



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:33 am GMT

PDB ID : 4V8Z  
EMDB ID : EMD-2422  
Title : Cryo-EM reconstruction of the 80S-eIF5B-Met-itRNAMet Eukaryotic Translation Initiation Complex  
Authors : Fernandez, I.S.; Bai, X.C.; Hussain, T.; Kelley, A.C.; Lorsch, J.R.; Ramakrishnan, V.; Scheres, S.H.W.  
Deposited on : 2013-07-20  
Resolution : 6.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

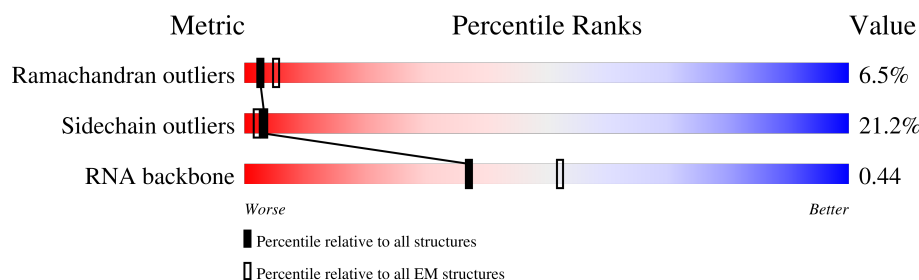
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A0	119	<div> <div>51%</div> <div>58% 18% 6% 18%</div> </div>
2	A1	82	<div> <div>48%</div> <div>83% 15% ..</div> </div>
3	A2	67	<div> <div>82%</div> <div>60% 34% 6%</div> </div>
4	A3	56	<div> <div>48%</div> <div>77% 14% . 5%</div> </div>
5	A4	63	<div> <div>52%</div> <div>81% 13% . 5%</div> </div>
6	A5	152	<div> <div>44%</div> <div>33% 11% . 53%</div> </div>
7	A6	319	<div> <div>73%</div> <div>85% 14% .</div> </div>
8	A7	273	<div> <div>50%</div> <div>47% 9% . 42%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	AA	252	
10	AB	255	
11	AC	254	
12	AD	240	
13	AE	261	
14	AF	225	
15	AG	236	
16	AH	190	
17	AI	200	
18	AJ	197	
19	AK	105	
20	AL	156	
21	AM	143	
22	AN	151	
23	AO	137	
24	AP	142	
25	AQ	143	
26	AR	136	
27	AS	146	
28	AT	144	
29	AU	121	
30	AV	87	
31	AW	130	
32	AX	145	
33	AY	135	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	AZ	108	
35	BA	253	
36	BB	386	
37	BC	361	
38	BD	296	
39	BE	175	
40	BF	243	
41	BG	255	
42	BH	191	
43	BI	220	
44	BJ	173	
45	BK	174	
46	BL	198	
47	BM	137	
48	BN	203	
49	BO	218	
50	BP	183	
51	BQ	185	
52	BR	188	
53	BS	172	
54	BT	159	
55	BU	120	
56	BV	136	
57	BW	155	
58	BX	141	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	BY	126	<div> <div>33%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
60	BZ	135	<div> <div>44%</div> <div>74%</div> <div>21%</div> <div>5%</div> </div>
61	Ba	148	<div> <div>39%</div> <div>76%</div> <div>22%</div> <div>..</div> </div>
62	Bb	58	<div> <div>41%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
63	Bc	104	<div> <div>45%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
64	Bd	112	<div> <div>40%</div> <div>73%</div> <div>21%</div> <div>..</div> </div>
65	Be	129	<div> <div>33%</div> <div>76%</div> <div>20%</div> <div>...</div> </div>
66	Bf	106	<div> <div>28%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
67	Bg	120	<div> <div>50%</div> <div>71%</div> <div>22%</div> <div>7%</div> </div>
68	Bh	119	<div> <div>34%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
69	Bi	99	<div> <div>45%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
70	Bj	87	<div> <div>46%</div> <div>75%</div> <div>25%</div> </div>
71	Bk	77	<div> <div>52%</div> <div>77%</div> <div>23%</div> </div>
72	Bl	50	<div> <div>58%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
73	Bm	128	<div> <div>14%</div> <div>30%</div> <div>9%</div> <div>59%</div> </div>
74	Bn	25	<div> <div>80%</div> <div>72%</div> <div>20%</div> <div>8%</div> </div>
75	Bo	105	<div> <div>38%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
76	Bq	312	<div> <div>21%</div> <div>34%</div> <div>11%</div> <div>54%</div> </div>
77	Br	47	<div> <div>91%</div> <div>98%</div> </div>
78	Bs	46	<div> <div>87%</div> <div>100%</div> </div>
79	B2	1800	<div> <div>30%</div> <div>54%</div> <div>36%</div> <div>9%</div> </div>
80	B5	3396	<div> <div>6%</div> <div>34%</div> <div>48%</div> <div>10%</div> <div>7%</div> </div>
81	B7	121	<div> <div>45%</div> <div>46%</div> <div>9%</div> </div>
82	B8	158	<div> <div>7%</div> <div>49%</div> <div>41%</div> <div>10%</div> </div>
83	CV	586	<div> <div>43%</div> <div>78%</div> <div>16%</div> <div>...</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
84	CW	76	<div><div></div><div>20%</div><div></div><div>34%</div><div></div><div>51%</div><div></div><div>11%</div></div>
85	CX	3	<div><div></div><div>33%</div><div></div><div>67%</div></div>

