
32	2a	555	C	N3-C4-C5	-5.06	119.88	121.90
32	2a	872	A	N7-C8-N9	5.06	116.33	113.80
1	1A	125	A	C6-N1-C2	-5.05	115.57	118.60
1	1A	2294	G	N1-C2-N3	-5.05	120.87	123.90
1	1A	2826	C	C5-C6-N1	-5.05	118.47	121.00
13	1R	33	ARG	NE-CZ-NH2	-5.05	117.77	120.30
32	1a	438	G	O5'-P-OP2	-5.05	101.15	105.70
32	1a	802	A	C4-C5-N7	5.05	113.23	110.70
32	1a	903	G	OP2-P-O3'	5.05	116.32	105.20
32	1a	1197	G	N3-C2-N2	5.05	123.44	119.90
1	2A	2821	A	C2-N3-C4	-5.05	108.07	110.60
32	2a	913	A	C2-N3-C4	5.05	113.13	110.60
1	1A	748	G	C5-C6-O6	5.05	131.63	128.60
1	1A	1977	U	N1-C2-N3	5.05	117.93	114.90
1	1A	2038	U	N1-C2-O2	5.05	126.34	122.80
1	1A	2874	G	N1-C6-O6	-5.05	116.87	119.90
1	2A	2102	U	N1-C2-O2	5.05	126.34	122.80
1	2A	2595	G	N1-C2-N3	5.05	126.93	123.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	36	G	C5-N7-C8	5.05	106.83	104.30
1	1A	762	G	C5-C6-O6	-5.05	125.57	128.60
1	1A	1047	A	C2-N3-C4	5.05	113.13	110.60
1	1A	2038	U	N3-C2-O2	-5.05	118.66	122.20
1	2A	1607	C	O5'-P-OP1	-5.05	101.16	105.70
32	2a	1146	A	N9-C4-C5	-5.05	103.78	105.80
1	1A	837	C	N3-C4-N4	5.05	121.53	118.00
1	1A	1079	U	C2-N3-C4	-5.05	123.97	127.00
1	1A	2229	A	C4-N9-C1'	5.05	135.39	126.30
1	1A	2312	G	OP1-P-OP2	-5.05	112.03	119.60
1	1A	2897	U	OP1-P-OP2	5.05	127.17	119.60
32	1a	484	G	N1-C6-O6	-5.05	116.87	119.90
32	1a	1516	G	O5'-P-OP1	-5.05	101.16	105.70
1	2A	1904	G	C4-C5-N7	-5.05	108.78	110.80
2	2B	55	U	N1-C2-O2	-5.05	119.27	122.80
32	2a	273	A	C8-N9-C4	5.05	107.82	105.80
32	2a	677	U	N3-C4-C5	-5.05	111.57	114.60
32	2a	749	C	O5'-P-OP2	5.05	116.76	110.70
1	1A	462	C	C5-C4-N4	-5.05	116.67	120.20
27	15	15	ARG	CA-CB-CG	-5.05	102.29	113.40
32	1a	908	A	C8-N9-C4	-5.05	103.78	105.80
1	2A	495	G	N1-C6-O6	-5.05	116.87	119.90
32	2a	1163	C	C6-N1-C2	-5.05	118.28	120.30
1	1A	581	G	N9-C4-C5	5.05	107.42	105.40
1	1A	1033	G	N3-C2-N2	-5.05	116.37	119.90
1	1A	1514	C	OP1-P-OP2	-5.05	112.03	119.60
1	1A	1631	C	O4'-C1'-N1	5.05	112.24	108.20
32	1a	1255	G	C8-N9-C4	5.05	108.42	106.40
1	2A	1052	C	C2-N1-C1'	5.05	124.35	118.80
1	2A	1450	G	OP1-P-OP2	5.05	127.17	119.60
1	2A	2042	A	C8-N9-C4	5.05	107.82	105.80
1	2A	2163	C	N3-C4-N4	5.05	121.53	118.00
1	2A	2378	A	C8-N9-C4	5.05	107.82	105.80
1	1A	1190	G	N1-C6-O6	-5.04	116.87	119.90
1	1A	1706	U	C2-N3-C4	-5.04	123.97	127.00
1	1A	1845	G	C4-C5-N7	5.04	112.82	110.80
32	1a	880	C	N3-C4-C5	5.04	123.92	121.90
1	2A	1440	G	N1-C6-O6	-5.04	116.87	119.90
1	2A	2146	C	O4'-C1'-N1	-5.04	104.16	108.20
1	2A	1903	G	N3-C4-N9	-5.04	122.97	126.00
1	2A	2489	G	OP2-P-O3'	5.04	116.30	105.20
1	1A	101	A	C8-N9-C1'	-5.04	118.62	127.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	150	C	N3-C4-C5	5.04	123.92	121.90
1	1A	153	C	OP2-P-O3'	5.04	116.29	105.20
1	1A	192	C	C5-C6-N1	-5.04	118.48	121.00
1	1A	499	G	N1-C2-N2	-5.04	111.66	116.20
1	1A	814	U	C4-C5-C6	5.04	122.72	119.70
1	1A	1953	U	N1-C2-O2	5.04	126.33	122.80
1	1A	2022	G	O5'-P-OP2	-5.04	101.16	105.70
1	2A	1760	A	C8-N9-C4	5.04	107.82	105.80
1	2A	1799	G	C5-N7-C8	5.04	106.82	104.30
32	2a	346	G	N3-C4-N9	5.04	129.03	126.00
1	2A	12	U	N1-C2-O2	5.04	126.33	122.80
1	2A	1241	A	O5'-P-OP2	5.04	116.75	110.70
1	2A	1919	A	C8-N9-C4	-5.04	103.78	105.80
1	2A	2623	G	N1-C6-O6	5.04	122.92	119.90
32	2a	1072	G	N1-C6-O6	-5.04	116.88	119.90
1	1A	376	G	OP2-P-O3'	5.04	116.28	105.20
1	1A	1305	G	N1-C6-O6	-5.04	116.88	119.90
1	1A	1835	C	C6-N1-C2	5.04	122.31	120.30
1	1A	2046	G	OP2-P-O3'	5.04	116.28	105.20
1	1A	2101	U	C6-N1-C2	-5.04	117.98	121.00
1	1A	2678	C	N1-C2-O2	5.04	121.92	118.90
1	1A	2830	A	N7-C8-N9	5.04	116.32	113.80
32	1a	158	G	C8-N9-C4	-5.04	104.38	106.40
32	1a	949	A	C8-N9-C4	-5.04	103.78	105.80
1	2A	2017	U	C4-C5-C6	5.04	122.72	119.70
1	2A	2123	G	N3-C2-N2	5.04	123.43	119.90
1	2A	2244	U	C5-C6-N1	-5.04	120.18	122.70
1	2A	2516	G	N1-C2-N3	5.04	126.92	123.90
1	2A	2705	A	C2-N3-C4	-5.04	108.08	110.60
1	1A	760	G	C6-C5-N7	-5.04	127.38	130.40
1	1A	1481	G	N1-C6-O6	-5.04	116.88	119.90
1	1A	2393	C	N1-C2-O2	-5.04	115.88	118.90
32	1a	119	A	O5'-P-OP2	-5.04	101.17	105.70
1	2A	1799	G	N7-C8-N9	-5.04	110.58	113.10
1	1A	466	G	OP1-P-OP2	-5.04	112.05	119.60
1	1A	507	G	O4'-C1'-N9	5.04	112.23	108.20
1	1A	1598	C	C5-C6-N1	-5.04	118.48	121.00
1	1A	2289	G	C5-N7-C8	5.04	106.82	104.30
2	1B	52	A	N9-C4-C5	-5.04	103.79	105.80
32	1a	557	G	N1-C2-N2	-5.04	111.67	116.20
32	1a	619	U	C5-C4-O4	5.04	128.92	125.90
32	1a	1131	G	C5-C6-O6	-5.04	125.58	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	188	G	C4-C5-N7	5.04	112.81	110.80
1	2A	1000	A	OP1-P-OP2	-5.04	112.05	119.60
1	2A	1404	C	OP2-P-O3'	5.04	116.28	105.20
1	2A	2228	G	C5-C6-O6	5.04	131.62	128.60
1	2A	2837	G	C5-C6-O6	-5.04	125.58	128.60
32	2a	299	G	C5-N7-C8	-5.04	101.78	104.30
32	2a	435	C	C2-N3-C4	5.04	122.42	119.90
1	1A	136	G	OP1-P-OP2	5.03	127.15	119.60
1	1A	805	C	C2-N3-C4	-5.03	117.38	119.90
1	1A	1295	U	C5-C6-N1	-5.03	120.18	122.70
1	1A	1664	A	N1-C6-N6	-5.03	115.58	118.60
1	1A	1717	C	C4-C5-C6	5.03	119.92	117.40
1	1A	1982	A	C4-C5-C6	-5.03	114.48	117.00
1	1A	2053	A	C5-C6-N6	5.03	127.73	123.70
1	1A	2290	A	C4-C5-N7	-5.03	108.18	110.70
1	1A	2495	C	N3-C4-C5	-5.03	119.89	121.90
1	1A	2735	G	C5-C6-O6	-5.03	125.58	128.60
32	1a	175	C	N3-C4-C5	-5.03	119.89	121.90
32	1a	504	C	N1-C2-O2	5.03	121.92	118.90
32	1a	620	C	OP1-P-O3'	5.03	116.27	105.20
32	1a	819	A	N3-C4-N9	5.03	131.43	127.40
32	1a	836	G	N9-C4-C5	-5.03	103.39	105.40
1	2A	109	G	C6-N1-C2	-5.03	122.08	125.10
1	2A	350	U	N3-C2-O2	-5.03	118.68	122.20
1	2A	885	C	C6-N1-C2	-5.03	118.29	120.30
1	2A	2816	C	O5'-P-OP2	-5.03	101.17	105.70
1	1A	1364	C	O5'-P-OP1	-5.03	101.17	105.70
1	1A	2230	U	C6-N1-C1'	-5.03	114.16	121.20
1	2A	82	G	C8-N9-C4	5.03	108.41	106.40
1	2A	2063	C	OP2-P-O3'	5.03	116.27	105.20
1	1A	355	A	C8-N9-C4	5.03	107.81	105.80
1	1A	2249	G	N1-C6-O6	-5.03	116.88	119.90
1	1A	2274	U	C5-C4-O4	-5.03	122.88	125.90
1	1A	2586	G	C6-C5-N7	5.03	133.42	130.40
2	1B	93	G	C4-C5-C6	-5.03	115.78	118.80
32	1a	809	G	C2-N3-C4	-5.03	109.39	111.90
32	1a	1134	G	N7-C8-N9	5.03	115.61	113.10
50	1r	26	LEU	CA-CB-CG	5.03	126.87	115.30
1	2A	1164	G	C5-C6-O6	5.03	131.62	128.60
1	2A	2743	C	N1-C2-O2	-5.03	115.88	118.90
32	2a	887	G	C4-C5-N7	5.03	112.81	110.80
32	2a	1356	G	N1-C6-O6	5.03	122.92	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	74	G	C5-C6-N1	5.03	114.01	111.50
1	1A	1258	A	N1-C2-N3	5.03	131.81	129.30
32	1a	689	C	O5'-P-OP1	-5.03	101.17	105.70
32	2a	616	G	N9-C4-C5	5.03	107.41	105.40
1	1A	34	C	C6-N1-C1'	5.03	126.83	120.80
1	1A	742	G	C4-C5-C6	-5.03	115.78	118.80
1	1A	1539	C	C5-C6-N1	-5.03	118.49	121.00
1	1A	2394	G	N7-C8-N9	5.03	115.61	113.10
1	1A	2442	A	C4-C5-C6	-5.03	114.49	117.00
1	1A	2828	G	N3-C2-N2	5.03	123.42	119.90
32	1a	189(C)	C	C6-N1-C2	-5.03	118.29	120.30
32	1a	1446	U	O4'-C1'-N1	5.03	112.22	108.20
1	2A	769	G	N3-C2-N2	-5.03	116.38	119.90
1	2A	866	A	C8-N9-C1'	-5.03	118.65	127.70
1	2A	1297	C	C4-C5-C6	5.03	119.91	117.40
1	2A	1740	G	N9-C4-C5	-5.03	103.39	105.40
1	2A	1863	G	C2-N3-C4	-5.03	109.39	111.90
32	2a	1145	C	O5'-P-OP2	-5.03	101.17	105.70
1	1A	215	G	C8-N9-C4	-5.03	104.39	106.40
1	1A	1613	A	C8-N9-C4	5.03	107.81	105.80
1	1A	1874	C	C5-C4-N4	-5.03	116.68	120.20
1	1A	2055	A	C6-N1-C2	-5.03	115.58	118.60
1	1A	2450	U	OP2-P-O3'	5.03	116.26	105.20
32	1a	419	C	OP1-P-O3'	5.03	116.25	105.20
1	1A	1322	A	O4'-C1'-N9	-5.02	104.18	108.20
1	2A	174	C	N3-C4-C5	-5.02	119.89	121.90
32	2a	306	G	N1-C2-N2	5.02	120.72	116.20
1	1A	548	C	OP2-P-O3'	5.02	116.25	105.20
1	1A	783	C	O5'-P-OP1	-5.02	101.18	105.70
1	1A	877	G	OP1-P-OP2	-5.02	112.07	119.60
1	1A	1676	G	N3-C4-N9	-5.02	122.99	126.00
1	1A	2384	G	N1-C6-O6	5.02	122.91	119.90
1	1A	2565	G	N3-C4-C5	-5.02	126.09	128.60
1	1A	2844	G	C6-C5-N7	5.02	133.41	130.40
32	1a	73	G	O4'-C1'-N9	5.02	112.22	108.20
32	1a	641	U	N3-C4-O4	5.02	122.92	119.40
1	2A	2582	G	N3-C2-N2	5.02	123.42	119.90
32	2a	902	G	C5-C6-N1	5.02	114.01	111.50
32	2a	1495	U	N3-C4-C5	-5.02	111.59	114.60
1	1A	385	G	C4-C5-N7	5.02	112.81	110.80
1	1A	1155	C	C5-C4-N4	-5.02	116.69	120.20
1	1A	1659	G	C2-N3-C4	-5.02	109.39	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2204	G	C8-N9-C1'	5.02	133.53	127.00
1	1A	2498	G	C8-N9-C1'	-5.02	120.47	127.00
1	2A	525	U	C5-C4-O4	5.02	128.91	125.90
32	2a	1335	C	C6-N1-C1'	-5.02	114.78	120.80
1	1A	484	G	OP1-P-OP2	5.02	127.13	119.60
1	1A	822	G	O5'-P-OP1	-5.02	101.18	105.70
1	1A	1976	G	N3-C2-N2	-5.02	116.39	119.90
1	1A	2134	G	C6-N1-C2	-5.02	122.09	125.10
1	1A	2270	C	C6-N1-C2	-5.02	118.29	120.30
1	1A	2348	A	C4-C5-N7	5.02	113.21	110.70
1	1A	2702	C	OP1-P-O3'	5.02	116.24	105.20
1	1A	2748	G	C5-C6-O6	5.02	131.61	128.60
32	1a	792	A	C4-N9-C1'	-5.02	117.26	126.30
32	1a	1286	A	O5'-P-OP2	5.02	116.72	110.70
1	2A	114	U	C2-N1-C1'	5.02	123.72	117.70
1	2A	1041	C	N3-C2-O2	-5.02	118.39	121.90
1	2A	1084	A	N3-C4-C5	5.02	130.31	126.80
1	2A	2816	C	OP1-P-OP2	5.02	127.13	119.60
32	2a	108	G	C5-C6-O6	-5.02	125.59	128.60
1	1A	555	G	N9-C4-C5	-5.02	103.39	105.40
1	1A	613	A	OP1-P-OP2	-5.02	112.08	119.60
1	1A	1708	G	C4-C5-N7	-5.02	108.79	110.80
1	1A	2233	G	N9-C4-C5	5.02	107.41	105.40
1	1A	2450	U	C2-N3-C4	-5.02	123.99	127.00
32	1a	330	C	C6-N1-C2	-5.02	118.29	120.30
1	2A	882	G	N1-C2-N2	5.02	120.72	116.20
1	2A	989	G	C4-C5-N7	5.02	112.81	110.80
1	2A	1292	U	O5'-P-OP2	-5.02	101.18	105.70
1	2A	1913	A	C4-N9-C1'	5.02	135.33	126.30
1	2A	2302	G	C5-C6-O6	5.02	131.61	128.60
32	2a	604	G	C8-N9-C4	5.02	108.41	106.40
32	2a	1487	G	OP1-P-OP2	-5.02	112.07	119.60
1	1A	236	G	C5-N7-C8	-5.02	101.79	104.30
1	1A	874	U	C3'-C2'-C1'	5.02	105.51	101.50
1	1A	1873	G	C4-C5-N7	5.02	112.81	110.80
1	2A	666	G	N9-C4-C5	-5.02	103.39	105.40
32	2a	1469	G	N3-C2-N2	-5.02	116.39	119.90
1	1A	799	A	N1-C2-N3	5.01	131.81	129.30
1	1A	839	G	N1-C6-O6	-5.01	116.89	119.90
1	1A	1051	C	N3-C4-N4	-5.01	114.49	118.00
1	1A	1918	G	N1-C6-O6	-5.01	116.89	119.90
1	1A	2085	C	OP2-P-O3'	5.01	116.23	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2261	U	N3-C4-C5	5.01	117.61	114.60
1	1A	2609	G	C2-N3-C4	-5.01	109.39	111.90
32	1a	120	A	O5'-P-OP2	5.01	116.72	110.70
32	1a	595	G	N3-C4-N9	5.01	129.01	126.00
32	1a	1285	A	P-O3'-C3'	5.01	125.72	119.70
1	2A	277	C	P-O3'-C3'	5.01	125.72	119.70
1	2A	958	U	C4-C5-C6	5.01	122.71	119.70
32	2a	663	A	O5'-P-OP1	-5.01	101.19	105.70
1	1A	1504	A	N1-C6-N6	5.01	121.61	118.60
1	1A	2480	G	O4'-C1'-N9	5.01	112.21	108.20
1	1A	2762	A	N1-C6-N6	-5.01	115.59	118.60
32	1a	361	G	C4-C5-N7	5.01	112.81	110.80
1	2A	1844	C	C5-C6-N1	-5.01	118.49	121.00
32	2a	189(E)	U	N1-C2-O2	5.01	126.31	122.80
1	1A	425	G	C5-C6-N1	-5.01	109.00	111.50
1	1A	1340	U	N1-C2-N3	5.01	117.91	114.90
1	1A	1439	A	C5-C6-N6	5.01	127.71	123.70
1	1A	1694	G	O4'-C1'-N9	-5.01	104.19	108.20
1	1A	2261	U	OP1-P-OP2	-5.01	112.08	119.60
1	1A	2357	G	N1-C2-N2	-5.01	111.69	116.20
1	2A	209	C	N1-C2-O2	5.01	121.91	118.90
1	2A	1966	A	N9-C4-C5	5.01	107.81	105.80
32	2a	1086	U	N3-C2-O2	-5.01	118.69	122.20
32	2a	1370	G	C4-C5-N7	5.01	112.81	110.80
1	1A	25	U	C5-C6-N1	5.01	125.20	122.70
1	1A	1768	U	C5-C6-N1	5.01	125.20	122.70
1	1A	2348	A	N7-C8-N9	-5.01	111.30	113.80
1	1A	2459	G	C6-N1-C2	-5.01	122.09	125.10
1	1A	2625	U	O5'-P-OP2	-5.01	101.19	105.70
1	1A	2844	G	N1-C6-O6	-5.01	116.89	119.90
32	1a	183	G	N3-C4-C5	-5.01	126.09	128.60
32	1a	802	A	N1-C6-N6	5.01	121.61	118.60
32	1a	1158	C	N3-C4-C5	-5.01	119.90	121.90
1	2A	882	G	C6-C5-N7	5.01	133.41	130.40
1	2A	1128	A	N7-C8-N9	-5.01	111.30	113.80
1	2A	2058	A	N3-C4-N9	5.01	131.41	127.40
1	2A	2877	G	C8-N9-C4	5.01	108.40	106.40
32	2a	22	G	C5-C6-N1	5.01	114.00	111.50
1	1A	2476	C	C5-C4-N4	-5.01	116.69	120.20
2	1B	77	U	N3-C4-O4	5.01	122.91	119.40
27	15	20	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	2A	65	C	C6-N1-C2	-5.01	118.30	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1122	G	C5-C6-O6	-5.01	125.59	128.60
1	2A	1508	A	N9-C4-C5	-5.01	103.80	105.80
32	2a	563	A	C2-N3-C4	-5.01	108.10	110.60
1	1A	23	G	N1-C2-N2	5.01	120.71	116.20
1	1A	330	U	C6-N1-C2	-5.01	118.00	121.00
1	1A	741	U	C4-C5-C6	5.01	122.70	119.70
1	1A	950	C	N3-C4-C5	5.01	123.90	121.90
1	1A	1042	A	O5'-P-OP2	5.01	116.71	110.70
1	1A	2644	A	OP1-P-OP2	5.01	127.11	119.60
32	1a	157	G	N9-C4-C5	5.01	107.40	105.40
32	1a	557	G	C8-N9-C1'	-5.01	120.49	127.00
32	1a	766	A	C5-C6-N6	-5.01	119.69	123.70
1	2A	764	A	O4'-C1'-N9	5.01	112.21	108.20
1	2A	909	A	N1-C6-N6	-5.01	115.60	118.60
1	2A	1682	G	C5-C6-O6	5.01	131.60	128.60
32	2a	1079	G	C8-N9-C4	-5.01	104.40	106.40
1	1A	2723	A	C5-N7-C8	-5.00	101.40	103.90
32	1a	821	G	O5'-P-OP2	5.00	116.71	110.70
1	2A	1563	G	N1-C2-N2	-5.00	111.70	116.20
1	1A	1006	C	OP1-P-O3'	5.00	116.21	105.20
9	1N	35	ARG	CA-CB-CG	5.00	124.41	113.40
32	1a	896	C	C5-C6-N1	-5.00	118.50	121.00
32	1a	905	U	C5-C6-N1	-5.00	120.20	122.70
1	2A	1001	A	N1-C6-N6	5.00	121.60	118.60
1	2A	1353	A	N7-C8-N9	-5.00	111.30	113.80
1	2A	1547	C	C4-C5-C6	5.00	119.90	117.40
1	2A	1774	C	C2-N3-C4	5.00	122.40	119.90
32	2a	578	C	C5-C4-N4	5.00	123.70	120.20
1	1A	200	A	N7-C8-N9	-5.00	111.30	113.80
1	1A	524	U	C2-N3-C4	-5.00	124.00	127.00
1	1A	1090	G	O5'-P-OP2	-5.00	101.20	105.70
3	1D	242	ARG	CG-CD-NE	5.00	122.31	111.80
32	1a	204	U	C6-N1-C1'	-5.00	114.20	121.20
1	2A	139(A)	G	N3-C4-N9	5.00	129.00	126.00
1	2A	452	G	C5-C6-O6	-5.00	125.60	128.60
1	2A	1844	C	N3-C4-C5	5.00	123.90	121.90
1	2A	2371	G	C8-N9-C4	5.00	108.40	106.40
1	2A	2783	G	OP2-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	18	13	ARG	Peptide
19	1X	93	GLU	Peptide
19	2X	93	GLU	Peptide
44	2l	86	ARG	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
3	1D	273/275 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/204 (99%)	194 (96%)	7 (4%)	1 (0%)	29	61
4	2E	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	29	61
5	1F	201/203 (99%)	194 (96%)	6 (3%)	1 (0%)	29	61
5	2F	201/203 (99%)	195 (97%)	4 (2%)	2 (1%)	15	44
6	1G	179/181 (99%)	164 (92%)	12 (7%)	3 (2%)	9	29
6	2G	179/181 (99%)	163 (91%)	14 (8%)	2 (1%)	14	41
7	1H	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
7	2H	171/174 (98%)	160 (94%)	11 (6%)	0	100	100
8	1I	145/147 (99%)	128 (88%)	15 (10%)	2 (1%)	11	34
8	2I	144/147 (98%)	125 (87%)	18 (12%)	1 (1%)	22	53
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	49
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
11	2P	147/149 (99%)	140 (95%)	6 (4%)	1 (1%)	22	53
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	53
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	53
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	17	46
14	2S	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	17	46
15	1T	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
15	2T	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/116 (98%)	114 (100%)	0	0	100	100
16	2U	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	44
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	44
18	1W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
21	1Z	201/203 (99%)	190 (94%)	10 (5%)	1 (0%)	29	61
21	2Z	199/203 (98%)	187 (94%)	12 (6%)	0	100	100
22	10	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
22	20	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
23	11	95/97 (98%)	94 (99%)	0	1 (1%)	14	41
23	21	95/97 (98%)	92 (97%)	2 (2%)	1 (1%)	14	41
24	12	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
24	22	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
25	13	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
25	23	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
26	14	67/69 (97%)	55 (82%)	9 (13%)	3 (4%)	2	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/69 (97%)	54 (81%)	6 (9%)	7 (10%)	0	1
27	15	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
27	25	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
28	16	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
28	26	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
29	17	46/48 (96%)	46 (100%)	0	0	100	100
29	27	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
30	18	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
30	28	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1x	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
33	2x	94/97 (97%)	92 (98%)	2 (2%)	0	100	100
34	1b	229/231 (99%)	193 (84%)	27 (12%)	9 (4%)	3	10
34	2b	229/231 (99%)	194 (85%)	28 (12%)	7 (3%)	4	14
35	1c	204/206 (99%)	177 (87%)	26 (13%)	1 (0%)	29	61
35	2c	204/206 (99%)	177 (87%)	23 (11%)	4 (2%)	7	24
36	1d	206/208 (99%)	187 (91%)	16 (8%)	3 (2%)	10	33
36	2d	206/208 (99%)	187 (91%)	16 (8%)	3 (2%)	10	33
37	1e	146/148 (99%)	136 (93%)	9 (6%)	1 (1%)	22	53
37	2e	146/148 (99%)	135 (92%)	11 (8%)	0	100	100
38	1f	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
38	2f	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
39	1g	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
39	2g	153/155 (99%)	146 (95%)	4 (3%)	3 (2%)	7	24
40	1h	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
40	2h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
41	1i	125/127 (98%)	109 (87%)	14 (11%)	2 (2%)	9	31
41	2i	124/127 (98%)	106 (86%)	14 (11%)	4 (3%)	4	13
42	1j	95/97 (98%)	79 (83%)	13 (14%)	3 (3%)	4	13
42	2j	94/97 (97%)	79 (84%)	12 (13%)	3 (3%)	4	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1k	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	46
43	2k	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
44	1l	119/122 (98%)	112 (94%)	6 (5%)	1 (1%)	19	49
44	2l	119/122 (98%)	108 (91%)	9 (8%)	2 (2%)	9	29
45	1m	114/116 (98%)	103 (90%)	9 (8%)	2 (2%)	8	28
45	2m	112/116 (97%)	102 (91%)	8 (7%)	2 (2%)	8	28
46	1n	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
46	2n	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
47	1o	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
47	2o	86/88 (98%)	80 (93%)	5 (6%)	1 (1%)	13	39
48	1p	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
48	2p	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
49	1q	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	44
49	2q	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
50	1r	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
50	2r	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
51	1s	81/83 (98%)	71 (88%)	8 (10%)	2 (2%)	5	19
51	2s	81/83 (98%)	72 (89%)	6 (7%)	3 (4%)	3	11
52	1t	94/98 (96%)	88 (94%)	3 (3%)	3 (3%)	4	13
52	2t	96/98 (98%)	87 (91%)	6 (6%)	3 (3%)	4	14
53	1u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2	7
53	2u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2	7
54	1y	14/16 (88%)	14 (100%)	0	0	100	100
54	2y	14/16 (88%)	14 (100%)	0	0	100	100
All	All	11657/11874 (98%)	10874 (93%)	682 (6%)	101 (1%)	17	46

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	52	LEU
6	1G	49	ASP
6	1G	51	ARG
8	1I	73	GLU
14	1S	59	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	1V	79	VAL
23	11	3	LYS
34	1b	17	PHE
34	1b	22	LYS
34	1b	125	PRO
34	1b	231	GLU
42	1j	79	ARG
51	1s	12	ASP
52	1t	95	ALA
5	2F	21	ALA
5	2F	130	ALA
6	2G	81	LYS
8	2I	10	GLU
23	21	3	LYS
26	24	45	GLY
26	24	47	GLN
26	24	60	GLN
26	24	65	ASP
41	2i	44	VAL
41	2i	54	ASP
42	2j	79	ARG
45	2m	67	GLU
51	2s	28	LYS
52	2t	95	ALA
5	1F	130	ALA
26	14	45	GLY
26	14	49	PHE
34	1b	37	ASN
34	1b	127	ILE
36	1d	171	GLY
41	1i	44	VAL
42	1j	32	ALA
53	1u	3	LYS
6	2G	78	SER
10	2O	5	GLN
17	2V	79	VAL
34	2b	17	PHE
34	2b	123	ALA
34	2b	125	PRO
34	2b	127	ILE
34	2b	228	GLY
35	2c	61	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2d	171	GLY
41	2i	11	LYS
44	2l	87	GLY
44	2l	88	GLY
8	1I	105	HIS
10	1O	5	GLN
12	1Q	59	ARG
26	14	55	ARG
4	2E	51	PHE
12	2Q	59	ARG
26	24	49	PHE
26	24	62	ARG
34	2b	232	PRO
39	2g	6	ARG
39	2g	7	ALA
45	2m	5	ALA
52	2t	100	ILE
52	2t	102	GLY
6	1G	78	SER
43	1k	117	ASN
45	1m	67	GLU
51	1s	27	GLU
42	2j	32	ALA
51	2s	27	GLU
53	2u	7	ARG
34	1b	83	MET
35	1c	144	SER
41	1i	109	VAL
45	1m	46	LYS
49	1q	49	GLU
52	1t	10	LEU
11	2P	29	LYS
14	2S	89	ARG
34	2b	120	ALA
35	2c	108	ASN
35	2c	144	SER
35	2c	156	ARG
47	2o	88	ARG
51	2s	29	ARG
36	1d	136	PRO
37	1e	147	ASP
44	1l	91	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	24	55	ARG
36	2d	136	PRO
41	2i	109	VAL
52	1t	100	ILE
36	1d	5	ILE
42	1j	82	ILE
42	2j	77	PRO
21	1Z	158	PRO
34	1b	202	PRO
36	2d	5	ILE
39	2g	55	GLY
34	1b	124	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
3	1D	214/217 (99%)	194 (91%)	20 (9%)	9	26
3	2D	215/217 (99%)	189 (88%)	26 (12%)	5	15
4	1E	164/165 (99%)	148 (90%)	16 (10%)	8	24
4	2E	164/165 (99%)	147 (90%)	17 (10%)	7	21
5	1F	160/161 (99%)	137 (86%)	23 (14%)	3	10
5	2F	159/161 (99%)	142 (89%)	17 (11%)	6	20
6	1G	144/155 (93%)	132 (92%)	12 (8%)	11	32
6	2G	142/155 (92%)	132 (93%)	10 (7%)	15	40
7	1H	144/145 (99%)	132 (92%)	12 (8%)	11	32
7	2H	143/145 (99%)	130 (91%)	13 (9%)	9	27
8	1I	111/123 (90%)	96 (86%)	15 (14%)	4	11
8	2I	108/123 (88%)	95 (88%)	13 (12%)	5	15
9	1N	119/119 (100%)	106 (89%)	13 (11%)	6	19
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1O	100/100 (100%)	92 (92%)	8 (8%)	12	34
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19	48
11	1P	115/116 (99%)	108 (94%)	7 (6%)	18	48
11	2P	115/116 (99%)	105 (91%)	10 (9%)	10	30
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	14	38
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
13	1R	101/101 (100%)	89 (88%)	12 (12%)	5	16
13	2R	101/101 (100%)	87 (86%)	14 (14%)	3	11
14	1S	87/87 (100%)	76 (87%)	11 (13%)	4	14
14	2S	85/87 (98%)	76 (89%)	9 (11%)	6	20
15	1T	115/115 (100%)	107 (93%)	8 (7%)	15	40
15	2T	113/115 (98%)	107 (95%)	6 (5%)	22	54
16	1U	93/93 (100%)	82 (88%)	11 (12%)	5	16
16	2U	93/93 (100%)	87 (94%)	6 (6%)	17	44
17	1V	81/82 (99%)	71 (88%)	10 (12%)	4	15
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6	18
18	1W	90/91 (99%)	81 (90%)	9 (10%)	7	22
18	2W	90/91 (99%)	82 (91%)	8 (9%)	9	28
19	1X	77/77 (100%)	73 (95%)	4 (5%)	23	55
19	2X	77/77 (100%)	73 (95%)	4 (5%)	23	55
20	1Y	86/88 (98%)	81 (94%)	5 (6%)	20	50
20	2Y	86/88 (98%)	81 (94%)	5 (6%)	20	50
21	1Z	169/176 (96%)	152 (90%)	17 (10%)	7	22
21	2Z	165/176 (94%)	149 (90%)	16 (10%)	8	24
22	10	61/62 (98%)	54 (88%)	7 (12%)	5	17
22	20	61/62 (98%)	56 (92%)	5 (8%)	11	33
23	11	79/82 (96%)	75 (95%)	4 (5%)	24	55
23	21	81/82 (99%)	72 (89%)	9 (11%)	6	19
24	12	65/66 (98%)	61 (94%)	4 (6%)	18	47
24	22	66/66 (100%)	65 (98%)	1 (2%)	65	89
25	13	51/51 (100%)	48 (94%)	3 (6%)	19	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	23	50/51 (98%)	47 (94%)	3 (6%)	19	48
26	14	58/62 (94%)	49 (84%)	9 (16%)	2	8
26	24	54/62 (87%)	48 (89%)	6 (11%)	6	19
27	15	51/51 (100%)	49 (96%)	2 (4%)	32	66
27	25	50/51 (98%)	47 (94%)	3 (6%)	19	48
28	16	51/51 (100%)	44 (86%)	7 (14%)	3	11
28	26	50/51 (98%)	46 (92%)	4 (8%)	12	34
29	17	41/41 (100%)	37 (90%)	4 (10%)	8	24
29	27	41/41 (100%)	39 (95%)	2 (5%)	25	57
30	18	54/54 (100%)	48 (89%)	6 (11%)	6	19
30	28	54/54 (100%)	49 (91%)	5 (9%)	9	26
31	19	34/34 (100%)	32 (94%)	2 (6%)	19	49
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1x	82/83 (99%)	77 (94%)	5 (6%)	18	48
33	2x	79/83 (95%)	69 (87%)	10 (13%)	4	14
34	1b	191/199 (96%)	162 (85%)	29 (15%)	3	8
34	2b	187/199 (94%)	164 (88%)	23 (12%)	4	15
35	1c	144/160 (90%)	141 (98%)	3 (2%)	53	84
35	2c	140/160 (88%)	126 (90%)	14 (10%)	7	22
36	1d	171/180 (95%)	155 (91%)	16 (9%)	8	26
36	2d	172/180 (96%)	157 (91%)	15 (9%)	10	30
37	1e	114/114 (100%)	104 (91%)	10 (9%)	10	29
37	2e	114/114 (100%)	105 (92%)	9 (8%)	12	34
38	1f	85/90 (94%)	81 (95%)	4 (5%)	26	59
38	2f	85/90 (94%)	79 (93%)	6 (7%)	14	39
39	1g	120/126 (95%)	113 (94%)	7 (6%)	20	50
39	2g	119/126 (94%)	112 (94%)	7 (6%)	19	49
40	1h	116/118 (98%)	108 (93%)	8 (7%)	15	41
40	2h	114/118 (97%)	108 (95%)	6 (5%)	22	54
41	1i	91/98 (93%)	83 (91%)	8 (9%)	10	29
41	2i	88/98 (90%)	80 (91%)	8 (9%)	9	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	1j	68/87 (78%)	62 (91%)	6 (9%)	10	29
42	2j	68/87 (78%)	64 (94%)	4 (6%)	19	49
43	1k	83/86 (96%)	80 (96%)	3 (4%)	35	69
43	2k	83/86 (96%)	74 (89%)	9 (11%)	6	19
44	1l	96/102 (94%)	92 (96%)	4 (4%)	30	63
44	2l	96/102 (94%)	89 (93%)	7 (7%)	14	38
45	1m	90/94 (96%)	81 (90%)	9 (10%)	7	22
45	2m	87/94 (93%)	77 (88%)	10 (12%)	5	17
46	1n	49/49 (100%)	43 (88%)	6 (12%)	5	15
46	2n	49/49 (100%)	46 (94%)	3 (6%)	18	48
47	1o	78/79 (99%)	72 (92%)	6 (8%)	13	35
47	2o	78/79 (99%)	73 (94%)	5 (6%)	17	45
48	1p	69/71 (97%)	60 (87%)	9 (13%)	4	13
48	2p	68/71 (96%)	57 (84%)	11 (16%)	2	7
49	1q	94/94 (100%)	91 (97%)	3 (3%)	39	73
49	2q	94/94 (100%)	87 (93%)	7 (7%)	13	37
50	1r	59/59 (100%)	54 (92%)	5 (8%)	10	31
50	2r	59/59 (100%)	55 (93%)	4 (7%)	16	42
51	1s	68/72 (94%)	60 (88%)	8 (12%)	5	16
51	2s	67/72 (93%)	62 (92%)	5 (8%)	13	37
52	1t	71/76 (93%)	65 (92%)	6 (8%)	10	31
52	2t	70/76 (92%)	62 (89%)	8 (11%)	5	18
53	1u	18/18 (100%)	16 (89%)	2 (11%)	6	19
53	2u	18/18 (100%)	18 (100%)	0	100	100
54	1y	14/15 (93%)	13 (93%)	1 (7%)	14	39
54	2y	14/15 (93%)	12 (86%)	2 (14%)	3	10
All	All	9552/9892 (97%)	8702 (91%)	850 (9%)	9	28