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 219371 atoms, of which 8407 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S RIBOSOMAL PROTEIN S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A4	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 6 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A5	71	Total	C	N	O	S	0	0
			516	328	93	91	4		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	82	UNK	LYS	SEE REMARK 999	UNP P05759
A5	83	UNK	LYS	SEE REMARK 999	UNP P05759
A5	84	UNK	VAL	SEE REMARK 999	UNP P05759
A5	85	UNK	TYR	SEE REMARK 999	UNP P05759
A5	86	UNK	THR	SEE REMARK 999	UNP P05759
A5	87	UNK	THR	SEE REMARK 999	UNP P05759
A5	88	UNK	PRO	SEE REMARK 999	UNP P05759
A5	89	UNK	LYS	SEE REMARK 999	UNP P05759
A5	90	UNK	LYS	SEE REMARK 999	UNP P05759
A5	91	UNK	ILE	SEE REMARK 999	UNP P05759
A5	92	UNK	LYS	SEE REMARK 999	UNP P05759
A5	93	UNK	HIS	SEE REMARK 999	UNP P05759
A5	94	UNK	LYS	SEE REMARK 999	UNP P05759
A5	95	UNK	HIS	SEE REMARK 999	UNP P05759
A5	96	UNK	LYS	SEE REMARK 999	UNP P05759
A5	97	UNK	LYS	SEE REMARK 999	UNP P05759
A5	98	UNK	VAL	SEE REMARK 999	UNP P05759
A5	99	UNK	LYS	SEE REMARK 999	UNP P05759
A5	100	UNK	LEU	SEE REMARK 999	UNP P05759
A5	101	UNK	ALA	SEE REMARK 999	UNP P05759

- Molecule 7 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

- Molecule 8 is a protein called SUPPRESSOR PROTEIN STM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	A7	159	Total	C	N	O	0	0
			1105	653	221	231		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A7	9	UNK	GLY	SEE REMARK 999	UNP P39015
A7	10	UNK	ASN	SEE REMARK 999	UNP P39015
A7	11	UNK	ASP	SEE REMARK 999	UNP P39015
A7	12	UNK	VAL	SEE REMARK 999	UNP P39015