All (850) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	13	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1D	37	LEU
3	1D	61	LEU
3	1D	69	ARG
3	1D	89	SER
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	106	ILE
3	1D	111	LEU
3	1D	113	VAL
3	1D	141	VAL
3	1D	142	VAL
3	1D	155	LEU
3	1D	211	ARG
3	1D	217	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	1	MET
4	1E	7	VAL
4	1E	9	VAL
4	1E	34	VAL
4	1E	49	LEU
4	1E	73	GLU
4	1E	75	VAL
4	1E	78	LEU
4	1E	89	ASP
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	154	LYS
4	1E	175	VAL
4	1E	181	LEU
5	1F	12	LEU
5	1F	18	ARG
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	74	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	94	PRO
5	1F	110	LEU
5	1F	125	LEU
5	1F	127	GLU
5	1F	132	VAL
5	1F	137	LYS
5	1F	140	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	170	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	197	ASP
5	1F	200	GLU
5	1F	201	VAL
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	43	LEU
6	1G	78	SER
6	1G	79	ASN
6	1G	126	ASP
6	1G	140	ILE
6	1G	148	MET
6	1G	153	ARG
6	1G	165	THR
6	1G	170	ARG
7	1H	2	SER
7	1H	6	ARG
7	1H	13	LYS
7	1H	44	VAL
7	1H	45	VAL
7	1H	71	LEU
7	1H	85	LYS
7	1H	105	LEU
7	1H	119	GLU
7	1H	134	SER
7	1H	139	GLN
7	1H	153	LYS
8	1I	5	LEU
8	1I	9	LEU
8	1I	10	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	15	VAL
8	1I	38	LEU
8	1I	50	ARG
8	1I	64	GLU
8	1I	69	LYS
8	1I	78	THR
8	1I	85	GLU
8	1I	92	VAL
8	1I	101	LEU
8	1I	104	GLN
8	1I	109	ILE
8	1I	140	LEU
9	1N	1	MET
9	1N	9	VAL
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	62	VAL
9	1N	67	LEU
9	1N	73	THR
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	121	LYS
10	1O	8	LEU
10	1O	10	VAL
10	1O	20	MET
10	1O	64	ARG
10	1O	94	ARG
10	1O	107	ARG
10	1O	108	GLU
10	1O	113	LYS
11	1P	1	MET
11	1P	3	LEU
11	1P	59	LEU
11	1P	83	VAL
11	1P	99	LEU
11	1P	112	LEU
11	1P	125	VAL
12	1Q	2	LEU
12	1Q	6	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	1Q	7	MET
12	1Q	18	LYS
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	130	LYS
12	1Q	133	ARG
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	75	LEU
13	1R	86	ARG
13	1R	96	ARG
13	1R	111	LEU
13	1R	114	VAL
13	1R	117	VAL
14	1S	14	VAL
14	1S	17	ARG
14	1S	21	THR
14	1S	25	ARG
14	1S	36	TYR
14	1S	49	VAL
14	1S	50	SER
14	1S	52	SER
14	1S	59	LYS
14	1S	68	GLN
14	1S	69	VAL
15	1T	13	ARG
15	1T	28	VAL
15	1T	34	VAL
15	1T	39	ARG
15	1T	59	THR
15	1T	78	LEU
15	1T	96	ARG
15	1T	108	ARG
16	1U	5	LYS
16	1U	8	VAL
16	1U	31	SER
16	1U	50	ARG
16	1U	52	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1U	59	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	95	LEU
16	1U	104	GLN
16	1U	117	GLN
17	1V	28	GLU
17	1V	35	LEU
17	1V	46	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	82	ARG
17	1V	100	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	27	LYS
18	1W	67	ASP
18	1W	100	THR
18	1W	107	LEU
19	1X	45	THR
19	1X	57	LEU
19	1X	66	LEU
19	1X	88	LYS
20	1Y	6	HIS
20	1Y	7	VAL
20	1Y	43	ASN
20	1Y	90	LEU
20	1Y	92	ASN
21	1Z	11	GLU
21	1Z	31	ARG
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	61	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	93	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	94	GLU
21	1Z	102	LEU
21	1Z	126	VAL
21	1Z	135	GLU
21	1Z	150	LEU
21	1Z	161	VAL
21	1Z	162	GLU
21	1Z	170	THR
21	1Z	203	GLU
22	10	10	THR
22	10	11	ARG
22	10	14	ARG
22	10	39	ARG
22	10	55	ARG
22	10	59	LEU
22	10	82	ARG
23	11	21	ARG
23	11	30	VAL
23	11	59	THR
23	11	95	LEU
24	12	3	LEU
24	12	8	LYS
24	12	53	LEU
24	12	70	GLN
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
26	14	13	ARG
26	14	23	GLU
26	14	30	GLU
26	14	49	PHE
26	14	56	VAL
26	14	57	GLU
26	14	59	PHE
26	14	65	ASP
26	14	69	LYS
27	15	16	ARG
27	15	29	THR
28	16	6	ARG
28	16	14	THR
28	16	19	ARG
28	16	28	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	16	40	CYS
28	16	48	VAL
28	16	52	VAL
29	17	1	MET
29	17	10	ARG
29	17	24	THR
29	17	43	THR
30	18	14	VAL
30	18	23	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	52	LYS
31	19	27	CYS
31	19	35	ARG
33	2x	3	MET
33	2x	9	GLN
33	2x	11	GLU
33	2x	13	THR
33	2x	24	LEU
33	2x	32	THR
33	2x	41	LEU
33	2x	60	VAL
33	2x	62	VAL
33	2x	96	ARG
34	1b	9	GLU
34	1b	17	PHE
34	1b	19	HIS
34	1b	21	ARG
34	1b	22	LYS
34	1b	24	TRP
34	1b	28	PHE
34	1b	35	GLU
34	1b	44	LEU
34	1b	45	GLN
34	1b	67	THR
34	1b	71	VAL
34	1b	73	THR
34	1b	76	GLN
34	1b	82	ARG
34	1b	111	ARG
34	1b	122	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1b	128	GLU
34	1b	130	ARG
34	1b	136	VAL
34	1b	157	ARG
34	1b	160	ASP
34	1b	178	ARG
34	1b	185	ILE
34	1b	187	LEU
34	1b	200	ILE
34	1b	201	ILE
34	1b	208	ILE
34	1b	226	ARG
35	1c	36	ASP
35	1c	38	ARG
35	1c	104	GLN
36	1d	8	VAL
36	1d	25	ARG
36	1d	28	SER
36	1d	31	CYS
36	1d	58	LEU
36	1d	59	ARG
36	1d	86	LYS
36	1d	107	ARG
36	1d	110	PHE
36	1d	127	THR
36	1d	135	LEU
36	1d	168	ARG
36	1d	173	TRP
36	1d	182	LYS
36	1d	194	LEU
36	1d	196	LEU
37	1e	9	LYS
37	1e	20	GLN
37	1e	24	ARG
37	1e	31	LEU
37	1e	34	VAL
37	1e	41	VAL
37	1e	75	THR
37	1e	91	LEU
37	1e	116	THR
37	1e	120	THR
38	1f	17	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	1f	40	VAL
38	1f	57	GLN
38	1f	73	ASN
39	1g	9	VAL
39	1g	15	ASP
39	1g	21	VAL
39	1g	97	GLN
39	1g	110	GLN
39	1g	115	ARG
39	1g	144	MET
40	1h	39	LEU
40	1h	52	ASP
40	1h	63	LEU
40	1h	68	ARG
40	1h	97	VAL
40	1h	104	ARG
40	1h	112	LEU
40	1h	120	THR
41	1i	42	ARG
41	1i	50	LEU
41	1i	53	VAL
41	1i	60	ASP
41	1i	81	ILE
41	1i	92	TYR
41	1i	103	THR
41	1i	125	TYR
42	1j	5	ARG
42	1j	42	THR
42	1j	56	HIS
42	1j	67	THR
42	1j	84	GLN
42	1j	100	THR
43	1k	31	THR
43	1k	70	LYS
43	1k	109	VAL
44	1l	18	VAL
44	1l	27	LEU
44	1l	33	ARG
44	1l	60	LEU
45	1m	8	GLU
45	1m	12	ASN
45	1m	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	1m	49	THR
45	1m	55	ARG
45	1m	56	LEU
45	1m	70	LEU
45	1m	80	ARG
45	1m	102	ARG
46	1n	3	ARG
46	1n	12	ARG
46	1n	18	VAL
46	1n	32	SER
46	1n	33	VAL
46	1n	44	LEU
47	1o	3	ILE
47	1o	5	LYS
47	1o	28	GLN
47	1o	39	LEU
47	1o	66	LEU
47	1o	88	ARG
48	1p	2	VAL
48	1p	5	ARG
48	1p	8	ARG
48	1p	42	ARG
48	1p	45	THR
48	1p	54	GLU
48	1p	62	VAL
48	1p	67	THR
48	1p	69	THR
49	1q	9	VAL
49	1q	63	ARG
49	1q	70	ARG
50	1r	31	LEU
50	1r	37	VAL
50	1r	47	THR
50	1r	76	LEU
50	1r	85	LEU
51	1s	4	SER
51	1s	16	LEU
51	1s	28	LYS
51	1s	37	ARG
51	1s	40	ILE
51	1s	41	VAL
51	1s	77	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1s	79	THR
52	1t	9	ASN
52	1t	10	LEU
52	1t	34	LYS
52	1t	58	LYS
52	1t	62	LEU
52	1t	84	LEU
53	1u	9	ARG
53	1u	24	ARG
33	1x	3	MET
33	1x	23	ARG
33	1x	24	LEU
33	1x	46	GLN
33	1x	87	LYS
54	1y	6	TYR
3	2D	3	VAL
3	2D	37	LEU
3	2D	38	LYS
3	2D	61	LEU
3	2D	89	SER
3	2D	94	LEU
3	2D	99	ASP
3	2D	103	ARG
3	2D	106	ILE
3	2D	111	LEU
3	2D	113	VAL
3	2D	116	GLN
3	2D	138	VAL
3	2D	141	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	169	GLU
3	2D	211	ARG
3	2D	217	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	274	ARG
3	2D	275	LYS
3	2D	276	LYS
4	2E	7	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	24	THR
4	2E	33	VAL
4	2E	34	VAL
4	2E	49	LEU
4	2E	75	VAL
4	2E	78	LEU
4	2E	87	GLU
4	2E	113	PHE
4	2E	116	VAL
4	2E	144	ARG
4	2E	154	LYS
4	2E	163	GLU
4	2E	170	LEU
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
5	2F	24	LEU
5	2F	33	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	60	SER
5	2F	74	ARG
5	2F	88	VAL
5	2F	125	LEU
5	2F	132	VAL
5	2F	140	LEU
5	2F	144	LYS
5	2F	170	LEU
5	2F	175	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	28	VAL
6	2G	49	ASP
6	2G	60	LEU
6	2G	71	THR
6	2G	79	ASN
6	2G	126	ASP
6	2G	159	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	165	THR
7	2H	6	ARG
7	2H	13	LYS
7	2H	15	VAL
7	2H	23	ARG
7	2H	33	LEU
7	2H	47	GLU
7	2H	85	LYS
7	2H	88	LEU
7	2H	105	LEU
7	2H	122	THR
7	2H	134	SER
7	2H	136	ILE
7	2H	139	GLN
8	2I	5	LEU
8	2I	9	LEU
8	2I	15	VAL
8	2I	38	LEU
8	2I	44	LEU
8	2I	69	LYS
8	2I	75	LEU
8	2I	87	LYS
8	2I	99	GLU
8	2I	116	LEU
8	2I	121	LYS
8	2I	123	LEU
8	2I	140	LEU
9	2N	12	ARG
9	2N	28	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	46	VAL
9	2N	48	MET
9	2N	59	LYS
9	2N	62	VAL
9	2N	67	LEU
9	2N	68	GLU
9	2N	73	THR
9	2N	87	LEU
9	2N	97	ARG
9	2N	99	LEU
10	2O	10	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	2O	24	VAL
10	2O	66	LYS
10	2O	90	GLN
10	2O	98	VAL
10	2O	108	GLU
11	2P	2	LYS
11	2P	3	LEU
11	2P	30	THR
11	2P	32	THR
11	2P	59	LEU
11	2P	76	LYS
11	2P	83	VAL
11	2P	99	LEU
11	2P	112	LEU
11	2P	125	VAL
12	2Q	2	LEU
12	2Q	7	MET
12	2Q	16	ARG
12	2Q	18	LYS
12	2Q	21	THR
12	2Q	22	LYS
12	2Q	59	ARG
12	2Q	75	THR
12	2Q	106	VAL
13	2R	18	LEU
13	2R	29	LEU
13	2R	36	THR
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	75	LEU
13	2R	79	LEU
13	2R	86	ARG
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
13	2R	117	VAL
14	2S	14	VAL
14	2S	17	ARG
14	2S	21	THR
14	2S	36	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2S	50	SER
14	2S	52	SER
14	2S	68	GLN
14	2S	75	GLU
14	2S	85	VAL
15	2T	28	VAL
15	2T	39	ARG
15	2T	49	VAL
15	2T	65	LYS
15	2T	74	ARG
15	2T	96	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	59	ARG
16	2U	74	LEU
16	2U	83	LEU
16	2U	89	GLU
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	52	VAL
17	2V	53	GLU
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
17	2V	98	GLU
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	27	LYS
18	2W	100	THR
18	2W	107	LEU
19	2X	57	LEU
19	2X	66	LEU
19	2X	88	LYS
19	2X	92	LEU
20	2Y	6	HIS
20	2Y	7	VAL
20	2Y	57	GLN
20	2Y	73	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	2Y	88	LYS
21	2Z	18	LEU
21	2Z	33	LEU
21	2Z	41	LEU
21	2Z	42	VAL
21	2Z	46	LYS
21	2Z	61	LEU
21	2Z	72	ARG
21	2Z	86	VAL
21	2Z	107	THR
21	2Z	131	ARG
21	2Z	136	PHE
21	2Z	150	LEU
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	182	LYS
21	2Z	193	GLU
22	20	9	SER
22	20	10	THR
22	20	14	ARG
22	20	39	ARG
22	20	55	ARG
23	21	3	LYS
23	21	4	VAL
23	21	21	ARG
23	21	30	VAL
23	21	59	THR
23	21	62	VAL
23	21	75	GLU
23	21	85	LEU
23	21	95	LEU
24	22	53	LEU
25	23	23	LEU
25	23	31	LEU
25	23	54	VAL
26	24	13	ARG
26	24	53	GLU
26	24	56	VAL
26	24	61	ARG
26	24	63	TYR
26	24	69	LYS
27	25	15	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	25	16	ARG
27	25	29	THR
28	26	6	ARG
28	26	14	THR
28	26	19	ARG
28	26	48	VAL
29	27	1	MET
29	27	43	THR
30	28	14	VAL
30	28	23	VAL
30	28	31	HIS
30	28	34	TRP
30	28	46	ARG
34	2b	10	LEU
34	2b	17	PHE
34	2b	23	ARG
34	2b	24	TRP
34	2b	28	PHE
34	2b	45	GLN
34	2b	82	ARG
34	2b	94	ASN
34	2b	111	ARG
34	2b	114	ARG
34	2b	126	GLU
34	2b	128	GLU
34	2b	135	GLN
34	2b	154	LEU
34	2b	157	ARG
34	2b	158	LEU
34	2b	175	ARG
34	2b	200	ILE
34	2b	208	ILE
34	2b	222	ILE
34	2b	224	GLN
34	2b	226	ARG
34	2b	230	VAL
35	2c	3	ASN
35	2c	15	THR
35	2c	16	ARG
35	2c	32	LEU
35	2c	44	GLU
35	2c	45	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2c	82	GLU
35	2c	105	GLU
35	2c	115	LEU
35	2c	127	ARG
35	2c	131	ARG
35	2c	152	ILE
35	2c	162	GLN
35	2c	192	THR
36	2d	8	VAL
36	2d	13	ARG
36	2d	28	SER
36	2d	31	CYS
36	2d	34	GLU
36	2d	58	LEU
36	2d	59	ARG
36	2d	65	ARG
36	2d	107	ARG
36	2d	108	LEU
36	2d	127	THR
36	2d	135	LEU
36	2d	150	GLU
36	2d	178	VAL
36	2d	194	LEU
37	2e	24	ARG
37	2e	31	LEU
37	2e	34	VAL
37	2e	40	ARG
37	2e	41	VAL
37	2e	69	VAL
37	2e	72	GLN
37	2e	91	LEU
37	2e	150	ARG
38	2f	17	SER
38	2f	40	VAL
38	2f	63	TYR
38	2f	72	VAL
38	2f	73	ASN
38	2f	94	GLN
39	2g	13	GLN
39	2g	15	ASP
39	2g	50	ILE
39	2g	104	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	2g	113	GLU
39	2g	115	ARG
39	2g	138	LYS
40	2h	54	ASP
40	2h	63	LEU
40	2h	91	ARG
40	2h	97	VAL
40	2h	104	ARG
40	2h	112	LEU
41	2i	7	THR
41	2i	64	THR
41	2i	65	VAL
41	2i	66	ARG
41	2i	87	GLN
41	2i	103	THR
41	2i	125	TYR
41	2i	127	LYS
42	2j	25	GLU
42	2j	38	ILE
42	2j	45	ARG
42	2j	92	THR
43	2k	14	VAL
43	2k	18	ARG
43	2k	28	THR
43	2k	48	ILE
43	2k	84	VAL
43	2k	103	LEU
43	2k	109	VAL
43	2k	112	THR
43	2k	114	VAL
44	2l	18	VAL
44	2l	33	ARG
44	2l	52	LEU
44	2l	60	LEU
44	2l	89	ARG
44	2l	116	SER
44	2l	117	ARG
45	2m	3	ARG
45	2m	4	ILE
45	2m	12	ASN
45	2m	14	ARG
45	2m	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	2m	63	THR
45	2m	65	LYS
45	2m	70	LEU
45	2m	88	ARG
45	2m	110	ARG
46	2n	12	ARG
46	2n	32	SER
46	2n	44	LEU
47	2o	5	LYS
47	2o	10	LYS
47	2o	39	LEU
47	2o	64	ARG
47	2o	66	LEU
48	2p	2	VAL
48	2p	8	ARG
48	2p	25	ARG
48	2p	42	ARG
48	2p	45	THR
48	2p	54	GLU
48	2p	62	VAL
48	2p	67	THR
48	2p	69	THR
48	2p	72	ARG
48	2p	76	GLN
49	2q	6	LEU
49	2q	9	VAL
49	2q	16	GLN
49	2q	63	ARG
49	2q	70	ARG
49	2q	74	LEU
49	2q	87	LYS
50	2r	25	THR
50	2r	76	LEU
50	2r	85	LEU
50	2r	86	VAL
51	2s	13	ASP
51	2s	27	GLU
51	2s	56	GLN
51	2s	77	THR
51	2s	79	THR
52	2t	15	ARG
52	2t	24	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	2t	38	LYS
52	2t	45	GLN
52	2t	62	LEU
52	2t	74	LYS
52	2t	84	LEU
52	2t	89	ARG
54	2y	5	SER
54	2y	6	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	143	HIS
3	1D	253	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	75	HIS
5	1F	203	GLN
6	1G	108	ASN
7	1H	139	GLN
8	1I	105	HIS
10	1O	3	GLN
10	1O	5	GLN
14	1S	95	HIS
15	1T	58	ASN
16	1U	104	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	34	ASN
21	1Z	73	GLN
21	1Z	151	HIS
24	12	9	GLN
25	13	32	GLN
26	14	60	GLN
33	2x	33	HIS
33	2x	79	ASN
35	1c	6	HIS
35	1c	102	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1c	104	GLN
36	1d	77	ASN
36	1d	119	GLN
36	1d	123	HIS
36	1d	125	HIS
36	1d	129	ASN
38	1f	73	ASN
38	1f	100	ASN
39	1g	28	ASN
39	1g	110	GLN
40	1h	82	HIS
41	1i	3	GLN
41	1i	58	HIS
41	1i	73	GLN
42	1j	56	HIS
42	1j	84	GLN
44	1l	99	HIS
47	1o	28	GLN
48	1p	13	HIS
49	1q	16	GLN
49	1q	26	GLN
51	1s	69	HIS
51	1s	83	HIS
52	1t	18	GLN
33	1x	38	HIS
3	2D	87	ASN
3	2D	126	GLN
3	2D	253	GLN
5	2F	69	HIS
5	2F	75	HIS
6	2G	26	GLN
9	2N	8	GLN
12	2Q	12	GLN
12	2Q	123	HIS
15	2T	58	ASN
16	2U	104	GLN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	34	ASN
21	2Z	73	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	20	50	ASN
22	20	70	GLN
25	23	32	GLN
26	24	46	GLN
34	2b	19	HIS
34	2b	78	GLN
35	2c	6	HIS
35	2c	162	GLN
36	2d	77	ASN
36	2d	116	GLN
36	2d	119	GLN
36	2d	123	HIS
36	2d	125	HIS
36	2d	161	ASN
37	2e	72	GLN
38	2f	94	GLN
38	2f	100	ASN
39	2g	28	ASN
39	2g	86	GLN
41	2i	3	GLN
41	2i	58	HIS
41	2i	117	HIS
42	2j	69	ASN
43	2k	117	ASN
44	2l	99	HIS
47	2o	28	GLN
48	2p	16	HIS
49	2q	26	GLN
51	2s	14	HIS
51	2s	65	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	396 (13%)	51 (1%)
1	2A	2856/2915 (97%)	414 (14%)	49 (1%)
2	1B	119/120 (99%)	5 (4%)	0
2	2B	118/120 (98%)	5 (4%)	0
32	1a	1494/1521 (98%)	319 (21%)	0
32	2a	1498/1521 (98%)	305 (20%)	0
All	All	8950/9112 (98%)	1444 (16%)	100 (1%)

All (1444) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	60	G
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	185	A
1	1A	188	A
1	1A	189	U
1	1A	194	G
1	1A	202	A
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	255	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	288	U
1	1A	289	G
1	1A	303	C
1	1A	304	C
1	1A	335	A
1	1A	354	A
1	1A	376	G
1	1A	386	U
1	1A	387	G
1	1A	413	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	455	A
1	1A	474	U
1	1A	480	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	530	A
1	1A	534	C
1	1A	543	G
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	574	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	609	A
1	1A	615	G
1	1A	618	C
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	633	G
1	1A	639	G
1	1A	641	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	693	G
1	1A	697	C
1	1A	698	G
1	1A	715	G
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	811	A
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	831	A
1	1A	832	G
1	1A	836	A
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	927	G
1	1A	934	A
1	1A	936	C
1	1A	937	A
1	1A	938	G
1	1A	942	A
1	1A	956	A
1	1A	977	G
1	1A	983	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1079	U
1	1A	1089	C
1	1A	1090	G
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1106	U
1	1A	1107	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1108	G
1	1A	1109	G
1	1A	1111	U
1	1A	1113	A
1	1A	1114	G
1	1A	1115	A
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1121	C
1	1A	1122	C
1	1A	1123	A
1	1A	1124	U
1	1A	1125	C
1	1A	1129	U
1	1A	1131	A
1	1A	1134	A
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1142	A
1	1A	1143	U
1	1A	1154	U
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1174	A
1	1A	1180	C
1	1A	1181	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1232	G
1	1A	1256	U
1	1A	1263	C
1	1A	1265	A
1	1A	1299	A
1	1A	1302	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1352	C
1	1A	1354	A
1	1A	1367	A
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1430	A
1	1A	1431	G
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1500	A
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1571	G
1	1A	1578	C
1	1A	1589	A
1	1A	1590	C
1	1A	1594	C
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1626	A
1	1A	1628	G
1	1A	1631	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1695	C
1	1A	1700	G
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1767	A
1	1A	1776	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1800	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1918	G
1	1A	1922	A
1	1A	1927	C
1	1A	1928	G
1	1A	1935	A
1	1A	1936	C
1	1A	1937	5MU
1	1A	1942	OMC
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2102	G
1	1A	2125	C
1	1A	2126	G
1	1A	2129	C
1	1A	2130	C
1	1A	2132	G
1	1A	2134	G
1	1A	2138	G
1	1A	2139	A
1	1A	2141	A
1	1A	2148	A
1	1A	2149	G
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2170	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2194	U
1	1A	2195	A
1	1A	2206	G
1	1A	2208	G
1	1A	2209	G
1	1A	2211	U
1	1A	2212	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2291	G
1	1A	2295	C
1	1A	2298	A
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2333	G
1	1A	2334	A
1	1A	2337	G
1	1A	2346	G
1	1A	2347	A
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2395	G
1	1A	2397	C
1	1A	2405	A
1	1A	2418	U
1	1A	2426	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2434	A
1	1A	2435	U
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2480	G
1	1A	2481	A
1	1A	2486	C
1	1A	2488	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2541	G
1	1A	2561	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2597	U
1	1A	2598	C
1	1A	2614	A
1	1A	2615	G
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2642	G
1	1A	2666	A
1	1A	2675	G
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2746	A
1	1A	2770	A
1	1A	2771	A
1	1A	2774	G
1	1A	2777	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2903	G
2	1B	45	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	33	A
32	1a	39	G
32	1a	44	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	101	A
32	1a	105	G
32	1a	110	C
32	1a	115	G
32	1a	116	A
32	1a	121	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	131	C
32	1a	135	C
32	1a	143	A
32	1a	163	C
32	1a	164	U
32	1a	166	G
32	1a	173	U
32	1a	174	C
32	1a	179	A
32	1a	181	G
32	1a	182	U
32	1a	189(D)	C
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	218	C
32	1a	219	C
32	1a	222	U
32	1a	227	G
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	270	A
32	1a	289	G
32	1a	298	A
32	1a	301	G
32	1a	309	G
32	1a	321	A
32	1a	328	C
32	1a	331	G
32	1a	332	G
32	1a	346	G
32	1a	348	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	385	C
32	1a	388	G
32	1a	398	C
32	1a	406	G
32	1a	410	G
32	1a	411	A
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	436	C
32	1a	439	A
32	1a	452	A
32	1a	454	C
32	1a	455	C
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	475	G
32	1a	480	U
32	1a	485	G
32	1a	487	A
32	1a	490	G
32	1a	495	A
32	1a	496	A
32	1a	498	U
32	1a	499	A
32	1a	500	G
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	563	A
32	1a	570	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	590	C
32	1a	592	G
32	1a	618	C
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	633	G
32	1a	634	C
32	1a	639	G
32	1a	653	A
32	1a	659	U
32	1a	660	G
32	1a	661	G
32	1a	665	A
32	1a	666	G
32	1a	671	G
32	1a	672	U
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	692	U
32	1a	722	A
32	1a	723	U
32	1a	733	A
32	1a	755	G
32	1a	759	A
32	1a	765	G
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	802	A
32	1a	805	C
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	853	G
32	1a	863	U
32	1a	872	A
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	933	G
32	1a	934	C
32	1a	935	A
32	1a	937	A
32	1a	938	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	966	M2G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	984	C
32	1a	990	C
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	1006	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1009	G
32	1a	1012	U
32	1a	1017	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1034	G
32	1a	1037	C
32	1a	1042	G
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1056	U
32	1a	1063	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1101	A
32	1a	1117	G
32	1a	1120	G
32	1a	1123	A
32	1a	1125	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1135	U
32	1a	1136	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1145	C
32	1a	1146	A
32	1a	1150	U
32	1a	1152	A
32	1a	1155	G
32	1a	1157	A
32	1a	1159	U
32	1a	1168	A
32	1a	1176	A
32	1a	1183	A
32	1a	1184	G
32	1a	1189	C
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1204	A
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1218	C
32	1a	1223	C
32	1a	1224	G
32	1a	1227	A
32	1a	1232	U
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1269	A
32	1a	1270	C
32	1a	1272	G
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1303	C
32	1a	1305	G
32	1a	1317	C
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1361	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1368	G
32	1a	1370	G
32	1a	1377	A
32	1a	1378	C
32	1a	1383	C
32	1a	1397	C
32	1a	1409	C
32	1a	1418	A
32	1a	1419	G
32	1a	1441	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1452	C
32	1a	1456	G
32	1a	1464	G
32	1a	1479	C
32	1a	1487	G
32	1a	1491	G
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1517	G
32	1a	1520	G
32	1a	1523	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	11	G
1	2A	12	U
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	157	U
1	2A	196	A
1	2A	199	A
1	2A	200	U
1	2A	205	G
1	2A	213	A
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	280	C
1	2A	311	A
1	2A	327	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	386	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	505	A
1	2A	509	C
1	2A	518	G
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	592	G
1	2A	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	610	G
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	652(U)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1033	U
1	2A	1042	G
1	2A	1043	C
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1080	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1093	G
1	2A	1094	U
1	2A	1095	A
1	2A	1096	A
1	2A	1097	U
1	2A	1108	U
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1128	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1187	G
1	2A	1211	U
1	2A	1218	C
1	2A	1220	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1306	C
1	2A	1308	A
1	2A	1321	A
1	2A	1352	U
1	2A	1359	A
1	2A	1365	A
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1450	G
1	2A	1452	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1494	A
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G
1	2A	1531	C
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1579	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1839	G
1	2A	1847	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1896	G
1	2A	1900	A
1	2A	1905	C
1	2A	1906	G
1	2A	1914	C
1	2A	1915	5MU
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2039	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2101	G
1	2A	2103	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2138	C
1	2A	2142	C
1	2A	2144	U
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2158	A
1	2A	2159	G
1	2A	2160	G
1	2A	2161	C
1	2A	2162	G
1	2A	2172	U
1	2A	2173	A
1	2A	2178	C
1	2A	2184	G
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2190	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2225	A
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2286	A
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2347	C
1	2A	2350	C
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U
1	2A	2586	C
1	2A	2601	C
1	2A	2602	A
1	2A	2603	G
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	45	A
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	110	G
32	2a	5	U
32	2a	7	G
32	2a	9	G
32	2a	13	U
32	2a	25	C
32	2a	26	A
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	59	A
32	2a	60	A
32	2a	61	G
32	2a	65	U
32	2a	66	G
32	2a	80	G
32	2a	89	C
32	2a	91	C
32	2a	98	G
32	2a	105	G
32	2a	112	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	143	A
32	2a	144	G
32	2a	146	G
32	2a	151	A
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	195	A
32	2a	197	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	240	C
32	2a	245	C
32	2a	247	G
32	2a	251	G
32	2a	257	G
32	2a	258	G
32	2a	262	A
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
32	2a	309	G
32	2a	320	C
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	388	G
32	2a	393	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	410	G
32	2a	411	A
32	2a	412	A
32	2a	413	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	445	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	450	G
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	473	G
32	2a	474	G
32	2a	476	G
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	500	G
32	2a	502	G
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	558	G
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	570	G
32	2a	571	U
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	587	G
32	2a	596	C
32	2a	597	G
32	2a	606	G
32	2a	608	A
32	2a	616	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	618	C
32	2a	630	G
32	2a	632	A
32	2a	633	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	693	G
32	2a	702	A
32	2a	718	G
32	2a	723	U
32	2a	724	G
32	2a	728	A
32	2a	731	G
32	2a	737	A
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	777	A
32	2a	782	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	829	G
32	2a	830	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	870	U
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	934	C
32	2a	935	A
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	1001(A)	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1012	U
32	2a	1020	U
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1031	G
32	2a	1041	A
32	2a	1044	A
32	2a	1052	U
32	2a	1054	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1063	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1079	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1115	C
32	2a	1117	G
32	2a	1123	A
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1162	C
32	2a	1165	C
32	2a	1170	A
32	2a	1171	G
32	2a	1183	A
32	2a	1184	G
32	2a	1189	C
32	2a	1196	U
32	2a	1197	G
32	2a	1213	A
32	2a	1217	C
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1250	A
32	2a	1256	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1267	C
32	2a	1270	C
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1293	G
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1312	G
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1381	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1445	C
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1487	G
32	2a	1489	G
32	2a	1492	A
32	2a	1493	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1528	U
32	2a	1529	G
32	2a	1530	G
32	2a	1532	U

All (100) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	184	A
1	1A	185	A
1	1A	188	A
1	1A	238	C
1	1A	302	A
1	1A	334	A
1	1A	509	A
1	1A	572	A
1	1A	596	G
1	1A	732	A
1	1A	793	A
1	1A	811	A
1	1A	823	G
1	1A	874	U
1	1A	913	A
1	1A	934	A
1	1A	935	C
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1099	C
1	1A	1115	A
1	1A	1116	A
1	1A	1157	A
1	1A	1188	A
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1346	U
1	1A	1425	A
1	1A	1466	U
1	1A	1654	A
1	1A	1655	A
1	1A	1700	G
1	1A	1793	A
1	1A	2148	A
1	1A	2194	U
1	1A	2227	G
1	1A	2347	A
1	1A	2418	U
1	1A	2434	A
1	1A	2442	A
1	1A	2451	A
1	1A	2613	C
1	1A	2623	U
1	1A	2701	U
1	1A	2769	U
1	2A	195	A
1	2A	196	A
1	2A	199	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	310	A
1	2A	573	G
1	2A	685	A
1	2A	746	A
1	2A	752	A
1	2A	764	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	776	G
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	974	G
1	2A	1047	G
1	2A	1053	C
1	2A	1057	A
1	2A	1063	G
1	2A	1065	U
1	2A	1067	A
1	2A	1071	G
1	2A	1073	A
1	2A	1076	C
1	2A	1111	A
1	2A	1142(A)	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1608	A
1	2A	1992	G
1	2A	1997	G
1	2A	2126	A
1	2A	2158	A
1	2A	2172	U
1	2A	2308	G
1	2A	2335	A
1	2A	2406	U
1	2A	2422	A
1	2A	2439	A
1	2A	2601	C
1	2A	2611	U
1	2A	2689	U
1	2A	2756	U

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

48 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	2A	1962	55,1	18,22,23	1.16	4 (22%)	26,32,35	1.49	4 (15%)
32	5MC	2a	1400	32	18,22,23	0.90	0	26,32,35	1.36	5 (19%)
32	MA6	2a	1519	32	19,26,27	1.13	2 (10%)	18,38,41	4.93	3 (16%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	22,30,33	1.71	5 (22%)
1	OMU	1A	2564	55,1	19,22,23	6.38	9 (47%)	26,31,34	2.90	11 (42%)
32	4OC	2a	1402	32	20,23,24	2.61	7 (35%)	26,32,35	1.13	2 (7%)
32	5MC	1a	1404	32	18,22,23	1.23	3 (16%)	26,32,35	1.41	3 (11%)
32	G7M	1a	527	55,32	20,26,27	2.89	4 (20%)	17,39,42	0.81	1 (5%)
1	PSU	2A	1911	1	18,21,22	1.42	3 (16%)	22,30,33	1.38	2 (9%)
32	M2G	1a	966	32	20,27,28	2.87	5 (25%)	22,40,43	1.46	6 (27%)
1	OMG	1A	2263	55,1	18,26,27	1.77	6 (33%)	19,38,41	1.51	5 (26%)
1	OMU	2A	2552	55,1	19,22,23	6.64	10 (52%)	26,31,34	2.69	8 (30%)
1	5MC	1A	1964	1	18,22,23	0.99	1 (5%)	26,32,35	1.16	3 (11%)
32	UR3	1a	1498	32	19,22,23	1.89	4 (21%)	26,32,35	1.40	3 (11%)
1	5MC	2A	1942	1	18,22,23	1.02	1 (5%)	26,32,35	1.14	3 (11%)
1	2MA	1A	2515	55,1	17,25,26	1.58	5 (29%)	17,37,40	1.93	3 (17%)
1	PSU	1A	1933	1	18,21,22	1.41	3 (16%)	22,30,33	1.47	3 (13%)
32	5MC	1a	967	32	18,22,23	1.04	2 (11%)	26,32,35	1.33	4 (15%)
32	5MC	2a	1404	32	18,22,23	1.06	2 (11%)	26,32,35	1.44	4 (15%)
1	PSU	1A	2617	1	18,21,22	1.64	4 (22%)	22,30,33	1.78	5 (22%)
32	MA6	1a	1518	32	19,26,27	1.05	1 (5%)	18,38,41	4.70	3 (16%)
32	PSU	1a	516	32	18,21,22	1.43	3 (16%)	22,30,33	2.05	4 (18%)
32	2MG	1a	1207	55,32	18,26,27	1.97	4 (22%)	16,38,41	1.83	5 (31%)
1	5MU	2A	1915	1	19,22,23	1.75	3 (15%)	28,32,35	1.59	5 (17%)
1	OMC	2A	1920	1	19,22,23	2.43	7 (36%)	26,31,34	1.01	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.72	5 (22%)
32	G7M	2a	527	32	20,26,27	3.15	6 (30%)	17,39,42	0.97	2 (11%)
32	5MC	2a	1407	32	18,22,23	1.24	1 (5%)	26,32,35	1.42	3 (11%)
1	5MU	1A	1961	55,1	19,22,23	1.00	2 (10%)	28,32,35	1.48	4 (14%)
44	0TD	1l	92	44	7,9,10	2.06	2 (28%)	6,11,13	4.14	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	4OC	1a	1402	32	20,23,24	2.41	7 (35%)	26,32,35	0.78	0
32	5MC	2a	967	32	18,22,23	0.97	1 (5%)	26,32,35	1.66	4 (15%)
1	OMG	2A	2251	55,1	18,26,27	1.73	3 (16%)	19,38,41	1.64	5 (26%)
32	PSU	2a	516	32	18,21,22	1.84	3 (16%)	22,30,33	2.03	5 (22%)
1	OMC	1A	1942	55,1	19,22,23	2.18	6 (31%)	26,31,34	1.01	3 (11%)
1	PSU	1A	1939	55,1	18,21,22	1.35	2 (11%)	22,30,33	1.75	5 (22%)
32	MA6	2a	1518	32	19,26,27	1.05	1 (5%)	18,38,41	4.81	3 (16%)
32	2MG	2a	1207	32	18,26,27	1.92	4 (22%)	16,38,41	1.12	2 (12%)
1	5MU	2A	1939	55,1	19,22,23	0.91	1 (5%)	28,32,35	1.37	4 (14%)
1	5MC	1A	1984	1	18,22,23	1.11	2 (11%)	26,32,35	1.68	5 (19%)
32	5MC	1a	1400	32	18,22,23	1.03	1 (5%)	26,32,35	1.61	6 (23%)
32	5MC	1a	1407	32	18,22,23	1.37	1 (5%)	26,32,35	1.51	5 (19%)
32	MA6	1a	1519	32	19,26,27	1.03	2 (10%)	18,38,41	4.46	3 (16%)
1	5MU	1A	1937	1	19,22,23	1.43	2 (10%)	28,32,35	1.58	6 (21%)
32	M2G	2a	966	32	20,27,28	3.02	7 (35%)	22,40,43	1.37	3 (13%)
44	0TD	2l	92	44	7,9,10	2.21	1 (14%)	6,11,13	2.99	4 (66%)
32	UR3	2a	1498	32	19,22,23	1.89	4 (21%)	26,32,35	1.48	4 (15%)
1	2MA	2A	2503	55,1	17,25,26	1.54	2 (11%)	17,37,40	1.11	2 (11%)

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
1	5MC	2A	1962	55,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2564	55,1	-	0/9/27/28	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	55,32	-	1/3/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	OMG	1A	2263	55,1	-	0/5/27/28	0/3/3/3
1	OMU	2A	2552	55,1	-	0/9/27/28	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	55,1	-	1/3/25/26	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	55,32	-	0/5/27/28	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	1/3/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	55,1	-	0/7/25/26	0/2/2/2
44	0TD	1l	92	44	-	4/7/12/14	-
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32	-	3/7/25/26	0/2/2/2
1	OMC	1A	1942	55,1	-	3/9/27/28	0/2/2/2
1	PSU	1A	1939	55,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	5MU	2A	1939	55,1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	5/7/29/30	0/3/3/3
1	5MU	1A	1937	1	-	4/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
44	0TD	2l	92	44	-	2/7/12/14	-
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	55,1	-	1/3/25/26	0/3/3/3

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C4-N3	-15.09	1.11	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	C4-N3	-14.97	1.11	1.38
1	2A	2552	OMU	C5-C4	14.92	1.76	1.43
1	1A	2564	OMU	C5-C4	13.65	1.73	1.43
1	1A	2564	OMU	C6-C5	-11.10	1.09	1.35
1	2A	2552	OMU	C6-C5	-10.45	1.10	1.35
32	2a	966	M2G	C2-N3	10.42	1.43	1.30
32	1a	966	M2G	C2-N3	10.26	1.43	1.30
32	2a	527	G7M	C8-N9	8.77	1.49	1.33
32	1a	527	G7M	C8-N9	8.59	1.48	1.33
1	2A	2552	OMU	C3'-C2'	-8.50	1.34	1.52
32	2a	527	G7M	C8-N7	8.13	1.48	1.33
1	2A	2552	OMU	C6-N1	8.05	1.57	1.38
1	1A	2564	OMU	C6-N1	7.45	1.56	1.38
1	1A	2564	OMU	C3'-C2'	-7.40	1.36	1.52
32	1a	527	G7M	C8-N7	7.27	1.46	1.33
1	2A	2552	OMU	O4'-C4'	-6.78	1.29	1.45
1	1A	2564	OMU	O4'-C4'	-6.33	1.30	1.45
1	2A	2552	OMU	O4'-C1'	6.14	1.56	1.42
1	1A	2564	OMU	O4'-C1'	6.04	1.56	1.42
32	2a	1402	4OC	C4-N4	5.91	1.48	1.35
32	2a	516	PSU	C2-N1	5.79	1.44	1.36
32	1a	1402	4OC	C4-N4	5.76	1.47	1.35
1	2A	1915	5MU	C2-N1	5.75	1.47	1.38
1	1A	2564	OMU	C1'-N1	-5.74	1.31	1.47
1	2A	1920	OMC	C4-N4	5.68	1.47	1.33
1	2A	2552	OMU	C1'-N1	-5.40	1.32	1.47
1	1A	1942	OMC	C4-N4	5.19	1.46	1.33
32	2a	1498	UR3	C6-C5	5.12	1.46	1.35
32	2a	1402	4OC	C2-N3	4.99	1.46	1.36
32	2a	966	M2G	C2-N2	4.89	1.44	1.35
1	1A	1937	5MU	C2-N1	4.82	1.46	1.38
1	2A	1920	OMC	C6-C5	4.75	1.46	1.35
32	1a	1498	UR3	C6-C5	4.74	1.46	1.35
44	2l	92	0TD	CB-SB	-4.73	1.77	1.82
32	1a	1207	2MG	C2-N1	4.72	1.44	1.36
32	2a	1207	2MG	C2-N1	4.66	1.44	1.36
32	2a	1402	4OC	C6-C5	4.65	1.45	1.35
32	1a	1407	5MC	C2-N1	4.60	1.50	1.40
32	1a	1207	2MG	C2-N2	4.52	1.43	1.33
32	1a	966	M2G	C2-N2	4.44	1.43	1.35
1	2A	1920	OMC	C2-N3	4.41	1.45	1.36
32	2a	1207	2MG	C2-N2	4.38	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	527	G7M	C2-N3	4.37	1.43	1.33
1	2A	1917	PSU	C2-N1	4.30	1.42	1.36
1	1A	1942	OMC	C6-C5	4.14	1.44	1.35
32	1a	1498	UR3	C2-N1	4.09	1.44	1.38
44	1l	92	0TD	CB-SB	-4.09	1.78	1.82
32	2a	1402	4OC	C4-N3	4.07	1.39	1.32
32	2a	1498	UR3	C2-N3	4.06	1.46	1.39
32	1a	1402	4OC	C4-N3	4.02	1.39	1.32
1	2A	2251	OMG	C2-N3	3.95	1.42	1.33
1	1A	1942	OMC	C2-N3	3.89	1.44	1.36
1	2A	2503	2MA	C2-N3	3.84	1.39	1.31
32	1a	1402	4OC	C6-C5	3.80	1.43	1.35
32	1a	527	G7M	C2-N3	3.80	1.42	1.33
1	2A	2552	OMU	C3'-C4'	3.79	1.62	1.53
32	2a	1407	5MC	C2-N1	3.79	1.48	1.40
1	2A	1911	PSU	C2-N1	3.77	1.41	1.36
1	1A	1939	PSU	C2-N1	3.75	1.41	1.36
32	1a	1498	UR3	C2-N3	3.69	1.46	1.39
32	1a	1402	4OC	O2-C2	-3.67	1.16	1.23
1	2A	1920	OMC	C2-N1	3.61	1.47	1.40
32	1a	1402	4OC	C5-C4	3.61	1.48	1.40
32	1a	1402	4OC	C2-N3	3.61	1.43	1.36
32	2a	1402	4OC	C5-C4	3.59	1.48	1.40
1	1A	1933	PSU	C4-N3	3.57	1.45	1.38
1	1A	2564	OMU	C3'-C4'	3.55	1.62	1.53
1	1A	2263	OMG	C2-N3	3.49	1.41	1.33
1	1A	2263	OMG	C5-C4	-3.47	1.34	1.43
32	2a	527	G7M	C2-N2	3.45	1.42	1.34
32	2a	1207	2MG	C4-N3	3.43	1.45	1.37
32	2a	516	PSU	C6-N1	3.42	1.41	1.36
1	2A	2251	OMG	C5-C4	-3.41	1.34	1.43
32	1a	516	PSU	C6-N1	3.36	1.41	1.36
32	1a	516	PSU	C2-N1	3.35	1.41	1.36
32	2a	1402	4OC	O2-C2	-3.32	1.17	1.23
32	1a	966	M2G	C4-N3	3.31	1.45	1.37
1	1A	1942	OMC	C2-N1	3.28	1.47	1.40
1	1A	2515	2MA	C2-N3	3.27	1.38	1.31
1	2A	2503	2MA	C5-C4	-3.26	1.34	1.43
1	1A	2617	PSU	C6-C5	-3.20	1.31	1.35
32	2a	966	M2G	C4-N3	3.18	1.45	1.37
1	2A	2605	PSU	C2-N1	3.15	1.41	1.36
1	1A	1933	PSU	C2-N1	3.14	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1920	OMC	O2-C2	-3.12	1.17	1.23
1	2A	1915	5MU	C2-N3	3.09	1.43	1.38
32	1a	1207	2MG	C4-N3	3.07	1.44	1.37
32	2a	527	G7M	C4-N3	3.04	1.44	1.37
1	1A	2617	PSU	C1'-C5	-3.02	1.43	1.50
1	1A	1942	OMC	O2-C2	-3.00	1.18	1.23
32	2a	966	M2G	C2-N1	2.96	1.44	1.36
32	1a	1400	5MC	C2-N1	2.95	1.46	1.40
32	1a	966	M2G	C5-C4	-2.92	1.35	1.43
32	1a	527	G7M	C4-N3	2.91	1.44	1.37
1	1A	2617	PSU	C6-N1	2.90	1.41	1.36
32	1a	1404	5MC	CM5-C5	-2.85	1.43	1.50
32	2a	1402	4OC	C2-N1	2.82	1.46	1.40
32	2a	516	PSU	O4'-C1'	-2.82	1.39	1.43
32	2a	1519	MA6	C2-N3	2.77	1.36	1.32
1	1A	1937	5MU	C2-N3	2.75	1.42	1.38
32	2a	1404	5MC	C6-C5	2.73	1.39	1.34
32	1a	1518	MA6	C5-C4	-2.67	1.33	1.40
1	2A	1920	OMC	C5-C4	2.67	1.49	1.42
1	2A	1911	PSU	C6-N1	2.66	1.40	1.36
1	1A	2515	2MA	C5-C4	-2.66	1.36	1.43
32	2a	966	M2G	C6-N1	2.65	1.41	1.37
32	2a	966	M2G	C5-C6	2.64	1.52	1.47
32	2a	966	M2G	C5-C4	-2.64	1.36	1.43
1	1A	2263	OMG	C4-N3	2.64	1.43	1.37
32	1a	966	M2G	C2-N1	2.64	1.43	1.36
32	2a	1519	MA6	C5-C4	-2.61	1.34	1.40
32	2a	527	G7M	C2-N1	2.59	1.44	1.37
1	2A	2605	PSU	C6-N1	2.58	1.40	1.36
1	2A	1911	PSU	C4-N3	2.58	1.43	1.38
32	2a	1518	MA6	C2-N3	2.56	1.36	1.32
1	1A	1964	5MC	C6-C5	2.52	1.38	1.34
1	1A	2617	PSU	O3'-C3'	-2.51	1.37	1.43
1	2A	1962	5MC	CM5-C5	-2.50	1.44	1.50
32	1a	967	5MC	C6-C5	2.48	1.38	1.34
32	2a	1207	2MG	CM2-N2	-2.44	1.41	1.45
1	1A	1961	5MU	C4-C5	-2.43	1.40	1.44
32	2a	1498	UR3	C3U-N3	-2.41	1.42	1.47
1	2A	1917	PSU	C6-N1	2.41	1.40	1.36
1	1A	1939	PSU	C6-N1	2.41	1.40	1.36
1	2A	1962	5MC	C4-N4	2.40	1.40	1.34
32	1a	967	5MC	C2-N3	2.40	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	967	5MC	C6-C5	2.39	1.38	1.34
32	1a	1519	MA6	C2-N3	2.37	1.35	1.32
1	1A	2263	OMG	C2-N2	2.35	1.39	1.34
32	2a	1498	UR3	C2-N1	2.35	1.41	1.38
32	1a	1404	5MC	C4-N4	2.34	1.40	1.34
32	1a	1402	4OC	CM4-N4	-2.33	1.41	1.45
32	1a	1207	2MG	C5-C4	-2.33	1.37	1.43
1	1A	2515	2MA	C2-N1	2.31	1.43	1.36
1	2A	1939	5MU	C5M-C5	-2.30	1.45	1.50
32	1a	1519	MA6	C5-C4	-2.29	1.34	1.40
1	1A	1984	5MC	CM5-C5	-2.27	1.45	1.50
1	2A	1915	5MU	C6-C5	2.26	1.38	1.34
32	1a	516	PSU	O4'-C1'	-2.25	1.40	1.43
1	2A	1942	5MC	C2-N3	2.25	1.40	1.36
1	1A	1942	OMC	C5-C4	2.21	1.48	1.42
1	2A	2552	OMU	O2'-C2'	2.20	1.48	1.42
1	1A	2515	2MA	C8-N7	2.20	1.38	1.35
1	2A	1962	5MC	C2-N3	2.17	1.40	1.36
1	2A	1920	OMC	C4-N3	2.17	1.39	1.34
1	1A	1961	5MU	C5M-C5	-2.16	1.45	1.50
1	1A	2515	2MA	O2'-C2'	-2.16	1.37	1.43
1	2A	2251	OMG	C4-N3	2.16	1.42	1.37
32	1a	1404	5MC	C2-N3	2.15	1.40	1.36
32	2a	1404	5MC	CM5-C5	-2.13	1.45	1.50
44	1l	92	0TD	CA-N	-2.12	1.41	1.47
1	1A	2263	OMG	C8-N7	2.10	1.38	1.35
1	2A	1962	5MC	O2-C2	-2.10	1.19	1.23
1	1A	1933	PSU	C6-N1	2.07	1.39	1.36
1	1A	2263	OMG	C2-N1	2.06	1.42	1.37
32	1a	1498	UR3	O2-C2	-2.03	1.18	1.22
1	1A	1984	5MC	C6-N1	-2.01	1.34	1.38

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1519	MA6	N1-C6-N6	-19.44	96.59	117.06
32	2a	1518	MA6	N1-C6-N6	-19.01	97.05	117.06
32	1a	1518	MA6	N1-C6-N6	-18.08	98.03	117.06
32	1a	1519	MA6	N1-C6-N6	-17.64	98.49	117.06
1	2A	2552	OMU	C5-C4-N3	7.23	125.65	114.84
44	1l	92	0TD	CSB-SB-CB	7.18	115.42	102.44
32	2a	516	PSU	C6-C5-C4	6.82	122.96	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	516	PSU	C6-C5-C4	6.74	122.91	118.20
1	1A	2564	OMU	C5-C4-N3	6.60	124.70	114.84
1	2A	2552	OMU	C4-N3-C2	-6.12	118.51	126.58
32	1a	1518	MA6	C1'-N9-C4	-6.00	116.09	126.64
1	1A	2564	OMU	O4-C4-C5	-5.79	114.98	125.16
32	2a	1518	MA6	C1'-N9-C4	-5.72	116.60	126.64
1	1A	2564	OMU	O2'-C2'-C1'	-5.55	98.25	109.08
1	1A	2515	2MA	CM2-C2-N1	5.47	128.40	116.23
1	1A	2617	PSU	C6-C5-C4	5.45	122.01	118.20
44	1l	92	0TD	CB-CA-N	-5.38	97.63	109.10
32	1a	1498	UR3	C4-N3-C2	-5.27	119.60	124.56
1	1A	1939	PSU	C6-C5-C4	5.23	121.85	118.20
32	1a	1518	MA6	N3-C2-N1	-5.19	120.57	128.68
32	2a	967	5MC	C5-C6-N1	-5.14	118.05	123.34
32	2a	1519	MA6	N3-C2-N1	-5.12	120.68	128.68
1	2A	2605	PSU	C6-C5-C4	4.98	121.68	118.20
32	2a	1519	MA6	C1'-N9-C4	-4.90	118.03	126.64
32	1a	1519	MA6	N3-C2-N1	-4.89	121.04	128.68
44	2l	92	0TD	CSB-SB-CB	4.84	111.20	102.44
1	2A	2552	OMU	O2-C2-N1	-4.84	116.36	122.79
1	2A	1917	PSU	C6-C5-C4	4.77	121.53	118.20
1	1A	1984	5MC	C5-C6-N1	-4.72	118.48	123.34
1	2A	2552	OMU	N3-C2-N1	4.64	121.06	114.89
1	1A	2564	OMU	C4-N3-C2	-4.59	120.52	126.58
32	1a	1404	5MC	C5-C6-N1	-4.37	118.84	123.34
32	2a	1498	UR3	C4-N3-C2	-4.30	120.52	124.56
32	2a	1518	MA6	N3-C2-N1	-4.23	122.07	128.68
1	1A	2515	2MA	C5-C6-N1	4.06	121.03	114.02
32	1a	1519	MA6	C1'-N9-C4	-4.06	119.51	126.64
1	1A	1984	5MC	C4-N3-C2	-4.05	115.21	120.69
1	2A	1962	5MC	C5-C6-N1	-4.05	119.17	123.34
1	1A	1961	5MU	C4-N3-C2	-4.03	122.14	127.35
32	2a	1404	5MC	C5-C6-N1	-4.00	119.22	123.34
32	2a	966	M2G	N1-C2-N2	3.99	121.44	118.04
1	2A	1962	5MC	C4-N3-C2	-3.97	115.33	120.69
32	1a	1407	5MC	C5-C4-N3	3.90	125.89	121.67
1	1A	1933	PSU	C6-C5-C4	3.84	120.88	118.20
1	1A	1984	5MC	C5-C4-N3	3.78	125.75	121.67
1	1A	2564	OMU	C6-C5-C4	-3.77	114.36	119.52
32	1a	967	5MC	C5-C4-N3	3.76	125.73	121.67
44	1l	92	0TD	OD2-CG-CB	3.76	121.27	113.15
32	2a	1407	5MC	C5-C4-N3	3.76	125.73	121.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1961	5MU	C5-C4-N3	3.75	118.51	115.31
32	2a	1402	4OC	C6-C5-C4	3.68	121.46	116.96
32	1a	516	PSU	C6-N1-C2	-3.66	118.94	122.68
32	1a	1404	5MC	C4-N3-C2	-3.66	115.74	120.69
1	2A	1911	PSU	C6-C5-C4	3.61	120.72	118.20
32	1a	967	5MC	C5-C6-N1	-3.58	119.65	123.34
44	2l	92	0TD	OD2-CG-CB	3.57	120.86	113.15
1	2A	2552	OMU	O4-C4-C5	-3.56	118.91	125.16
32	2a	1400	5MC	C5-C6-N1	-3.55	119.69	123.34
32	1a	1400	5MC	C5-C4-N3	3.53	125.48	121.67
32	1a	1207	2MG	C8-N7-C5	3.52	109.70	102.99
1	2A	1939	5MU	C4-N3-C2	-3.49	122.83	127.35
32	2a	967	5MC	C4-N3-C2	-3.48	115.98	120.69
1	1A	2263	OMG	C8-N7-C5	3.48	109.61	102.99
32	1a	1400	5MC	C1'-N1-C6	-3.42	115.43	121.12
32	2a	1498	UR3	O2-C2-N1	-3.41	114.73	122.72
1	1A	2515	2MA	CM2-C2-N3	-3.33	109.63	119.47
1	1A	2564	OMU	C2'-C1'-N1	-3.33	107.76	114.22
1	1A	2564	OMU	N3-C2-N1	3.31	119.28	114.89
1	1A	2564	OMU	C1'-N1-C2	3.30	123.55	117.57
32	2a	1404	5MC	C4-N3-C2	-3.29	116.24	120.69
1	2A	2251	OMG	C5-C6-N1	3.28	119.73	113.95
1	1A	1937	5MU	C4-N3-C2	-3.26	123.13	127.35
1	2A	2251	OMG	C2-N1-C6	-3.23	119.16	125.10
1	2A	1939	5MU	C6-C5-C4	3.19	120.70	118.03
44	2l	92	0TD	CB-CA-N	-3.19	102.30	109.10
1	2A	1915	5MU	C1'-N1-C2	3.18	123.32	117.57
1	2A	2251	OMG	C8-N7-C5	3.17	109.03	102.99
32	1a	966	M2G	C5-C6-N1	3.17	119.55	113.95
1	1A	2564	OMU	C3'-C2'-C1'	3.16	108.84	102.89
1	2A	1939	5MU	C5-C6-N1	-3.16	120.08	123.34
1	2A	2552	OMU	C6-C5-C4	-3.13	115.23	119.52
1	2A	1917	PSU	O2-C2-N1	-3.13	119.34	122.79
32	2a	1407	5MC	C5-C6-N1	-3.12	120.12	123.34
1	1A	1937	5MU	C6-C5-C4	3.12	120.64	118.03
1	1A	1937	5MU	C1'-N1-C2	3.12	123.22	117.57
32	1a	516	PSU	N1-C2-N3	3.12	118.66	115.13
32	2a	967	5MC	C5-C4-N3	3.11	125.03	121.67
1	1A	1939	PSU	O2-C2-N1	-3.10	119.38	122.79
1	1A	2564	OMU	O2-C2-N1	-3.09	118.68	122.79
32	2a	1400	5MC	C5-C4-N3	3.08	125.00	121.67
32	2a	1404	5MC	C5-C4-N3	3.06	124.97	121.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2503	2MA	C5-C6-N1	3.04	119.26	114.02
32	1a	966	M2G	N1-C2-N2	3.03	120.62	118.04
1	2A	1915	5MU	C6-C5-C4	3.01	120.55	118.03
32	1a	1207	2MG	C5-C6-N1	3.00	119.25	113.95
32	1a	1400	5MC	CM5-C5-C6	-2.93	118.93	122.85
1	1A	1964	5MC	C5-C6-N1	-2.91	120.35	123.34
1	2A	1942	5MC	C5-C4-N3	2.86	124.76	121.67
32	1a	1400	5MC	C5-C6-N1	-2.84	120.42	123.34
1	1A	1961	5MU	C5-C6-N1	-2.83	120.43	123.34
1	1A	1933	PSU	O2-C2-N1	-2.82	119.69	122.79
32	1a	1207	2MG	O3'-C3'-C4'	2.82	119.20	111.05
32	1a	1407	5MC	N4-C4-N3	-2.81	113.35	118.48
1	1A	2617	PSU	O4-C4-N3	-2.79	114.76	120.12
1	2A	1942	5MC	C5-C6-N1	-2.79	120.47	123.34
32	2a	967	5MC	N4-C4-N3	-2.78	113.40	118.48
32	1a	967	5MC	C4-N3-C2	-2.78	116.93	120.69
1	2A	1915	5MU	C4-N3-C2	-2.77	123.76	127.35
1	1A	1984	5MC	CM5-C5-C6	-2.76	119.16	122.85
32	2a	1407	5MC	C4-N3-C2	-2.75	116.97	120.69
1	1A	1961	5MU	C6-C5-C4	2.73	120.31	118.03
1	2A	1920	OMC	O2-C2-N3	-2.72	117.91	122.33
32	2a	1400	5MC	C4-N3-C2	-2.69	117.05	120.69
32	1a	1400	5MC	C4-N3-C2	-2.68	117.06	120.69
32	1a	1407	5MC	C4-N3-C2	-2.67	117.07	120.69
1	1A	1942	OMC	C2'-C1'-N1	-2.67	109.05	114.22
32	1a	966	M2G	C2-N1-C6	-2.66	119.29	123.71
1	1A	2564	OMU	O4'-C1'-C2'	-2.66	101.91	106.57
1	1A	2263	OMG	N2-C2-N1	2.66	122.37	116.71
32	2a	1207	2MG	C8-N7-C5	2.64	108.03	102.99
44	1l	92	0TD	OD2-CG-OD1	-2.64	118.10	124.09
1	2A	2552	OMU	O4-C4-N3	-2.63	115.44	119.31
32	1a	1407	5MC	CM5-C5-C6	-2.63	119.33	122.85
32	2a	966	M2G	C8-N7-C5	2.62	107.97	102.99
1	2A	2552	OMU	O2'-C2'-C1'	-2.61	103.99	109.08
32	2a	516	PSU	N1-C2-N3	2.60	118.07	115.13
1	1A	2263	OMG	C5-C6-N1	2.60	118.54	113.95
1	1A	1964	5MC	C4-N3-C2	-2.58	117.20	120.69
1	1A	1937	5MU	C1'-N1-C6	-2.58	116.83	121.12
1	1A	1942	OMC	O2-C2-N3	-2.58	118.14	122.33
1	2A	2605	PSU	N1-C2-N3	2.58	118.05	115.13
32	2a	1498	UR3	O2-C2-N3	2.57	124.96	121.34
32	1a	1498	UR3	C3U-N3-C2	2.53	121.75	117.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2263	OMG	O6-C6-N1	-2.53	117.67	120.65
1	1A	1937	5MU	C5M-C5-C6	-2.52	119.48	122.85
32	1a	1207	2MG	O3'-C3'-C2'	2.52	119.98	111.82
32	2a	516	PSU	C6-N1-C2	-2.51	120.11	122.68
32	1a	516	PSU	O4'-C1'-C2'	2.51	108.68	105.14
1	2A	1939	5MU	C5-C4-N3	2.50	117.45	115.31
1	1A	1984	5MC	N4-C4-N3	-2.50	113.92	118.48
32	2a	1400	5MC	CM5-C5-C6	-2.48	119.53	122.85
1	2A	2605	PSU	O4-C4-N3	-2.47	115.39	120.12
32	2a	516	PSU	O4'-C1'-C2'	2.46	108.62	105.14
32	2a	1498	UR3	C3U-N3-C4	2.46	121.41	117.89
1	2A	1962	5MC	CM5-C5-C6	-2.45	119.58	122.85
1	2A	1915	5MU	C1'-N1-C6	-2.43	117.07	121.12
1	1A	1964	5MC	C5-C4-N3	2.43	124.30	121.67
1	1A	1939	PSU	N1-C2-N3	2.43	117.88	115.13
32	1a	966	M2G	C8-N7-C5	2.42	107.60	102.99
1	1A	2617	PSU	O2'-C2'-C1'	-2.40	105.50	111.23
32	1a	527	G7M	C2-N1-C6	-2.40	120.67	125.10
1	2A	2251	OMG	O6-C6-N1	-2.40	117.82	120.65
1	2A	1911	PSU	O4-C4-N3	-2.39	115.54	120.12
1	1A	2617	PSU	C6-N1-C2	-2.38	120.25	122.68
1	1A	2617	PSU	O4-C4-C5	2.37	130.25	124.05
32	2a	1404	5MC	N4-C4-N3	-2.36	114.16	118.48
32	2a	1402	4OC	C5-C4-N3	-2.35	118.81	122.59
1	2A	1917	PSU	O4-C4-N3	-2.34	115.64	120.12
32	2a	1400	5MC	N4-C4-N3	-2.32	114.24	118.48
32	2a	1207	2MG	C5-C6-N1	2.30	118.02	113.95
32	2a	966	M2G	C5-C6-N1	2.30	118.01	113.95
44	2l	92	0TD	OD2-CG-OD1	-2.27	118.94	124.09
32	1a	1400	5MC	N4-C4-N3	-2.26	114.35	118.48
1	1A	1942	OMC	CM2-O2'-C2'	-2.26	108.61	114.52
32	1a	967	5MC	N4-C4-N3	-2.25	114.37	118.48
1	2A	1917	PSU	N1-C2-N3	2.23	117.66	115.13
32	1a	1498	UR3	C5-C6-N1	-2.21	118.10	121.81
32	2a	516	PSU	O4-C4-N3	-2.20	115.90	120.12
1	1A	1937	5MU	C5-C4-N3	2.16	117.16	115.31
32	1a	1404	5MC	C5-C4-N3	2.16	124.00	121.67
1	2A	1917	PSU	C4-N3-C2	-2.12	123.29	126.34
1	2A	2605	PSU	C4-N3-C2	-2.12	123.29	126.34
32	1a	1207	2MG	C3'-C2'-C1'	-2.09	97.83	100.98
32	2a	527	G7M	C2-N1-C6	-2.09	121.26	125.10
1	2A	1962	5MC	C5-C4-N3	2.09	123.92	121.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	966	M2G	O6-C6-C5	-2.07	120.33	124.37
1	1A	1933	PSU	C4-N3-C2	-2.07	123.36	126.34
1	1A	1939	PSU	C4-N3-C2	-2.07	123.36	126.34
1	2A	2605	PSU	O2-C2-N1	-2.07	120.52	122.79
1	2A	2251	OMG	CM2-O2'-C2'	-2.06	109.11	114.52
32	1a	1407	5MC	O2-C2-N3	-2.06	118.97	122.33
1	2A	1920	OMC	C2'-C1'-N1	-2.04	110.26	114.22
32	1a	966	M2G	CM2-N2-CM1	2.04	122.09	115.77
1	1A	1939	PSU	O4-C4-N3	-2.03	116.23	120.12
1	2A	1942	5MC	C4-N3-C2	-2.03	117.95	120.69
1	2A	2503	2MA	C8-N7-C5	2.02	106.84	102.99
1	1A	2263	OMG	N1-C2-N3	-2.01	119.57	123.32
32	2a	527	G7M	N1-C2-N3	-2.00	119.58	123.32
1	2A	1915	5MU	O4'-C1'-N1	2.00	112.94	108.36

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6
1	1A	1937	5MU	C3'-C4'-C5'-O5'
1	1A	1937	5MU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C9
44	1l	92	0TD	CA-CB-SB-CSB
44	1l	92	0TD	SB-CB-CG-OD2
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	2a	516	PSU	C2'-C1'-C5-C4
32	2a	1518	MA6	C5-C6-N6-C9
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	N1-C6-N6-C9
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	527	G7M	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
44	2l	92	0TD	CG-CB-SB-CSB
44	1l	92	0TD	SB-CB-CG-OD1
44	2l	92	0TD	CA-CB-CG-OD2
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	516	PSU	O4'-C1'-C5-C4
32	2a	516	PSU	O4'-C1'-C5-C4
1	1A	1942	OMC	O4'-C4'-C5'-O5'
1	1A	1942	OMC	C3'-C4'-C5'-O5'
32	1a	516	PSU	O4'-C1'-C5-C6
44	1l	92	0TD	CG-CB-SB-CSB
32	2a	516	PSU	O4'-C1'-C5-C6
1	1A	1942	OMC	C2'-C1'-N1-C2
1	2A	1920	OMC	C2'-C1'-N1-C2
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2435 ligands modelled in this entry, 2432 are monoatomic and 1 is modelled with single atom - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	SF4	1d	501	36	0,12,12	-	-	-		
57	SF4	2d	501	36	0,12,12	-	-	-		

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
57	SF4	1d	501	36	-	-	0/6/5/5
57	SF4	2d	501	36	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2A	2801(A):A	O3'	2802:G	P	3.56

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1A	2861/2915 (98%)	0.20	153 (5%)	26	17	18, 37, 90, 99	0
1	2A	2856/2915 (97%)	0.13	161 (5%)	24	16	33, 58, 91, 100	0
2	1B	120/120 (100%)	-0.35	0	100	100	33, 56, 67, 89	0
2	2B	120/120 (100%)	-0.34	0	100	100	63, 76, 81, 86	0
3	1D	275/275 (100%)	-0.29	0	100	100	17, 38, 53, 70	0
3	2D	275/275 (100%)	-0.25	0	100	100	32, 52, 64, 74	0
4	1E	204/204 (100%)	-0.40	0	100	100	19, 41, 61, 70	0
4	2E	204/204 (100%)	-0.23	1 (0%)	91	88	34, 57, 70, 78	0
5	1F	203/203 (100%)	-0.28	2 (0%)	82	77	17, 44, 70, 86	0
5	2F	203/203 (100%)	-0.28	0	100	100	38, 64, 78, 84	0
6	1G	181/181 (100%)	-0.42	2 (1%)	80	75	52, 68, 78, 88	0
6	2G	181/181 (100%)	0.56	15 (8%)	11	6	74, 80, 86, 91	0
7	1H	174/174 (100%)	-0.47	1 (0%)	89	86	39, 55, 66, 70	0
7	2H	173/174 (99%)	0.77	27 (15%)	2	1	65, 79, 85, 87	0
8	1I	147/147 (100%)	-0.26	0	100	100	41, 70, 78, 81	0
8	2I	146/147 (99%)	0.24	5 (3%)	45	35	53, 74, 82, 87	0
9	1N	140/140 (100%)	-0.39	0	100	100	23, 39, 62, 75	0
9	2N	140/140 (100%)	-0.26	0	100	100	48, 63, 73, 82	0
10	1O	122/122 (100%)	-0.33	0	100	100	30, 43, 59, 64	0
10	2O	122/122 (100%)	-0.36	0	100	100	44, 55, 67, 73	0
11	1P	149/149 (100%)	-0.25	0	100	100	19, 46, 65, 78	0
11	2P	149/149 (100%)	0.23	3 (2%)	65	56	42, 66, 79, 82	0
12	1Q	141/141 (100%)	-0.18	0	100	100	28, 43, 56, 69	0
12	2Q	141/141 (100%)	-0.38	2 (1%)	75	70	47, 63, 74, 77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.16	0	100	100	26, 38, 55, 63	0
13	2R	118/118 (100%)	-0.21	0	100	100	40, 54, 64, 70	0
14	1S	110/110 (100%)	-0.36	0	100	100	44, 55, 67, 71	0
14	2S	110/110 (100%)	0.21	3 (2%)	54	44	64, 72, 78, 82	0
15	1T	131/131 (100%)	-0.34	1 (0%)	86	81	34, 47, 70, 79	0
15	2T	131/131 (100%)	-0.36	0	100	100	50, 60, 75, 83	0
16	1U	116/116 (100%)	-0.25	0	100	100	22, 32, 48, 64	0
16	2U	116/116 (100%)	-0.12	0	100	100	45, 60, 72, 81	0
17	1V	101/101 (100%)	-0.41	0	100	100	22, 41, 60, 71	0
17	2V	101/101 (100%)	-0.24	0	100	100	42, 68, 76, 83	0
18	1W	112/112 (100%)	-0.35	2 (1%)	68	61	22, 32, 54, 85	0
18	2W	112/112 (100%)	-0.30	0	100	100	39, 52, 66, 81	0
19	1X	95/95 (100%)	-0.31	0	100	100	28, 42, 64, 72	0
19	2X	95/95 (100%)	-0.06	1 (1%)	80	75	48, 62, 72, 76	0
20	1Y	107/107 (100%)	-0.35	1 (0%)	84	80	38, 51, 67, 75	0
20	2Y	107/107 (100%)	0.34	12 (11%)	5	3	53, 68, 79, 86	0
21	1Z	203/203 (100%)	-0.40	1 (0%)	91	88	45, 62, 74, 82	0
21	2Z	201/203 (99%)	0.11	3 (1%)	73	68	65, 75, 82, 87	0
22	10	77/77 (100%)	-0.28	0	100	100	29, 41, 58, 63	0
22	20	77/77 (100%)	0.16	2 (2%)	56	46	52, 63, 71, 75	0
23	11	97/97 (100%)	-0.11	1 (1%)	82	77	27, 45, 68, 77	0
23	21	97/97 (100%)	-0.14	1 (1%)	82	77	46, 59, 75, 79	0
24	12	70/70 (100%)	-0.28	0	100	100	40, 51, 63, 77	0
24	22	70/70 (100%)	-0.07	0	100	100	60, 69, 77, 79	0
25	13	59/59 (100%)	-0.32	0	100	100	28, 40, 62, 77	0
25	23	59/59 (100%)	0.32	2 (3%)	45	35	54, 63, 74, 79	0
26	14	69/69 (100%)	0.34	12 (17%)	1	1	64, 79, 87, 91	0
26	24	69/69 (100%)	1.28	21 (30%)	0	0	76, 85, 89, 94	0
27	15	59/59 (100%)	-0.30	0	100	100	18, 38, 57, 66	0
27	25	59/59 (100%)	-0.20	0	100	100	38, 55, 71, 75	0
28	16	53/53 (100%)	-0.43	0	100	100	38, 48, 60, 63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	26	53/53 (100%)	-0.21	0	100	100	56, 64, 71, 77	0
29	17	48/48 (100%)	-0.16	0	100	100	20, 27, 58, 68	0
29	27	48/48 (100%)	-0.10	0	100	100	34, 44, 67, 78	0
30	18	64/64 (100%)	-0.17	0	100	100	28, 35, 46, 59	0
30	28	64/64 (100%)	0.04	0	100	100	46, 58, 65, 70	0
31	19	37/37 (100%)	-0.11	0	100	100	35, 46, 63, 70	0
31	29	37/37 (100%)	0.28	1 (2%)	54	44	63, 69, 75, 75	0
32	1a	1488/1521 (97%)	0.02	59 (3%)	38	28	35, 72, 91, 100	0
32	2a	1492/1521 (98%)	0.01	58 (3%)	39	29	44, 74, 91, 97	0
33	1x	97/97 (100%)	-0.08	1 (1%)	82	77	55, 67, 76, 80	0
33	2x	96/97 (98%)	1.75	40 (41%)	0	0	70, 78, 87, 89	0
34	1b	231/231 (100%)	0.15	18 (7%)	13	7	65, 77, 84, 90	0
34	2b	231/231 (100%)	0.23	14 (6%)	21	13	66, 79, 85, 89	0
35	1c	206/206 (100%)	0.25	13 (6%)	20	12	67, 78, 84, 90	0
35	2c	206/206 (100%)	0.52	16 (7%)	13	7	72, 81, 86, 90	0
36	1d	208/208 (100%)	-0.13	2 (0%)	82	77	59, 73, 80, 87	0
36	2d	208/208 (100%)	-0.16	3 (1%)	75	70	58, 71, 80, 84	0
37	1e	148/148 (100%)	-0.24	0	100	100	45, 68, 75, 89	0
37	2e	148/148 (100%)	-0.27	0	100	100	57, 70, 77, 82	0
38	1f	100/100 (100%)	-0.44	0	100	100	54, 72, 77, 80	0
38	2f	100/100 (100%)	-0.48	0	100	100	59, 68, 78, 80	0
39	1g	155/155 (100%)	-0.03	4 (2%)	56	46	66, 74, 82, 85	0
39	2g	155/155 (100%)	0.35	14 (9%)	9	5	69, 77, 82, 87	0
40	1h	137/137 (100%)	-0.05	1 (0%)	87	84	58, 68, 74, 82	0
40	2h	137/137 (100%)	-0.19	0	100	100	62, 69, 76, 80	0
41	1i	127/127 (100%)	0.58	8 (6%)	20	12	67, 80, 86, 89	0
41	2i	126/127 (99%)	1.16	34 (26%)	0	0	72, 81, 86, 89	0
42	1j	97/97 (100%)	1.13	20 (20%)	1	0	68, 81, 87, 90	0
42	2j	96/97 (98%)	1.06	19 (19%)	1	0	73, 82, 87, 89	0
43	1k	114/114 (100%)	-0.38	0	100	100	44, 64, 75, 81	0
43	2k	114/114 (100%)	-0.29	1 (0%)	84	80	54, 69, 80, 82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	1l	121/122 (99%)	-0.23	2 (1%)	70	63	51, 64, 72, 79	0
44	2l	121/122 (99%)	-0.17	1 (0%)	86	81	56, 66, 74, 77	0
45	1m	116/116 (100%)	0.33	8 (6%)	16	10	69, 77, 82, 83	0
45	2m	114/116 (98%)	0.48	11 (9%)	8	4	75, 81, 85, 88	0
46	1n	60/60 (100%)	0.35	4 (6%)	17	10	69, 77, 81, 83	0
46	2n	60/60 (100%)	0.83	10 (16%)	1	1	73, 81, 84, 88	0
47	1o	88/88 (100%)	-0.01	1 (1%)	80	75	52, 66, 76, 82	0
47	2o	88/88 (100%)	-0.17	1 (1%)	80	75	54, 69, 78, 81	0
48	1p	82/82 (100%)	0.15	3 (3%)	41	31	63, 74, 80, 87	0
48	2p	82/82 (100%)	0.15	2 (2%)	59	49	58, 69, 76, 84	0
49	1q	99/99 (100%)	-0.12	2 (2%)	65	56	54, 68, 77, 79	0
49	2q	99/99 (100%)	-0.26	0	100	100	57, 68, 76, 78	0
50	1r	68/68 (100%)	0.11	5 (7%)	14	8	57, 67, 75, 80	0
50	2r	68/68 (100%)	-0.07	2 (2%)	51	41	62, 69, 77, 79	0
51	1s	83/83 (100%)	0.88	16 (19%)	1	0	73, 79, 84, 85	0
51	2s	83/83 (100%)	1.73	32 (38%)	0	0	77, 83, 88, 90	0
52	1t	96/98 (97%)	0.17	3 (3%)	49	39	63, 72, 81, 83	0
52	2t	98/98 (100%)	0.10	1 (1%)	82	77	59, 69, 78, 80	0
53	1u	23/23 (100%)	1.18	5 (21%)	0	0	72, 75, 78, 81	0
53	2u	23/23 (100%)	1.71	9 (39%)	0	0	76, 79, 82, 84	0
54	1y	16/16 (100%)	0.46	2 (12%)	3	2	36, 50, 60, 61	0
54	2y	16/16 (100%)	1.09	5 (31%)	0	0	53, 59, 69, 72	0
All	All	20798/20986 (99%)	0.04	886 (4%)	35	25	17, 64, 85, 100	0