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A7	13	UNK	GLU	SEE REMARK 999	UNP P39015
A7	14	UNK	ASP	SEE REMARK 999	UNP P39015
A7	15	UNK	ALA	SEE REMARK 999	UNP P39015
A7	16	UNK	ASP	SEE REMARK 999	UNP P39015
A7	17	UNK	VAL	SEE REMARK 999	UNP P39015
A7	18	UNK	VAL	SEE REMARK 999	UNP P39015
A7	19	UNK	VAL	SEE REMARK 999	UNP P39015
A7	20	UNK	LEU	SEE REMARK 999	UNP P39015
A7	151	UNK	LEU	SEE REMARK 999	UNP P39015
A7	152	UNK	GLN	SEE REMARK 999	UNP P39015
A7	153	UNK	ASP	SEE REMARK 999	UNP P39015
A7	154	UNK	TYR	SEE REMARK 999	UNP P39015
A7	155	UNK	LEU	SEE REMARK 999	UNP P39015
A7	156	UNK	ASN	SEE REMARK 999	UNP P39015
A7	157	UNK	GLN	SEE REMARK 999	UNP P39015
A7	158	UNK	GLN	SEE REMARK 999	UNP P39015
A7	159	UNK	ALA	SEE REMARK 999	UNP P39015
A7	160	UNK	ASN	SEE REMARK 999	UNP P39015
A7	161	UNK	ASN	SEE REMARK 999	UNP P39015
A7	162	UNK	GLN	SEE REMARK 999	UNP P39015
A7	163	UNK	PHE	SEE REMARK 999	UNP P39015
A7	164	UNK	ASN	SEE REMARK 999	UNP P39015
A7	165	UNK	LYS	SEE REMARK 999	UNP P39015
A7	166	UNK	VAL	SEE REMARK 999	UNP P39015
A7	167	UNK	PRO	SEE REMARK 999	UNP P39015
A7	168	UNK	GLU	SEE REMARK 999	UNP P39015
A7	169	UNK	ALA	SEE REMARK 999	UNP P39015
A7	170	UNK	LYS	SEE REMARK 999	UNP P39015
A7	171	UNK	LYS	SEE REMARK 999	UNP P39015
A7	172	UNK	VAL	SEE REMARK 999	UNP P39015
A7	173	UNK	GLU	SEE REMARK 999	UNP P39015
A7	174	UNK	LEU	SEE REMARK 999	UNP P39015
A7	175	UNK	ASP	SEE REMARK 999	UNP P39015

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AA	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AG	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	AH	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AK	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AL	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AM	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AO	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AP	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AQ	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AR	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AT	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 33 is a protein called 40S RIBOSOMAL PROTEIN S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AY	134	Total	C	N	O		0	0
			1073	676	208	189			

- Molecule 34 is a protein called 40S RIBOSOMAL PROTEIN S25-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AZ	70	Total	C	N	O		0	0
			563	360	104	99			

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L2-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	252	Total	C	N	O	S	0	0
			1912	1190	388	333	1		

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 38 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BI	213	Total	C	N	O	S	0	0
			1722	1094	325	297	6		

- Molecule 44 is a protein called 60S RIBOSOMAL PROTEIN L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BK	153	Total	C	H	N	O	0	3
			1509	450	756	153	150		

- Molecule 46 is a protein called 60S RIBOSOMAL PROTEIN L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	BL	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 47 is a protein called 60S RIBOSOMAL PROTEIN L14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BM	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	89	ALA	GLY	conflict	UNP P38754

- Molecule 48 is a protein called 60S RIBOSOMAL PROTEIN L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 49 is a protein called 60S RIBOSOMAL PROTEIN L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BO	197	Total	C	N	O	S	197	0
			3119	2008	581	528	2		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	3	VAL	SER	microheterogeneity	UNP P26784
BO	4	GLU	GLN	microheterogeneity	UNP P26784
BO	11	GLY	ALA	microheterogeneity	UNP P26784
BO	13	GLY	ASP	microheterogeneity	UNP P26784
BO	16	VAL	LEU	microheterogeneity	UNP P26784
BO	22	VAL	THR	microheterogeneity	UNP P26784
BO	23	VAL	ILE	microheterogeneity	UNP P26784

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
BO	27	LEU	VAL	microheterogeneity	UNP P26784
BO	40	GLU	ALA	microheterogeneity	UNP P26784
BO	80	PHE	LEU	microheterogeneity	UNP P26784
BO	84	LEU	ILE	microheterogeneity	UNP P26784
BO	104	VAL	ILE	microheterogeneity	UNP P26784
BO	158	ALA	ASP	microheterogeneity	UNP P26784
BO	163	SER	ARG	microheterogeneity	UNP P26784
BO	179	ALA	SER	microheterogeneity	UNP P26784
BO	182	ASN	SER	microheterogeneity	UNP P26784
BO	184	THR	ALA	microheterogeneity	UNP P26784
BO	186	ALA	SER	microheterogeneity	UNP P26784
BO	196	ALA	SER	microheterogeneity	UNP P26784
BO	197	LEU	PHE	microheterogeneity	UNP P26784

- Molecule 50 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BP	155	Total	C	N	O	0	0
			1227	764	238	225		

- Molecule 51 is a protein called 60S RIBOSOMAL PROTEIN L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 52 is a protein called 60S RIBOSOMAL PROTEIN L19-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	BR	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 53 is a protein called 60S RIBOSOMAL PROTEIN L20-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 54 is a protein called 60S RIBOSOMAL PROTEIN L21-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
54	BT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 55 is a protein called 60S RIBOSOMAL PROTEIN L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BU	98	Total	C	N	O		0	0
			778	505	127	146			

- Molecule 56 is a protein called 60S RIBOSOMAL PROTEIN L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 57 is a protein called 60S RIBOSOMAL PROTEIN L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BW	135	Total	C	N	O	S	0	0
			1038	651	206	180	1		

- Molecule 58 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BX	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 59 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BY	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 60 is a protein called 60S RIBOSOMAL PROTEIN L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BZ	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 61 is a protein called 60S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ba	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 62 is a protein called 60S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bb	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 63 is a protein called 60S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bc	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 64 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bd	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 65 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Be	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 66 is a protein called 60S RIBOSOMAL PROTEIN L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bf	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 67 is a protein called 60S RIBOSOMAL PROTEIN L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bg	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 68 is a protein called 60S RIBOSOMAL PROTEIN L35-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bh	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 69 is a protein called 60S RIBOSOMAL PROTEIN L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bi	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 70 is a protein called 60S RIBOSOMAL PROTEIN L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 71 is a protein called 60S RIBOSOMAL PROTEIN L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bk	77	Total	C	N	O		0	0
			608	388	114	106			

- Molecule 72 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bl	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 73 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bm	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 74 is a protein called 60S RIBOSOMAL PROTEIN L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bn	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 75 is a protein called 60S RIBOSOMAL PROTEIN L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bo	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 76 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P0.

Mol	Chain	Residues	Atoms					AltConf	Trace	
76	Bq	145	Total	C	H	N	O	S	0	2
			2185	683	1110	194	195	3		

- Molecule 77 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Br	47	Total	C	H	N	O	0	0
			473	141	237	47	48		

- Molecule 78 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P2.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bs	46	Total	C	H	N	O	0	0
			463	138	232	46	47		

- Molecule 79 is a RNA chain called 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	B2	1781	Total	C	N	O	P	1	0
			37835	16910	6661	12482	1782		

- Molecule 80 is a RNA chain called 25S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	B5	3147	Total	C	H	N	O	P	0	0
			67972	30066	664	12132	21965	3145		

- Molecule 81 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	B7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 82 is a RNA chain called 5.8S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	B8	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 83 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 5B, PROBABLE TRANSLATION INITIATION FACTOR IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
83	CV	570	Total	C	H	N	O	S	0	2
			9036	2819	4585	766	847	19		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CV	340	ASP	-	linker	UNP P39730
CV	341	LEU	-	linker	UNP P39730
CV	342	THR	-	linker	UNP P39730
CV	343	GLY	-	linker	UNP P39730
CV	344	LEU	-	linker	UNP P39730
CV	345	LEU	-	linker	UNP P39730
CV	346	ASP	-	linker	UNP P39730
CV	347	SER	-	linker	UNP P39730
CV	348	VAL	-	linker	UNP P39730
CV	349	ASP	-	linker	UNP P39730
CV	350	THR	-	linker	UNP P39730

- Molecule 84 is a RNA chain called EUKARYOTIC RIBOSOMAL PI TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
84	CW	76	Total	C	H	N	O	P	0	0
			2403	721	789	285	533	75		