All (886) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1133	G	17.3
1	1A	1135	G	15.6
1	1A	1137	G	14.1
1	1A	1118	C	12.4
1	1A	1136	U	11.7
1	1A	1149	A	11.4
1	1A	1120	G	11.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1127	U	10.5
1	1A	1132	A	10.3
1	1A	1134	A	10.1
1	1A	1123	A	10.1
1	1A	1121	C	10.0
1	1A	1139	G	9.8
1	1A	1126	C	9.7
1	1A	1109	G	9.6
1	1A	1113	A	9.5
1	1A	1125	C	9.3
1	1A	1110	C	9.1
1	1A	1122	C	9.0
1	1A	1117	G	8.7
1	1A	1138	C	8.7
1	1A	1128	U	8.6
1	1A	1112	U	8.2
32	2a	1001(A)	G	8.1
1	1A	1129	U	8.1
32	2a	1030(B)	C	8.0
1	2A	2125	G	7.9
32	1a	1036	G	7.9
1	2A	2802	G	7.9
1	1A	1124	U	7.8
1	1A	1119	A	7.7
32	1a	1030(B)	C	7.6
1	2A	2147	G	7.6
1	2A	2123	G	7.5
32	2a	1030(A)	G	7.4
33	2x	9	GLN	7.3
42	1j	10	GLY	7.3
1	1A	1148	C	7.2
32	2a	1001	A	7.2
26	14	52	THR	7.2
1	1A	1150	C	7.1
1	2A	2126	A	6.9
1	2A	2139	C	6.9
1	2A	2162	G	6.7
1	1A	1103	A	6.6
1	2A	2169	A	6.6
1	2A	2174	C	6.6
1	2A	1046	A	6.5
1	2A	1085	A	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1031	G	6.5
1	2A	2124	G	6.4
33	2x	64	SER	6.3
1	1A	2139	A	6.3
1	2A	2168	G	6.3
1	2A	2146	C	6.2
32	1a	1001	A	6.1
1	1A	1111	U	6.1
1	1A	2138	G	6.1
32	1a	1034	G	6.1
32	1a	1001(A)	G	6.0
45	1m	115	LYS	6.0
1	1A	2145	G	5.9
32	1a	1030(C)	G	5.9
1	2A	1064	C	5.9
1	2A	2803	C	5.9
1	2A	2118	U	5.9
1	2A	2801(A)	A	5.8
1	2A	2131	G	5.8
1	2A	2154	G	5.8
1	2A	2155	G	5.8
32	2a	80	G	5.8
1	1A	1114	G	5.7
33	2x	73	ALA	5.7
32	1a	1037	C	5.7
32	2a	1036	G	5.7
1	1A	1131	A	5.6
1	2A	1067	A	5.6
1	2A	2176	A	5.6
1	2A	2173	A	5.6
32	1a	1002	G	5.5
1	2A	2107	C	5.5
32	2a	1257	U	5.5
20	2Y	1	MET	5.5
1	2A	2179	C	5.5
32	2a	1030(C)	G	5.5
1	2A	888	C	5.5
1	2A	2145	C	5.5
1	2A	2153	G	5.4
1	2A	2133	G	5.4
1	2A	2141	G	5.4
1	1A	2166	U	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2i	102	LEU	5.3
1	2A	2165	G	5.3
1	1A	2806	G	5.3
1	1A	2188	G	5.3
1	2A	229	A	5.2
32	1a	1035	A	5.2
1	1A	935	C	5.2
51	2s	71	LEU	5.2
26	24	49	PHE	5.2
42	2j	6	ILE	5.2
34	1b	136	VAL	5.2
41	1i	15	ALA	5.2
33	2x	42	SER	5.2
26	24	63	TYR	5.2
1	1A	1130	A	5.2
1	1A	2195	A	5.1
1	2A	2128	C	5.1
1	2A	2127	G	5.1
32	2a	1026	G	5.1
1	2A	1083	U	5.1
1	2A	2119	A	5.1
32	2a	1027	C	5.1
1	1A	2816	G	5.1
42	1j	100	THR	5.1
32	2a	1030(D)	A	5.1
32	1a	1005	A	5.0
1	2A	2106	G	5.0
39	2g	156	TRP	5.0
39	2g	154	TYR	5.0
1	1A	2161	C	5.0
1	2A	2157	G	5.0
32	1a	1032	G	5.0
1	2A	2896	C	5.0
32	1a	1003	G	4.9
35	1c	193	TYR	4.9
1	1A	2169	G	4.9
26	24	45	GLY	4.9
1	2A	1095	A	4.9
1	2A	2138	C	4.9
32	2a	1034	G	4.9
1	1A	2183	C	4.9
1	1A	2154	U	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2159	G	4.8
32	1a	1026	G	4.8
32	1a	1286	A	4.8
23	11	2	SER	4.8
1	2A	1082	U	4.8
39	2g	82	GLY	4.8
1	2A	2166	G	4.8
32	1a	1030	C	4.7
32	2a	1002	G	4.7
1	1A	2134	G	4.7
1	2A	2132	U	4.7
1	2A	2120	G	4.7
1	1A	2807	C	4.6
1	2A	2804	C	4.6
42	2j	74	ILE	4.6
1	2A	2110	G	4.6
32	2a	1035	A	4.6
1	1A	1108	G	4.6
1	1A	1141	A	4.6
39	1g	156	TRP	4.6
1	1A	2163	G	4.6
32	1a	1028	C	4.6
33	2x	41	LEU	4.5
51	1s	40	ILE	4.5
1	2A	1079	C	4.5
1	2A	2148	G	4.5
51	2s	12	ASP	4.5
1	2A	2142	C	4.5
32	1a	1024	G	4.5
32	2a	1031	G	4.5
32	1a	1004	A	4.4
1	1A	2814	C	4.4
1	2A	1076	C	4.4
1	2A	2164	C	4.4
32	2a	998	G	4.4
1	2A	1088	A	4.4
1	1A	2147	G	4.4
1	2A	2112	G	4.4
1	2A	2140	C	4.4
33	2x	10	MET	4.4
33	2x	46	GLN	4.4
41	1i	106	ALA	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2121	G	4.4
32	1a	1257	U	4.3
32	1a	1033	G	4.3
45	1m	2	ALA	4.3
1	1A	1555	C	4.3
1	1A	2151	C	4.3
1	2A	2793	G	4.3
32	2a	1040	U	4.3
14	2S	58	LEU	4.3
51	1s	56	GLN	4.3
1	1A	2148	A	4.3
26	14	54	GLY	4.3
32	1a	1030(A)	G	4.3
41	2i	72	GLY	4.3
32	1a	202	U	4.3
46	2n	13	THR	4.3
1	1A	2181	G	4.3
32	1a	1027	C	4.3
32	2a	1033	G	4.3
1	2A	2897	U	4.3
51	2s	64	GLU	4.3
34	1b	133	LYS	4.3
1	2A	2143	C	4.2
1	1A	2137	G	4.2
1	2A	2152	G	4.2
1	1A	2177	G	4.2
26	24	69	LYS	4.2
1	1A	2162	C	4.2
1	1A	2175	G	4.2
1	2A	1509	C	4.2
1	1A	2149	G	4.1
1	2A	2170	A	4.1
26	24	50	VAL	4.1
1	2A	2122	U	4.1
1	2A	2144	U	4.1
1	2A	2792	G	4.1
33	2x	63	ALA	4.1
32	1a	1030(D)	A	4.1
1	2A	2111	C	4.1
41	1i	78	LYS	4.1
1	2A	2136	C	4.1
53	1u	18	TYR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2198	A	4.1
1	1A	2160	C	4.1
1	1A	2165	C	4.1
1	2A	2134	A	4.1
42	2j	36	GLY	4.0
1	1A	2191	A	4.0
1	1A	2130	C	4.0
32	1a	1038	C	4.0
32	2a	1030	C	4.0
42	2j	85	LEU	4.0
1	2A	652(B)	A	4.0
1	2A	2137	C	4.0
1	2A	2175	C	4.0
1	2A	6	A	4.0
32	2a	1041	A	4.0
32	1a	1006	C	4.0
6	2G	62	LEU	4.0
1	1A	2194	U	4.0
1	1A	2189	U	4.0
1	2A	2158	A	3.9
1	1A	2167	C	3.9
34	1b	135	GLN	3.9
26	14	59	PHE	3.9
33	2x	65	GLY	3.9
33	2x	50	ALA	3.9
26	24	68	ARG	3.9
1	2A	1104	C	3.9
32	1a	1029	C	3.9
1	1A	2141	A	3.9
1	1A	1104	G	3.9
1	2A	2805	G	3.9
32	1a	204	U	3.9
1	2A	2105	C	3.9
33	2x	38	HIS	3.9
1	1A	2190	G	3.9
42	1j	8	LEU	3.9
51	2s	13	ASP	3.9
46	2n	12	ARG	3.9
1	1A	1221	G	3.9
1	1A	2182	G	3.9
1	1A	2178	G	3.9
32	2a	1003	G	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2151	G	3.8
26	24	64	GLY	3.8
7	2H	103	LEU	3.8
1	2A	2167	U	3.8
1	2A	2108	C	3.8
34	2b	232	PRO	3.8
42	2j	20	ALA	3.8
1	1A	2813	G	3.8
51	2s	48	THR	3.8
1	1A	2164	C	3.8
26	14	65	ASP	3.8
46	2n	38	GLY	3.8
32	2a	1286	A	3.7
32	2a	1042	G	3.7
1	1A	2815	C	3.7
32	2a	89	C	3.7
42	1j	5	ARG	3.7
33	2x	49	VAL	3.7
54	2y	16	ILE	3.7
7	2H	29	PRO	3.7
1	2A	2109	U	3.7
35	2c	158	GLY	3.7
1	2A	2178	C	3.7
1	1A	2187	G	3.7
7	2H	128	PRO	3.7
42	1j	96	ILE	3.7
1	2A	2171	A	3.7
7	2H	30	LYS	3.7
1	2A	2156	G	3.7
1	1A	2168	C	3.7
1	2A	2163	C	3.7
32	2a	1029	C	3.7
1	2A	889	C	3.6
1	2A	2116	G	3.6
52	1t	55	ILE	3.6
34	1b	130	ARG	3.6
1	2A	2177	C	3.6
20	2Y	90	LEU	3.6
1	2A	1080	C	3.6
1	2A	2794	C	3.6
35	2c	190	ARG	3.6
33	2x	75	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1037	C	3.6
34	1b	129	GLU	3.6
33	2x	68	GLU	3.6
7	2H	82	GLY	3.6
34	1b	128	GLU	3.6
33	2x	8	LYS	3.5
1	1A	2180	A	3.5
32	2a	1004	A	3.5
34	1b	131	PRO	3.5
1	1A	2186	C	3.5
11	2P	91	PHE	3.5
33	2x	11	GLU	3.5
6	2G	49	ASP	3.5
41	2i	7	THR	3.5
8	2I	74	ASN	3.5
1	2A	2172	U	3.5
51	2s	53	ASN	3.5
33	1x	95	ARG	3.5
32	2a	90	U	3.5
51	2s	16	LEU	3.5
1	1A	1099	C	3.4
35	1c	101	LEU	3.4
46	2n	25	VAL	3.4
32	1a	1039	C	3.4
1	1A	2170	G	3.4
1	1A	2129	C	3.4
6	2G	2	PRO	3.4
26	24	66	SER	3.4
34	1b	232	PRO	3.4
33	2x	45	PRO	3.4
1	2A	2160	G	3.4
34	2b	133	LYS	3.4
23	21	2	SER	3.4
1	2A	2149	G	3.4
6	2G	48	GLU	3.4
7	2H	50	VAL	3.4
43	2k	13	GLN	3.3
39	2g	32	ARG	3.3
1	2A	2150	U	3.3
7	2H	48	GLY	3.3
42	1j	98	ILE	3.3
42	1j	85	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2b	123	ALA	3.3
41	2i	30	GLY	3.3
32	2a	1024	G	3.3
32	1a	841	U	3.3
14	2S	20	ARG	3.3
42	1j	75	ILE	3.3
39	1g	16	LEU	3.3
32	2a	79	G	3.3
1	1A	1116	A	3.3
1	1A	1143	U	3.3
53	2u	11	GLY	3.3
1	1A	2171	G	3.3
1	2A	2894	G	3.3
32	2a	1032	G	3.3
34	2b	70	PHE	3.3
51	2s	63	THR	3.3
1	2A	2129	C	3.2
1	1A	2193	A	3.2
32	2a	848	C	3.2
51	1s	58	VAL	3.2
1	1A	2155	G	3.2
1	1A	2905	C	3.2
1	2A	11	G	3.2
7	2H	47	GLU	3.2
34	1b	123	ALA	3.2
32	2a	1006	C	3.2
42	2j	40	LEU	3.2
1	1A	2152	U	3.2
26	24	67	TYR	3.2
1	1A	2131	U	3.2
26	24	52	THR	3.2
53	1u	19	GLY	3.2
6	1G	80	PHE	3.2
46	2n	11	LYS	3.1
45	2m	82	MET	3.1
33	2x	20	VAL	3.1
49	1q	98	LEU	3.1
1	2A	1075	C	3.1
1	2A	2113	U	3.1
26	14	64	GLY	3.1
51	2s	82	GLY	3.1
7	2H	159	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2x	48	PHE	3.1
1	1A	1105	G	3.1
32	2a	1021	G	3.1
1	1A	2202	U	3.1
26	24	54	GLY	3.1
1	2A	887	A	3.1
34	1b	228	GLY	3.1
1	1A	2176	G	3.1
33	2x	77	LEU	3.1
32	1a	203	U	3.1
41	1i	46	ALA	3.1
35	1c	87	LEU	3.1
54	2y	13	PRO	3.1
1	1A	2812	A	3.1
41	2i	127	LYS	3.1
53	2u	14	TRP	3.1
6	2G	19	LEU	3.0
53	2u	6	ARG	3.0
32	1a	1000	U	3.0
33	2x	88	LEU	3.0
6	2G	67	LYS	3.0
35	2c	124	ILE	3.0
42	2j	72	VAL	3.0
1	1A	2150	C	3.0
1	2A	1086	A	3.0
32	2a	202	U	3.0
39	2g	79	ARG	3.0
1	2A	1087	G	3.0
42	2j	89	ASP	3.0
51	2s	49	ILE	3.0
54	2y	15	PRO	3.0
32	2a	994	A	3.0
20	2Y	58	GLY	3.0
1	1A	2173	G	3.0
1	1A	2906	U	3.0
32	2a	841	U	3.0
46	2n	10	ALA	3.0
1	1A	2140	U	3.0
1	2A	614(A)	U	3.0
1	1A	696	C	3.0
1	1A	1144	A	3.0
46	1n	17	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1025	U	3.0
32	2a	723	U	3.0
1	2A	2161	C	3.0
32	2a	1039	C	3.0
42	2j	98	ILE	3.0
35	2c	64	VAL	3.0
42	2j	27	ALA	2.9
7	2H	95	ARG	2.9
51	1s	71	LEU	2.9
33	2x	39	ILE	2.9
51	2s	81	ARG	2.9
1	1A	1220	U	2.9
50	1r	24	ALA	2.9
1	1A	1145	G	2.9
19	2X	68	ARG	2.9
34	2b	124	SER	2.9
7	2H	102	ALA	2.9
1	1A	1147	U	2.9
1	1A	2144	U	2.9
45	1m	87	TYR	2.9
1	2A	652(T)	C	2.9
32	1a	1007	C	2.9
41	1i	47	LEU	2.9
1	1A	2179	G	2.9
32	1a	216	G	2.9
50	2r	58	LEU	2.9
32	1a	1136	U	2.9
26	14	45	GLY	2.9
26	24	56	VAL	2.9
1	1A	2196	C	2.9
1	1A	1140	U	2.9
51	1s	60	VAL	2.9
32	2a	1023	G	2.9
42	1j	7	LYS	2.8
14	2S	35	ILE	2.8
42	2j	86	MET	2.8
1	2A	890	A	2.8
1	2A	2807	G	2.8
18	1W	111	HIS	2.8
34	2b	122	PHE	2.8
41	2i	18	PHE	2.8
51	2s	20	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2130	U	2.8
26	24	27	THR	2.8
36	1d	23	GLY	2.8
1	2A	614(B)	G	2.8
45	2m	87	TYR	2.8
42	1j	77	PRO	2.8
1	1A	697	C	2.8
51	2s	80	TYR	2.8
1	1A	2174	G	2.8
1	2A	1057	A	2.8
20	2Y	91	GLU	2.8
32	1a	217	C	2.8
51	1s	47	HIS	2.8
7	2H	18	GLU	2.8
45	2m	116	THR	2.8
1	2A	1043	C	2.8
51	2s	52	TYR	2.8
1	1A	2146	G	2.8
1	2A	10	G	2.8
53	1u	22	ARG	2.8
1	1A	2135	U	2.7
1	2A	2180	U	2.7
35	1c	96	GLY	2.7
45	2m	78	ILE	2.7
1	2A	1044	G	2.7
11	2P	125	VAL	2.7
41	2i	27	THR	2.7
1	2A	2135	A	2.7
7	2H	13	LYS	2.7
33	2x	58	ASN	2.7
33	2x	92	GLY	2.7
6	2G	82	LEU	2.7
1	1A	2153	G	2.7
45	2m	92	HIS	2.7
1	1A	218	A	2.7
50	1r	29	PHE	2.7
1	1A	2805	G	2.7
21	2Z	143	GLY	2.7
1	2A	645	C	2.7
26	24	59	PHE	2.7
51	2s	15	LEU	2.7
35	1c	2	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	1081	U	2.7
45	2m	84	ILE	2.7
6	2G	75	LYS	2.7
21	2Z	199	LYS	2.7
33	2x	80	LYS	2.7
7	2H	113	VAL	2.7
46	2n	8	GLU	2.7
35	2c	159	GLY	2.7
1	2A	1066	U	2.7
41	2i	83	ARG	2.7
7	2H	43	VAL	2.7
20	2Y	55	TYR	2.7
20	2Y	89	PHE	2.7
39	1g	154	TYR	2.7
1	1A	1151	U	2.7
32	2a	84	U	2.7
39	2g	6	ARG	2.7
6	1G	49	ASP	2.7
1	2A	2181	G	2.7
34	1b	125	PRO	2.7
34	2b	227	GLY	2.7
32	2a	1005	A	2.7
45	1m	116	THR	2.7
1	2A	1068	G	2.7
42	2j	29	ARG	2.7
53	1u	6	ARG	2.7
32	1a	1020	U	2.6
32	2a	1136	U	2.6
40	1h	58	TYR	2.6
26	14	50	VAL	2.6
32	2a	91	C	2.6
39	2g	155	ARG	2.6
53	2u	10	ARG	2.6
1	1A	2203	G	2.6
32	2a	1020	U	2.6
11	2P	122	PRO	2.6
32	1a	1137	C	2.6
20	1Y	1	MET	2.6
51	2s	40	ILE	2.6
1	2A	1059	G	2.6
32	1a	1023	G	2.6
41	2i	8	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2b	33	TYR	2.6
42	1j	30	SER	2.6
44	1l	64	TYR	2.6
46	2n	35	ARG	2.6
51	2s	30	LEU	2.6
18	1W	112	GLY	2.6
42	1j	72	VAL	2.6
1	2A	652(C)	G	2.6
1	2A	1042	G	2.6
1	2A	1103	A	2.6
32	1a	344	A	2.6
32	1a	201	C	2.6
51	2s	11	VAL	2.6
6	2G	79	ASN	2.6
1	1A	2136	A	2.6
39	2g	81	GLY	2.6
41	2i	54	ASP	2.6
46	1n	25	VAL	2.6
20	2Y	56	PRO	2.6
44	2l	28	LYS	2.6
39	2g	86	GLN	2.6
42	2j	87	THR	2.6
1	1A	2192	A	2.6
1	2A	2602	A	2.6
7	2H	41	MET	2.6
7	2H	105	LEU	2.6
32	2a	1000	U	2.6
8	2I	3	VAL	2.6
39	2g	33	ASP	2.6
45	2m	80	ARG	2.6
33	2x	15	ALA	2.6
33	2x	70	MET	2.5
51	1s	66	MET	2.5
1	1A	2185	C	2.5
26	24	57	GLU	2.5
33	2x	76	GLU	2.5
35	2c	89	GLU	2.5
53	2u	8	THR	2.5
33	2x	95	ARG	2.5
41	2i	59	PHE	2.5
46	2n	2	ALA	2.5
1	2A	2114	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2j	84	GLN	2.5
1	2A	2187	G	2.5
46	1n	55	GLY	2.5
46	1n	11	LYS	2.5
42	1j	90	LEU	2.5
50	1r	78	LEU	2.5
32	1a	77	G	2.5
1	1A	2199	C	2.5
1	1A	2803	A	2.5
32	1a	161	A	2.5
51	2s	66	MET	2.5
1	1A	2126	G	2.5
39	2g	8	GLU	2.5
42	1j	40	LEU	2.5
53	2u	13	ILE	2.5
42	2j	34	VAL	2.5
33	2x	67	HIS	2.5
42	2j	68	HIS	2.5
41	2i	5	TYR	2.5
34	2b	130	ARG	2.5
51	2s	45	VAL	2.5
1	2A	2117	A	2.5
1	1A	1101	G	2.5
35	2c	8	ILE	2.5
41	2i	79	LEU	2.5
1	1A	2200	C	2.4
32	2a	1043	C	2.4
33	2x	7	SER	2.4
1	1A	934	A	2.4
35	1c	206	GLU	2.4
42	1j	70	ARG	2.4
45	2m	94	ARG	2.4
45	2m	102	ARG	2.4
1	2A	2104	G	2.4
32	1a	78	G	2.4
1	1A	34	C	2.4
4	2E	1	MET	2.4
20	2Y	60	PHE	2.4
32	2a	1018	C	2.4
32	2a	1028	C	2.4
1	1A	2156	A	2.4
34	2b	201	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	1c	124	ILE	2.4
39	1g	42	ILE	2.4
1	2A	652(V)	C	2.4
1	2A	2895	U	2.4
26	24	46	GLN	2.4
21	2Z	201	LYS	2.4
33	2x	12	ILE	2.4
45	2m	41	PRO	2.4
54	1y	10	PRO	2.4
1	1A	2172	U	2.4
32	2a	1019	C	2.4
1	1A	2206	G	2.4
26	24	44	THR	2.4
33	2x	71	TYR	2.4
8	2I	142	VAL	2.4
41	2i	90	PRO	2.4
41	2i	92	TYR	2.4
41	2i	103	THR	2.4
42	2j	21	GLN	2.4
1	2A	1106	G	2.4
1	2A	2100	G	2.4
7	2H	115	VAL	2.4
26	14	56	VAL	2.4
26	24	7	PRO	2.4
51	2s	84	GLY	2.4
20	2Y	65	ALA	2.4
41	2i	45	ALA	2.4
1	1A	2210	C	2.4
48	2p	19	ILE	2.4
50	1r	31	LEU	2.4
1	1A	2184	G	2.4
41	2i	42	ARG	2.4
34	1b	227	GLY	2.4
35	2c	206	GLU	2.4
36	2d	180	GLY	2.4
1	1A	2157	A	2.4
1	2A	34	C	2.4
51	1s	30	LEU	2.4
20	2Y	57	GLN	2.4
41	2i	36	TYR	2.4
1	2A	1084	A	2.4
48	1p	50	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	218	C	2.4
20	2Y	45	VAL	2.3
26	24	19	GLY	2.3
35	2c	71	ALA	2.3
45	2m	93	ARG	2.3
35	1c	39	ILE	2.3
7	2H	34	GLU	2.3
1	1A	2197	C	2.3
32	1a	91	C	2.3
51	2s	68	GLY	2.3
53	1u	9	ARG	2.3
1	1A	2128	G	2.3
52	1t	9	ASN	2.3
33	2x	47	GLY	2.3
35	1c	194	GLY	2.3
39	2g	141	VAL	2.3
22	20	74	ARG	2.3
51	1s	59	PRO	2.3
41	2i	88	TYR	2.3
51	1s	61	TYR	2.3
44	1l	61	THR	2.3
51	2s	28	LYS	2.3
1	2A	1056	G	2.3
35	1c	180	ALA	2.3
35	2c	189	ALA	2.3
1	2A	652(U)	G	2.3
32	1a	999	C	2.3
35	2c	193	TYR	2.3
51	2s	24	ALA	2.3
45	1m	114	ARG	2.3
5	1F	15	SER	2.3
21	1Z	192	ALA	2.3
51	1s	74	PHE	2.3
41	2i	87	GLN	2.3
41	2i	105	ASP	2.3
41	2i	94	ALA	2.3
33	2x	87	LYS	2.3
33	2x	91	LYS	2.3
1	1A	2204	G	2.3
8	2I	81	VAL	2.2
33	2x	79	ASN	2.2
50	1r	25	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	2u	15	ARG	2.2
31	29	37	GLY	2.2
41	1i	81	ILE	2.2
51	2s	32	LYS	2.2
1	1A	1146	C	2.2
42	1j	47	PHE	2.2
26	14	55	ARG	2.2
1	1A	2142	G	2.2
32	1a	1040	U	2.2
32	2a	204	U	2.2
6	2G	152	LEU	2.2
22	20	76	GLY	2.2
41	2i	19	LEU	2.2
32	2a	1038	C	2.2
6	2G	136	ARG	2.2
25	23	59	VAL	2.2
35	1c	64	VAL	2.2
41	2i	86	VAL	2.2
1	1A	6	A	2.2
32	2a	1531	A	2.2
6	2G	3	LEU	2.2
51	2s	8	GLY	2.2
1	1A	2201	C	2.2
1	2A	2892	A	2.2
32	1a	162	A	2.2
34	2b	43	ASP	2.2
41	1i	30	GLY	2.2
51	1s	57	HIS	2.2
1	1A	2132	G	2.2
1	2A	2184	G	2.2
46	2n	24	CYS	2.2
1	2A	1041	C	2.2
32	1a	840	C	2.2
25	23	26	LEU	2.2
34	1b	134	GLU	2.2
51	2s	17	GLU	2.2
12	2Q	5	ARG	2.2
42	1j	27	ALA	2.2
42	2j	35	SER	2.2
36	2d	158	ILE	2.2
51	1s	50	ALA	2.2
1	1A	694	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	698	G	2.2
1	2A	2893	G	2.2
26	24	43	TYR	2.2
32	2a	1017	G	2.2
26	14	57	GLU	2.2
32	1a	163	C	2.2
32	2a	1007	C	2.2
32	2a	1045	C	2.2
41	2i	110	GLU	2.2
41	2i	75	ASP	2.2
1	1A	2143	G	2.2
1	2A	1062	G	2.2
1	2A	1089	G	2.2
32	2a	1022	G	2.2
47	2o	6	GLU	2.2
34	2b	228	GLY	2.2
1	1A	936	C	2.2
26	14	68	ARG	2.2
41	2i	66	ARG	2.2
48	2p	48	TRP	2.2
26	14	18	CYS	2.2
50	2r	24	ALA	2.2
33	2x	72	THR	2.2
49	1q	99	SER	2.2
51	1s	69	HIS	2.2
12	2Q	59	ARG	2.2
41	1i	80	GLY	2.2
42	1j	9	ARG	2.2
41	2i	52	ALA	2.2
42	2j	47	PHE	2.2
26	24	29	PRO	2.2
39	2g	153	HIS	2.2
34	1b	126	GLU	2.2
36	1d	135	LEU	2.1
1	2A	1058	G	2.1
1	2A	2115	G	2.1
35	1c	89	GLU	2.1
7	2H	106	THR	2.1
6	2G	25	TYR	2.1
41	2i	62	TYR	2.1
34	1b	132	LYS	2.1
35	2c	65	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	1t	100	ILE	2.1
52	2t	55	ILE	2.1
34	2b	131	PRO	2.1
1	1A	1102	G	2.1
51	2s	69	HIS	2.1
7	2H	114	VAL	2.1
39	2g	80	VAL	2.1
1	2A	653	A	2.1
34	1b	122	PHE	2.1
1	2A	1065	U	2.1
6	2G	39	ILE	2.1
7	2H	97	ARG	2.1
54	2y	12	PRO	2.1
7	1H	2	SER	2.1
1	2A	1533	G	2.1
32	1a	156	G	2.1
6	2G	146	TYR	2.1
48	1p	39	TYR	2.1
20	2Y	50	ARG	2.1
42	1j	33	GLN	2.1
51	2s	36	ARG	2.1
15	1T	38	ASN	2.1
32	2a	999	C	2.1
34	1b	121	LEU	2.1
1	2A	1099	G	2.1
32	1a	1212	U	2.1
33	2x	40	ILE	2.1
33	2x	74	ILE	2.1
35	2c	157	ILE	2.1
7	2H	25	LYS	2.1
47	1o	89	GLY	2.1
1	1A	2158	C	2.1
35	2c	154	SER	2.1
51	2s	35	SER	2.1
51	2s	47	HIS	2.1
5	1F	16	GLY	2.1
1	2A	1045	A	2.1
7	2H	6	ARG	2.1
7	2H	101	ARG	2.1
1	2A	652(D)	C	2.1
1	2A	886	C	2.1
1	2A	2103	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1b	231	GLU	2.1
41	2i	4	TYR	2.1
51	1s	12	ASP	2.1
34	2b	137	ARG	2.1
45	1m	93	ARG	2.1
1	2A	2629	A	2.1
35	2c	87	LEU	2.1
45	1m	90	LEU	2.1
51	2s	56	GLN	2.1
8	2I	144	VAL	2.1
45	1m	117	VAL	2.1
51	1s	38	SER	2.0
41	2i	82	ALA	2.0
53	2u	9	ARG	2.0
54	2y	14	ARG	2.0
7	2H	44	VAL	2.0
1	2A	2182	G	2.0
32	1a	79	G	2.0
1	1A	1115	A	2.0
1	2A	1054	A	2.0
32	1a	723	U	2.0
35	2c	160	ALA	2.0
36	2d	149	ALA	2.0
42	1j	36	GLY	2.0
7	2H	45	VAL	2.0
35	1c	63	ASN	2.0
1	1A	2207	C	2.0
1	2A	1170	G	2.0
32	1a	1021	G	2.0
32	1a	1493	A	2.0
54	1y	11	THR	2.0
41	2i	6	GLY	2.0
1	1A	1072	U	2.0
1	2A	1060	U	2.0
1	2A	883	G	2.0
1	2A	2186	G	2.0
48	1p	57	ARG	2.0
53	2u	17	THR	2.0
41	2i	21	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	1A	1939	20/21	0.91	0.22	60,73,87,88	0
1	5MU	1A	1937	21/22	0.92	0.23	73,79,94,111	0
32	2MG	2a	1207	24/25	0.92	0.21	76,85,87,93	0
32	5MC	2a	967	21/22	0.93	0.15	67,70,79,85	0
32	M2G	2a	966	25/26	0.93	0.14	64,71,79,91	0
32	PSU	2a	516	20/21	0.94	0.16	70,80,85,85	0
32	PSU	1a	516	20/21	0.94	0.15	62,72,77,77	0
1	PSU	2A	1911	20/21	0.94	0.11	68,72,78,81	0
1	PSU	2A	1917	20/21	0.94	0.14	67,76,84,95	0
32	2MG	1a	1207	24/25	0.95	0.12	71,78,82,84	0
32	G7M	2a	527	24/25	0.95	0.17	64,71,75,80	0
32	M2G	1a	966	25/26	0.95	0.14	58,63,73,75	0
1	5MU	2A	1915	21/22	0.95	0.18	76,82,87,102	0
32	5MC	1a	967	21/22	0.95	0.14	62,67,74,77	0
32	5MC	2a	1404	21/22	0.95	0.16	51,55,61,66	0
32	5MC	1a	1407	21/22	0.96	0.17	42,55,59,61	0
32	5MC	2a	1400	21/22	0.96	0.18	61,70,74,75	0
32	4OC	2a	1402	22/23	0.96	0.16	54,61,66,70	0
1	OMC	2A	1920	21/22	0.96	0.15	59,65,69,74	0
44	0TD	2l	92	10/11	0.96	0.12	68,70,74,84	0
1	5MC	2A	1962	21/22	0.97	0.14	38,46,53,61	0
1	2MA	2A	2503	23/24	0.97	0.23	33,38,41,42	0
1	PSU	2A	2605	20/21	0.97	0.18	34,38,44,44	0
32	UR3	1a	1498	21/22	0.97	0.18	48,53,58,64	0
32	MA6	1a	1518	24/25	0.97	0.20	42,51,58,62	0
32	MA6	1a	1519	24/25	0.97	0.18	46,53,58,61	0
44	0TD	1l	92	10/11	0.97	0.13	64,65,70,78	0
1	PSU	1A	1933	20/21	0.97	0.14	62,68,71,72	0
32	G7M	1a	527	24/25	0.97	0.16	50,60,66,69	0
32	4OC	1a	1402	22/23	0.97	0.17	50,53,57,60	0
1	OMC	1A	1942	21/22	0.97	0.14	51,61,63,67	0
32	5MC	2a	1407	21/22	0.97	0.14	51,59,66,69	0
32	UR3	2a	1498	21/22	0.97	0.15	50,60,64,67	0
32	MA6	2a	1518	24/25	0.97	0.17	54,63,68,69	0
32	MA6	2a	1519	24/25	0.97	0.19	51,61,65,68	0
1	5MC	2A	1942	21/22	0.97	0.16	47,52,55,56	0
1	5MU	1A	1961	21/22	0.98	0.17	24,28,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	2A	1939	21/22	0.98	0.16	36,39,45,46	0
1	5MC	1A	1964	21/22	0.98	0.13	29,37,42,45	0
1	5MC	1A	1984	21/22	0.98	0.14	31,37,39,44	0
1	OMG	2A	2251	24/25	0.98	0.16	37,44,46,51	0
1	OMG	1A	2263	24/25	0.98	0.18	19,25,27,30	0
1	OMU	1A	2564	21/22	0.98	0.18	23,29,31,33	0
32	5MC	1a	1400	21/22	0.98	0.14	57,61,66,67	0
1	PSU	1A	2617	20/21	0.98	0.21	23,27,33,34	0
32	5MC	1a	1404	21/22	0.98	0.15	45,50,54,55	0
1	2MA	1A	2515	23/24	0.99	0.21	16,20,24,24	0
1	OMU	2A	2552	21/22	0.99	0.16	32,43,45,45	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3411	1/1	0.20	0.94	88,88,88,88	0
55	MG	2A	3090	1/1	0.34	0.34	78,78,78,78	0
55	MG	2a	1791	1/1	0.34	0.31	102,102,102,102	0
55	MG	2A	3532	1/1	0.38	0.28	87,87,87,87	0
55	MG	1A	3898	1/1	0.44	0.53	53,53,53,53	0
55	MG	2A	3549	1/1	0.46	0.47	72,72,72,72	0
55	MG	2A	3554	1/1	0.48	0.75	62,62,62,62	0
55	MG	2A	3506	1/1	0.48	0.52	72,72,72,72	0
55	MG	2N	201	1/1	0.49	0.43	90,90,90,90	0
55	MG	2A	3717	1/1	0.50	0.15	89,89,89,89	0
55	MG	1B	206	1/1	0.52	0.17	66,66,66,66	0
55	MG	2A	3454	1/1	0.52	1.21	67,67,67,67	0
55	MG	1A	3758	1/1	0.52	0.60	60,60,60,60	0
55	MG	1A	3496	1/1	0.53	0.08	73,73,73,73	0
55	MG	1A	3185	1/1	0.53	0.18	74,74,74,74	0
55	MG	1A	3359	1/1	0.54	0.12	80,80,80,80	0
55	MG	1a	3078	1/1	0.54	0.71	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1722	1/1	0.54	0.12	77,77,77,77	0
55	MG	2a	1750	1/1	0.54	0.20	103,103,103,103	0
55	MG	1A	3254	1/1	0.54	0.52	59,59,59,59	0
55	MG	2a	1741	1/1	0.55	0.46	91,91,91,91	0
55	MG	2A	3475	1/1	0.55	0.53	66,66,66,66	0
55	MG	1a	3151	1/1	0.55	0.14	81,81,81,81	0
55	MG	2A	3562	1/1	0.56	0.46	81,81,81,81	0
55	MG	1A	3712	1/1	0.56	0.23	96,96,96,96	0
55	MG	2A	3791	1/1	0.56	0.76	73,73,73,73	0
55	MG	2A	3555	1/1	0.56	0.68	70,70,70,70	0
55	MG	1a	3077	1/1	0.57	0.76	68,68,68,68	0
55	MG	1A	3854	1/1	0.57	0.14	74,74,74,74	0
55	MG	2A	3810	1/1	0.58	0.15	68,68,68,68	0
55	MG	1a	3058	1/1	0.58	0.58	81,81,81,81	0
55	MG	1a	3168	1/1	0.58	0.07	75,75,75,75	0
55	MG	2d	504	1/1	0.58	0.25	93,93,93,93	0
55	MG	1A	3213	1/1	0.59	0.52	56,56,56,56	0
55	MG	1A	3886	1/1	0.59	0.22	39,39,39,39	0
55	MG	2A	3113	1/1	0.59	0.23	66,66,66,66	0
55	MG	2B	3013	1/1	0.60	0.06	77,77,77,77	0
55	MG	2a	1719	1/1	0.61	0.23	75,75,75,75	0
55	MG	2A	3103	1/1	0.61	0.25	64,64,64,64	0
55	MG	2A	3773	1/1	0.61	0.10	81,81,81,81	0
55	MG	1A	3609	1/1	0.62	0.40	63,63,63,63	0
55	MG	1D	313	1/1	0.62	0.25	54,54,54,54	0
55	MG	2A	3133	1/1	0.62	0.48	64,64,64,64	0
55	MG	2A	3610	1/1	0.62	0.10	82,82,82,82	0
55	MG	2n	502	1/1	0.62	0.48	77,77,77,77	0
55	MG	2A	3178	1/1	0.63	0.23	73,73,73,73	0
55	MG	1B	220	1/1	0.63	0.22	57,57,57,57	0
55	MG	1A	3721	1/1	0.63	0.24	71,71,71,71	0
55	MG	2A	3635	1/1	0.63	0.23	97,97,97,97	0
55	MG	2A	3695	1/1	0.63	0.10	82,82,82,82	0
55	MG	1H	8001	1/1	0.63	0.23	91,91,91,91	0
55	MG	1A	3608	1/1	0.64	0.18	76,76,76,76	0
55	MG	1A	3839	1/1	0.64	0.18	68,68,68,68	0
55	MG	2A	3574	1/1	0.65	0.31	99,99,99,99	0
55	MG	2A	3727	1/1	0.65	0.61	64,64,64,64	0
55	MG	2A	3128	1/1	0.65	0.59	83,83,83,83	0
55	MG	2a	1731	1/1	0.65	0.13	88,88,88,88	0
55	MG	2A	3627	1/1	0.65	0.19	67,67,67,67	0
55	MG	2A	3049	1/1	0.65	1.70	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3813	1/1	0.65	0.49	59,59,59,59	0
55	MG	1A	3095	1/1	0.65	0.41	58,58,58,58	0
55	MG	2D	302	1/1	0.65	0.35	67,67,67,67	0
55	MG	1B	222	1/1	0.66	0.10	78,78,78,78	0
55	MG	2a	1753	1/1	0.66	0.22	84,84,84,84	0
55	MG	2A	3752	1/1	0.66	0.41	77,77,77,77	0
55	MG	2d	503	1/1	0.66	0.24	72,72,72,72	0
55	MG	2A	3136	1/1	0.66	0.47	59,59,59,59	0
55	MG	2l	201	1/1	0.66	0.80	106,106,106,106	0
55	MG	2P	202	1/1	0.66	0.31	74,74,74,74	0
55	MG	2A	3473	1/1	0.67	0.13	71,71,71,71	0
55	MG	2A	3675	1/1	0.67	0.16	75,75,75,75	0
55	MG	2A	3474	1/1	0.67	0.10	78,78,78,78	0
55	MG	1A	3201	1/1	0.67	0.30	61,61,61,61	0
55	MG	1a	3210	1/1	0.67	0.15	76,76,76,76	0
55	MG	1A	3112	1/1	0.68	0.38	50,50,50,50	0
55	MG	1B	207	1/1	0.68	0.24	60,60,60,60	0
55	MG	2B	3012	1/1	0.68	0.07	80,80,80,80	0
55	MG	1A	3135	1/1	0.69	0.17	71,71,71,71	0
55	MG	2A	3501	1/1	0.69	0.21	57,57,57,57	0
55	MG	1E	303	1/1	0.69	0.29	64,64,64,64	0
55	MG	2A	3376	1/1	0.69	0.15	89,89,89,89	0
55	MG	2A	3672	1/1	0.69	0.32	67,67,67,67	0
55	MG	1F	309	1/1	0.69	0.25	59,59,59,59	0
55	MG	1A	3912	1/1	0.69	0.26	52,52,52,52	0
55	MG	2B	3017	1/1	0.69	0.21	91,91,91,91	0
55	MG	1A	3701	1/1	0.69	0.35	44,44,44,44	0
55	MG	2A	3042	1/1	0.69	0.63	59,59,59,59	0
55	MG	2A	3748	1/1	0.69	0.11	66,66,66,66	0
55	MG	1A	3130	1/1	0.70	0.24	65,65,65,65	0
55	MG	1A	3855	1/1	0.70	0.23	51,51,51,51	0
55	MG	2A	3678	1/1	0.70	0.09	91,91,91,91	0
55	MG	2A	3131	1/1	0.70	0.51	71,71,71,71	0
55	MG	1A	3861	1/1	0.70	0.08	75,75,75,75	0
55	MG	2B	3015	1/1	0.70	0.12	79,79,79,79	0
55	MG	1A	3530	1/1	0.70	0.17	63,63,63,63	0
55	MG	1A	3832	1/1	0.70	0.08	72,72,72,72	0
55	MG	2A	3258	1/1	0.70	0.21	84,84,84,84	0
55	MG	1A	3243	1/1	0.70	0.26	62,62,62,62	0
55	MG	2a	1654	1/1	0.70	0.69	79,79,79,79	0
58	A	2A	3816	1/23	0.70	1.02	85,85,85,85	0
55	MG	1a	3140	1/1	0.71	0.20	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3484	1/1	0.71	0.32	62,62,62,62	0
55	MG	1a	3149	1/1	0.71	0.24	97,97,97,97	0
55	MG	1A	3072	1/1	0.71	0.38	42,42,42,42	0
55	MG	2a	1604	1/1	0.71	0.17	61,61,61,61	0
55	MG	2A	3602	1/1	0.71	0.14	73,73,73,73	0
55	MG	2A	3606	1/1	0.71	0.15	69,69,69,69	0
55	MG	1A	3514	1/1	0.71	0.43	38,38,38,38	0
55	MG	2A	3340	1/1	0.71	0.18	72,72,72,72	0
55	MG	2a	1643	1/1	0.72	0.16	78,78,78,78	0
55	MG	2A	3255	1/1	0.72	0.40	67,67,67,67	0
55	MG	1A	3531	1/1	0.72	0.20	68,68,68,68	0
55	MG	2A	3834	1/1	0.72	0.27	68,68,68,68	0
55	MG	2B	3011	1/1	0.72	0.15	88,88,88,88	0
55	MG	1a	3063	1/1	0.72	0.89	65,65,65,65	0
55	MG	1a	3176	1/1	0.72	0.17	91,91,91,91	0
55	MG	1a	3049	1/1	0.72	0.67	78,78,78,78	0
55	MG	2A	3509	1/1	0.72	0.16	99,99,99,99	0
55	MG	2A	3444	1/1	0.72	0.29	57,57,57,57	0
55	MG	2A	3170	1/1	0.72	0.21	71,71,71,71	0
55	MG	2A	3028	1/1	0.72	0.40	61,61,61,61	0
55	MG	2A	3801	1/1	0.72	0.31	86,86,86,86	0
55	MG	2a	1624	1/1	0.72	0.14	78,78,78,78	0
55	MG	2A	3138	1/1	0.73	0.42	53,53,53,53	0
55	MG	1A	3030	1/1	0.73	0.20	39,39,39,39	0
55	MG	1A	3642	1/1	0.73	0.34	28,28,28,28	0
55	MG	2A	3814	1/1	0.73	0.20	76,76,76,76	0
55	MG	1A	3661	1/1	0.73	0.11	55,55,55,55	0
55	MG	2A	3057	1/1	0.73	0.38	48,48,48,48	0
55	MG	2A	3276	1/1	0.73	0.10	61,61,61,61	0
55	MG	1A	3700	1/1	0.73	0.42	47,47,47,47	0
55	MG	1A	3062	1/1	0.73	0.63	49,49,49,49	0
55	MG	1A	3433	1/1	0.73	0.07	81,81,81,81	0
55	MG	1A	3195	1/1	0.73	0.28	46,46,46,46	0
55	MG	2D	304	1/1	0.73	0.87	58,58,58,58	0
55	MG	1A	3887	1/1	0.73	0.19	58,58,58,58	0
55	MG	1A	3757	1/1	0.73	0.40	59,59,59,59	0
55	MG	1A	3904	1/1	0.73	0.58	53,53,53,53	0
55	MG	1A	3805	1/1	0.74	0.14	72,72,72,72	0
55	MG	2A	3519	1/1	0.74	0.17	68,68,68,68	0
55	MG	1a	3038	1/1	0.74	0.77	78,78,78,78	0
55	MG	2a	1603	1/1	0.74	0.74	65,65,65,65	0
55	MG	2A	3075	1/1	0.74	0.30	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1620	1/1	0.74	0.45	76,76,76,76	0
55	MG	1A	3226	1/1	0.74	0.29	31,31,31,31	0
55	MG	1A	3728	1/1	0.74	0.17	53,53,53,53	0
55	MG	2A	3104	1/1	0.74	0.34	57,57,57,57	0
55	MG	1A	3311	1/1	0.74	0.29	52,52,52,52	0
55	MG	2A	3589	1/1	0.74	0.28	80,80,80,80	0
55	MG	2a	1727	1/1	0.74	0.24	92,92,92,92	0
55	MG	1a	3069	1/1	0.74	0.29	65,65,65,65	0
55	MG	1a	3217	1/1	0.74	0.17	81,81,81,81	0
55	MG	2A	3815	1/1	0.74	0.43	79,79,79,79	0
55	MG	1a	3218	1/1	0.74	0.24	82,82,82,82	0
55	MG	2A	3013	1/1	0.74	0.23	65,65,65,65	0
55	MG	2A	3631	1/1	0.74	0.44	80,80,80,80	0
55	MG	1A	3035	1/1	0.74	0.21	42,42,42,42	0
55	MG	2A	3150	1/1	0.74	0.26	50,50,50,50	0
55	MG	2A	3160	1/1	0.74	0.39	52,52,52,52	0
55	MG	1A	3760	1/1	0.74	0.12	60,60,60,60	0
55	MG	1A	3150	1/1	0.75	0.23	62,62,62,62	0
55	MG	2A	3804	1/1	0.75	0.10	75,75,75,75	0
55	MG	2A	3101	1/1	0.75	0.27	66,66,66,66	0
55	MG	1A	3219	1/1	0.75	0.87	76,76,76,76	0
55	MG	1a	3066	1/1	0.75	0.11	75,75,75,75	0
55	MG	1A	3454	1/1	0.75	0.39	61,61,61,61	0
55	MG	2a	1655	1/1	0.75	0.37	70,70,70,70	0
55	MG	2a	1718	1/1	0.75	0.17	88,88,88,88	0
55	MG	2A	3829	1/1	0.75	0.39	60,60,60,60	0
55	MG	1A	3665	1/1	0.75	0.22	49,49,49,49	0
55	MG	1a	3005	1/1	0.75	0.17	67,67,67,67	0
55	MG	1a	3013	1/1	0.75	0.10	79,79,79,79	0
55	MG	2A	3412	1/1	0.75	0.17	72,72,72,72	0
55	MG	2a	1746	1/1	0.75	0.12	89,89,89,89	0
55	MG	1A	3093	1/1	0.75	0.24	41,41,41,41	0
55	MG	1a	3039	1/1	0.75	0.43	68,68,68,68	0
55	MG	2a	1773	1/1	0.75	0.10	91,91,91,91	0
55	MG	2B	3018	1/1	0.75	0.19	74,74,74,74	0
55	MG	2A	3464	1/1	0.75	0.15	83,83,83,83	0
55	MG	2A	3582	1/1	0.75	0.28	67,67,67,67	0
55	MG	2A	3058	1/1	0.75	0.20	60,60,60,60	0
55	MG	1A	3845	1/1	0.75	0.18	47,47,47,47	0
55	MG	2Q	204	1/1	0.75	0.51	69,69,69,69	0
55	MG	2A	3299	1/1	0.76	0.15	46,46,46,46	0
55	MG	2a	1633	1/1	0.76	0.36	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3302	1/1	0.76	0.14	47,47,47,47	0
55	MG	1a	3150	1/1	0.76	0.23	94,94,94,94	0
55	MG	2A	3141	1/1	0.76	0.48	51,51,51,51	0
55	MG	2A	3533	1/1	0.76	1.28	79,79,79,79	0
55	MG	2A	3694	1/1	0.76	0.10	61,61,61,61	0
55	MG	2A	3148	1/1	0.76	0.27	72,72,72,72	0
55	MG	1A	3171	1/1	0.76	0.29	48,48,48,48	0
55	MG	2A	3151	1/1	0.76	0.92	50,50,50,50	0
55	MG	2a	1732	1/1	0.76	0.13	83,83,83,83	0
55	MG	1A	3319	1/1	0.76	0.21	64,64,64,64	0
55	MG	2A	3457	1/1	0.76	0.16	77,77,77,77	0
55	MG	1A	3877	1/1	0.76	0.14	69,69,69,69	0
55	MG	1a	3136	1/1	0.76	0.57	82,82,82,82	0
55	MG	1A	3880	1/1	0.76	0.09	73,73,73,73	0
55	MG	1A	3724	1/1	0.76	0.41	40,40,40,40	0
55	MG	2X	102	1/1	0.76	0.44	82,82,82,82	0
55	MG	28	101	1/1	0.76	0.60	67,67,67,67	0
55	MG	2A	3808	1/1	0.76	0.31	73,73,73,73	0
55	MG	2A	3260	1/1	0.76	0.31	74,74,74,74	0
55	MG	1d	505	1/1	0.76	0.10	76,76,76,76	0
55	MG	2A	3594	1/1	0.77	0.12	55,55,55,55	0
55	MG	1A	3766	1/1	0.77	0.08	58,58,58,58	0
55	MG	2A	3337	1/1	0.77	0.04	74,74,74,74	0
55	MG	1a	3175	1/1	0.77	0.17	87,87,87,87	0
55	MG	10	101	1/1	0.77	0.38	51,51,51,51	0
55	MG	2a	1729	1/1	0.77	0.19	68,68,68,68	0
55	MG	1a	3074	1/1	0.77	0.48	70,70,70,70	0
55	MG	1A	3139	1/1	0.77	0.30	38,38,38,38	0
55	MG	2a	1733	1/1	0.77	0.53	66,66,66,66	0
55	MG	2A	3424	1/1	0.77	0.21	76,76,76,76	0
55	MG	1B	216	1/1	0.77	0.17	74,74,74,74	0
55	MG	2a	1601	1/1	0.77	0.31	59,59,59,59	0
55	MG	1a	3117	1/1	0.77	0.32	71,71,71,71	0
55	MG	2a	1771	1/1	0.77	0.37	83,83,83,83	0
55	MG	1A	3890	1/1	0.77	0.20	45,45,45,45	0
55	MG	1A	3396	1/1	0.77	0.32	40,40,40,40	0
55	MG	2A	3706	1/1	0.77	0.07	93,93,93,93	0
55	MG	1A	3899	1/1	0.77	0.10	52,52,52,52	0
55	MG	2a	1641	1/1	0.77	0.96	65,65,65,65	0
55	MG	1A	3685	1/1	0.77	0.13	31,31,31,31	0
55	MG	1A	3567	1/1	0.77	0.18	51,51,51,51	0
55	MG	2A	3183	1/1	0.78	0.58	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3188	1/1	0.78	0.43	57,57,57,57	0
55	MG	1a	3114	1/1	0.78	0.10	79,79,79,79	0
55	MG	1a	3048	1/1	0.78	0.13	75,75,75,75	0
55	MG	1a	3129	1/1	0.78	0.11	83,83,83,83	0
55	MG	2a	1659	1/1	0.78	0.13	76,76,76,76	0
55	MG	2A	3008	1/1	0.78	0.37	68,68,68,68	0
55	MG	2A	3292	1/1	0.78	0.08	55,55,55,55	0
55	MG	1F	301	1/1	0.78	0.20	51,51,51,51	0
55	MG	1A	3131	1/1	0.78	0.21	44,44,44,44	0
55	MG	1A	3816	1/1	0.78	0.27	72,72,72,72	0
55	MG	1A	3179	1/1	0.78	0.35	44,44,44,44	0
55	MG	2A	3538	1/1	0.78	0.07	73,73,73,73	0
55	MG	1A	3725	1/1	0.78	0.25	33,33,33,33	0
55	MG	2G	3003	1/1	0.78	0.10	83,83,83,83	0
55	MG	1a	3152	1/1	0.78	0.14	90,90,90,90	0
55	MG	1a	3073	1/1	0.78	0.17	75,75,75,75	0
55	MG	2A	3754	1/1	0.78	0.18	85,85,85,85	0
55	MG	2A	3416	1/1	0.78	0.53	50,50,50,50	0
55	MG	27	102	1/1	0.78	0.17	72,72,72,72	0
55	MG	2A	3787	1/1	0.78	0.18	84,84,84,84	0
55	MG	2A	3422	1/1	0.78	0.12	71,71,71,71	0
55	MG	1A	3123	1/1	0.78	0.18	61,61,61,61	0
55	MG	2A	3161	1/1	0.78	0.28	83,83,83,83	0
55	MG	1A	3848	1/1	0.78	0.27	60,60,60,60	0
55	MG	1A	3920	1/1	0.78	0.40	45,45,45,45	0
55	MG	2A	3132	1/1	0.79	0.72	68,68,68,68	0
55	MG	2A	3263	1/1	0.79	0.17	65,65,65,65	0
55	MG	2A	3811	1/1	0.79	0.48	57,57,57,57	0
55	MG	1A	3647	1/1	0.79	0.05	85,85,85,85	0
55	MG	2a	1636	1/1	0.79	0.30	67,67,67,67	0
55	MG	1A	3655	1/1	0.79	0.18	72,72,72,72	0
55	MG	1B	224	1/1	0.79	0.18	55,55,55,55	0
55	MG	1A	3169	1/1	0.79	0.36	37,37,37,37	0
55	MG	2A	3303	1/1	0.79	0.09	73,73,73,73	0
55	MG	1A	3174	1/1	0.79	0.71	60,60,60,60	0
55	MG	2a	1714	1/1	0.79	0.36	73,73,73,73	0
55	MG	2A	3682	1/1	0.79	0.21	68,68,68,68	0
55	MG	1A	3501	1/1	0.79	0.19	58,58,58,58	0
55	MG	1a	3194	1/1	0.79	0.11	80,80,80,80	0
55	MG	2a	1725	1/1	0.79	0.12	89,89,89,89	0
55	MG	1A	3729	1/1	0.79	0.17	68,68,68,68	0
55	MG	1A	3622	1/1	0.79	0.27	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3561	1/1	0.79	0.17	55,55,55,55	0
55	MG	1a	3144	1/1	0.79	0.39	74,74,74,74	0
55	MG	2F	305	1/1	0.79	0.19	51,51,51,51	0
55	MG	2A	3105	1/1	0.79	0.14	83,83,83,83	0
55	MG	2A	3439	1/1	0.79	0.15	73,73,73,73	0
55	MG	2A	3765	1/1	0.79	0.42	60,60,60,60	0
55	MG	2A	3766	1/1	0.79	0.13	78,78,78,78	0
55	MG	2R	8001	1/1	0.79	0.35	77,77,77,77	0
55	MG	2V	202	1/1	0.79	0.17	70,70,70,70	0
55	MG	2A	3002	1/1	0.79	0.23	68,68,68,68	0
55	MG	20	103	1/1	0.79	0.20	77,77,77,77	0
55	MG	2A	3228	1/1	0.79	0.33	84,84,84,84	0
55	MG	10	103	1/1	0.79	0.11	51,51,51,51	0
55	MG	2A	3011	1/1	0.79	0.41	57,57,57,57	0
55	MG	2A	3605	1/1	0.79	0.38	68,68,68,68	0
55	MG	1A	3723	1/1	0.80	0.10	77,77,77,77	0
55	MG	1A	3482	1/1	0.80	0.27	64,64,64,64	0
55	MG	2A	3795	1/1	0.80	0.59	61,61,61,61	0
55	MG	2A	3798	1/1	0.80	0.14	81,81,81,81	0
55	MG	1a	3022	1/1	0.80	0.68	66,66,66,66	0
55	MG	2A	3250	1/1	0.80	0.15	68,68,68,68	0
55	MG	2A	3109	1/1	0.80	0.50	63,63,63,63	0
55	MG	2A	3461	1/1	0.80	0.25	72,72,72,72	0
55	MG	1A	3806	1/1	0.80	0.18	59,59,59,59	0
55	MG	1A	3143	1/1	0.80	0.48	69,69,69,69	0
55	MG	2a	1644	1/1	0.80	0.29	71,71,71,71	0
55	MG	1A	3824	1/1	0.80	0.15	57,57,57,57	0
55	MG	1D	303	1/1	0.80	0.62	48,48,48,48	0
55	MG	2A	3819	1/1	0.80	0.86	51,51,51,51	0
55	MG	2A	3671	1/1	0.80	0.14	76,76,76,76	0
55	MG	1a	3057	1/1	0.80	0.48	89,89,89,89	0
55	MG	2B	3005	1/1	0.80	0.14	71,71,71,71	0
55	MG	1A	3536	1/1	0.80	0.17	56,56,56,56	0
55	MG	2A	3041	1/1	0.80	0.83	62,62,62,62	0
55	MG	2A	3681	1/1	0.80	0.06	65,65,65,65	0
55	MG	1A	3628	1/1	0.80	0.20	66,66,66,66	0
55	MG	2A	3513	1/1	0.80	0.85	62,62,62,62	0
55	MG	2A	3327	1/1	0.80	0.20	88,88,88,88	0
55	MG	1A	3752	1/1	0.80	0.14	65,65,65,65	0
55	MG	1a	3157	1/1	0.80	0.11	75,75,75,75	0
55	MG	2F	303	1/1	0.80	0.31	57,57,57,57	0
55	MG	2a	1747	1/1	0.80	0.15	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3725	1/1	0.80	0.09	58,58,58,58	0
55	MG	2A	3343	1/1	0.80	0.29	79,79,79,79	0
55	MG	1A	3547	1/1	0.80	0.23	29,29,29,29	0
55	MG	1A	3021	1/1	0.80	0.12	50,50,50,50	0
55	MG	2A	3076	1/1	0.80	0.34	50,50,50,50	0
55	MG	2A	3558	1/1	0.80	0.19	67,67,67,67	0
55	MG	1A	3258	1/1	0.80	0.14	53,53,53,53	0
55	MG	1A	3856	1/1	0.80	0.26	53,53,53,53	0
55	MG	2A	3777	1/1	0.80	0.21	83,83,83,83	0
55	MG	2A	3785	1/1	0.80	0.08	53,53,53,53	0
55	MG	2A	3803	1/1	0.81	0.20	47,47,47,47	0
55	MG	1A	3528	1/1	0.81	0.20	61,61,61,61	0
55	MG	2A	3129	1/1	0.81	0.17	64,64,64,64	0
55	MG	2A	3130	1/1	0.81	0.41	66,66,66,66	0
55	MG	2A	3668	1/1	0.81	0.14	72,72,72,72	0
55	MG	2A	3481	1/1	0.81	0.56	57,57,57,57	0
55	MG	1A	3849	1/1	0.81	0.23	86,86,86,86	0
55	MG	1A	3026	1/1	0.81	0.21	59,59,59,59	0
55	MG	1a	3146	1/1	0.81	0.12	71,71,71,71	0
55	MG	2a	1645	1/1	0.81	0.21	64,64,64,64	0
55	MG	2A	3035	1/1	0.81	0.16	53,53,53,53	0
55	MG	2A	3305	1/1	0.81	0.09	52,52,52,52	0
55	MG	2A	3686	1/1	0.81	0.10	93,93,93,93	0
55	MG	2a	1682	1/1	0.81	0.16	78,78,78,78	0
55	MG	2a	1708	1/1	0.81	0.10	89,89,89,89	0
55	MG	1A	3170	1/1	0.81	0.31	40,40,40,40	0
55	MG	1A	3374	1/1	0.81	0.08	74,74,74,74	0
55	MG	1A	3240	1/1	0.81	0.31	42,42,42,42	0
55	MG	2A	3712	1/1	0.81	0.14	69,69,69,69	0
55	MG	2A	3050	1/1	0.81	0.20	63,63,63,63	0
55	MG	1A	3862	1/1	0.81	0.36	55,55,55,55	0
55	MG	1A	3550	1/1	0.81	0.37	47,47,47,47	0
55	MG	1A	3878	1/1	0.81	0.13	36,36,36,36	0
55	MG	1A	3697	1/1	0.81	0.31	64,64,64,64	0
55	MG	1A	3147	1/1	0.81	0.21	62,62,62,62	0
55	MG	2G	3002	1/1	0.81	0.18	79,79,79,79	0
55	MG	2A	3564	1/1	0.81	0.13	58,58,58,58	0
55	MG	1A	3246	1/1	0.81	0.12	87,87,87,87	0
55	MG	2P	201	1/1	0.81	0.33	67,67,67,67	0
55	MG	2A	3771	1/1	0.81	0.15	65,65,65,65	0
55	MG	2A	3427	1/1	0.81	0.43	81,81,81,81	0
55	MG	1A	3252	1/1	0.81	0.80	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3200	1/1	0.81	0.53	65,65,65,65	0
55	MG	1A	3101	1/1	0.81	0.52	55,55,55,55	0
55	MG	1A	3209	1/1	0.81	0.43	49,49,49,49	0
55	MG	1A	3623	1/1	0.81	0.34	43,43,43,43	0
55	MG	1A	3177	1/1	0.81	0.54	54,54,54,54	0
56	ZN	14	501	1/1	0.81	0.05	149,149,149,149	0
55	MG	2A	3621	1/1	0.81	0.73	64,64,64,64	0
55	MG	1a	3197	1/1	0.82	0.12	78,78,78,78	0
55	MG	2A	3380	1/1	0.82	0.10	83,83,83,83	0
55	MG	2A	3690	1/1	0.82	0.22	82,82,82,82	0
55	MG	2A	3821	1/1	0.82	0.30	54,54,54,54	0
55	MG	2A	3545	1/1	0.82	0.07	84,84,84,84	0
55	MG	2A	3173	1/1	0.82	0.97	72,72,72,72	0
55	MG	2B	3002	1/1	0.82	0.12	67,67,67,67	0
55	MG	2a	1652	1/1	0.82	0.11	65,65,65,65	0
55	MG	1A	3267	1/1	0.82	0.12	77,77,77,77	0
55	MG	1A	3166	1/1	0.82	0.18	54,54,54,54	0
55	MG	2a	1657	1/1	0.82	0.34	64,64,64,64	0
55	MG	1A	3167	1/1	0.82	0.11	54,54,54,54	0
55	MG	2A	3194	1/1	0.82	0.08	83,83,83,83	0
55	MG	2a	1696	1/1	0.82	0.07	78,78,78,78	0
55	MG	2a	1697	1/1	0.82	0.07	79,79,79,79	0
55	MG	1A	3207	1/1	0.82	0.29	35,35,35,35	0
55	MG	2a	1710	1/1	0.82	0.16	84,84,84,84	0
55	MG	1A	3236	1/1	0.82	0.27	53,53,53,53	0
55	MG	1A	3382	1/1	0.82	0.54	58,58,58,58	0
55	MG	2A	3009	1/1	0.82	0.69	64,64,64,64	0
55	MG	1A	3632	1/1	0.82	0.29	53,53,53,53	0
55	MG	2F	301	1/1	0.82	0.30	52,52,52,52	0
55	MG	1A	3257	1/1	0.82	0.54	44,44,44,44	0
55	MG	2A	3019	1/1	0.82	0.20	43,43,43,43	0
55	MG	1A	3118	1/1	0.82	0.31	39,39,39,39	0
55	MG	2A	3774	1/1	0.82	0.22	81,81,81,81	0
55	MG	1A	3444	1/1	0.82	0.22	57,57,57,57	0
55	MG	1A	3260	1/1	0.82	0.18	75,75,75,75	0
55	MG	2A	3479	1/1	0.82	0.11	73,73,73,73	0
55	MG	1A	3907	1/1	0.82	0.44	58,58,58,58	0
55	MG	1A	3477	1/1	0.82	0.17	40,40,40,40	0
55	MG	2A	3647	1/1	0.82	0.19	77,77,77,77	0
55	MG	2a	1755	1/1	0.82	0.13	66,66,66,66	0
55	MG	2A	3650	1/1	0.82	0.35	57,57,57,57	0
55	MG	2A	3802	1/1	0.82	0.68	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	21	102	1/1	0.82	0.19	66,66,66,66	0
55	MG	1A	3670	1/1	0.82	0.27	51,51,51,51	0
55	MG	1a	3184	1/1	0.82	0.15	82,82,82,82	0
55	MG	2A	3329	1/1	0.82	0.44	72,72,72,72	0
55	MG	1a	3186	1/1	0.82	0.08	69,69,69,69	0
55	MG	1A	3683	1/1	0.82	0.16	50,50,50,50	0
55	MG	1a	3196	1/1	0.82	0.13	82,82,82,82	0
55	MG	20	102	1/1	0.83	0.31	63,63,63,63	0
55	MG	1g	3001	1/1	0.83	0.25	79,79,79,79	0
55	MG	1h	3001	1/1	0.83	0.56	52,52,52,52	0
55	MG	2A	3768	1/1	0.83	0.44	94,94,94,94	0
55	MG	2A	3326	1/1	0.83	0.13	69,69,69,69	0
55	MG	1A	3039	1/1	0.83	0.34	55,55,55,55	0
55	MG	1a	3131	1/1	0.83	0.17	70,70,70,70	0
55	MG	2A	3336	1/1	0.83	0.80	76,76,76,76	0
55	MG	1A	3558	1/1	0.83	0.19	72,72,72,72	0
55	MG	2A	3010	1/1	0.83	0.20	62,62,62,62	0
55	MG	1A	3431	1/1	0.83	0.58	53,53,53,53	0
55	MG	2A	3585	1/1	0.83	0.19	75,75,75,75	0
55	MG	2a	1638	1/1	0.83	0.86	70,70,70,70	0
55	MG	1A	3142	1/1	0.83	0.47	43,43,43,43	0
55	MG	1a	3019	1/1	0.83	0.15	67,67,67,67	0
55	MG	2A	3385	1/1	0.83	0.23	86,86,86,86	0
55	MG	2A	3027	1/1	0.83	0.35	66,66,66,66	0
55	MG	2a	1646	1/1	0.83	0.41	62,62,62,62	0
55	MG	1A	3919	1/1	0.83	0.45	33,33,33,33	0
55	MG	1A	3786	1/1	0.83	0.30	58,58,58,58	0
55	MG	2A	3162	1/1	0.83	0.76	79,79,79,79	0
55	MG	1A	3803	1/1	0.83	0.10	78,78,78,78	0
55	MG	2A	3172	1/1	0.83	0.39	64,64,64,64	0
55	MG	2A	3431	1/1	0.83	0.15	74,74,74,74	0
55	MG	2A	3638	1/1	0.83	0.19	85,85,85,85	0
55	MG	2A	3641	1/1	0.83	0.16	72,72,72,72	0
55	MG	2A	3643	1/1	0.83	0.51	56,56,56,56	0
55	MG	1A	3857	1/1	0.83	0.16	67,67,67,67	0
55	MG	1A	3804	1/1	0.83	0.10	71,71,71,71	0
55	MG	2A	3655	1/1	0.83	0.24	60,60,60,60	0
55	MG	2A	3179	1/1	0.83	0.72	63,63,63,63	0
55	MG	2B	3007	1/1	0.83	0.14	79,79,79,79	0
55	MG	1B	217	1/1	0.83	0.08	57,57,57,57	0
55	MG	1A	3603	1/1	0.83	0.48	46,46,46,46	0
55	MG	2A	3674	1/1	0.83	0.12	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2B	3014	1/1	0.83	0.09	73,73,73,73	0
55	MG	1A	3188	1/1	0.83	0.35	44,44,44,44	0
55	MG	1A	3034	1/1	0.83	0.19	60,60,60,60	0
55	MG	2a	1737	1/1	0.83	0.84	87,87,87,87	0
55	MG	2A	3203	1/1	0.83	1.25	58,58,58,58	0
55	MG	2A	3209	1/1	0.83	0.07	89,89,89,89	0
55	MG	1A	3468	1/1	0.83	0.17	30,30,30,30	0
55	MG	2A	3243	1/1	0.83	0.46	55,55,55,55	0
55	MG	2a	1752	1/1	0.83	0.49	69,69,69,69	0
55	MG	1A	3882	1/1	0.83	0.19	67,67,67,67	0
55	MG	2A	3486	1/1	0.83	0.15	57,57,57,57	0
55	MG	1A	3215	1/1	0.83	0.21	51,51,51,51	0
55	MG	2A	3707	1/1	0.83	0.15	73,73,73,73	0
55	MG	1A	3245	1/1	0.83	0.10	74,74,74,74	0
55	MG	1A	3840	1/1	0.83	0.26	64,64,64,64	0
55	MG	1a	3216	1/1	0.83	0.11	96,96,96,96	0
55	MG	1a	3079	1/1	0.83	0.14	54,54,54,54	0
55	MG	1A	3843	1/1	0.83	0.22	47,47,47,47	0
55	MG	1a	3226	1/1	0.83	0.41	74,74,74,74	0
55	MG	1P	202	1/1	0.83	0.19	85,85,85,85	0
55	MG	1A	3903	1/1	0.84	0.10	34,34,34,34	0
55	MG	2A	3612	1/1	0.84	0.18	41,41,41,41	0
55	MG	2a	1607	1/1	0.84	0.88	73,73,73,73	0
55	MG	2A	3229	1/1	0.84	0.46	64,64,64,64	0
55	MG	1A	3552	1/1	0.84	0.20	64,64,64,64	0
55	MG	2A	3030	1/1	0.84	0.25	66,66,66,66	0
55	MG	1a	3208	1/1	0.84	0.29	70,70,70,70	0
55	MG	2A	3462	1/1	0.84	0.19	62,62,62,62	0
55	MG	1A	3164	1/1	0.84	0.29	78,78,78,78	0
55	MG	1A	3182	1/1	0.84	0.41	38,38,38,38	0
55	MG	1A	3259	1/1	0.84	0.24	36,36,36,36	0
55	MG	2A	3147	1/1	0.84	0.17	81,81,81,81	0
55	MG	2A	3277	1/1	0.84	0.17	54,54,54,54	0
55	MG	1F	302	1/1	0.84	0.43	37,37,37,37	0
55	MG	2A	3297	1/1	0.84	0.13	68,68,68,68	0
55	MG	2A	3053	1/1	0.84	0.96	60,60,60,60	0
55	MG	2A	3835	1/1	0.84	1.05	65,65,65,65	0
55	MG	2A	3838	1/1	0.84	0.38	54,54,54,54	0
55	MG	1a	3222	1/1	0.84	0.35	72,72,72,72	0
55	MG	2A	3154	1/1	0.84	0.73	53,53,53,53	0
55	MG	1A	3572	1/1	0.84	0.23	67,67,67,67	0
55	MG	1A	3932	1/1	0.84	0.33	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1B	204	1/1	0.84	0.27	72,72,72,72	0
55	MG	2A	3169	1/1	0.84	0.29	73,73,73,73	0
55	MG	2A	3085	1/1	0.84	0.17	67,67,67,67	0
55	MG	2A	3534	1/1	0.84	0.16	82,82,82,82	0
55	MG	1a	3071	1/1	0.84	0.28	56,56,56,56	0
55	MG	2A	3542	1/1	0.84	0.23	75,75,75,75	0
55	MG	1y	101	1/1	0.84	0.35	50,50,50,50	0
55	MG	2A	3177	1/1	0.84	0.98	50,50,50,50	0
55	MG	2a	1730	1/1	0.84	0.13	84,84,84,84	0
55	MG	2A	3716	1/1	0.84	0.10	85,85,85,85	0
55	MG	2A	3553	1/1	0.84	0.13	66,66,66,66	0
55	MG	2A	3347	1/1	0.84	0.05	72,72,72,72	0
55	MG	2F	309	1/1	0.84	0.14	72,72,72,72	0
55	MG	2A	3374	1/1	0.84	0.59	60,60,60,60	0
55	MG	1A	3218	1/1	0.84	0.22	53,53,53,53	0
55	MG	2A	3378	1/1	0.84	0.07	58,58,58,58	0
55	MG	1A	3253	1/1	0.84	0.42	63,63,63,63	0
55	MG	1A	3541	1/1	0.84	0.30	55,55,55,55	0
55	MG	1A	3671	1/1	0.84	0.17	46,46,46,46	0
55	MG	2A	3192	1/1	0.84	0.66	64,64,64,64	0
55	MG	2a	1769	1/1	0.84	0.23	83,83,83,83	0
55	MG	1A	3211	1/1	0.84	0.40	41,41,41,41	0
55	MG	2A	3197	1/1	0.84	0.28	53,53,53,53	0
55	MG	2a	1785	1/1	0.84	0.17	83,83,83,83	0
55	MG	2A	3115	1/1	0.84	0.29	65,65,65,65	0
55	MG	2A	3603	1/1	0.84	0.12	70,70,70,70	0
55	MG	2A	3604	1/1	0.84	0.30	77,77,77,77	0
55	MG	2g	3001	1/1	0.84	0.18	75,75,75,75	0
55	MG	27	101	1/1	0.84	0.33	57,57,57,57	0
55	MG	1A	3315	1/1	0.84	0.07	74,74,74,74	0
55	MG	1a	3036	1/1	0.84	0.20	50,50,50,50	0
55	MG	2A	3608	1/1	0.84	0.15	63,63,63,63	0
55	MG	1A	3566	1/1	0.85	0.18	70,70,70,70	0
55	MG	2A	3644	1/1	0.85	0.44	66,66,66,66	0
55	MG	2A	3499	1/1	0.85	0.38	51,51,51,51	0
55	MG	2A	3159	1/1	0.85	0.43	53,53,53,53	0
55	MG	1A	3876	1/1	0.85	0.07	61,61,61,61	0
55	MG	2A	3658	1/1	0.85	0.26	76,76,76,76	0
55	MG	2A	3054	1/1	0.85	0.34	54,54,54,54	0
55	MG	18	3302	1/1	0.85	0.60	43,43,43,43	0
55	MG	2A	3166	1/1	0.85	0.28	54,54,54,54	0
55	MG	1A	3287	1/1	0.85	0.17	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3162	1/1	0.85	0.24	62,62,62,62	0
55	MG	2A	3338	1/1	0.85	0.22	55,55,55,55	0