- Molecule 85 is a RNA chain called 5'-R(\*AP\*UP\*GP)-3'.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	CX	3	Total	C	H	N	O	P	0	0
			96	29	34	12	19	2		

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	A0	1	Total	Zn	0
			1	1	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
86	A1	1	Total 1	Zn 1	0
86	A3	1	Total 1	Zn 1	0
86	A5	1	Total 1	Zn 1	0
86	Bj	1	Total 1	Zn 1	0
86	Bm	1	Total 1	Zn 1	0

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

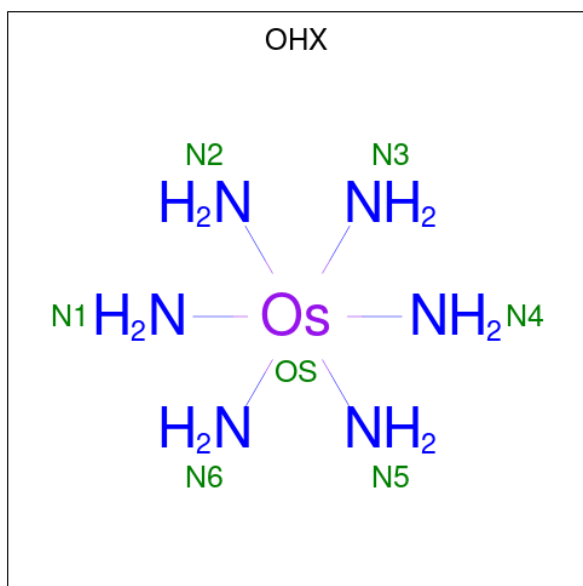
Mol	Chain	Residues	Atoms		AltConf
87	A0	2	Total 2	Mg 2	0
87	A3	3	Total 3	Mg 3	0
87	A5	1	Total 1	Mg 1	0
87	AB	1	Total 1	Mg 1	0
87	AC	2	Total 2	Mg 2	0
87	AE	1	Total 1	Mg 1	0
87	AG	1	Total 1	Mg 1	0
87	AI	1	Total 1	Mg 1	0
87	AJ	1	Total 1	Mg 1	0
87	AL	2	Total 2	Mg 2	0
87	AN	1	Total 1	Mg 1	0
87	AP	1	Total 1	Mg 1	0
87	AS	1	Total 1	Mg 1	0
87	AU	1	Total 1	Mg 1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	BD	4	Total	Mg	0
			4	4	
87	BF	1	Total	Mg	0
			1	1	
87	BS	3	Total	Mg	0
			3	3	
87	B2	168	Total	Mg	0
			168	168	
87	B5	3	Total	Mg	0
			3	3	
87	B7	27	Total	Mg	0
			27	27	
87	CW	1	Total	Mg	0
			1	1	

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			AltConf
88	A3	1	Total	N	Os	0
			7	6	1	
88	A6	1	Total	N	Os	0
			7	6	1	
88	AC	1	Total	N	Os	0
			7	6	1	
88	AI	1	Total	N	Os	0
			14	12	2	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
88	AI	1	Total 14	N 12	Os 2	0
88	AL	1	Total 7	N 6	Os 1	0
88	AN	1	Total 7	N 6	Os 1	0
88	AP	1	Total 7	N 6	Os 1	0
88	BR	1	Total 7	N 6	Os 1	0
88	Bn	1	Total 7	N 6	Os 1	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0

*Continued on next page...*



[illegible]

[illegible]

[illegible]

[illegible]

Continued from previous page...

[illegible]

*Continued on next page...*

[illegible]

Continued from previous page...