55	MG	1a	3018	1/1	0.85	0.11	66,66,66,66	0
55	MG	2A	3077	1/1	0.85	0.34	58,58,58,58	0
55	MG	1A	3472	1/1	0.85	0.15	64,64,64,64	0
55	MG	1d	502	1/1	0.85	0.28	71,71,71,71	0
55	MG	1d	504	1/1	0.85	0.21	77,77,77,77	0
55	MG	1A	3837	1/1	0.85	0.13	78,78,78,78	0
55	MG	2A	3184	1/1	0.85	0.64	57,57,57,57	0
55	MG	1a	3033	1/1	0.85	0.12	56,56,56,56	0
55	MG	1A	3392	1/1	0.85	0.37	57,57,57,57	0
55	MG	1A	3148	1/1	0.85	0.47	48,48,48,48	0
55	MG	2a	1721	1/1	0.85	0.14	86,86,86,86	0
55	MG	2A	3110	1/1	0.85	0.61	58,58,58,58	0
55	MG	2A	3579	1/1	0.85	0.17	61,61,61,61	0
55	MG	2a	1726	1/1	0.85	0.15	73,73,73,73	0
55	MG	2A	3581	1/1	0.85	0.09	73,73,73,73	0
55	MG	2A	3737	1/1	0.85	0.12	79,79,79,79	0
55	MG	1A	3104	1/1	0.85	0.21	42,42,42,42	0
55	MG	2A	3749	1/1	0.85	0.06	81,81,81,81	0
55	MG	1a	3041	1/1	0.85	0.11	76,76,76,76	0
55	MG	2A	3587	1/1	0.85	0.06	63,63,63,63	0
55	MG	1D	301	1/1	0.85	0.45	54,54,54,54	0
55	MG	1A	3499	1/1	0.85	0.13	62,62,62,62	0
55	MG	1D	312	1/1	0.85	0.26	65,65,65,65	0
55	MG	2A	3240	1/1	0.85	0.15	50,50,50,50	0
55	MG	1A	3551	1/1	0.85	0.27	36,36,36,36	0
55	MG	1A	3357	1/1	0.85	0.06	75,75,75,75	0
55	MG	20	101	1/1	0.85	0.27	84,84,84,84	0
55	MG	2A	3458	1/1	0.85	0.12	74,74,74,74	0
55	MG	2a	1759	1/1	0.85	0.04	86,86,86,86	0
55	MG	1A	3706	1/1	0.85	0.40	70,70,70,70	0
55	MG	1a	3180	1/1	0.85	0.20	97,97,97,97	0
55	MG	1A	3793	1/1	0.85	0.33	60,60,60,60	0
55	MG	2a	1780	1/1	0.85	0.27	73,73,73,73	0
55	MG	1a	3070	1/1	0.85	0.35	60,60,60,60	0
55	MG	1A	3505	1/1	0.85	0.38	50,50,50,50	0
55	MG	1A	3720	1/1	0.85	0.36	64,64,64,64	0
55	MG	2A	3634	1/1	0.85	0.20	81,81,81,81	0
55	MG	2e	202	1/1	0.85	0.31	73,73,73,73	0
55	MG	2A	3045	1/1	0.85	0.11	75,75,75,75	0
55	MG	2h	3002	1/1	0.85	0.24	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3280	1/1	0.85	0.16	33,33,33,33	0
55	MG	2a	1608	1/1	0.85	0.30	57,57,57,57	0
55	MG	2a	1610	1/1	0.85	0.96	70,70,70,70	0
55	MG	2A	3152	1/1	0.85	0.24	66,66,66,66	0
55	MG	25	104	1/1	0.86	0.16	83,83,83,83	0
55	MG	1A	3002	1/1	0.86	0.23	55,55,55,55	0
55	MG	2A	3731	1/1	0.86	0.07	65,65,65,65	0
55	MG	1A	3834	1/1	0.86	0.17	73,73,73,73	0
55	MG	2A	3266	1/1	0.86	0.20	66,66,66,66	0
55	MG	1a	3020	1/1	0.86	0.34	71,71,71,71	0
55	MG	1A	3036	1/1	0.86	0.25	40,40,40,40	0
55	MG	1A	3152	1/1	0.86	0.17	46,46,46,46	0
55	MG	1A	3518	1/1	0.86	0.21	71,71,71,71	0
55	MG	1A	3073	1/1	0.86	0.19	44,44,44,44	0
55	MG	2a	1612	1/1	0.86	0.19	54,54,54,54	0
55	MG	2a	1615	1/1	0.86	1.49	78,78,78,78	0
55	MG	1a	3201	1/1	0.86	0.10	80,80,80,80	0
55	MG	1A	3180	1/1	0.86	0.15	64,64,64,64	0
55	MG	1A	3629	1/1	0.86	0.16	63,63,63,63	0
55	MG	1a	3046	1/1	0.86	0.30	50,50,50,50	0
55	MG	1A	3138	1/1	0.86	0.29	57,57,57,57	0
55	MG	1A	3636	1/1	0.86	0.41	27,27,27,27	0
55	MG	1a	3050	1/1	0.86	0.25	54,54,54,54	0
55	MG	1a	3223	1/1	0.86	0.22	65,65,65,65	0
55	MG	1a	3056	1/1	0.86	0.09	74,74,74,74	0
55	MG	1A	3733	1/1	0.86	0.26	42,42,42,42	0
55	MG	2a	1648	1/1	0.86	0.08	82,82,82,82	0
55	MG	2A	3142	1/1	0.86	0.77	57,57,57,57	0
55	MG	2A	3599	1/1	0.86	0.10	78,78,78,78	0
55	MG	1A	3734	1/1	0.86	0.25	29,29,29,29	0
55	MG	1A	3113	1/1	0.86	0.25	26,26,26,26	0
55	MG	1A	3013	1/1	0.86	0.16	62,62,62,62	0
55	MG	2a	1667	1/1	0.86	0.25	75,75,75,75	0
55	MG	1a	3068	1/1	0.86	0.23	71,71,71,71	0
55	MG	1B	225	1/1	0.86	0.34	68,68,68,68	0
55	MG	1A	3436	1/1	0.86	0.16	58,58,58,58	0
55	MG	1A	3869	1/1	0.86	0.19	40,40,40,40	0
55	MG	1A	3270	1/1	0.86	0.33	60,60,60,60	0
55	MG	1A	3190	1/1	0.86	0.17	72,72,72,72	0
55	MG	1A	3669	1/1	0.86	0.30	62,62,62,62	0
55	MG	2A	3825	1/1	0.86	1.51	60,60,60,60	0
55	MG	2A	3165	1/1	0.86	0.35	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3191	1/1	0.86	0.28	39,39,39,39	0
55	MG	1A	3881	1/1	0.86	0.20	51,51,51,51	0
55	MG	1F	308	1/1	0.86	0.56	62,62,62,62	0
55	MG	1A	3058	1/1	0.86	0.08	50,50,50,50	0
55	MG	2B	3003	1/1	0.86	0.16	71,71,71,71	0
55	MG	1A	3199	1/1	0.86	0.63	41,41,41,41	0
55	MG	2A	3032	1/1	0.86	0.35	63,63,63,63	0
55	MG	1A	3316	1/1	0.86	0.40	69,69,69,69	0
55	MG	1A	3127	1/1	0.86	0.14	36,36,36,36	0
55	MG	1A	3895	1/1	0.86	0.37	45,45,45,45	0
55	MG	2A	3463	1/1	0.86	0.18	77,77,77,77	0
55	MG	2A	3664	1/1	0.86	0.13	81,81,81,81	0
55	MG	1a	3143	1/1	0.86	0.10	82,82,82,82	0
55	MG	11	102	1/1	0.86	0.22	56,56,56,56	0
55	MG	11	103	1/1	0.86	0.20	50,50,50,50	0
55	MG	17	101	1/1	0.86	0.28	64,64,64,64	0
55	MG	1A	3809	1/1	0.86	0.14	35,35,35,35	0
55	MG	18	3303	1/1	0.86	0.04	63,63,63,63	0
55	MG	1a	3004	1/1	0.86	0.19	67,67,67,67	0
55	MG	2A	3065	1/1	0.86	0.08	70,70,70,70	0
55	MG	2A	3488	1/1	0.86	0.17	75,75,75,75	0
55	MG	2a	1775	1/1	0.86	0.10	74,74,74,74	0
55	MG	2A	3223	1/1	0.86	0.16	68,68,68,68	0
55	MG	2A	3691	1/1	0.86	0.08	75,75,75,75	0
55	MG	2a	1786	1/1	0.86	0.12	72,72,72,72	0
55	MG	2A	3693	1/1	0.86	0.06	78,78,78,78	0
55	MG	1a	3153	1/1	0.86	0.12	66,66,66,66	0
55	MG	1A	3322	1/1	0.86	0.17	49,49,49,49	0
55	MG	1a	3164	1/1	0.86	0.20	68,68,68,68	0
55	MG	2A	3512	1/1	0.86	0.59	59,59,59,59	0
55	MG	2A	3078	1/1	0.86	0.23	50,50,50,50	0
55	MG	1a	3007	1/1	0.86	0.28	71,71,71,71	0
55	MG	1A	3602	1/1	0.86	0.18	56,56,56,56	0
55	MG	2A	3721	1/1	0.86	0.23	50,50,50,50	0
55	MG	2A	3098	1/1	0.86	0.23	60,60,60,60	0
55	MG	1A	3217	1/1	0.87	0.45	35,35,35,35	0
55	MG	28	102	1/1	0.87	0.07	73,73,73,73	0
55	MG	2A	3139	1/1	0.87	0.20	51,51,51,51	0
55	MG	2A	3140	1/1	0.87	0.34	56,56,56,56	0
55	MG	1A	3859	1/1	0.87	0.19	81,81,81,81	0
55	MG	2A	3756	1/1	0.87	0.64	86,86,86,86	0
55	MG	2A	3563	1/1	0.87	0.28	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1a	3139	1/1	0.87	0.28	67,67,67,67	0
55	MG	1A	3607	1/1	0.87	0.19	67,67,67,67	0
55	MG	1A	3049	1/1	0.87	0.57	36,36,36,36	0
55	MG	2a	1618	1/1	0.87	0.59	66,66,66,66	0
55	MG	1A	3866	1/1	0.87	0.25	62,62,62,62	0
55	MG	1A	3532	1/1	0.87	0.13	56,56,56,56	0
55	MG	2A	3583	1/1	0.87	0.11	72,72,72,72	0
55	MG	2A	3782	1/1	0.87	0.19	79,79,79,79	0
55	MG	2A	3783	1/1	0.87	0.31	93,93,93,93	0
55	MG	1a	3028	1/1	0.87	0.30	63,63,63,63	0
55	MG	2a	1642	1/1	0.87	0.16	82,82,82,82	0
55	MG	1A	3870	1/1	0.87	0.36	54,54,54,54	0
55	MG	1A	3063	1/1	0.87	0.52	45,45,45,45	0
55	MG	2A	3033	1/1	0.87	0.62	66,66,66,66	0
55	MG	1A	3255	1/1	0.87	0.23	41,41,41,41	0
55	MG	2A	3037	1/1	0.87	0.43	48,48,48,48	0
55	MG	1A	3546	1/1	0.87	0.24	40,40,40,40	0
55	MG	1a	3040	1/1	0.87	0.25	73,73,73,73	0
55	MG	2A	3043	1/1	0.87	0.18	68,68,68,68	0
55	MG	1a	3163	1/1	0.87	0.16	79,79,79,79	0
55	MG	1A	3052	1/1	0.87	0.54	24,24,24,24	0
55	MG	1D	306	1/1	0.87	0.22	45,45,45,45	0
55	MG	2a	1676	1/1	0.87	0.14	65,65,65,65	0
55	MG	1D	310	1/1	0.87	0.13	68,68,68,68	0
55	MG	1A	3235	1/1	0.87	0.42	72,72,72,72	0
55	MG	1A	3054	1/1	0.87	0.22	41,41,41,41	0
55	MG	2a	1707	1/1	0.87	0.10	82,82,82,82	0
55	MG	2A	3445	1/1	0.87	0.41	61,61,61,61	0
55	MG	2A	3448	1/1	0.87	0.15	80,80,80,80	0
55	MG	1a	3054	1/1	0.87	0.19	79,79,79,79	0
55	MG	2a	1717	1/1	0.87	0.06	71,71,71,71	0
55	MG	2A	3063	1/1	0.87	0.22	65,65,65,65	0
55	MG	1A	3638	1/1	0.87	0.25	35,35,35,35	0
55	MG	1A	3836	1/1	0.87	0.14	54,54,54,54	0
55	MG	1A	3889	1/1	0.87	0.09	55,55,55,55	0
55	MG	1A	3239	1/1	0.87	0.45	50,50,50,50	0
55	MG	1a	3199	1/1	0.87	0.14	71,71,71,71	0
55	MG	1A	3089	1/1	0.87	0.19	48,48,48,48	0
55	MG	1A	3090	1/1	0.87	0.22	41,41,41,41	0
55	MG	2A	3661	1/1	0.87	0.11	88,88,88,88	0
55	MG	2A	3094	1/1	0.87	1.35	58,58,58,58	0
55	MG	1A	3044	1/1	0.87	0.23	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1R	203	1/1	0.87	0.26	48,48,48,48	0
55	MG	2a	1734	1/1	0.87	0.06	73,73,73,73	0
55	MG	1A	3406	1/1	0.87	0.21	37,37,37,37	0
55	MG	2A	3673	1/1	0.87	0.22	70,70,70,70	0
55	MG	1A	3568	1/1	0.87	0.29	53,53,53,53	0
55	MG	2A	3244	1/1	0.87	0.06	87,87,87,87	0
55	MG	1A	3193	1/1	0.87	0.36	29,29,29,29	0
55	MG	2A	3254	1/1	0.87	0.12	87,87,87,87	0
55	MG	1A	3853	1/1	0.87	0.09	22,22,22,22	0
55	MG	2A	3256	1/1	0.87	0.14	61,61,61,61	0
55	MG	1a	3225	1/1	0.87	0.10	74,74,74,74	0
55	MG	2G	3001	1/1	0.87	0.19	82,82,82,82	0
55	MG	1A	3579	1/1	0.87	0.52	41,41,41,41	0
55	MG	2A	3114	1/1	0.87	0.40	62,62,62,62	0
55	MG	2A	3528	1/1	0.87	0.09	67,67,67,67	0
55	MG	1A	3764	1/1	0.87	0.09	41,41,41,41	0
55	MG	2A	3705	1/1	0.87	0.21	65,65,65,65	0
55	MG	1a	3096	1/1	0.87	0.17	81,81,81,81	0
55	MG	1a	3097	1/1	0.87	0.10	58,58,58,58	0
55	MG	2a	1792	1/1	0.87	0.20	74,74,74,74	0
55	MG	2A	3536	1/1	0.87	0.15	62,62,62,62	0
55	MG	2A	3537	1/1	0.87	0.73	65,65,65,65	0
55	MG	1A	3929	1/1	0.87	0.64	40,40,40,40	0
55	MG	2A	3540	1/1	0.87	0.07	70,70,70,70	0
55	MG	1A	3299	1/1	0.87	0.21	37,37,37,37	0
55	MG	1a	3124	1/1	0.87	0.30	88,88,88,88	0
55	MG	1B	203	1/1	0.87	0.25	66,66,66,66	0
55	MG	2q	201	1/1	0.87	0.39	63,63,63,63	0
55	MG	2A	3736	1/1	0.87	0.14	88,88,88,88	0
55	MG	2A	3004	1/1	0.87	0.23	52,52,52,52	0
55	MG	2A	3134	1/1	0.88	0.89	70,70,70,70	0
55	MG	1a	3133	1/1	0.88	0.42	77,77,77,77	0
55	MG	1A	3594	1/1	0.88	0.18	59,59,59,59	0
55	MG	1A	3922	1/1	0.88	0.21	39,39,39,39	0
55	MG	1A	3159	1/1	0.88	0.87	40,40,40,40	0
55	MG	2A	3732	1/1	0.88	0.56	60,60,60,60	0
55	MG	2A	3544	1/1	0.88	0.14	89,89,89,89	0
55	MG	1A	3176	1/1	0.88	0.29	45,45,45,45	0
55	MG	2A	3547	1/1	0.88	0.06	67,67,67,67	0
55	MG	2A	3318	1/1	0.88	0.06	77,77,77,77	0
55	MG	1A	3940	1/1	0.88	0.23	40,40,40,40	0
55	MG	2A	3753	1/1	0.88	0.09	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1616	1/1	0.88	0.12	55,55,55,55	0
55	MG	2A	3144	1/1	0.88	0.15	78,78,78,78	0
55	MG	1A	3606	1/1	0.88	0.23	62,62,62,62	0
55	MG	2a	1621	1/1	0.88	0.11	80,80,80,80	0
55	MG	2A	3757	1/1	0.88	0.25	64,64,64,64	0
55	MG	2A	3762	1/1	0.88	0.63	57,57,57,57	0
55	MG	1A	3220	1/1	0.88	0.22	61,61,61,61	0
55	MG	2a	1637	1/1	0.88	0.48	87,87,87,87	0
55	MG	1A	3515	1/1	0.88	0.28	63,63,63,63	0
55	MG	1A	3517	1/1	0.88	0.20	51,51,51,51	0
55	MG	1a	3035	1/1	0.88	1.05	69,69,69,69	0
55	MG	2A	3568	1/1	0.88	0.31	46,46,46,46	0
55	MG	1A	3198	1/1	0.88	0.26	30,30,30,30	0
55	MG	2A	3576	1/1	0.88	0.52	57,57,57,57	0
55	MG	2A	3157	1/1	0.88	0.26	63,63,63,63	0
55	MG	2a	1647	1/1	0.88	0.23	60,60,60,60	0
55	MG	1a	3154	1/1	0.88	0.12	90,90,90,90	0
55	MG	2a	1649	1/1	0.88	0.11	71,71,71,71	0
55	MG	1A	3521	1/1	0.88	0.30	66,66,66,66	0
55	MG	1A	3384	1/1	0.88	0.11	70,70,70,70	0
55	MG	1A	3234	1/1	0.88	0.26	43,43,43,43	0
55	MG	2A	3794	1/1	0.88	0.10	70,70,70,70	0
55	MG	1A	3737	1/1	0.88	0.39	38,38,38,38	0
55	MG	2A	3400	1/1	0.88	0.28	77,77,77,77	0
55	MG	1A	3749	1/1	0.88	0.10	50,50,50,50	0
55	MG	2A	3596	1/1	0.88	0.16	63,63,63,63	0
55	MG	1A	3160	1/1	0.88	0.26	52,52,52,52	0
55	MG	1a	3179	1/1	0.88	0.04	73,73,73,73	0
55	MG	2A	3420	1/1	0.88	0.15	58,58,58,58	0
55	MG	1A	3032	1/1	0.88	0.39	53,53,53,53	0
55	MG	1A	3203	1/1	0.88	0.36	38,38,38,38	0
55	MG	2A	3174	1/1	0.88	0.39	47,47,47,47	0
55	MG	1D	308	1/1	0.88	0.13	46,46,46,46	0
55	MG	2A	3437	1/1	0.88	0.06	75,75,75,75	0
55	MG	1A	3285	1/1	0.88	0.22	49,49,49,49	0
55	MG	1A	3644	1/1	0.88	0.43	51,51,51,51	0
55	MG	1A	3206	1/1	0.88	0.28	42,42,42,42	0
55	MG	2A	3446	1/1	0.88	0.13	78,78,78,78	0
55	MG	1A	3774	1/1	0.88	0.22	79,79,79,79	0
55	MG	2A	3185	1/1	0.88	0.44	65,65,65,65	0
55	MG	2A	3637	1/1	0.88	0.05	63,63,63,63	0
55	MG	2A	3455	1/1	0.88	0.25	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1a	3200	1/1	0.88	0.08	87,87,87,87	0
55	MG	2A	3642	1/1	0.88	0.07	80,80,80,80	0
55	MG	2A	3080	1/1	0.88	0.26	66,66,66,66	0
55	MG	1A	3442	1/1	0.88	0.13	80,80,80,80	0
55	MG	1A	3792	1/1	0.88	0.08	63,63,63,63	0
55	MG	1A	3443	1/1	0.88	0.27	59,59,59,59	0
55	MG	2A	3653	1/1	0.88	0.23	70,70,70,70	0
55	MG	1A	3078	1/1	0.88	0.29	50,50,50,50	0
55	MG	2B	3016	1/1	0.88	0.29	81,81,81,81	0
55	MG	2a	1751	1/1	0.88	0.12	77,77,77,77	0
55	MG	1A	3667	1/1	0.88	0.09	74,74,74,74	0
55	MG	2A	3102	1/1	0.88	0.39	55,55,55,55	0
55	MG	1a	3072	1/1	0.88	0.09	59,59,59,59	0
55	MG	2a	1756	1/1	0.88	0.17	76,76,76,76	0
55	MG	1A	3079	1/1	0.88	0.78	45,45,45,45	0
55	MG	2A	3234	1/1	0.88	0.10	71,71,71,71	0
55	MG	1R	201	1/1	0.88	0.22	59,59,59,59	0
55	MG	1A	3312	1/1	0.88	0.17	61,61,61,61	0
55	MG	1W	3001	1/1	0.88	0.31	44,44,44,44	0
55	MG	2A	3498	1/1	0.88	0.11	68,68,68,68	0
55	MG	1A	3080	1/1	0.88	0.32	45,45,45,45	0
55	MG	1A	3682	1/1	0.88	0.44	61,61,61,61	0
55	MG	2a	1788	1/1	0.88	0.10	83,83,83,83	0
55	MG	1A	3823	1/1	0.88	0.16	32,32,32,32	0
55	MG	2A	3127	1/1	0.88	0.18	76,76,76,76	0
55	MG	1a	3106	1/1	0.88	0.06	56,56,56,56	0
55	MG	1A	3476	1/1	0.88	0.10	33,33,33,33	0
55	MG	1A	3011	1/1	0.88	0.49	48,48,48,48	0
55	MG	2A	3520	1/1	0.88	0.15	70,70,70,70	0
55	MG	2A	3523	1/1	0.88	0.07	65,65,65,65	0
55	MG	2A	3524	1/1	0.88	0.10	47,47,47,47	0
55	MG	1A	3038	1/1	0.88	0.23	50,50,50,50	0
55	MG	1A	3116	1/1	0.88	0.14	49,49,49,49	0
55	MG	1A	3348	1/1	0.88	0.09	42,42,42,42	0
55	MG	2A	3291	1/1	0.88	0.17	40,40,40,40	0
55	MG	2A	3005	1/1	0.89	0.20	47,47,47,47	0
55	MG	1A	3328	1/1	0.89	0.10	40,40,40,40	0
55	MG	1a	3084	1/1	0.89	0.30	58,58,58,58	0
55	MG	2A	3646	1/1	0.89	0.36	57,57,57,57	0
55	MG	1A	3790	1/1	0.89	0.07	38,38,38,38	0
55	MG	1A	3333	1/1	0.89	0.19	29,29,29,29	0
55	MG	2U	201	1/1	0.89	0.15	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3225	1/1	0.89	0.20	32,32,32,32	0
55	MG	1A	3074	1/1	0.89	0.68	39,39,39,39	0
55	MG	2A	3026	1/1	0.89	0.14	37,37,37,37	0
55	MG	1A	3204	1/1	0.89	0.30	43,43,43,43	0
55	MG	1a	3120	1/1	0.89	0.08	65,65,65,65	0
55	MG	20	105	1/1	0.89	0.21	80,80,80,80	0
55	MG	1A	3571	1/1	0.89	0.45	33,33,33,33	0
55	MG	25	101	1/1	0.89	0.31	58,58,58,58	0
55	MG	2A	3456	1/1	0.89	0.25	91,91,91,91	0
55	MG	1A	3263	1/1	0.89	0.15	48,48,48,48	0
55	MG	15	202	1/1	0.89	0.25	39,39,39,39	0
55	MG	1a	3132	1/1	0.89	0.11	71,71,71,71	0
55	MG	1A	3902	1/1	0.89	0.32	25,25,25,25	0
55	MG	1A	3576	1/1	0.89	0.16	77,77,77,77	0
55	MG	2a	1602	1/1	0.89	0.40	76,76,76,76	0
55	MG	1A	3577	1/1	0.89	0.18	68,68,68,68	0
55	MG	2A	3469	1/1	0.89	0.09	62,62,62,62	0
55	MG	1a	3001	1/1	0.89	0.07	73,73,73,73	0
55	MG	2A	3689	1/1	0.89	0.18	66,66,66,66	0
55	MG	1A	3906	1/1	0.89	0.36	40,40,40,40	0
55	MG	2A	3046	1/1	0.89	0.10	72,72,72,72	0
55	MG	1A	3504	1/1	0.89	0.12	66,66,66,66	0
55	MG	2A	3480	1/1	0.89	0.16	65,65,65,65	0
55	MG	1A	3586	1/1	0.89	0.19	60,60,60,60	0
55	MG	2A	3189	1/1	0.89	0.33	53,53,53,53	0
55	MG	2A	3051	1/1	0.89	0.42	53,53,53,53	0
55	MG	1A	3830	1/1	0.89	0.07	51,51,51,51	0
55	MG	2a	1630	1/1	0.89	0.16	83,83,83,83	0
55	MG	2A	3195	1/1	0.89	0.18	60,60,60,60	0
55	MG	1A	3588	1/1	0.89	0.06	41,41,41,41	0
55	MG	2A	3055	1/1	0.89	0.30	56,56,56,56	0
55	MG	2A	3502	1/1	0.89	0.52	69,69,69,69	0
55	MG	2A	3505	1/1	0.89	0.25	44,44,44,44	0
55	MG	2A	3201	1/1	0.89	0.27	50,50,50,50	0
55	MG	1A	3704	1/1	0.89	0.34	57,57,57,57	0
55	MG	2A	3207	1/1	0.89	0.15	65,65,65,65	0
55	MG	1A	3205	1/1	0.89	0.19	34,34,34,34	0
55	MG	1A	3598	1/1	0.89	0.13	76,76,76,76	0
55	MG	2A	3740	1/1	0.89	0.26	78,78,78,78	0
55	MG	2A	3742	1/1	0.89	0.59	61,61,61,61	0
55	MG	1A	3838	1/1	0.89	0.22	46,46,46,46	0
55	MG	2a	1651	1/1	0.89	0.77	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3521	1/1	0.89	0.13	74,74,74,74	0
55	MG	2A	3522	1/1	0.89	0.15	67,67,67,67	0
55	MG	2A	3066	1/1	0.89	0.29	64,64,64,64	0
55	MG	1a	3029	1/1	0.89	0.14	55,55,55,55	0
55	MG	2A	3525	1/1	0.89	0.18	77,77,77,77	0
55	MG	2A	3236	1/1	0.89	0.09	65,65,65,65	0
55	MG	1a	3030	1/1	0.89	1.08	75,75,75,75	0
55	MG	2A	3242	1/1	0.89	0.07	75,75,75,75	0
55	MG	1a	3032	1/1	0.89	0.16	39,39,39,39	0
55	MG	1a	3166	1/1	0.89	0.13	70,70,70,70	0
55	MG	1A	3944	1/1	0.89	0.77	47,47,47,47	0
55	MG	2A	3083	1/1	0.89	0.29	60,60,60,60	0
55	MG	1a	3170	1/1	0.89	0.22	80,80,80,80	0
55	MG	1a	3173	1/1	0.89	0.23	68,68,68,68	0
55	MG	2A	3091	1/1	0.89	0.23	52,52,52,52	0
55	MG	1A	3717	1/1	0.89	0.16	69,69,69,69	0
55	MG	2A	3095	1/1	0.89	0.23	58,58,58,58	0
55	MG	1A	3719	1/1	0.89	0.10	70,70,70,70	0
55	MG	2A	3552	1/1	0.89	0.55	57,57,57,57	0
55	MG	2A	3271	1/1	0.89	0.10	58,58,58,58	0
55	MG	1A	3507	1/1	0.89	0.32	32,32,32,32	0
55	MG	1A	3055	1/1	0.89	0.21	48,48,48,48	0
55	MG	1B	213	1/1	0.89	0.09	54,54,54,54	0
55	MG	1A	3273	1/1	0.89	0.11	35,35,35,35	0
55	MG	1A	3004	1/1	0.89	0.16	50,50,50,50	0
55	MG	2A	3107	1/1	0.89	0.12	58,58,58,58	0
55	MG	2A	3567	1/1	0.89	0.22	72,72,72,72	0
55	MG	1A	3404	1/1	0.89	0.15	62,62,62,62	0
55	MG	2a	1735	1/1	0.89	0.17	74,74,74,74	0
55	MG	2A	3569	1/1	0.89	0.17	56,56,56,56	0
55	MG	1A	3050	1/1	0.89	0.25	37,37,37,37	0
55	MG	2A	3112	1/1	0.89	1.04	68,68,68,68	0
55	MG	2A	3315	1/1	0.89	0.12	68,68,68,68	0
55	MG	1A	3084	1/1	0.89	0.56	43,43,43,43	0
55	MG	2A	3322	1/1	0.89	0.21	69,69,69,69	0
55	MG	1a	3052	1/1	0.89	0.30	59,59,59,59	0
55	MG	1A	3732	1/1	0.89	0.70	34,34,34,34	0
55	MG	1a	3055	1/1	0.89	0.32	44,44,44,44	0
55	MG	2A	3588	1/1	0.89	0.17	66,66,66,66	0
55	MG	2A	3332	1/1	0.89	0.18	63,63,63,63	0
55	MG	2A	3593	1/1	0.89	0.23	72,72,72,72	0
55	MG	1A	3172	1/1	0.89	0.53	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3308	1/1	0.89	0.31	38,38,38,38	0
55	MG	1A	3441	1/1	0.89	0.17	21,21,21,21	0
55	MG	2a	1776	1/1	0.89	0.09	74,74,74,74	0
55	MG	1A	3214	1/1	0.89	0.23	33,33,33,33	0
55	MG	1a	3064	1/1	0.89	0.34	82,82,82,82	0
55	MG	1a	3065	1/1	0.89	0.53	67,67,67,67	0
55	MG	2A	3359	1/1	0.89	0.08	64,64,64,64	0
55	MG	1A	3865	1/1	0.89	0.11	82,82,82,82	0
55	MG	1A	3173	1/1	0.89	0.22	45,45,45,45	0
55	MG	1A	3051	1/1	0.89	0.17	35,35,35,35	0
55	MG	1A	3031	1/1	0.89	0.21	27,27,27,27	0
55	MG	1E	304	1/1	0.89	0.25	35,35,35,35	0
55	MG	2A	3393	1/1	0.89	0.14	67,67,67,67	0
55	MG	1A	3465	1/1	0.89	0.18	28,28,28,28	0
55	MG	1A	3163	1/1	0.89	0.27	69,69,69,69	0
55	MG	1o	3001	1/1	0.89	0.46	62,62,62,62	0
55	MG	1A	3029	1/1	0.89	0.17	39,39,39,39	0
55	MG	1A	3773	1/1	0.89	0.15	53,53,53,53	0
55	MG	1A	3659	1/1	0.89	0.33	61,61,61,61	0
55	MG	1A	3457	1/1	0.90	0.48	70,70,70,70	0
55	MG	2A	3320	1/1	0.90	0.17	71,71,71,71	0
55	MG	1A	3244	1/1	0.90	0.28	49,49,49,49	0
55	MG	2A	3021	1/1	0.90	0.27	50,50,50,50	0
55	MG	2A	3719	1/1	0.90	0.07	67,67,67,67	0
55	MG	1A	3937	1/1	0.90	1.57	52,52,52,52	0
55	MG	1A	3161	1/1	0.90	0.66	38,38,38,38	0
55	MG	1A	3584	1/1	0.90	0.08	48,48,48,48	0
55	MG	2A	3729	1/1	0.90	0.42	72,72,72,72	0
55	MG	1A	3755	1/1	0.90	0.18	44,44,44,44	0
55	MG	1a	3148	1/1	0.90	0.23	88,88,88,88	0
55	MG	1A	3756	1/1	0.90	0.16	38,38,38,38	0
55	MG	2a	1614	1/1	0.90	0.42	61,61,61,61	0
55	MG	1A	3402	1/1	0.90	0.07	62,62,62,62	0
55	MG	1a	3031	1/1	0.90	0.12	71,71,71,71	0
55	MG	2A	3550	1/1	0.90	0.11	75,75,75,75	0
55	MG	2a	1619	1/1	0.90	0.57	76,76,76,76	0
55	MG	2A	3744	1/1	0.90	0.26	72,72,72,72	0
55	MG	2A	3344	1/1	0.90	0.12	78,78,78,78	0
55	MG	1A	3474	1/1	0.90	0.20	50,50,50,50	0
55	MG	1A	3759	1/1	0.90	0.19	61,61,61,61	0
55	MG	1A	3077	1/1	0.90	0.29	48,48,48,48	0
55	MG	2a	1634	1/1	0.90	0.34	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1635	1/1	0.90	0.60	81,81,81,81	0
55	MG	2A	3556	1/1	0.90	0.15	63,63,63,63	0
55	MG	1A	3674	1/1	0.90	0.39	51,51,51,51	0
55	MG	1a	3161	1/1	0.90	0.60	67,67,67,67	0
55	MG	1A	3067	1/1	0.90	0.74	47,47,47,47	0
55	MG	1A	3600	1/1	0.90	0.46	81,81,81,81	0
55	MG	1A	3534	1/1	0.90	0.09	40,40,40,40	0
55	MG	2A	3395	1/1	0.90	0.12	76,76,76,76	0
55	MG	2A	3398	1/1	0.90	0.10	45,45,45,45	0
55	MG	1A	3782	1/1	0.90	0.14	59,59,59,59	0
55	MG	2A	3403	1/1	0.90	0.05	67,67,67,67	0
55	MG	2A	3404	1/1	0.90	0.11	47,47,47,47	0
55	MG	1B	226	1/1	0.90	0.11	72,72,72,72	0
55	MG	2a	1650	1/1	0.90	0.08	84,84,84,84	0
55	MG	1A	3689	1/1	0.90	0.16	62,62,62,62	0
55	MG	1a	3174	1/1	0.90	0.11	70,70,70,70	0
55	MG	2A	3417	1/1	0.90	0.12	52,52,52,52	0
55	MG	1A	3874	1/1	0.90	0.17	67,67,67,67	0
55	MG	2A	3059	1/1	0.90	1.20	55,55,55,55	0
55	MG	2A	3180	1/1	0.90	0.43	72,72,72,72	0
55	MG	2A	3590	1/1	0.90	0.38	63,63,63,63	0
55	MG	2a	1671	1/1	0.90	0.16	80,80,80,80	0
55	MG	1A	3478	1/1	0.90	0.12	33,33,33,33	0
55	MG	1A	3791	1/1	0.90	0.16	58,58,58,58	0
55	MG	2a	1686	1/1	0.90	0.20	61,61,61,61	0
55	MG	1A	3409	1/1	0.90	0.17	48,48,48,48	0
55	MG	2A	3072	1/1	0.90	0.64	64,64,64,64	0
55	MG	2A	3074	1/1	0.90	0.39	51,51,51,51	0
55	MG	1a	3183	1/1	0.90	0.15	82,82,82,82	0
55	MG	2a	1709	1/1	0.90	0.16	87,87,87,87	0
55	MG	1A	3493	1/1	0.90	0.14	46,46,46,46	0
55	MG	2a	1712	1/1	0.90	0.40	68,68,68,68	0
55	MG	1A	3237	1/1	0.90	0.28	42,42,42,42	0
55	MG	2A	3452	1/1	0.90	0.11	63,63,63,63	0
55	MG	1A	3498	1/1	0.90	0.41	67,67,67,67	0
55	MG	1A	3621	1/1	0.90	0.14	58,58,58,58	0
55	MG	2A	3611	1/1	0.90	0.30	79,79,79,79	0
55	MG	2A	3822	1/1	0.90	0.78	65,65,65,65	0
55	MG	2a	1723	1/1	0.90	0.21	98,98,98,98	0
55	MG	1A	3087	1/1	0.90	0.46	34,34,34,34	0
55	MG	1A	3888	1/1	0.90	0.28	54,54,54,54	0
55	MG	2A	3832	1/1	0.90	0.90	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3500	1/1	0.90	0.14	67,67,67,67	0
55	MG	1A	3553	1/1	0.90	0.06	47,47,47,47	0
55	MG	2A	3211	1/1	0.90	0.15	64,64,64,64	0
55	MG	1F	311	1/1	0.90	0.22	67,67,67,67	0
55	MG	1A	3369	1/1	0.90	0.16	70,70,70,70	0
55	MG	2A	3097	1/1	0.90	0.23	39,39,39,39	0
55	MG	2A	3470	1/1	0.90	0.17	75,75,75,75	0
55	MG	1a	3213	1/1	0.90	0.16	67,67,67,67	0
55	MG	2a	1740	1/1	0.90	0.06	73,73,73,73	0
55	MG	1A	3722	1/1	0.90	0.08	50,50,50,50	0
55	MG	1A	3371	1/1	0.90	0.12	62,62,62,62	0
55	MG	1A	3900	1/1	0.90	0.45	57,57,57,57	0
55	MG	1U	203	1/1	0.90	0.19	51,51,51,51	0
55	MG	2A	3649	1/1	0.90	0.38	52,52,52,52	0
55	MG	1A	3831	1/1	0.90	0.20	43,43,43,43	0
55	MG	1A	3098	1/1	0.90	0.21	37,37,37,37	0
55	MG	1A	3833	1/1	0.90	0.13	70,70,70,70	0
55	MG	10	107	1/1	0.90	0.43	46,46,46,46	0
55	MG	1A	3276	1/1	0.90	0.23	35,35,35,35	0
55	MG	2a	1765	1/1	0.90	0.07	88,88,88,88	0
55	MG	2a	1767	1/1	0.90	0.09	74,74,74,74	0
55	MG	1A	3508	1/1	0.90	0.12	72,72,72,72	0
55	MG	2A	3666	1/1	0.90	0.07	63,63,63,63	0
55	MG	2A	3500	1/1	0.90	0.11	78,78,78,78	0
55	MG	1A	3909	1/1	0.90	0.28	38,38,38,38	0
55	MG	1A	3383	1/1	0.90	0.14	53,53,53,53	0
55	MG	2a	1777	1/1	0.90	0.05	85,85,85,85	0
55	MG	2A	3118	1/1	0.90	0.39	54,54,54,54	0
55	MG	2A	3267	1/1	0.90	0.13	50,50,50,50	0
55	MG	2A	3508	1/1	0.90	0.97	52,52,52,52	0
55	MG	1l	201	1/1	0.90	0.14	71,71,71,71	0
55	MG	2a	1789	1/1	0.90	0.53	82,82,82,82	0
55	MG	2A	3511	1/1	0.90	0.17	54,54,54,54	0
55	MG	18	3301	1/1	0.90	0.62	64,64,64,64	0
55	MG	1A	3914	1/1	0.90	0.33	68,68,68,68	0
55	MG	2A	3001	1/1	0.90	0.18	50,50,50,50	0
55	MG	1A	3730	1/1	0.90	0.10	75,75,75,75	0
55	MG	1A	3061	1/1	0.90	0.14	36,36,36,36	0
55	MG	2h	3001	1/1	0.90	0.56	64,64,64,64	0
55	MG	1A	3921	1/1	0.90	0.44	40,40,40,40	0
55	MG	1a	3130	1/1	0.90	0.34	75,75,75,75	0
55	MG	2l	202	1/1	0.90	0.09	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3575	1/1	0.90	0.56	45,45,45,45	0
55	MG	2A	3700	1/1	0.90	0.15	79,79,79,79	0
55	MG	1A	3926	1/1	0.90	0.64	44,44,44,44	0
55	MG	1a	3009	1/1	0.90	0.89	62,62,62,62	0
55	MG	1A	3549	1/1	0.91	0.24	52,52,52,52	0
55	MG	1A	3489	1/1	0.91	0.19	46,46,46,46	0
55	MG	2A	3146	1/1	0.91	0.66	57,57,57,57	0
55	MG	1A	3913	1/1	0.91	0.42	64,64,64,64	0
55	MG	2A	3720	1/1	0.91	0.36	58,58,58,58	0
55	MG	2A	3541	1/1	0.91	0.14	85,85,85,85	0
55	MG	1A	3146	1/1	0.91	0.19	39,39,39,39	0
55	MG	2a	1609	1/1	0.91	0.20	46,46,46,46	0
55	MG	1A	3047	1/1	0.91	0.37	45,45,45,45	0
55	MG	1a	3135	1/1	0.91	0.26	77,77,77,77	0
55	MG	1A	3064	1/1	0.91	0.39	59,59,59,59	0
55	MG	1A	3426	1/1	0.91	0.12	72,72,72,72	0
55	MG	1A	3183	1/1	0.91	0.21	44,44,44,44	0
55	MG	2A	3358	1/1	0.91	0.15	59,59,59,59	0
55	MG	2A	3158	1/1	0.91	0.74	56,56,56,56	0
55	MG	1A	3924	1/1	0.91	0.93	43,43,43,43	0
55	MG	2A	3743	1/1	0.91	0.22	48,48,48,48	0
55	MG	1A	3565	1/1	0.91	0.17	26,26,26,26	0
55	MG	2A	3747	1/1	0.91	0.09	78,78,78,78	0
55	MG	1A	3168	1/1	0.91	0.27	56,56,56,56	0
55	MG	1A	3931	1/1	0.91	0.32	35,35,35,35	0
55	MG	2A	3559	1/1	0.91	0.10	51,51,51,51	0
55	MG	1a	3017	1/1	0.91	0.40	75,75,75,75	0
55	MG	1A	3132	1/1	0.91	0.60	34,34,34,34	0
55	MG	2A	3167	1/1	0.91	0.60	56,56,56,56	0
55	MG	1A	3934	1/1	0.91	0.30	30,30,30,30	0
55	MG	1A	3744	1/1	0.91	0.05	55,55,55,55	0
55	MG	1A	3747	1/1	0.91	0.14	66,66,66,66	0
55	MG	2A	3572	1/1	0.91	0.16	51,51,51,51	0
55	MG	1a	3026	1/1	0.91	0.30	64,64,64,64	0
55	MG	2A	3769	1/1	0.91	0.13	66,66,66,66	0
55	MG	2A	3405	1/1	0.91	0.23	60,60,60,60	0
55	MG	1A	3657	1/1	0.91	0.32	45,45,45,45	0
55	MG	1A	3151	1/1	0.91	0.27	48,48,48,48	0
55	MG	1A	3133	1/1	0.91	0.13	62,62,62,62	0
55	MG	1A	3275	1/1	0.91	0.20	38,38,38,38	0
55	MG	1a	3165	1/1	0.91	0.78	74,74,74,74	0
55	MG	2a	1653	1/1	0.91	0.44	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3115	1/1	0.91	0.14	69,69,69,69	0
55	MG	2A	3062	1/1	0.91	0.29	56,56,56,56	0
55	MG	1A	3668	1/1	0.91	0.55	63,63,63,63	0
55	MG	1A	3453	1/1	0.91	0.08	51,51,51,51	0
55	MG	2a	1661	1/1	0.91	0.17	74,74,74,74	0
55	MG	1A	3277	1/1	0.91	0.20	56,56,56,56	0
55	MG	1A	3863	1/1	0.91	0.28	68,68,68,68	0
55	MG	2A	3799	1/1	0.91	0.25	97,97,97,97	0
55	MG	2A	3440	1/1	0.91	0.11	78,78,78,78	0
55	MG	2a	1683	1/1	0.91	0.21	79,79,79,79	0
55	MG	2A	3193	1/1	0.91	0.09	80,80,80,80	0
55	MG	2A	3073	1/1	0.91	0.35	52,52,52,52	0
55	MG	1A	3455	1/1	0.91	0.15	21,21,21,21	0
55	MG	1A	3216	1/1	0.91	0.46	50,50,50,50	0
55	MG	1A	3526	1/1	0.91	0.08	52,52,52,52	0
55	MG	1A	3527	1/1	0.91	0.22	56,56,56,56	0
55	MG	2A	3812	1/1	0.91	0.53	68,68,68,68	0
55	MG	2A	3202	1/1	0.91	0.25	59,59,59,59	0
55	MG	1A	3593	1/1	0.91	0.05	63,63,63,63	0
55	MG	1A	3372	1/1	0.91	0.11	68,68,68,68	0
55	MG	1A	3789	1/1	0.91	0.12	89,89,89,89	0
55	MG	2A	3615	1/1	0.91	0.23	59,59,59,59	0
55	MG	1a	3188	1/1	0.91	0.24	65,65,65,65	0
55	MG	2A	3824	1/1	0.91	0.38	55,55,55,55	0
55	MG	2A	3624	1/1	0.91	0.34	55,55,55,55	0
55	MG	2A	3221	1/1	0.91	0.49	68,68,68,68	0
55	MG	2A	3831	1/1	0.91	1.10	52,52,52,52	0
55	MG	1D	307	1/1	0.91	0.38	22,22,22,22	0
55	MG	1a	3053	1/1	0.91	0.23	76,76,76,76	0
55	MG	1A	3529	1/1	0.91	0.07	45,45,45,45	0
55	MG	2A	3636	1/1	0.91	0.06	67,67,67,67	0
55	MG	1A	3281	1/1	0.91	0.14	31,31,31,31	0
55	MG	2A	3472	1/1	0.91	0.11	55,55,55,55	0
55	MG	1A	3014	1/1	0.91	0.40	41,41,41,41	0
55	MG	1A	3068	1/1	0.91	0.51	41,41,41,41	0
55	MG	1A	3883	1/1	0.91	0.06	58,58,58,58	0
55	MG	1A	3885	1/1	0.91	0.21	33,33,33,33	0
55	MG	1A	3802	1/1	0.91	0.09	41,41,41,41	0
55	MG	1A	3705	1/1	0.91	0.12	53,53,53,53	0
55	MG	2A	3648	1/1	0.91	0.08	39,39,39,39	0
55	MG	1A	3289	1/1	0.91	0.19	33,33,33,33	0
55	MG	1A	3711	1/1	0.91	0.14	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3651	1/1	0.91	0.23	56,56,56,56	0
55	MG	2A	3487	1/1	0.91	0.23	75,75,75,75	0
55	MG	1F	310	1/1	0.91	0.40	43,43,43,43	0
55	MG	2D	310	1/1	0.91	0.27	61,61,61,61	0
55	MG	2E	301	1/1	0.91	0.15	47,47,47,47	0
55	MG	2a	1764	1/1	0.91	0.50	70,70,70,70	0
55	MG	1A	3110	1/1	0.91	0.29	41,41,41,41	0
55	MG	2A	3660	1/1	0.91	0.15	80,80,80,80	0
55	MG	1A	3893	1/1	0.91	0.23	66,66,66,66	0
55	MG	1A	3111	1/1	0.91	0.22	55,55,55,55	0
55	MG	1A	3812	1/1	0.91	0.09	32,32,32,32	0
55	MG	1A	3718	1/1	0.91	0.11	46,46,46,46	0
55	MG	2A	3268	1/1	0.91	0.18	54,54,54,54	0
55	MG	2H	201	1/1	0.91	0.72	95,95,95,95	0
55	MG	2a	1779	1/1	0.91	0.20	85,85,85,85	0
55	MG	1U	202	1/1	0.91	0.32	34,34,34,34	0
55	MG	2A	3124	1/1	0.91	0.95	53,53,53,53	0
55	MG	1A	3545	1/1	0.91	0.21	30,30,30,30	0
55	MG	2A	3288	1/1	0.91	0.32	67,67,67,67	0
55	MG	1A	3615	1/1	0.91	0.04	50,50,50,50	0
55	MG	2a	1790	1/1	0.91	0.23	72,72,72,72	0
55	MG	1W	3002	1/1	0.91	0.27	51,51,51,51	0
55	MG	2A	3296	1/1	0.91	0.16	60,60,60,60	0
55	MG	2b	3001	1/1	0.91	0.18	79,79,79,79	0
55	MG	1a	3092	1/1	0.91	0.09	86,86,86,86	0
55	MG	2X	103	1/1	0.91	0.13	58,58,58,58	0
55	MG	1A	3825	1/1	0.91	0.08	67,67,67,67	0
55	MG	10	102	1/1	0.91	0.26	69,69,69,69	0
55	MG	1A	3826	1/1	0.91	0.07	65,65,65,65	0
55	MG	1a	3113	1/1	0.91	0.26	65,65,65,65	0
55	MG	10	105	1/1	0.91	0.14	63,63,63,63	0
55	MG	2A	3526	1/1	0.91	0.19	64,64,64,64	0
55	MG	10	106	1/1	0.91	0.06	73,73,73,73	0
55	MG	1A	3178	1/1	0.91	0.53	37,37,37,37	0
55	MG	1A	3488	1/1	0.91	0.22	64,64,64,64	0
56	ZN	24	501	1/1	0.91	0.14	132,132,132,132	0
55	MG	1a	3127	1/1	0.91	0.16	52,52,52,52	0
55	MG	2W	3001	1/1	0.92	0.25	57,57,57,57	0
55	MG	2A	3485	1/1	0.92	0.81	57,57,57,57	0
55	MG	1A	3037	1/1	0.92	0.11	51,51,51,51	0
55	MG	2A	3092	1/1	0.92	0.52	49,49,49,49	0
55	MG	1a	3185	1/1	0.92	0.21	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3493	1/1	0.92	0.09	75,75,75,75	0
55	MG	1A	3688	1/1	0.92	0.17	76,76,76,76	0
55	MG	1a	3051	1/1	0.92	0.39	59,59,59,59	0
55	MG	1A	3192	1/1	0.92	0.32	51,51,51,51	0
55	MG	1A	3690	1/1	0.92	0.14	21,21,21,21	0
55	MG	1A	3692	1/1	0.92	0.09	40,40,40,40	0
55	MG	1A	3800	1/1	0.92	0.06	65,65,65,65	0
55	MG	1A	3695	1/1	0.92	0.09	33,33,33,33	0
55	MG	1F	305	1/1	0.92	0.11	35,35,35,35	0
55	MG	1A	3241	1/1	0.92	0.28	32,32,32,32	0
55	MG	1a	3060	1/1	0.92	0.41	74,74,74,74	0
55	MG	1A	3596	1/1	0.92	0.17	83,83,83,83	0
55	MG	2A	3702	1/1	0.92	0.17	38,38,38,38	0
55	MG	1a	3215	1/1	0.92	0.23	74,74,74,74	0
55	MG	1A	3048	1/1	0.92	0.16	29,29,29,29	0
55	MG	1A	3894	1/1	0.92	0.04	87,87,87,87	0
55	MG	1A	3467	1/1	0.92	0.23	59,59,59,59	0
55	MG	1a	3067	1/1	0.92	0.06	66,66,66,66	0
55	MG	2A	3119	1/1	0.92	0.22	47,47,47,47	0
55	MG	1H	8002	1/1	0.92	0.19	58,58,58,58	0
55	MG	1N	8001	1/1	0.92	0.26	49,49,49,49	0
55	MG	1A	3144	1/1	0.92	0.26	33,33,33,33	0
55	MG	2A	3724	1/1	0.92	0.14	46,46,46,46	0
55	MG	1A	3145	1/1	0.92	0.15	60,60,60,60	0
55	MG	2A	3529	1/1	0.92	0.37	48,48,48,48	0
55	MG	1d	503	1/1	0.92	0.27	72,72,72,72	0
55	MG	1R	202	1/1	0.92	0.32	51,51,51,51	0
55	MG	2a	1631	1/1	0.92	0.42	52,52,52,52	0
55	MG	2A	3316	1/1	0.92	0.27	69,69,69,69	0
55	MG	1A	3814	1/1	0.92	0.25	46,46,46,46	0
55	MG	1A	3041	1/1	0.92	0.25	63,63,63,63	0
55	MG	1a	3076	1/1	0.92	0.20	69,69,69,69	0
55	MG	2A	3539	1/1	0.92	0.13	64,64,64,64	0
55	MG	1A	3820	1/1	0.92	0.24	45,45,45,45	0
55	MG	1A	3250	1/1	0.92	0.42	43,43,43,43	0
55	MG	1A	3714	1/1	0.92	0.04	80,80,80,80	0
55	MG	1A	3537	1/1	0.92	0.25	63,63,63,63	0
55	MG	1a	3087	1/1	0.92	0.11	63,63,63,63	0
55	MG	1A	3388	1/1	0.92	0.17	26,26,26,26	0
55	MG	2A	3548	1/1	0.92	0.05	72,72,72,72	0
55	MG	1A	3105	1/1	0.92	0.29	35,35,35,35	0
55	MG	1A	3480	1/1	0.92	0.28	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3342	1/1	0.92	0.19	49,49,49,49	0
55	MG	1a	3101	1/1	0.92	0.13	46,46,46,46	0
55	MG	2A	3764	1/1	0.92	0.13	80,80,80,80	0
55	MG	1A	3394	1/1	0.92	0.66	75,75,75,75	0
55	MG	2A	3149	1/1	0.92	0.23	58,58,58,58	0
55	MG	2A	3348	1/1	0.92	0.16	59,59,59,59	0
55	MG	2A	3355	1/1	0.92	0.14	58,58,58,58	0
55	MG	1A	3548	1/1	0.92	0.19	47,47,47,47	0
55	MG	2A	3772	1/1	0.92	0.10	68,68,68,68	0
55	MG	1A	3307	1/1	0.92	0.19	37,37,37,37	0
55	MG	2a	1662	1/1	0.92	0.30	61,61,61,61	0
55	MG	2A	3360	1/1	0.92	0.20	58,58,58,58	0
55	MG	2A	3015	1/1	0.92	0.36	46,46,46,46	0
55	MG	1A	3399	1/1	0.92	0.05	65,65,65,65	0
55	MG	2A	3155	1/1	0.92	0.64	42,42,42,42	0
55	MG	1A	3022	1/1	0.92	0.24	28,28,28,28	0
55	MG	2A	3786	1/1	0.92	0.14	66,66,66,66	0
55	MG	2a	1694	1/1	0.92	0.26	77,77,77,77	0
55	MG	2A	3025	1/1	0.92	0.23	53,53,53,53	0
55	MG	15	203	1/1	0.92	0.32	45,45,45,45	0
55	MG	2a	1699	1/1	0.92	0.14	67,67,67,67	0
55	MG	1A	3633	1/1	0.92	0.22	48,48,48,48	0
55	MG	2A	3396	1/1	0.92	0.04	64,64,64,64	0
55	MG	2A	3397	1/1	0.92	0.16	83,83,83,83	0
55	MG	1A	3221	1/1	0.92	0.60	32,32,32,32	0
55	MG	2A	3029	1/1	0.92	0.53	72,72,72,72	0
55	MG	2A	3584	1/1	0.92	0.18	65,65,65,65	0
55	MG	1A	3928	1/1	0.92	0.22	32,32,32,32	0
55	MG	1A	3405	1/1	0.92	0.08	59,59,59,59	0
55	MG	2A	3805	1/1	0.92	0.22	68,68,68,68	0
55	MG	19	103	1/1	0.92	0.21	63,63,63,63	0
55	MG	2A	3809	1/1	0.92	0.28	45,45,45,45	0
55	MG	2A	3034	1/1	0.92	0.17	58,58,58,58	0
55	MG	2a	1724	1/1	0.92	0.23	92,92,92,92	0
55	MG	1A	3639	1/1	0.92	0.28	30,30,30,30	0
55	MG	2A	3415	1/1	0.92	0.19	69,69,69,69	0
55	MG	1A	3554	1/1	0.92	0.18	15,15,15,15	0
55	MG	1A	3119	1/1	0.92	0.39	35,35,35,35	0
55	MG	2A	3419	1/1	0.92	0.18	58,58,58,58	0
55	MG	2A	3818	1/1	0.92	0.49	69,69,69,69	0
55	MG	1A	3136	1/1	0.92	0.62	42,42,42,42	0
55	MG	1A	3938	1/1	0.92	0.24	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3741	1/1	0.92	0.41	56,56,56,56	0
55	MG	2A	3823	1/1	0.92	0.79	53,53,53,53	0
55	MG	2A	3425	1/1	0.92	0.27	67,67,67,67	0
55	MG	1A	3942	1/1	0.92	0.32	32,32,32,32	0
55	MG	2A	3827	1/1	0.92	0.67	58,58,58,58	0
55	MG	2a	1744	1/1	0.92	0.36	69,69,69,69	0
55	MG	1A	3648	1/1	0.92	0.19	33,33,33,33	0
55	MG	2A	3830	1/1	0.92	0.70	65,65,65,65	0
55	MG	2a	1748	1/1	0.92	0.10	85,85,85,85	0
55	MG	2A	3432	1/1	0.92	0.15	58,58,58,58	0
55	MG	2A	3434	1/1	0.92	0.14	78,78,78,78	0
55	MG	2A	3181	1/1	0.92	0.58	67,67,67,67	0
55	MG	1A	3945	1/1	0.92	0.22	56,56,56,56	0
55	MG	2A	3616	1/1	0.92	0.06	57,57,57,57	0
55	MG	1A	3425	1/1	0.92	0.10	46,46,46,46	0
55	MG	2A	3441	1/1	0.92	0.29	88,88,88,88	0
55	MG	2A	3626	1/1	0.92	0.21	68,68,68,68	0
55	MG	1A	3228	1/1	0.92	0.20	76,76,76,76	0
55	MG	1a	3024	1/1	0.92	0.31	61,61,61,61	0
55	MG	2A	3632	1/1	0.92	0.37	94,94,94,94	0
55	MG	1A	3232	1/1	0.92	0.34	68,68,68,68	0
55	MG	2a	1772	1/1	0.92	0.10	81,81,81,81	0
55	MG	1a	3027	1/1	0.92	0.89	75,75,75,75	0
55	MG	2a	1774	1/1	0.92	0.07	65,65,65,65	0
55	MG	1A	3120	1/1	0.92	0.24	54,54,54,54	0
55	MG	1A	3860	1/1	0.92	0.22	56,56,56,56	0
55	MG	2A	3060	1/1	0.92	0.35	48,48,48,48	0
55	MG	2A	3640	1/1	0.92	0.17	76,76,76,76	0
55	MG	2A	3196	1/1	0.92	0.12	75,75,75,75	0
55	MG	2D	303	1/1	0.92	0.26	54,54,54,54	0
55	MG	1A	3186	1/1	0.92	0.10	58,58,58,58	0
55	MG	1A	3156	1/1	0.92	0.10	53,53,53,53	0
55	MG	1A	3344	1/1	0.92	0.20	54,54,54,54	0
55	MG	1A	3057	1/1	0.92	0.18	26,26,26,26	0
55	MG	1A	3353	1/1	0.92	0.25	62,62,62,62	0
55	MG	1A	3519	1/1	0.92	0.23	52,52,52,52	0
55	MG	2F	307	1/1	0.92	0.83	58,58,58,58	0
55	MG	1a	3169	1/1	0.92	0.25	90,90,90,90	0
55	MG	1A	3583	1/1	0.92	0.09	59,59,59,59	0
55	MG	1A	3772	1/1	0.92	0.11	48,48,48,48	0
55	MG	1A	3678	1/1	0.92	0.23	40,40,40,40	0
55	MG	1A	3679	1/1	0.92	0.07	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1a	3043	1/1	0.92	0.61	66,66,66,66	0
55	MG	2A	3476	1/1	0.92	0.17	67,67,67,67	0
55	MG	2A	3231	1/1	0.92	0.17	74,74,74,74	0
55	MG	1a	3044	1/1	0.92	0.17	62,62,62,62	0
55	MG	2A	3665	1/1	0.92	0.09	54,54,54,54	0
55	MG	1A	3238	1/1	0.92	0.15	37,37,37,37	0
55	MG	2U	202	1/1	0.92	0.54	60,60,60,60	0
55	MG	1A	3522	1/1	0.92	0.30	57,57,57,57	0
55	MG	2Q	202	1/1	0.93	0.13	65,65,65,65	0
55	MG	2A	3662	1/1	0.93	0.07	65,65,65,65	0
55	MG	1A	3395	1/1	0.93	0.05	68,68,68,68	0
55	MG	2A	3086	1/1	0.93	0.42	60,60,60,60	0
55	MG	2A	3483	1/1	0.93	0.26	44,44,44,44	0
55	MG	2A	3253	1/1	0.93	0.09	66,66,66,66	0
55	MG	2A	3089	1/1	0.93	0.15	58,58,58,58	0
55	MG	1F	307	1/1	0.93	0.69	34,34,34,34	0
55	MG	1A	3817	1/1	0.93	0.08	21,21,21,21	0
55	MG	1A	3247	1/1	0.93	0.26	47,47,47,47	0
55	MG	2A	3489	1/1	0.93	0.26	38,38,38,38	0
55	MG	2A	3492	1/1	0.93	0.28	46,46,46,46	0
55	MG	2A	3680	1/1	0.93	0.12	63,63,63,63	0
55	MG	1a	3189	1/1	0.93	0.17	81,81,81,81	0
55	MG	1a	3193	1/1	0.93	0.41	75,75,75,75	0
55	MG	25	102	1/1	0.93	0.31	63,63,63,63	0
55	MG	2A	3684	1/1	0.93	0.13	61,61,61,61	0
55	MG	1A	3821	1/1	0.93	0.13	64,64,64,64	0
55	MG	1A	3470	1/1	0.93	0.26	52,52,52,52	0
55	MG	1A	3006	1/1	0.93	0.20	26,26,26,26	0
55	MG	1A	3329	1/1	0.93	0.11	30,30,30,30	0
55	MG	1A	3523	1/1	0.93	0.40	70,70,70,70	0
55	MG	1A	3905	1/1	0.93	0.09	58,58,58,58	0
55	MG	2A	3278	1/1	0.93	0.13	53,53,53,53	0
55	MG	1a	3205	1/1	0.93	0.06	78,78,78,78	0
55	MG	2A	3701	1/1	0.93	0.09	59,59,59,59	0
55	MG	2A	3510	1/1	0.93	0.12	82,82,82,82	0
55	MG	1Q	203	1/1	0.93	0.19	49,49,49,49	0
55	MG	1Q	204	1/1	0.93	0.16	51,51,51,51	0
55	MG	2A	3293	1/1	0.93	0.30	72,72,72,72	0
55	MG	2a	1613	1/1	0.93	0.09	50,50,50,50	0
55	MG	2A	3514	1/1	0.93	0.30	50,50,50,50	0
55	MG	2A	3518	1/1	0.93	0.20	60,60,60,60	0
55	MG	2A	3295	1/1	0.93	0.10	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3649	1/1	0.93	0.39	52,52,52,52	0
55	MG	1A	3650	1/1	0.93	0.24	45,45,45,45	0
55	MG	1A	3652	1/1	0.93	0.08	67,67,67,67	0
55	MG	2A	3723	1/1	0.93	0.07	70,70,70,70	0
55	MG	1U	201	1/1	0.93	0.30	56,56,56,56	0
55	MG	1A	3100	1/1	0.93	0.33	31,31,31,31	0
55	MG	1a	3219	1/1	0.93	0.22	68,68,68,68	0
55	MG	1A	3017	1/1	0.93	0.25	31,31,31,31	0
55	MG	1A	3042	1/1	0.93	0.23	32,32,32,32	0
55	MG	1a	3224	1/1	0.93	0.25	60,60,60,60	0
55	MG	1A	3479	1/1	0.93	0.11	31,31,31,31	0
55	MG	1Y	502	1/1	0.93	0.07	68,68,68,68	0
55	MG	1A	3735	1/1	0.93	0.29	79,79,79,79	0
55	MG	2A	3535	1/1	0.93	0.08	67,67,67,67	0
55	MG	1A	3088	1/1	0.93	0.50	34,34,34,34	0
55	MG	1A	3355	1/1	0.93	0.17	22,22,22,22	0
55	MG	2A	3746	1/1	0.93	0.07	73,73,73,73	0
55	MG	1A	3483	1/1	0.93	0.32	56,56,56,56	0
55	MG	2A	3334	1/1	0.93	0.25	71,71,71,71	0
55	MG	1d	506	1/1	0.93	0.16	86,86,86,86	0
55	MG	2A	3750	1/1	0.93	0.14	60,60,60,60	0
55	MG	2A	3751	1/1	0.93	0.20	67,67,67,67	0
55	MG	1a	3081	1/1	0.93	0.23	76,76,76,76	0
55	MG	1A	3590	1/1	0.93	0.31	77,77,77,77	0
55	MG	1A	3485	1/1	0.93	0.30	56,56,56,56	0
55	MG	2A	3341	1/1	0.93	0.04	75,75,75,75	0
55	MG	1A	3750	1/1	0.93	0.21	55,55,55,55	0
55	MG	2A	3759	1/1	0.93	0.10	84,84,84,84	0
55	MG	1t	3001	1/1	0.93	0.21	64,64,64,64	0
55	MG	1A	3019	1/1	0.93	0.45	43,43,43,43	0
55	MG	2a	1660	1/1	0.93	0.15	74,74,74,74	0
55	MG	1A	3673	1/1	0.93	0.14	29,29,29,29	0
55	MG	1A	3595	1/1	0.93	0.43	35,35,35,35	0
55	MG	2a	1665	1/1	0.93	0.35	65,65,65,65	0
55	MG	2A	3354	1/1	0.93	0.19	41,41,41,41	0
55	MG	1a	3102	1/1	0.93	0.09	48,48,48,48	0
55	MG	2a	1675	1/1	0.93	0.22	83,83,83,83	0
55	MG	1A	3676	1/1	0.93	0.15	57,57,57,57	0
55	MG	2a	1677	1/1	0.93	0.16	61,61,61,61	0
55	MG	2a	1678	1/1	0.93	0.18	75,75,75,75	0
55	MG	2a	1681	1/1	0.93	0.10	53,53,53,53	0
55	MG	1a	3107	1/1	0.93	0.22	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3677	1/1	0.93	0.24	38,38,38,38	0
55	MG	2a	1685	1/1	0.93	0.09	77,77,77,77	0
55	MG	1A	3430	1/1	0.93	0.11	54,54,54,54	0
55	MG	2a	1688	1/1	0.93	0.09	58,58,58,58	0
55	MG	2a	1690	1/1	0.93	0.22	83,83,83,83	0
55	MG	2a	1691	1/1	0.93	0.18	64,64,64,64	0
55	MG	1A	3941	1/1	0.93	0.20	54,54,54,54	0
55	MG	2A	3780	1/1	0.93	0.08	54,54,54,54	0
55	MG	1A	3540	1/1	0.93	0.08	80,80,80,80	0
55	MG	1A	3490	1/1	0.93	0.21	50,50,50,50	0
55	MG	2a	1706	1/1	0.93	0.24	90,90,90,90	0
55	MG	2A	3017	1/1	0.93	0.37	65,65,65,65	0
55	MG	1a	3003	1/1	0.93	0.21	81,81,81,81	0
55	MG	1A	3543	1/1	0.93	0.30	39,39,39,39	0
55	MG	2A	3789	1/1	0.93	0.05	68,68,68,68	0
55	MG	2A	3024	1/1	0.93	0.76	60,60,60,60	0
55	MG	2A	3573	1/1	0.93	0.06	73,73,73,73	0
55	MG	1A	3770	1/1	0.93	0.05	64,64,64,64	0
55	MG	2A	3797	1/1	0.93	0.33	88,88,88,88	0
55	MG	1a	3006	1/1	0.93	0.16	72,72,72,72	0
55	MG	2A	3577	1/1	0.93	0.10	51,51,51,51	0
55	MG	1A	3864	1/1	0.93	0.05	53,53,53,53	0
55	MG	2A	3402	1/1	0.93	0.10	80,80,80,80	0
55	MG	1A	3358	1/1	0.93	0.13	24,24,24,24	0
55	MG	1a	3134	1/1	0.93	0.18	73,73,73,73	0
55	MG	1a	3010	1/1	0.93	0.25	60,60,60,60	0
55	MG	2A	3407	1/1	0.93	0.21	70,70,70,70	0
55	MG	2a	1728	1/1	0.93	0.18	81,81,81,81	0
55	MG	2A	3586	1/1	0.93	0.14	89,89,89,89	0
55	MG	2A	3409	1/1	0.93	0.10	88,88,88,88	0
55	MG	1A	3292	1/1	0.93	0.07	34,34,34,34	0
55	MG	1B	210	1/1	0.93	0.21	60,60,60,60	0
55	MG	1B	211	1/1	0.93	0.06	59,59,59,59	0
55	MG	1A	3297	1/1	0.93	0.25	26,26,26,26	0
55	MG	1A	3124	1/1	0.93	0.18	35,35,35,35	0
55	MG	2A	3040	1/1	0.93	0.18	53,53,53,53	0
55	MG	1a	3145	1/1	0.93	0.16	79,79,79,79	0
55	MG	2A	3601	1/1	0.93	0.13	59,59,59,59	0
55	MG	1a	3021	1/1	0.93	0.31	68,68,68,68	0
55	MG	1A	3053	1/1	0.93	0.38	32,32,32,32	0
55	MG	1B	219	1/1	0.93	0.13	47,47,47,47	0
55	MG	1A	3875	1/1	0.93	0.40	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2a	1749	1/1	0.93	0.04	72,72,72,72	0
55	MG	2A	3428	1/1	0.93	0.09	68,68,68,68	0
55	MG	2A	3048	1/1	0.93	0.14	46,46,46,46	0
55	MG	1A	3012	1/1	0.93	0.18	30,30,30,30	0
55	MG	1A	3617	1/1	0.93	0.42	47,47,47,47	0
55	MG	1A	3698	1/1	0.93	0.12	48,48,48,48	0
55	MG	1A	3310	1/1	0.93	0.15	64,64,64,64	0
55	MG	1A	3010	1/1	0.93	0.49	46,46,46,46	0
55	MG	2a	1760	1/1	0.93	0.23	71,71,71,71	0
55	MG	2a	1762	1/1	0.93	0.12	60,60,60,60	0
55	MG	2A	3837	1/1	0.93	0.77	53,53,53,53	0
55	MG	1D	302	1/1	0.93	0.33	44,44,44,44	0
55	MG	2A	3623	1/1	0.93	0.20	71,71,71,71	0
55	MG	2A	3056	1/1	0.93	0.22	47,47,47,47	0
55	MG	1a	3162	1/1	0.93	0.05	72,72,72,72	0
55	MG	1A	3222	1/1	0.93	0.12	46,46,46,46	0
55	MG	2B	3008	1/1	0.93	0.12	84,84,84,84	0
55	MG	2A	3447	1/1	0.93	0.39	47,47,47,47	0
55	MG	1a	3034	1/1	0.93	0.32	74,74,74,74	0
55	MG	1D	304	1/1	0.93	0.07	56,56,56,56	0
55	MG	2A	3061	1/1	0.93	0.87	71,71,71,71	0
55	MG	1A	3624	1/1	0.93	0.14	53,53,53,53	0
55	MG	1A	3884	1/1	0.93	0.12	22,22,22,22	0
55	MG	1A	3208	1/1	0.93	0.12	70,70,70,70	0
55	MG	2A	3214	1/1	0.93	0.16	76,76,76,76	0
55	MG	2A	3460	1/1	0.93	0.17	44,44,44,44	0
55	MG	1A	3707	1/1	0.93	0.18	55,55,55,55	0
55	MG	1a	3172	1/1	0.93	0.18	75,75,75,75	0
55	MG	2D	306	1/1	0.93	1.21	64,64,64,64	0
55	MG	2A	3225	1/1	0.93	0.11	52,52,52,52	0
55	MG	1A	3512	1/1	0.93	0.16	37,37,37,37	0
55	MG	2A	3468	1/1	0.93	0.15	64,64,64,64	0
55	MG	2F	302	1/1	0.93	0.26	58,58,58,58	0
55	MG	1A	3560	1/1	0.93	0.25	24,24,24,24	0
55	MG	1A	3114	1/1	0.93	0.08	59,59,59,59	0
55	MG	2A	3471	1/1	0.93	0.10	72,72,72,72	0
55	MG	2A	3233	1/1	0.93	0.19	48,48,48,48	0
55	MG	2A	3652	1/1	0.93	0.33	58,58,58,58	0
55	MG	1A	3634	1/1	0.93	0.13	44,44,44,44	0
55	MG	1A	3892	1/1	0.93	0.16	59,59,59,59	0
55	MG	2A	3657	1/1	0.93	0.09	55,55,55,55	0
55	MG	1A	3227	1/1	0.93	0.34	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1a	3182	1/1	0.93	0.65	76,76,76,76	0
55	MG	1F	304	1/1	0.93	0.67	41,41,41,41	0
55	MG	1A	3492	1/1	0.94	0.23	68,68,68,68	0
55	MG	2A	3018	1/1	0.94	0.80	48,48,48,48	0
55	MG	2A	3421	1/1	0.94	0.13	52,52,52,52	0
55	MG	1a	3109	1/1	0.94	0.30	60,60,60,60	0
55	MG	1A	3400	1/1	0.94	0.18	44,44,44,44	0
55	MG	1A	3401	1/1	0.94	0.12	43,43,43,43	0
55	MG	2A	3426	1/1	0.94	0.12	62,62,62,62	0
55	MG	2A	3175	1/1	0.94	0.26	50,50,50,50	0
55	MG	1a	3115	1/1	0.94	0.58	71,71,71,71	0
55	MG	2A	3430	1/1	0.94	0.30	54,54,54,54	0
55	MG	1a	3116	1/1	0.94	0.55	80,80,80,80	0
55	MG	2Q	201	1/1	0.94	0.05	77,77,77,77	0
55	MG	1A	3570	1/1	0.94	0.27	46,46,46,46	0
55	MG	2Q	203	1/1	0.94	0.34	55,55,55,55	0
55	MG	1a	3119	1/1	0.94	0.14	78,78,78,78	0
55	MG	2A	3436	1/1	0.94	0.12	82,82,82,82	0
55	MG	2S	201	1/1	0.94	0.52	70,70,70,70	0
55	MG	1A	3497	1/1	0.94	0.21	70,70,70,70	0
55	MG	1A	3256	1/1	0.94	0.35	47,47,47,47	0
55	MG	1A	3056	1/1	0.94	0.23	47,47,47,47	0