[illegible]

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B5	1	Total	N	Os	0
			21	18	3	

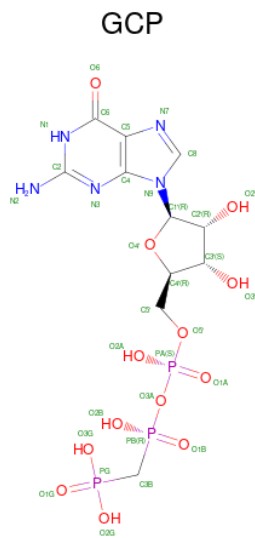
*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
88	B5	1	Total	N	Os	0
			21	18	3	
88	B5	1	Total	N	Os	0
			21	18	3	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	CV	1	Total	N	Os	0
			7	6	1	
88	CX	1	Total	N	Os	0
			7	6	1	

- Molecule 89 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

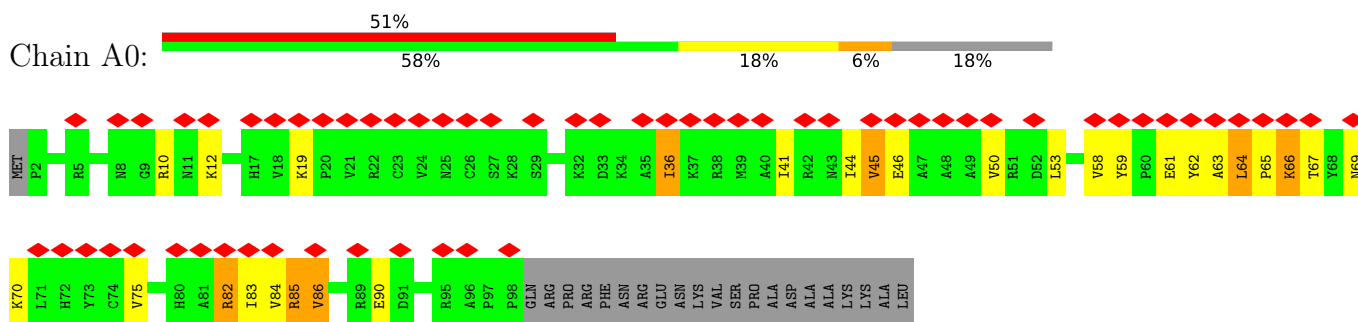