55	MG	1A	3794	1/1	0.94	0.26	46,46,46,46	0
55	MG	2A	3443	1/1	0.94	0.17	33,33,33,33	0
55	MG	2A	3186	1/1	0.94	0.40	72,72,72,72	0
55	MG	2A	3187	1/1	0.94	0.17	41,41,41,41	0
55	MG	1A	3033	1/1	0.94	0.42	52,52,52,52	0
55	MG	1A	3233	1/1	0.94	0.23	49,49,49,49	0
55	MG	2A	3191	1/1	0.94	0.20	64,64,64,64	0
55	MG	1A	3578	1/1	0.94	0.21	68,68,68,68	0
55	MG	2A	3453	1/1	0.94	0.12	74,74,74,74	0
55	MG	1A	3503	1/1	0.94	0.20	42,42,42,42	0
55	MG	1A	3580	1/1	0.94	0.24	70,70,70,70	0
55	MG	1A	3915	1/1	0.94	0.27	64,64,64,64	0
55	MG	1A	3408	1/1	0.94	0.21	43,43,43,43	0
55	MG	1A	3140	1/1	0.94	0.36	38,38,38,38	0
55	MG	2A	3198	1/1	0.94	0.23	19,19,19,19	0
55	MG	2A	3199	1/1	0.94	0.61	54,54,54,54	0
55	MG	1A	3506	1/1	0.94	0.18	51,51,51,51	0
55	MG	1a	3141	1/1	0.94	0.12	78,78,78,78	0
55	MG	1a	3002	1/1	0.94	0.21	44,44,44,44	0
55	MG	2A	3466	1/1	0.94	0.15	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3587	1/1	0.94	0.12	35,35,35,35	0
55	MG	1A	3420	1/1	0.94	0.17	37,37,37,37	0
55	MG	2A	3683	1/1	0.94	0.08	68,68,68,68	0
55	MG	2A	3052	1/1	0.94	0.23	59,59,59,59	0
55	MG	1A	3693	1/1	0.94	0.09	38,38,38,38	0
55	MG	2A	3687	1/1	0.94	0.18	46,46,46,46	0
55	MG	2A	3213	1/1	0.94	0.13	36,36,36,36	0
55	MG	1A	3262	1/1	0.94	0.15	41,41,41,41	0
55	MG	2a	1617	1/1	0.94	0.21	67,67,67,67	0
55	MG	2A	3219	1/1	0.94	0.14	64,64,64,64	0
55	MG	1A	3592	1/1	0.94	0.17	27,27,27,27	0
55	MG	1A	3930	1/1	0.94	0.22	25,25,25,25	0
55	MG	2A	3478	1/1	0.94	0.23	55,55,55,55	0
55	MG	2a	1622	1/1	0.94	0.39	61,61,61,61	0
55	MG	1A	3081	1/1	0.94	0.37	41,41,41,41	0
55	MG	2a	1626	1/1	0.94	0.51	68,68,68,68	0
55	MG	2a	1629	1/1	0.94	0.21	61,61,61,61	0
55	MG	2A	3227	1/1	0.94	0.28	50,50,50,50	0
55	MG	1a	3012	1/1	0.94	0.22	28,28,28,28	0
55	MG	2A	3704	1/1	0.94	0.08	57,57,57,57	0
55	MG	1A	3264	1/1	0.94	0.16	73,73,73,73	0
55	MG	1a	3014	1/1	0.94	0.17	67,67,67,67	0
55	MG	2A	3232	1/1	0.94	0.07	70,70,70,70	0
55	MG	2A	3709	1/1	0.94	0.12	49,49,49,49	0
55	MG	1a	3155	1/1	0.94	0.05	76,76,76,76	0
55	MG	1a	3016	1/1	0.94	0.24	77,77,77,77	0
55	MG	1a	3158	1/1	0.94	0.08	78,78,78,78	0
55	MG	2A	3239	1/1	0.94	0.18	38,38,38,38	0
55	MG	1a	3159	1/1	0.94	0.13	79,79,79,79	0
55	MG	1A	3265	1/1	0.94	0.17	81,81,81,81	0
55	MG	2A	3722	1/1	0.94	0.07	69,69,69,69	0
55	MG	2A	3496	1/1	0.94	0.16	85,85,85,85	0
55	MG	2A	3070	1/1	0.94	0.58	52,52,52,52	0
55	MG	1A	3516	1/1	0.94	0.15	77,77,77,77	0
55	MG	2A	3249	1/1	0.94	0.07	68,68,68,68	0
55	MG	1A	3341	1/1	0.94	0.15	31,31,31,31	0
55	MG	2A	3252	1/1	0.94	0.34	54,54,54,54	0
55	MG	1A	3599	1/1	0.94	0.54	46,46,46,46	0
55	MG	2A	3734	1/1	0.94	0.04	67,67,67,67	0
55	MG	2A	3735	1/1	0.94	0.16	55,55,55,55	0
55	MG	1A	3103	1/1	0.94	0.52	41,41,41,41	0
55	MG	1A	3709	1/1	0.94	0.08	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3345	1/1	0.94	0.14	24,24,24,24	0
55	MG	2A	3257	1/1	0.94	0.22	49,49,49,49	0
55	MG	1A	3835	1/1	0.94	0.07	51,51,51,51	0
55	MG	2a	1663	1/1	0.94	0.20	64,64,64,64	0
55	MG	1A	3347	1/1	0.94	0.23	28,28,28,28	0
55	MG	2a	1666	1/1	0.94	0.08	74,74,74,74	0
55	MG	1A	3605	1/1	0.94	0.05	63,63,63,63	0
55	MG	2a	1668	1/1	0.94	0.13	63,63,63,63	0
55	MG	1A	3122	1/1	0.94	0.58	27,27,27,27	0
55	MG	2a	1672	1/1	0.94	0.04	75,75,75,75	0
55	MG	1A	3351	1/1	0.94	0.08	66,66,66,66	0
55	MG	2A	3088	1/1	0.94	0.08	73,73,73,73	0
55	MG	1A	3524	1/1	0.94	0.17	55,55,55,55	0
55	MG	1A	3841	1/1	0.94	0.08	68,68,68,68	0
55	MG	2a	1679	1/1	0.94	0.43	64,64,64,64	0
55	MG	1A	3842	1/1	0.94	0.03	68,68,68,68	0
55	MG	1A	3450	1/1	0.94	0.31	71,71,71,71	0
55	MG	2A	3279	1/1	0.94	0.08	58,58,58,58	0
55	MG	2A	3755	1/1	0.94	0.20	63,63,63,63	0
55	MG	2A	3281	1/1	0.94	0.17	39,39,39,39	0
55	MG	2A	3283	1/1	0.94	0.15	47,47,47,47	0
55	MG	1a	3181	1/1	0.94	0.11	76,76,76,76	0
55	MG	1A	3612	1/1	0.94	0.12	77,77,77,77	0
55	MG	2A	3763	1/1	0.94	0.17	41,41,41,41	0
55	MG	2a	1695	1/1	0.94	0.31	65,65,65,65	0
55	MG	2A	3531	1/1	0.94	0.09	78,78,78,78	0
55	MG	1A	3847	1/1	0.94	0.14	61,61,61,61	0
55	MG	1A	3071	1/1	0.94	0.21	32,32,32,32	0
55	MG	2A	3099	1/1	0.94	0.23	52,52,52,52	0
55	MG	1A	3045	1/1	0.94	0.22	37,37,37,37	0
55	MG	1A	3851	1/1	0.94	0.08	29,29,29,29	0
55	MG	1A	3109	1/1	0.94	0.25	41,41,41,41	0
55	MG	1a	3042	1/1	0.94	0.20	63,63,63,63	0
55	MG	2a	1711	1/1	0.94	1.00	82,82,82,82	0
55	MG	1A	3128	1/1	0.94	0.17	33,33,33,33	0
55	MG	2a	1713	1/1	0.94	0.06	68,68,68,68	0
55	MG	1A	3726	1/1	0.94	0.28	39,39,39,39	0
55	MG	1A	3460	1/1	0.94	0.07	47,47,47,47	0
55	MG	1a	3047	1/1	0.94	0.15	64,64,64,64	0
55	MG	2A	3111	1/1	0.94	0.58	57,57,57,57	0
55	MG	2a	1720	1/1	0.94	0.18	66,66,66,66	0
55	MG	1A	3278	1/1	0.94	0.10	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3546	1/1	0.94	0.15	43,43,43,43	0
55	MG	1A	3046	1/1	0.94	0.24	13,13,13,13	0
55	MG	2A	3325	1/1	0.94	0.58	68,68,68,68	0
55	MG	1A	3194	1/1	0.94	0.16	54,54,54,54	0
55	MG	2A	3792	1/1	0.94	0.16	77,77,77,77	0
55	MG	1a	3204	1/1	0.94	0.05	70,70,70,70	0
55	MG	2A	3117	1/1	0.94	0.22	56,56,56,56	0
55	MG	1A	3469	1/1	0.94	0.16	62,62,62,62	0
55	MG	2A	3333	1/1	0.94	0.08	69,69,69,69	0
55	MG	1A	3016	1/1	0.94	0.26	18,18,18,18	0
55	MG	2A	3335	1/1	0.94	0.11	70,70,70,70	0
55	MG	2A	3557	1/1	0.94	0.07	55,55,55,55	0
55	MG	1D	309	1/1	0.94	0.23	31,31,31,31	0
55	MG	2A	3125	1/1	0.94	0.18	66,66,66,66	0
55	MG	2a	1736	1/1	0.94	0.34	74,74,74,74	0
55	MG	1A	3471	1/1	0.94	0.08	67,67,67,67	0
55	MG	2a	1738	1/1	0.94	0.05	77,77,77,77	0
55	MG	1A	3196	1/1	0.94	0.11	32,32,32,32	0
55	MG	1A	3740	1/1	0.94	0.09	63,63,63,63	0
55	MG	1E	301	1/1	0.94	0.36	40,40,40,40	0
55	MG	1A	3375	1/1	0.94	0.11	69,69,69,69	0
55	MG	1A	3742	1/1	0.94	0.12	55,55,55,55	0
55	MG	1a	3220	1/1	0.94	0.10	60,60,60,60	0
55	MG	1A	3076	1/1	0.94	0.48	43,43,43,43	0
55	MG	2A	3350	1/1	0.94	0.22	54,54,54,54	0
55	MG	1A	3872	1/1	0.94	0.12	32,32,32,32	0
55	MG	1F	303	1/1	0.94	0.28	44,44,44,44	0
55	MG	2A	3356	1/1	0.94	0.21	51,51,51,51	0
55	MG	1A	3873	1/1	0.94	0.11	59,59,59,59	0
55	MG	1A	3745	1/1	0.94	0.16	30,30,30,30	0
55	MG	1A	3746	1/1	0.94	0.05	52,52,52,52	0
55	MG	2A	3363	1/1	0.94	0.24	43,43,43,43	0
55	MG	2A	3364	1/1	0.94	0.07	34,34,34,34	0
55	MG	2a	1763	1/1	0.94	0.10	55,55,55,55	0
55	MG	2A	3373	1/1	0.94	0.15	76,76,76,76	0
55	MG	1A	3290	1/1	0.94	0.17	52,52,52,52	0
55	MG	1A	3018	1/1	0.94	0.19	30,30,30,30	0
55	MG	1A	3645	1/1	0.94	0.24	35,35,35,35	0
55	MG	2A	3833	1/1	0.94	0.19	57,57,57,57	0
55	MG	2A	3379	1/1	0.94	0.07	76,76,76,76	0
55	MG	1A	3294	1/1	0.94	0.13	25,25,25,25	0
55	MG	1A	3390	1/1	0.94	0.20	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3390	1/1	0.94	0.10	48,48,48,48	0
55	MG	2A	3598	1/1	0.94	0.15	70,70,70,70	0
55	MG	1A	3481	1/1	0.94	0.14	35,35,35,35	0
55	MG	1A	3251	1/1	0.94	0.30	34,34,34,34	0
55	MG	1P	201	1/1	0.94	0.23	30,30,30,30	0
55	MG	2a	1782	1/1	0.94	0.16	75,75,75,75	0
55	MG	1A	3393	1/1	0.94	0.17	48,48,48,48	0
55	MG	2B	3009	1/1	0.94	0.12	79,79,79,79	0
55	MG	1A	3653	1/1	0.94	0.15	42,42,42,42	0
55	MG	1A	3200	1/1	0.94	0.31	37,37,37,37	0
55	MG	1a	3082	1/1	0.94	0.24	58,58,58,58	0
55	MG	1A	3761	1/1	0.94	0.61	43,43,43,43	0
55	MG	1A	3486	1/1	0.94	0.30	43,43,43,43	0
55	MG	1A	3094	1/1	0.94	0.48	34,34,34,34	0
55	MG	1A	3202	1/1	0.94	0.43	49,49,49,49	0
55	MG	2A	3408	1/1	0.94	0.15	48,48,48,48	0
55	MG	2D	301	1/1	0.94	0.58	49,49,49,49	0
55	MG	2f	8001	1/1	0.94	0.16	56,56,56,56	0
55	MG	1A	3663	1/1	0.94	0.22	68,68,68,68	0
55	MG	2A	3617	1/1	0.94	0.14	35,35,35,35	0
55	MG	2A	3619	1/1	0.94	0.11	57,57,57,57	0
55	MG	2A	3163	1/1	0.94	0.26	60,60,60,60	0
55	MG	2D	307	1/1	0.94	0.41	60,60,60,60	0
55	MG	1A	3562	1/1	0.94	0.23	52,52,52,52	0
55	MG	2o	3001	1/1	0.94	0.13	57,57,57,57	0
55	MG	1A	3043	1/1	0.94	0.33	13,13,13,13	0
55	MG	2E	304	1/1	0.94	0.15	71,71,71,71	0
55	MG	1A	3775	1/1	0.94	0.06	47,47,47,47	0
55	MG	2A	3168	1/1	0.94	0.27	72,72,72,72	0
55	MG	1A	3274	1/1	0.95	0.29	8,8,8,8	0
55	MG	1A	3008	1/1	0.95	0.26	48,48,48,48	0
55	MG	1A	3415	1/1	0.95	0.11	26,26,26,26	0
55	MG	1a	3202	1/1	0.95	0.07	53,53,53,53	0
55	MG	2A	3467	1/1	0.95	0.16	76,76,76,76	0
55	MG	2A	3096	1/1	0.95	0.34	48,48,48,48	0
55	MG	1A	3828	1/1	0.95	0.19	70,70,70,70	0
55	MG	1A	3362	1/1	0.95	0.29	42,42,42,42	0
55	MG	1A	3184	1/1	0.95	0.72	38,38,38,38	0
55	MG	2A	3100	1/1	0.95	0.33	61,61,61,61	0
55	MG	1A	3097	1/1	0.95	0.36	42,42,42,42	0
55	MG	2A	3676	1/1	0.95	0.36	76,76,76,76	0
55	MG	2A	3677	1/1	0.95	0.17	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3429	1/1	0.95	0.12	41,41,41,41	0
55	MG	2A	3679	1/1	0.95	0.05	71,71,71,71	0
55	MG	1A	3153	1/1	0.95	0.47	36,36,36,36	0
55	MG	1A	3916	1/1	0.95	0.87	49,49,49,49	0
55	MG	2A	3477	1/1	0.95	0.12	81,81,81,81	0
55	MG	2A	3261	1/1	0.95	0.29	52,52,52,52	0
55	MG	2A	3262	1/1	0.95	0.19	71,71,71,71	0
55	MG	1A	3917	1/1	0.95	0.41	38,38,38,38	0
55	MG	2A	3264	1/1	0.95	0.16	61,61,61,61	0
55	MG	2A	3265	1/1	0.95	0.40	69,69,69,69	0
55	MG	2A	3106	1/1	0.95	0.31	67,67,67,67	0
55	MG	2a	1606	1/1	0.95	0.45	57,57,57,57	0
55	MG	1X	8001	1/1	0.95	0.11	27,27,27,27	0
55	MG	2A	3108	1/1	0.95	0.10	65,65,65,65	0
55	MG	2A	3269	1/1	0.95	0.18	38,38,38,38	0
55	MG	1A	3373	1/1	0.95	0.33	53,53,53,53	0
55	MG	2A	3274	1/1	0.95	0.16	51,51,51,51	0
55	MG	1a	3080	1/1	0.95	0.17	67,67,67,67	0
55	MG	1A	3601	1/1	0.95	0.07	38,38,38,38	0
55	MG	1A	3025	1/1	0.95	0.31	32,32,32,32	0
55	MG	1A	3675	1/1	0.95	0.12	65,65,65,65	0
55	MG	10	104	1/1	0.95	0.10	73,73,73,73	0
55	MG	1A	3434	1/1	0.95	0.14	46,46,46,46	0
55	MG	2A	3285	1/1	0.95	0.08	46,46,46,46	0
55	MG	2A	3711	1/1	0.95	0.08	67,67,67,67	0
55	MG	1a	3093	1/1	0.95	0.06	68,68,68,68	0
55	MG	2A	3715	1/1	0.95	0.07	63,63,63,63	0
55	MG	2A	3503	1/1	0.95	0.24	58,58,58,58	0
55	MG	1A	3925	1/1	0.95	0.17	42,42,42,42	0
55	MG	2A	3718	1/1	0.95	0.09	78,78,78,78	0
55	MG	1A	3320	1/1	0.95	0.30	52,52,52,52	0
55	MG	1A	3927	1/1	0.95	0.30	34,34,34,34	0
55	MG	1A	3379	1/1	0.95	0.19	67,67,67,67	0
55	MG	2A	3126	1/1	0.95	0.30	62,62,62,62	0
55	MG	1e	3001	1/1	0.95	0.26	61,61,61,61	0
55	MG	1f	8001	1/1	0.95	0.21	61,61,61,61	0
55	MG	15	201	1/1	0.95	0.57	46,46,46,46	0
55	MG	1A	3099	1/1	0.95	0.29	62,62,62,62	0
55	MG	2a	1640	1/1	0.95	0.52	50,50,50,50	0
55	MG	2A	3304	1/1	0.95	0.23	41,41,41,41	0
55	MG	1h	3002	1/1	0.95	0.12	73,73,73,73	0
55	MG	2A	3314	1/1	0.95	0.16	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3733	1/1	0.95	0.13	65,65,65,65	0
55	MG	1a	3108	1/1	0.95	0.04	75,75,75,75	0
55	MG	1A	3680	1/1	0.95	0.08	53,53,53,53	0
55	MG	15	205	1/1	0.95	0.09	62,62,62,62	0
55	MG	1A	3754	1/1	0.95	0.11	71,71,71,71	0
55	MG	2A	3738	1/1	0.95	0.07	62,62,62,62	0
55	MG	2A	3137	1/1	0.95	0.40	58,58,58,58	0
55	MG	1A	3846	1/1	0.95	0.14	53,53,53,53	0
55	MG	1A	3681	1/1	0.95	0.24	57,57,57,57	0
55	MG	2A	3003	1/1	0.95	0.08	35,35,35,35	0
55	MG	2A	3530	1/1	0.95	0.13	71,71,71,71	0
55	MG	1A	3325	1/1	0.95	0.19	22,22,22,22	0
55	MG	2a	1656	1/1	0.95	0.06	78,78,78,78	0
55	MG	1A	3060	1/1	0.95	0.26	38,38,38,38	0
55	MG	2A	3143	1/1	0.95	0.20	59,59,59,59	0
55	MG	2A	3007	1/1	0.95	0.25	61,61,61,61	0
55	MG	1A	3610	1/1	0.95	0.10	68,68,68,68	0
55	MG	1A	3852	1/1	0.95	0.21	22,22,22,22	0
55	MG	1A	3447	1/1	0.95	0.18	24,24,24,24	0
55	MG	1A	3448	1/1	0.95	0.17	19,19,19,19	0
55	MG	2A	3012	1/1	0.95	0.18	42,42,42,42	0
55	MG	1A	3616	1/1	0.95	0.08	63,63,63,63	0
55	MG	2A	3014	1/1	0.95	0.74	58,58,58,58	0
55	MG	1A	3763	1/1	0.95	0.10	70,70,70,70	0
55	MG	1A	3691	1/1	0.95	0.09	42,42,42,42	0
55	MG	2a	1673	1/1	0.95	0.16	59,59,59,59	0
55	MG	2A	3345	1/1	0.95	0.07	78,78,78,78	0
55	MG	1a	3008	1/1	0.95	0.21	76,76,76,76	0
55	MG	1A	3858	1/1	0.95	0.12	60,60,60,60	0
55	MG	2A	3020	1/1	0.95	0.10	42,42,42,42	0
55	MG	2A	3351	1/1	0.95	0.06	69,69,69,69	0
55	MG	2a	1680	1/1	0.95	0.10	63,63,63,63	0
55	MG	1A	3449	1/1	0.95	0.10	41,41,41,41	0
55	MG	2A	3770	1/1	0.95	0.04	74,74,74,74	0
55	MG	2A	3022	1/1	0.95	0.14	72,72,72,72	0
55	MG	2A	3023	1/1	0.95	0.53	47,47,47,47	0
55	MG	1B	208	1/1	0.95	0.23	68,68,68,68	0
55	MG	1a	3138	1/1	0.95	0.15	66,66,66,66	0
55	MG	1B	209	1/1	0.95	0.23	59,59,59,59	0
55	MG	2A	3361	1/1	0.95	0.15	53,53,53,53	0
55	MG	2a	1692	1/1	0.95	0.23	82,82,82,82	0
55	MG	2A	3781	1/1	0.95	0.12	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3362	1/1	0.95	0.10	56,56,56,56	0
55	MG	1A	3767	1/1	0.95	0.13	52,52,52,52	0
55	MG	2A	3561	1/1	0.95	0.06	82,82,82,82	0
55	MG	1A	3768	1/1	0.95	0.08	58,58,58,58	0
55	MG	2a	1701	1/1	0.95	0.23	85,85,85,85	0
55	MG	2a	1702	1/1	0.95	0.10	72,72,72,72	0
55	MG	2a	1704	1/1	0.95	0.18	76,76,76,76	0
55	MG	2A	3365	1/1	0.95	0.09	81,81,81,81	0
55	MG	2A	3369	1/1	0.95	0.08	81,81,81,81	0
55	MG	2A	3565	1/1	0.95	0.49	70,70,70,70	0
55	MG	2A	3372	1/1	0.95	0.14	54,54,54,54	0
55	MG	1A	3385	1/1	0.95	0.07	69,69,69,69	0
55	MG	1A	3771	1/1	0.95	0.21	38,38,38,38	0
55	MG	2A	3570	1/1	0.95	0.29	54,54,54,54	0
55	MG	2A	3171	1/1	0.95	0.34	45,45,45,45	0
55	MG	2A	3377	1/1	0.95	0.15	54,54,54,54	0
55	MG	2a	1716	1/1	0.95	0.23	75,75,75,75	0
55	MG	1A	3386	1/1	0.95	0.26	49,49,49,49	0
55	MG	1A	3069	1/1	0.95	0.32	34,34,34,34	0
55	MG	1A	3009	1/1	0.95	0.29	32,32,32,32	0
55	MG	2A	3384	1/1	0.95	0.18	37,37,37,37	0
55	MG	2A	3580	1/1	0.95	0.11	71,71,71,71	0
55	MG	1A	3456	1/1	0.95	0.16	49,49,49,49	0
55	MG	2A	3386	1/1	0.95	0.15	63,63,63,63	0
55	MG	2A	3388	1/1	0.95	0.17	47,47,47,47	0
55	MG	1A	3780	1/1	0.95	0.54	34,34,34,34	0
55	MG	2A	3038	1/1	0.95	0.22	54,54,54,54	0
55	MG	1A	3117	1/1	0.95	0.09	61,61,61,61	0
55	MG	1A	3783	1/1	0.95	0.17	44,44,44,44	0
55	MG	1A	3703	1/1	0.95	0.10	42,42,42,42	0
55	MG	1A	3787	1/1	0.95	0.08	48,48,48,48	0
55	MG	1A	3788	1/1	0.95	0.14	28,28,28,28	0
55	MG	1A	3459	1/1	0.95	0.08	65,65,65,65	0
55	MG	2A	3047	1/1	0.95	0.37	45,45,45,45	0
55	MG	2A	3595	1/1	0.95	0.16	52,52,52,52	0
55	MG	1A	3342	1/1	0.95	0.06	29,29,29,29	0
55	MG	2A	3597	1/1	0.95	0.10	47,47,47,47	0
55	MG	1A	3461	1/1	0.95	0.11	27,27,27,27	0
55	MG	2A	3406	1/1	0.95	0.56	81,81,81,81	0
55	MG	1a	3160	1/1	0.95	0.29	67,67,67,67	0
55	MG	2A	3190	1/1	0.95	0.73	66,66,66,66	0
55	MG	2a	1742	1/1	0.95	0.08	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3463	1/1	0.95	0.33	60,60,60,60	0
55	MG	1A	3092	1/1	0.95	0.14	33,33,33,33	0
55	MG	1A	3574	1/1	0.95	0.41	49,49,49,49	0
55	MG	1A	3799	1/1	0.95	0.11	57,57,57,57	0
55	MG	2A	3836	1/1	0.95	0.56	61,61,61,61	0
55	MG	1A	3231	1/1	0.95	0.60	25,25,25,25	0
55	MG	1D	314	1/1	0.95	0.32	77,77,77,77	0
55	MG	1A	3713	1/1	0.95	0.14	75,75,75,75	0
55	MG	1A	3346	1/1	0.95	0.20	69,69,69,69	0
55	MG	2a	1754	1/1	0.95	0.67	78,78,78,78	0
55	MG	2A	3614	1/1	0.95	0.09	56,56,56,56	0
55	MG	1A	3520	1/1	0.95	0.12	33,33,33,33	0
55	MG	2a	1757	1/1	0.95	0.26	66,66,66,66	0
55	MG	2a	1758	1/1	0.95	0.08	74,74,74,74	0
55	MG	1A	3165	1/1	0.95	0.38	41,41,41,41	0
55	MG	2A	3423	1/1	0.95	0.36	51,51,51,51	0
55	MG	2B	3010	1/1	0.95	0.05	73,73,73,73	0
55	MG	2A	3618	1/1	0.95	0.31	68,68,68,68	0
55	MG	1A	3001	1/1	0.95	0.14	38,38,38,38	0
55	MG	1A	3891	1/1	0.95	0.11	84,84,84,84	0
55	MG	2A	3622	1/1	0.95	0.13	52,52,52,52	0
55	MG	1A	3306	1/1	0.95	0.12	43,43,43,43	0
55	MG	2A	3206	1/1	0.95	0.10	64,64,64,64	0
55	MG	1A	3352	1/1	0.95	0.11	34,34,34,34	0
55	MG	2A	3208	1/1	0.95	0.10	80,80,80,80	0
55	MG	2A	3629	1/1	0.95	0.06	73,73,73,73	0
55	MG	2A	3630	1/1	0.95	0.39	56,56,56,56	0
55	MG	1F	306	1/1	0.95	0.20	25,25,25,25	0
55	MG	2A	3067	1/1	0.95	0.42	61,61,61,61	0
55	MG	2D	305	1/1	0.95	0.10	73,73,73,73	0
55	MG	2A	3212	1/1	0.95	0.14	36,36,36,36	0
55	MG	2a	1781	1/1	0.95	0.16	51,51,51,51	0
55	MG	1A	3651	1/1	0.95	0.14	34,34,34,34	0
55	MG	2a	1784	1/1	0.95	0.05	87,87,87,87	0
55	MG	2D	309	1/1	0.95	0.13	57,57,57,57	0
55	MG	1A	3473	1/1	0.95	0.48	32,32,32,32	0
55	MG	2A	3438	1/1	0.95	0.25	66,66,66,66	0
55	MG	2E	303	1/1	0.95	0.18	52,52,52,52	0
55	MG	2A	3215	1/1	0.95	0.31	42,42,42,42	0
55	MG	2A	3217	1/1	0.95	0.10	57,57,57,57	0
55	MG	1A	3896	1/1	0.95	0.48	38,38,38,38	0
55	MG	1A	3271	1/1	0.95	0.34	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3007	1/1	0.95	0.12	38,38,38,38	0
55	MG	2F	306	1/1	0.95	0.39	47,47,47,47	0
55	MG	1G	3003	1/1	0.95	0.09	49,49,49,49	0
55	MG	1A	3309	1/1	0.95	0.14	37,37,37,37	0
55	MG	1a	3187	1/1	0.95	0.07	82,82,82,82	0
55	MG	1A	3901	1/1	0.95	0.47	35,35,35,35	0
55	MG	2A	3081	1/1	0.95	0.32	39,39,39,39	0
55	MG	1A	3822	1/1	0.95	0.10	54,54,54,54	0
55	MG	1a	3190	1/1	0.95	0.07	73,73,73,73	0
55	MG	1a	3061	1/1	0.95	0.26	66,66,66,66	0
55	MG	2A	3235	1/1	0.95	0.08	77,77,77,77	0
55	MG	1N	8002	1/1	0.95	0.21	61,61,61,61	0
56	ZN	1Y	501	1/1	0.95	0.12	61,61,61,61	0
55	MG	2A	3237	1/1	0.95	0.14	45,45,45,45	0
56	ZN	2Y	501	1/1	0.95	0.06	91,91,91,91	0
55	MG	1N	8003	1/1	0.95	0.17	61,61,61,61	0
55	MG	1A	3658	1/1	0.95	0.04	50,50,50,50	0
55	MG	1G	3001	1/1	0.96	0.07	74,74,74,74	0
55	MG	1A	3065	1/1	0.96	0.35	33,33,33,33	0
55	MG	1a	3083	1/1	0.96	0.23	66,66,66,66	0
55	MG	1A	3502	1/1	0.96	0.19	16,16,16,16	0
55	MG	1A	3438	1/1	0.96	0.19	61,61,61,61	0
55	MG	1a	3088	1/1	0.96	0.37	61,61,61,61	0
55	MG	1A	3439	1/1	0.96	0.15	51,51,51,51	0
55	MG	1A	3125	1/1	0.96	0.19	30,30,30,30	0
55	MG	2A	3633	1/1	0.96	0.11	80,80,80,80	0
55	MG	2A	3414	1/1	0.96	0.07	77,77,77,77	0
55	MG	2A	3016	1/1	0.96	0.46	50,50,50,50	0
55	MG	1a	3094	1/1	0.96	0.06	47,47,47,47	0
55	MG	1a	3095	1/1	0.96	0.31	63,63,63,63	0
55	MG	2A	3418	1/1	0.96	0.11	44,44,44,44	0
55	MG	1A	3360	1/1	0.96	0.19	25,25,25,25	0
55	MG	1N	8004	1/1	0.96	0.22	71,71,71,71	0
55	MG	1A	3301	1/1	0.96	0.21	12,12,12,12	0
55	MG	1A	3777	1/1	0.96	0.06	73,73,73,73	0
55	MG	1a	3103	1/1	0.96	0.13	77,77,77,77	0
55	MG	2A	3645	1/1	0.96	0.07	64,64,64,64	0
55	MG	1a	3105	1/1	0.96	0.11	54,54,54,54	0
55	MG	2V	203	1/1	0.96	0.15	73,73,73,73	0
55	MG	1Q	202	1/1	0.96	0.29	51,51,51,51	0
55	MG	2X	101	1/1	0.96	0.30	77,77,77,77	0
55	MG	1A	3778	1/1	0.96	0.12	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3126	1/1	0.96	0.25	23,23,23,23	0
55	MG	1A	3509	1/1	0.96	0.21	31,31,31,31	0
55	MG	1a	3110	1/1	0.96	0.16	54,54,54,54	0
55	MG	1a	3112	1/1	0.96	0.24	85,85,85,85	0
55	MG	2A	3031	1/1	0.96	0.15	64,64,64,64	0
55	MG	21	101	1/1	0.96	0.12	66,66,66,66	0
55	MG	2A	3654	1/1	0.96	0.05	34,34,34,34	0
55	MG	2A	3433	1/1	0.96	0.19	81,81,81,81	0
55	MG	1A	3066	1/1	0.96	0.28	39,39,39,39	0
55	MG	1A	3785	1/1	0.96	0.17	24,24,24,24	0
55	MG	2A	3659	1/1	0.96	0.07	73,73,73,73	0
55	MG	1A	3513	1/1	0.96	0.16	53,53,53,53	0
55	MG	1A	3589	1/1	0.96	0.10	28,28,28,28	0
55	MG	2A	3205	1/1	0.96	0.15	44,44,44,44	0
55	MG	2A	3036	1/1	0.96	0.52	38,38,38,38	0
55	MG	1A	3023	1/1	0.96	0.15	21,21,21,21	0
55	MG	2A	3442	1/1	0.96	0.09	62,62,62,62	0
55	MG	1V	201	1/1	0.96	0.10	67,67,67,67	0
55	MG	2A	3039	1/1	0.96	0.23	25,25,25,25	0
55	MG	2A	3210	1/1	0.96	0.15	44,44,44,44	0
55	MG	1A	3591	1/1	0.96	0.08	26,26,26,26	0
55	MG	1A	3684	1/1	0.96	0.23	59,59,59,59	0
55	MG	1A	3040	1/1	0.96	0.19	40,40,40,40	0
55	MG	2a	1611	1/1	0.96	0.36	76,76,76,76	0
55	MG	1a	3128	1/1	0.96	0.20	75,75,75,75	0
55	MG	1A	3210	1/1	0.96	0.52	42,42,42,42	0
55	MG	1A	3451	1/1	0.96	0.16	23,23,23,23	0
55	MG	1A	3189	1/1	0.96	0.11	69,69,69,69	0
55	MG	1A	3795	1/1	0.96	0.13	48,48,48,48	0
55	MG	1A	3797	1/1	0.96	0.13	50,50,50,50	0
55	MG	2A	3224	1/1	0.96	0.15	55,55,55,55	0
55	MG	1A	3377	1/1	0.96	0.14	47,47,47,47	0
55	MG	2A	3226	1/1	0.96	0.12	70,70,70,70	0
55	MG	1A	3266	1/1	0.96	0.19	34,34,34,34	0
55	MG	1A	3908	1/1	0.96	0.24	40,40,40,40	0
55	MG	2a	1623	1/1	0.96	0.65	60,60,60,60	0
55	MG	1a	3137	1/1	0.96	0.29	63,63,63,63	0
55	MG	2a	1625	1/1	0.96	0.28	49,49,49,49	0
55	MG	1A	3313	1/1	0.96	0.22	39,39,39,39	0
55	MG	2a	1627	1/1	0.96	0.17	54,54,54,54	0
55	MG	1A	3694	1/1	0.96	0.24	46,46,46,46	0
55	MG	2A	3692	1/1	0.96	0.06	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3314	1/1	0.96	0.09	53,53,53,53	0
55	MG	2a	1632	1/1	0.96	0.46	73,73,73,73	0
55	MG	1A	3212	1/1	0.96	0.45	39,39,39,39	0
55	MG	1A	3027	1/1	0.96	0.17	31,31,31,31	0
55	MG	2A	3697	1/1	0.96	0.05	53,53,53,53	0
55	MG	1A	3808	1/1	0.96	0.23	19,19,19,19	0
55	MG	1A	3149	1/1	0.96	0.18	49,49,49,49	0
55	MG	17	102	1/1	0.96	0.15	55,55,55,55	0
55	MG	2A	3703	1/1	0.96	0.25	91,91,91,91	0
55	MG	1A	3918	1/1	0.96	0.22	28,28,28,28	0
55	MG	2A	3241	1/1	0.96	0.33	44,44,44,44	0
55	MG	1A	3810	1/1	0.96	0.06	63,63,63,63	0
55	MG	2A	3064	1/1	0.96	0.61	54,54,54,54	0
55	MG	2A	3708	1/1	0.96	0.12	69,69,69,69	0
55	MG	1A	3811	1/1	0.96	0.11	35,35,35,35	0
55	MG	2A	3710	1/1	0.96	0.14	62,62,62,62	0
55	MG	2A	3246	1/1	0.96	0.03	71,71,71,71	0
55	MG	2A	3247	1/1	0.96	0.20	38,38,38,38	0
55	MG	2A	3714	1/1	0.96	0.11	52,52,52,52	0
55	MG	19	101	1/1	0.96	0.39	52,52,52,52	0
55	MG	1A	3462	1/1	0.96	0.58	33,33,33,33	0
55	MG	2A	3069	1/1	0.96	0.23	54,54,54,54	0
55	MG	1A	3702	1/1	0.96	0.19	31,31,31,31	0
55	MG	2A	3071	1/1	0.96	0.28	38,38,38,38	0
55	MG	1A	3272	1/1	0.96	0.20	23,23,23,23	0
55	MG	1A	3464	1/1	0.96	0.22	61,61,61,61	0
55	MG	2a	1658	1/1	0.96	0.14	58,58,58,58	0
55	MG	1A	3818	1/1	0.96	0.09	52,52,52,52	0
55	MG	2A	3491	1/1	0.96	0.13	49,49,49,49	0
55	MG	1A	3819	1/1	0.96	0.52	45,45,45,45	0
55	MG	1A	3242	1/1	0.96	0.65	46,46,46,46	0
55	MG	1A	3324	1/1	0.96	0.17	24,24,24,24	0
55	MG	2A	3497	1/1	0.96	0.13	39,39,39,39	0
55	MG	1A	3070	1/1	0.96	0.22	37,37,37,37	0
55	MG	2A	3079	1/1	0.96	0.31	60,60,60,60	0
55	MG	1A	3708	1/1	0.96	0.23	51,51,51,51	0
55	MG	1A	3533	1/1	0.96	0.17	41,41,41,41	0
55	MG	2A	3082	1/1	0.96	0.30	60,60,60,60	0
55	MG	1a	3011	1/1	0.96	0.15	74,74,74,74	0
55	MG	2A	3504	1/1	0.96	0.24	58,58,58,58	0
55	MG	1A	3614	1/1	0.96	0.03	50,50,50,50	0
55	MG	2A	3739	1/1	0.96	0.10	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3936	1/1	0.96	0.28	55,55,55,55	0
55	MG	2A	3507	1/1	0.96	0.57	62,62,62,62	0
55	MG	1a	3167	1/1	0.96	0.09	79,79,79,79	0
55	MG	1A	3327	1/1	0.96	0.10	43,43,43,43	0
55	MG	1A	3005	1/1	0.96	0.16	22,22,22,22	0
55	MG	1A	3939	1/1	0.96	0.62	39,39,39,39	0
55	MG	2a	1684	1/1	0.96	0.19	64,64,64,64	0
55	MG	1a	3171	1/1	0.96	0.11	54,54,54,54	0
55	MG	2A	3093	1/1	0.96	0.50	56,56,56,56	0
55	MG	2a	1687	1/1	0.96	0.30	58,58,58,58	0
55	MG	2A	3280	1/1	0.96	0.15	35,35,35,35	0
55	MG	2a	1689	1/1	0.96	0.16	63,63,63,63	0
55	MG	2A	3515	1/1	0.96	0.09	50,50,50,50	0
55	MG	1A	3829	1/1	0.96	0.34	67,67,67,67	0
55	MG	1A	3134	1/1	0.96	0.12	40,40,40,40	0
55	MG	1A	3619	1/1	0.96	0.20	44,44,44,44	0
55	MG	1A	3943	1/1	0.96	0.30	37,37,37,37	0
55	MG	1A	3059	1/1	0.96	0.20	58,58,58,58	0
55	MG	1a	3178	1/1	0.96	0.07	70,70,70,70	0
55	MG	1A	3336	1/1	0.96	0.17	19,19,19,19	0
55	MG	1a	3025	1/1	0.96	0.08	51,51,51,51	0
55	MG	1B	202	1/1	0.96	0.21	60,60,60,60	0
55	MG	2a	1703	1/1	0.96	0.09	60,60,60,60	0
55	MG	1A	3338	1/1	0.96	0.14	24,24,24,24	0
55	MG	2a	1705	1/1	0.96	0.20	75,75,75,75	0
55	MG	2A	3298	1/1	0.96	0.17	37,37,37,37	0
55	MG	1A	3544	1/1	0.96	0.27	30,30,30,30	0
55	MG	2A	3767	1/1	0.96	0.06	69,69,69,69	0
55	MG	2A	3301	1/1	0.96	0.08	85,85,85,85	0
55	MG	1A	3627	1/1	0.96	0.15	49,49,49,49	0
55	MG	1A	3475	1/1	0.96	0.08	25,25,25,25	0
55	MG	1A	3339	1/1	0.96	0.12	23,23,23,23	0
55	MG	1A	3630	1/1	0.96	0.10	60,60,60,60	0
55	MG	2A	3306	1/1	0.96	0.33	62,62,62,62	0
55	MG	2A	3312	1/1	0.96	0.14	62,62,62,62	0
55	MG	2A	3313	1/1	0.96	0.20	65,65,65,65	0
55	MG	2A	3778	1/1	0.96	0.24	51,51,51,51	0
55	MG	2A	3779	1/1	0.96	0.15	36,36,36,36	0
55	MG	1A	3631	1/1	0.96	0.26	81,81,81,81	0
55	MG	1A	3727	1/1	0.96	0.09	48,48,48,48	0
55	MG	1A	3403	1/1	0.96	0.14	48,48,48,48	0
55	MG	2A	3317	1/1	0.96	0.05	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3543	1/1	0.96	0.04	85,85,85,85	0
55	MG	1a	3192	1/1	0.96	0.15	64,64,64,64	0
55	MG	1B	214	1/1	0.96	0.11	50,50,50,50	0
55	MG	2A	3788	1/1	0.96	0.19	66,66,66,66	0
55	MG	1A	3155	1/1	0.96	0.74	60,60,60,60	0
55	MG	2A	3323	1/1	0.96	0.11	59,59,59,59	0
55	MG	1a	3195	1/1	0.96	0.14	68,68,68,68	0
55	MG	2A	3116	1/1	0.96	0.21	56,56,56,56	0
55	MG	1A	3279	1/1	0.96	0.12	55,55,55,55	0
55	MG	1B	218	1/1	0.96	0.08	49,49,49,49	0
55	MG	2A	3331	1/1	0.96	0.18	45,45,45,45	0
55	MG	1A	3343	1/1	0.96	0.26	54,54,54,54	0
55	MG	2A	3120	1/1	0.96	0.07	75,75,75,75	0
55	MG	2A	3121	1/1	0.96	0.23	46,46,46,46	0
55	MG	1A	3637	1/1	0.96	0.14	45,45,45,45	0
55	MG	2a	1739	1/1	0.96	0.13	81,81,81,81	0
55	MG	1A	3407	1/1	0.96	0.12	58,58,58,58	0
55	MG	1B	223	1/1	0.96	0.32	61,61,61,61	0
55	MG	2A	3560	1/1	0.96	0.08	66,66,66,66	0
55	MG	2a	1743	1/1	0.96	0.32	65,65,65,65	0
55	MG	1a	3203	1/1	0.96	0.16	64,64,64,64	0
55	MG	2A	3339	1/1	0.96	0.17	37,37,37,37	0
55	MG	1a	3045	1/1	0.96	0.33	63,63,63,63	0
55	MG	1A	3249	1/1	0.96	0.23	10,10,10,10	0
55	MG	1A	3640	1/1	0.96	0.44	37,37,37,37	0
55	MG	1a	3209	1/1	0.96	0.14	56,56,56,56	0
55	MG	1A	3641	1/1	0.96	0.13	41,41,41,41	0
55	MG	2A	3817	1/1	0.96	1.18	56,56,56,56	0
55	MG	1a	3211	1/1	0.96	0.28	65,65,65,65	0
55	MG	2A	3346	1/1	0.96	0.05	77,77,77,77	0
55	MG	2A	3820	1/1	0.96	0.56	51,51,51,51	0
55	MG	1a	3212	1/1	0.96	0.05	56,56,56,56	0
55	MG	1A	3197	1/1	0.96	0.41	31,31,31,31	0
55	MG	2A	3349	1/1	0.96	0.14	80,80,80,80	0
55	MG	2A	3575	1/1	0.96	0.16	52,52,52,52	0
55	MG	1A	3411	1/1	0.96	0.04	48,48,48,48	0
55	MG	2a	1761	1/1	0.96	0.15	68,68,68,68	0
55	MG	2A	3826	1/1	0.96	1.08	56,56,56,56	0
55	MG	1A	3743	1/1	0.96	0.04	58,58,58,58	0
55	MG	2A	3828	1/1	0.96	0.69	65,65,65,65	0
55	MG	2A	3352	1/1	0.96	0.20	29,29,29,29	0
55	MG	2a	1766	1/1	0.96	0.25	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3555	1/1	0.96	0.12	28,28,28,28	0
55	MG	1A	3646	1/1	0.96	0.16	49,49,49,49	0
55	MG	2a	1770	1/1	0.96	0.06	61,61,61,61	0
55	MG	1A	3284	1/1	0.96	0.11	64,64,64,64	0
55	MG	1A	3559	1/1	0.96	0.18	56,56,56,56	0
55	MG	1a	3221	1/1	0.96	0.44	79,79,79,79	0
55	MG	1A	3107	1/1	0.96	0.23	25,25,25,25	0
55	MG	2A	3145	1/1	0.96	0.13	75,75,75,75	0
55	MG	1A	3158	1/1	0.96	0.13	31,31,31,31	0
55	MG	1D	311	1/1	0.96	0.09	61,61,61,61	0
55	MG	1a	3059	1/1	0.96	0.16	78,78,78,78	0
55	MG	1A	3349	1/1	0.96	0.38	62,62,62,62	0
55	MG	2A	3592	1/1	0.96	0.10	80,80,80,80	0
55	MG	2B	3006	1/1	0.96	0.44	80,80,80,80	0
55	MG	2a	1783	1/1	0.96	0.07	59,59,59,59	0
55	MG	1b	3001	1/1	0.96	0.07	71,71,71,71	0
55	MG	1A	3753	1/1	0.96	0.05	50,50,50,50	0
55	MG	1a	3062	1/1	0.96	0.62	81,81,81,81	0
55	MG	1A	3563	1/1	0.96	0.15	29,29,29,29	0
55	MG	1A	3564	1/1	0.96	0.13	28,28,28,28	0
55	MG	2A	3156	1/1	0.96	0.27	58,58,58,58	0
55	MG	1E	302	1/1	0.96	0.19	26,26,26,26	0
55	MG	2A	3600	1/1	0.96	0.38	53,53,53,53	0
55	MG	2a	1793	1/1	0.96	0.14	56,56,56,56	0
55	MG	2a	1794	1/1	0.96	0.06	74,74,74,74	0
55	MG	2a	1795	1/1	0.96	0.37	80,80,80,80	0
55	MG	2a	1796	1/1	0.96	0.12	58,58,58,58	0
55	MG	1A	3428	1/1	0.96	0.14	18,18,18,18	0
55	MG	1A	3867	1/1	0.96	0.34	45,45,45,45	0
55	MG	1A	3868	1/1	0.96	0.12	27,27,27,27	0
55	MG	2e	201	1/1	0.96	0.15	71,71,71,71	0
55	MG	1A	3656	1/1	0.96	0.11	57,57,57,57	0
55	MG	1A	3108	1/1	0.96	0.21	32,32,32,32	0
55	MG	2A	3387	1/1	0.96	0.08	58,58,58,58	0
55	MG	1A	3494	1/1	0.96	0.09	48,48,48,48	0
55	MG	1A	3082	1/1	0.96	0.76	47,47,47,47	0
55	MG	2A	3392	1/1	0.96	0.13	55,55,55,55	0
55	MG	1A	3291	1/1	0.96	0.10	72,72,72,72	0
55	MG	2A	3394	1/1	0.96	0.15	49,49,49,49	0
55	MG	1A	3762	1/1	0.96	0.17	19,19,19,19	0
55	MG	1a	3075	1/1	0.96	0.23	57,57,57,57	0
55	MG	1A	3096	1/1	0.96	0.35	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3181	1/1	0.96	0.42	43,43,43,43	0
56	ZN	1n	501	1/1	0.96	0.13	85,85,85,85	0
55	MG	1A	3573	1/1	0.96	0.19	21,21,21,21	0
55	MG	1A	3435	1/1	0.96	0.09	44,44,44,44	0
56	ZN	2n	501	1/1	0.96	0.06	94,94,94,94	0
55	MG	1F	312	1/1	0.96	0.11	47,47,47,47	0
55	MG	1A	3484	1/1	0.97	0.20	69,69,69,69	0
55	MG	2A	3353	1/1	0.97	0.06	70,70,70,70	0
55	MG	2A	3806	1/1	0.97	0.26	47,47,47,47	0
55	MG	2A	3807	1/1	0.97	0.43	57,57,57,57	0
55	MG	2A	3218	1/1	0.97	0.34	23,23,23,23	0
55	MG	1A	3230	1/1	0.97	0.67	35,35,35,35	0
55	MG	2A	3220	1/1	0.97	0.31	49,49,49,49	0
55	MG	1A	3157	1/1	0.97	0.20	33,33,33,33	0
55	MG	1A	3715	1/1	0.97	0.06	51,51,51,51	0
55	MG	1A	3716	1/1	0.97	0.12	31,31,31,31	0
55	MG	1A	3539	1/1	0.97	0.52	35,35,35,35	0
55	MG	1A	3389	1/1	0.97	0.18	21,21,21,21	0
55	MG	1A	3350	1/1	0.97	0.13	26,26,26,26	0
55	MG	2a	1664	1/1	0.97	0.34	68,68,68,68	0
55	MG	1A	3321	1/1	0.97	0.25	49,49,49,49	0
55	MG	1A	3597	1/1	0.97	0.05	49,49,49,49	0
55	MG	2A	3366	1/1	0.97	0.20	35,35,35,35	0
55	MG	2A	3230	1/1	0.97	0.18	44,44,44,44	0
55	MG	2a	1669	1/1	0.97	0.07	49,49,49,49	0
55	MG	2a	1670	1/1	0.97	0.10	49,49,49,49	0
55	MG	1A	3491	1/1	0.97	0.15	42,42,42,42	0
55	MG	1A	3075	1/1	0.97	0.47	33,33,33,33	0
55	MG	2A	3122	1/1	0.97	0.28	46,46,46,46	0
55	MG	2a	1674	1/1	0.97	0.19	71,71,71,71	0
55	MG	2A	3517	1/1	0.97	0.13	80,80,80,80	0
55	MG	2A	3123	1/1	0.97	0.22	52,52,52,52	0
55	MG	1A	3446	1/1	0.97	0.16	24,24,24,24	0
55	MG	1B	205	1/1	0.97	0.10	54,54,54,54	0
55	MG	1A	3798	1/1	0.97	0.14	46,46,46,46	0
55	MG	2A	3667	1/1	0.97	0.15	64,64,64,64	0
55	MG	1A	3323	1/1	0.97	0.07	29,29,29,29	0
55	MG	2A	3670	1/1	0.97	0.04	76,76,76,76	0
55	MG	2A	3381	1/1	0.97	0.11	66,66,66,66	0
55	MG	2A	3382	1/1	0.97	0.21	61,61,61,61	0
55	MG	2A	3383	1/1	0.97	0.14	66,66,66,66	0
55	MG	11	101	1/1	0.97	0.07	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3527	1/1	0.97	0.20	37,37,37,37	0
55	MG	1A	3020	1/1	0.97	0.42	38,38,38,38	0
55	MG	1A	3664	1/1	0.97	0.25	48,48,48,48	0
55	MG	1A	3356	1/1	0.97	0.14	23,23,23,23	0
55	MG	2B	3004	1/1	0.97	0.12	78,78,78,78	0
55	MG	1A	3666	1/1	0.97	0.23	53,53,53,53	0
55	MG	2a	1693	1/1	0.97	0.33	60,60,60,60	0
55	MG	2A	3389	1/1	0.97	0.18	51,51,51,51	0
55	MG	1B	212	1/1	0.97	0.18	56,56,56,56	0
55	MG	1A	3604	1/1	0.97	0.05	59,59,59,59	0
55	MG	2A	3248	1/1	0.97	0.07	28,28,28,28	0
55	MG	2a	1698	1/1	0.97	0.65	61,61,61,61	0
55	MG	1A	3398	1/1	0.97	0.24	66,66,66,66	0
55	MG	1A	3300	1/1	0.97	0.11	43,43,43,43	0
55	MG	1A	3452	1/1	0.97	0.07	55,55,55,55	0
55	MG	2A	3688	1/1	0.97	0.17	73,73,73,73	0
55	MG	1A	3261	1/1	0.97	0.19	17,17,17,17	0
55	MG	1A	3304	1/1	0.97	0.12	14,14,14,14	0
55	MG	1A	3738	1/1	0.97	0.17	23,23,23,23	0
55	MG	1B	221	1/1	0.97	0.35	79,79,79,79	0
55	MG	1a	3085	1/1	0.97	0.33	66,66,66,66	0
55	MG	1a	3086	1/1	0.97	0.45	64,64,64,64	0
55	MG	2A	3259	1/1	0.97	0.12	89,89,89,89	0
55	MG	2A	3044	1/1	0.97	0.38	38,38,38,38	0
55	MG	2A	3698	1/1	0.97	0.17	40,40,40,40	0
55	MG	2A	3699	1/1	0.97	0.15	37,37,37,37	0
55	MG	1A	3028	1/1	0.97	0.29	37,37,37,37	0
55	MG	2a	1715	1/1	0.97	0.17	81,81,81,81	0
55	MG	1a	3191	1/1	0.97	0.12	49,49,49,49	0
55	MG	2D	308	1/1	0.97	0.25	28,28,28,28	0
55	MG	1A	3815	1/1	0.97	0.16	25,25,25,25	0
55	MG	1A	3331	1/1	0.97	0.19	23,23,23,23	0
55	MG	1A	3365	1/1	0.97	0.22	30,30,30,30	0
55	MG	2A	3413	1/1	0.97	0.13	70,70,70,70	0
55	MG	1A	3368	1/1	0.97	0.11	47,47,47,47	0
55	MG	1A	3121	1/1	0.97	0.43	31,31,31,31	0
55	MG	1A	3370	1/1	0.97	0.21	26,26,26,26	0
55	MG	1a	3198	1/1	0.97	0.08	57,57,57,57	0
55	MG	2F	304	1/1	0.97	0.34	62,62,62,62	0
55	MG	1A	3223	1/1	0.97	0.08	72,72,72,72	0
55	MG	2A	3272	1/1	0.97	0.07	60,60,60,60	0
55	MG	1A	3620	1/1	0.97	0.09	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1D	305	1/1	0.97	0.35	42,42,42,42	0
55	MG	1A	3748	1/1	0.97	0.07	39,39,39,39	0
55	MG	1A	3510	1/1	0.97	0.40	44,44,44,44	0
55	MG	1A	3897	1/1	0.97	0.22	11,11,11,11	0
55	MG	1A	3337	1/1	0.97	0.18	18,18,18,18	0
55	MG	2A	3566	1/1	0.97	0.34	55,55,55,55	0
55	MG	1a	3206	1/1	0.97	0.04	74,74,74,74	0
55	MG	2A	3282	1/1	0.97	0.12	42,42,42,42	0
55	MG	2A	3164	1/1	0.97	0.29	41,41,41,41	0
55	MG	2A	3429	1/1	0.97	0.20	76,76,76,76	0
55	MG	1A	3224	1/1	0.97	0.14	35,35,35,35	0
55	MG	1A	3827	1/1	0.97	0.09	69,69,69,69	0
55	MG	2A	3726	1/1	0.97	0.11	38,38,38,38	0
55	MG	2R	8002	1/1	0.97	0.25	45,45,45,45	0
55	MG	2A	3290	1/1	0.97	0.22	71,71,71,71	0
55	MG	2A	3728	1/1	0.97	0.12	46,46,46,46	0
55	MG	1A	3413	1/1	0.97	0.09	28,28,28,28	0
55	MG	2V	201	1/1	0.97	0.72	54,54,54,54	0
55	MG	2A	3730	1/1	0.97	0.14	51,51,51,51	0
55	MG	1A	3686	1/1	0.97	0.29	55,55,55,55	0
55	MG	1A	3625	1/1	0.97	0.45	44,44,44,44	0
55	MG	2A	3578	1/1	0.97	0.09	61,61,61,61	0
55	MG	2A	3294	1/1	0.97	0.14	45,45,45,45	0
55	MG	1A	3466	1/1	0.97	0.11	53,53,53,53	0
55	MG	2A	3068	1/1	0.97	0.11	65,65,65,65	0
55	MG	1A	3414	1/1	0.97	0.15	31,31,31,31	0
55	MG	1a	3023	1/1	0.97	0.48	53,53,53,53	0
55	MG	1A	3283	1/1	0.97	0.23	40,40,40,40	0
55	MG	1A	3416	1/1	0.97	0.20	31,31,31,31	0
55	MG	1A	3417	1/1	0.97	0.16	37,37,37,37	0
55	MG	1a	3121	1/1	0.97	0.71	72,72,72,72	0
55	MG	1A	3187	1/1	0.97	0.56	35,35,35,35	0
55	MG	2A	3745	1/1	0.97	0.10	65,65,65,65	0
55	MG	1A	3910	1/1	0.97	0.38	36,36,36,36	0
55	MG	1A	3422	1/1	0.97	0.07	68,68,68,68	0
55	MG	2A	3307	1/1	0.97	0.16	63,63,63,63	0
55	MG	2A	3308	1/1	0.97	0.15	58,58,58,58	0
55	MG	2a	1768	1/1	0.97	0.21	74,74,74,74	0
55	MG	2A	3182	1/1	0.97	0.09	80,80,80,80	0
55	MG	1A	3696	1/1	0.97	0.16	25,25,25,25	0
55	MG	1A	3376	1/1	0.97	0.13	13,13,13,13	0
55	MG	1A	3765	1/1	0.97	0.05	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3635	1/1	0.97	0.08	29,29,29,29	0
55	MG	1A	3699	1/1	0.97	0.15	27,27,27,27	0
55	MG	1A	3102	1/1	0.97	0.34	34,34,34,34	0
55	MG	2A	3319	1/1	0.97	0.20	30,30,30,30	0
55	MG	2A	3084	1/1	0.97	0.30	49,49,49,49	0
55	MG	2a	1778	1/1	0.97	0.09	64,64,64,64	0
55	MG	2A	3761	1/1	0.97	0.17	38,38,38,38	0
55	MG	2A	3321	1/1	0.97	0.04	65,65,65,65	0
55	MG	1A	3844	1/1	0.97	0.09	25,25,25,25	0
55	MG	1a	3037	1/1	0.97	0.16	70,70,70,70	0
55	MG	2A	3087	1/1	0.97	0.17	61,61,61,61	0
55	MG	1A	3378	1/1	0.97	0.16	47,47,47,47	0
55	MG	1A	3269	1/1	0.97	0.09	26,26,26,26	0
55	MG	1A	3380	1/1	0.97	0.14	49,49,49,49	0
55	MG	2A	3330	1/1	0.97	0.13	45,45,45,45	0
55	MG	1A	3923	1/1	0.97	0.14	17,17,17,17	0
55	MG	1A	3581	1/1	0.97	0.22	39,39,39,39	0
55	MG	1a	3142	1/1	0.97	0.15	86,86,86,86	0
55	MG	1k	201	1/1	0.97	0.23	50,50,50,50	0
55	MG	1A	3381	1/1	0.97	0.17	23,23,23,23	0
55	MG	2A	3775	1/1	0.97	0.12	63,63,63,63	0
55	MG	1A	3850	1/1	0.97	0.12	23,23,23,23	0
55	MG	2A	3620	1/1	0.97	0.12	40,40,40,40	0
55	MG	2a	1797	1/1	0.97	0.09	75,75,75,75	0
55	MG	1A	3003	1/1	0.97	0.10	20,20,20,20	0
55	MG	1A	3776	1/1	0.97	0.06	43,43,43,43	0
55	MG	2A	3204	1/1	0.97	0.71	58,58,58,58	0
55	MG	2A	3482	1/1	0.97	0.66	56,56,56,56	0
55	MG	1a	3147	1/1	0.97	0.13	73,73,73,73	0
55	MG	2A	3784	1/1	0.97	0.16	64,64,64,64	0
55	MG	1A	3015	1/1	0.97	0.29	30,30,30,30	0
55	MG	2A	3628	1/1	0.97	0.22	57,57,57,57	0
55	MG	1A	3229	1/1	0.97	0.15	41,41,41,41	0
55	MG	1Q	201	1/1	0.97	0.12	51,51,51,51	0
55	MG	1A	3779	1/1	0.97	0.04	57,57,57,57	0
55	MG	2A	3006	1/1	0.97	0.13	40,40,40,40	0
55	MG	1A	3318	1/1	0.97	0.14	70,70,70,70	0
55	MG	1A	3933	1/1	0.97	0.15	28,28,28,28	0
55	MG	1A	3437	1/1	0.97	0.09	66,66,66,66	0
55	MG	1A	3935	1/1	0.97	0.14	27,27,27,27	0
55	MG	2A	3494	1/1	0.97	0.09	59,59,59,59	0
55	MG	2A	3495	1/1	0.97	0.16	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3639	1/1	0.97	0.19	79,79,79,79	0
56	ZN	25	103	1/1	0.97	0.08	64,64,64,64	0
55	MG	1a	3156	1/1	0.97	0.14	70,70,70,70	0
55	MG	2A	3216	1/1	0.97	0.14	37,37,37,37	0
55	MG	1a	3100	1/1	0.98	0.38	62,62,62,62	0
55	MG	1A	3731	1/1	0.98	0.09	25,25,25,25	0
55	MG	2A	3758	1/1	0.98	0.06	78,78,78,78	0
55	MG	1A	3796	1/1	0.98	0.08	33,33,33,33	0
55	MG	2A	3760	1/1	0.98	0.07	42,42,42,42	0
55	MG	1A	3303	1/1	0.98	0.20	16,16,16,16	0
55	MG	1a	3104	1/1	0.98	0.24	80,80,80,80	0
55	MG	1A	3618	1/1	0.98	0.07	51,51,51,51	0
55	MG	2a	1700	1/1	0.98	0.15	68,68,68,68	0
55	MG	1A	3154	1/1	0.98	0.39	31,31,31,31	0
55	MG	2A	3311	1/1	0.98	0.12	48,48,48,48	0
55	MG	1G	3002	1/1	0.98	0.09	67,67,67,67	0
55	MG	1A	3305	1/1	0.98	0.06	68,68,68,68	0
55	MG	1A	3801	1/1	0.98	0.16	32,32,32,32	0
55	MG	1A	3736	1/1	0.98	0.09	20,20,20,20	0
55	MG	1A	3569	1/1	0.98	0.45	48,48,48,48	0
55	MG	1A	3445	1/1	0.98	0.21	24,24,24,24	0
55	MG	1A	3129	1/1	0.98	0.26	33,33,33,33	0
55	MG	1A	3871	1/1	0.98	0.12	16,16,16,16	0
55	MG	1A	3525	1/1	0.98	0.13	27,27,27,27	0
55	MG	1A	3807	1/1	0.98	0.07	17,17,17,17	0
55	MG	2A	3776	1/1	0.98	0.07	44,44,44,44	0
55	MG	1a	3118	1/1	0.98	0.06	68,68,68,68	0
55	MG	2A	3222	1/1	0.98	0.16	56,56,56,56	0
55	MG	1A	3288	1/1	0.98	0.09	62,62,62,62	0
55	MG	1A	3626	1/1	0.98	0.06	42,42,42,42	0
55	MG	1a	3207	1/1	0.98	0.17	77,77,77,77	0
55	MG	2A	3663	1/1	0.98	0.12	53,53,53,53	0
55	MG	2A	3328	1/1	0.98	0.19	63,63,63,63	0
55	MG	1A	3326	1/1	0.98	0.11	28,28,28,28	0
55	MG	1a	3122	1/1	0.98	0.28	67,67,67,67	0
55	MG	1a	3123	1/1	0.98	0.23	79,79,79,79	0
55	MG	2A	3551	1/1	0.98	0.10	62,62,62,62	0
55	MG	1A	3487	1/1	0.98	0.10	32,32,32,32	0
55	MG	1a	3125	1/1	0.98	0.34	78,78,78,78	0
55	MG	2A	3790	1/1	0.98	0.12	39,39,39,39	0
55	MG	1B	201	1/1	0.98	0.70	48,48,48,48	0
55	MG	1A	3141	1/1	0.98	0.54	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	2A	3793	1/1	0.98	0.21	53,53,53,53	0
55	MG	1A	3879	1/1	0.98	0.11	47,47,47,47	0
55	MG	2a	1605	1/1	0.98	0.09	53,53,53,53	0
55	MG	1A	3813	1/1	0.98	0.12	22,22,22,22	0
55	MG	2A	3796	1/1	0.98	0.15	78,78,78,78	0
55	MG	1A	3410	1/1	0.98	0.18	8,8,8,8	0
55	MG	1A	3687	1/1	0.98	0.15	25,25,25,25	0
55	MG	1A	3086	1/1	0.98	0.10	55,55,55,55	0
55	MG	2A	3449	1/1	0.98	0.18	34,34,34,34	0
55	MG	2A	3238	1/1	0.98	0.17	46,46,46,46	0
55	MG	1A	3412	1/1	0.98	0.21	22,22,22,22	0
55	MG	1A	3751	1/1	0.98	0.08	24,24,24,24	0
55	MG	1A	3106	1/1	0.98	0.32	34,34,34,34	0
55	MG	1A	3354	1/1	0.98	0.14	26,26,26,26	0
55	MG	1A	3535	1/1	0.98	0.28	38,38,38,38	0
55	MG	2a	1745	1/1	0.98	0.04	77,77,77,77	0
55	MG	1A	3175	1/1	0.98	0.17	47,47,47,47	0
55	MG	2A	3459	1/1	0.98	0.06	64,64,64,64	0
55	MG	2A	3245	1/1	0.98	0.30	35,35,35,35	0
55	MG	1A	3495	1/1	0.98	0.23	66,66,66,66	0
55	MG	1A	3538	1/1	0.98	0.18	22,22,22,22	0
55	MG	1A	3332	1/1	0.98	0.19	23,23,23,23	0
55	MG	1A	3293	1/1	0.98	0.14	19,19,19,19	0
55	MG	1A	3418	1/1	0.98	0.12	34,34,34,34	0
55	MG	1A	3542	1/1	0.98	0.16	37,37,37,37	0
55	MG	2A	3696	1/1	0.98	0.05	61,61,61,61	0
55	MG	1A	3643	1/1	0.98	0.14	22,22,22,22	0
55	MG	1A	3419	1/1	0.98	0.17	28,28,28,28	0
55	MG	2A	3357	1/1	0.98	0.11	53,53,53,53	0
55	MG	13	101	1/1	0.98	0.30	42,42,42,42	0
55	MG	1A	3334	1/1	0.98	0.16	27,27,27,27	0
55	MG	1A	3421	1/1	0.98	0.16	23,23,23,23	0
55	MG	1A	3268	1/1	0.98	0.16	22,22,22,22	0
55	MG	1A	3423	1/1	0.98	0.18	23,23,23,23	0
55	MG	1A	3295	1/1	0.98	0.19	11,11,11,11	0
55	MG	1A	3769	1/1	0.98	0.16	31,31,31,31	0
55	MG	2a	1639	1/1	0.98	0.15	74,74,74,74	0
55	MG	1A	3361	1/1	0.98	0.10	28,28,28,28	0
55	MG	1A	3391	1/1	0.98	0.12	62,62,62,62	0
55	MG	2A	3367	1/1	0.98	0.09	46,46,46,46	0
55	MG	1A	3248	1/1	0.98	0.12	21,21,21,21	0
55	MG	2A	3371	1/1	0.98	0.18	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3363	1/1	0.98	0.15	39,39,39,39	0
55	MG	2A	3713	1/1	0.98	0.04	79,79,79,79	0
55	MG	2A	3176	1/1	0.98	0.61	43,43,43,43	0
55	MG	1A	3654	1/1	0.98	0.15	40,40,40,40	0
55	MG	1A	3364	1/1	0.98	0.12	26,26,26,26	0
55	MG	2B	3001	1/1	0.98	0.21	64,64,64,64	0
55	MG	1A	3137	1/1	0.98	0.22	43,43,43,43	0
55	MG	2A	3270	1/1	0.98	0.10	45,45,45,45	0
55	MG	1A	3911	1/1	0.98	0.21	33,33,33,33	0
55	MG	2A	3490	1/1	0.98	0.11	56,56,56,56	0
55	MG	1A	3511	1/1	0.98	0.12	25,25,25,25	0
55	MG	2A	3273	1/1	0.98	0.13	44,44,44,44	0
55	MG	1A	3556	1/1	0.98	0.13	32,32,32,32	0
55	MG	2A	3275	1/1	0.98	0.25	35,35,35,35	0
55	MG	1A	3557	1/1	0.98	0.23	29,29,29,29	0
55	MG	2a	1787	1/1	0.98	0.05	78,78,78,78	0
55	MG	2A	3607	1/1	0.98	0.06	74,74,74,74	0
55	MG	1A	3660	1/1	0.98	0.12	35,35,35,35	0
55	MG	1A	3366	1/1	0.98	0.25	31,31,31,31	0
55	MG	1A	3662	1/1	0.98	0.09	22,22,22,22	0
55	MG	1A	3397	1/1	0.98	0.26	17,17,17,17	0
55	MG	1A	3340	1/1	0.98	0.11	25,25,25,25	0
55	MG	1E	305	1/1	0.98	0.17	57,57,57,57	0
55	MG	2A	3391	1/1	0.98	0.22	38,38,38,38	0
55	MG	1A	3317	1/1	0.98	0.28	38,38,38,38	0
55	MG	1A	3611	1/1	0.98	0.05	81,81,81,81	0
55	MG	2A	3286	1/1	0.98	0.07	37,37,37,37	0
55	MG	2d	502	1/1	0.98	0.10	70,70,70,70	0
55	MG	1a	3015	1/1	0.98	0.29	71,71,71,71	0
55	MG	2A	3289	1/1	0.98	0.17	40,40,40,40	0
55	MG	1a	3089	1/1	0.98	0.09	52,52,52,52	0
55	MG	1a	3090	1/1	0.98	0.07	39,39,39,39	0
55	MG	2A	3741	1/1	0.98	0.05	70,70,70,70	0
55	MG	2A	3399	1/1	0.98	0.18	51,51,51,51	0
55	MG	1a	3091	1/1	0.98	0.11	40,40,40,40	0
55	MG	2A	3401	1/1	0.98	0.14	40,40,40,40	0
55	MG	2E	302	1/1	0.98	0.15	39,39,39,39	0
55	MG	1A	3091	1/1	0.98	0.32	17,17,17,17	0
55	MG	1A	3613	1/1	0.98	0.14	23,23,23,23	0
55	MG	1A	3083	1/1	0.98	0.06	50,50,50,50	0
55	MG	2A	3516	1/1	0.98	0.10	59,59,59,59	0
55	MG	1A	3440	1/1	0.98	0.10	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3302	1/1	0.98	0.12	51,51,51,51	0
56	ZN	16	101	1/1	0.98	0.12	62,62,62,62	0
56	ZN	19	102	1/1	0.98	0.13	68,68,68,68	0
55	MG	1A	3672	1/1	0.98	0.18	35,35,35,35	0
55	MG	1a	3098	1/1	0.98	0.24	59,59,59,59	0
55	MG	2A	3300	1/1	0.98	0.14	42,42,42,42	0
55	MG	2F	308	1/1	0.98	0.38	57,57,57,57	0
56	ZN	29	501	1/1	0.98	0.10	77,77,77,77	0
55	MG	2A	3410	1/1	0.98	0.11	59,59,59,59	0
55	MG	1a	3099	1/1	0.98	0.17	64,64,64,64	0
55	MG	1A	3582	1/1	0.99	0.11	40,40,40,40	0
55	MG	1a	3126	1/1	0.99	0.18	74,74,74,74	0
55	MG	1A	3784	1/1	0.99	0.15	32,32,32,32	0
55	MG	2A	3435	1/1	0.99	0.06	71,71,71,71	0
55	MG	1A	3298	1/1	0.99	0.10	49,49,49,49	0
55	MG	1A	3282	1/1	0.99	0.15	50,50,50,50	0
55	MG	1A	3585	1/1	0.99	0.10	49,49,49,49	0
55	MG	1a	3177	1/1	0.99	0.06	75,75,75,75	0
55	MG	2A	3135	1/1	0.99	0.21	71,71,71,71	0
55	MG	2Q	205	1/1	0.99	0.12	57,57,57,57	0
55	MG	2A	3368	1/1	0.99	0.13	63,63,63,63	0
55	MG	1A	3458	1/1	0.99	0.16	20,20,20,20	0
55	MG	2a	1628	1/1	0.99	0.22	80,80,80,80	0
55	MG	2A	3370	1/1	0.99	0.18	36,36,36,36	0
55	MG	1A	3432	1/1	0.99	0.18	14,14,14,14	0
55	MG	1A	3330	1/1	0.99	0.13	31,31,31,31	0
55	MG	1a	3111	1/1	0.99	0.15	55,55,55,55	0
55	MG	2A	3609	1/1	0.99	0.11	36,36,36,36	0
55	MG	1A	3286	1/1	0.99	0.17	25,25,25,25	0
55	MG	2A	3800	1/1	0.99	0.27	27,27,27,27	0
55	MG	2A	3656	1/1	0.99	0.11	45,45,45,45	0
55	MG	2A	3375	1/1	0.99	0.17	31,31,31,31	0
55	MG	1A	3024	1/1	0.99	0.30	34,34,34,34	0
55	MG	2A	3613	1/1	0.99	0.10	57,57,57,57	0
55	MG	2A	3450	1/1	0.99	0.33	62,62,62,62	0
55	MG	2A	3571	1/1	0.99	0.13	47,47,47,47	0
55	MG	20	104	1/1	0.99	0.07	68,68,68,68	0
55	MG	2A	3451	1/1	0.99	0.07	55,55,55,55	0
55	MG	1A	3296	1/1	0.99	0.20	31,31,31,31	0
55	MG	2A	3309	1/1	0.99	0.17	44,44,44,44	0
55	MG	2A	3310	1/1	0.99	0.21	46,46,46,46	0
55	MG	2A	3251	1/1	0.99	0.17	52,52,52,52	0

Continued on next page...

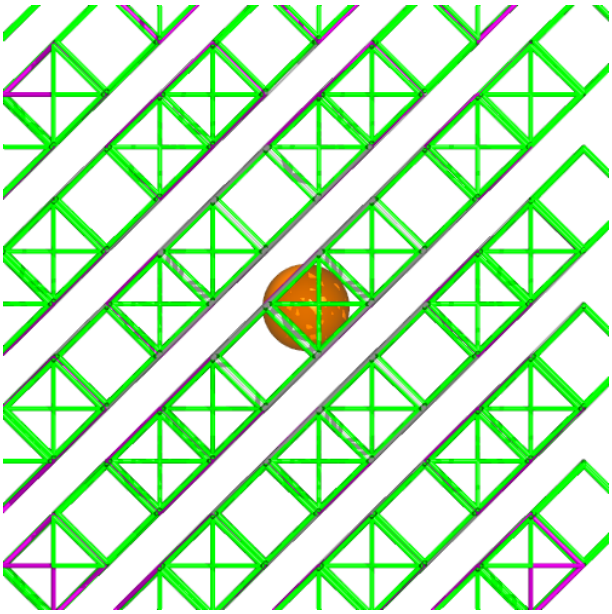
Continued from previous page...

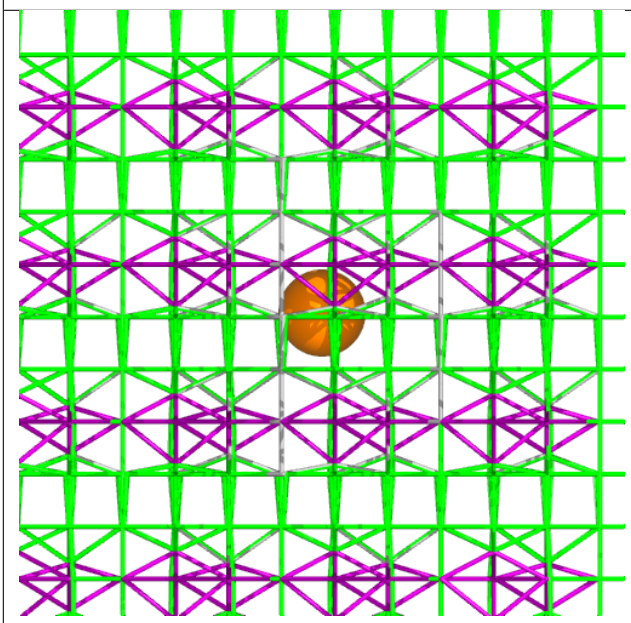
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	1A	3424	1/1	0.99	0.10	22,22,22,22	0
55	MG	1A	3739	1/1	0.99	0.08	19,19,19,19	0
55	MG	2A	3669	1/1	0.99	0.14	45,45,45,45	0
55	MG	1A	3085	1/1	0.99	0.22	38,38,38,38	0
55	MG	1A	3367	1/1	0.99	0.09	14,14,14,14	0
55	MG	2A	3625	1/1	0.99	0.06	67,67,67,67	0
55	MG	2A	3284	1/1	0.99	0.10	36,36,36,36	0
55	MG	1A	3427	1/1	0.99	0.14	27,27,27,27	0
55	MG	1a	3214	1/1	0.99	0.06	73,73,73,73	0
55	MG	2A	3287	1/1	0.99	0.21	57,57,57,57	0
55	MG	1A	3335	1/1	0.99	0.14	42,42,42,42	0
56	ZN	15	204	1/1	0.99	0.10	53,53,53,53	0
55	MG	2A	3465	1/1	0.99	0.18	34,34,34,34	0
55	MG	1B	215	1/1	0.99	0.15	50,50,50,50	0
55	MG	1A	3387	1/1	0.99	0.23	47,47,47,47	0
55	MG	1A	3781	1/1	0.99	0.08	36,36,36,36	0
55	MG	2A	3324	1/1	0.99	0.15	37,37,37,37	0
55	MG	2A	3591	1/1	0.99	0.18	56,56,56,56	0
56	ZN	26	101	1/1	0.99	0.12	66,66,66,66	0
55	MG	2A	3153	1/1	0.99	0.16	51,51,51,51	0
55	MG	2A	3685	1/1	0.99	0.34	55,55,55,55	0
57	SF4	1d	501	8/8	0.99	0.12	65,73,78,86	0
57	SF4	2d	501	8/8	0.99	0.09	67,72,87,89	0
55	MG	1A	3710	1/1	0.99	0.23	35,35,35,35	0

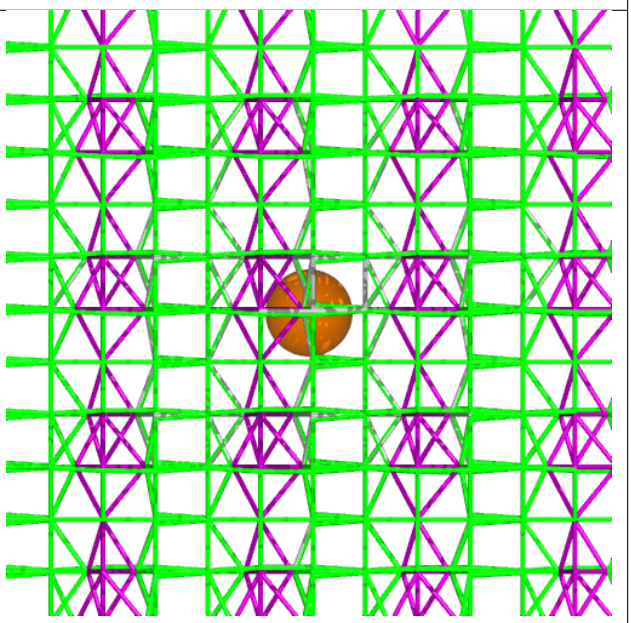
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A 2A 3816:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.