Mol	Chain	Residues	Atoms					AltConf
89	CV	1	Total	C	N	O	P	0
			32	11	5	13	3	

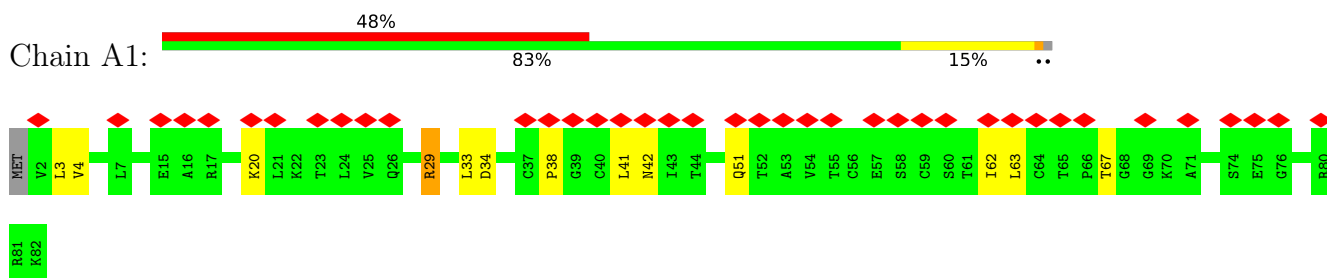
### 3 Residue-property plots

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

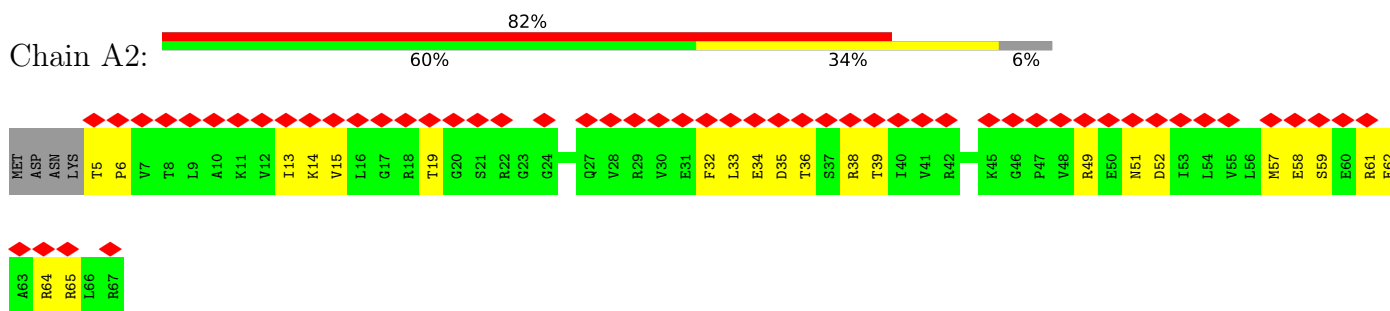
#### • Molecule 1: 40S RIBOSOMAL PROTEIN S26-A



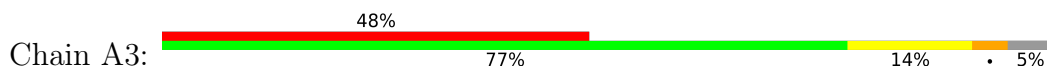
#### • Molecule 2: 40S RIBOSOMAL PROTEIN S27-A



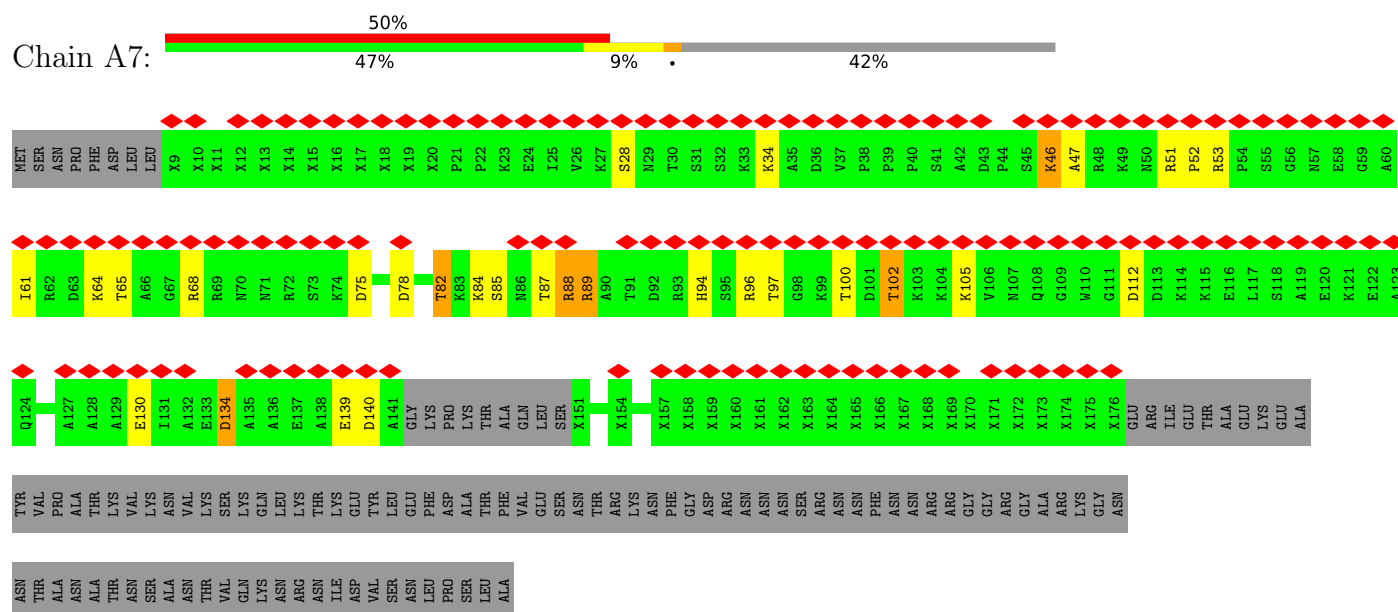
#### • Molecule 3: 40S RIBOSOMAL PROTEIN S28-A



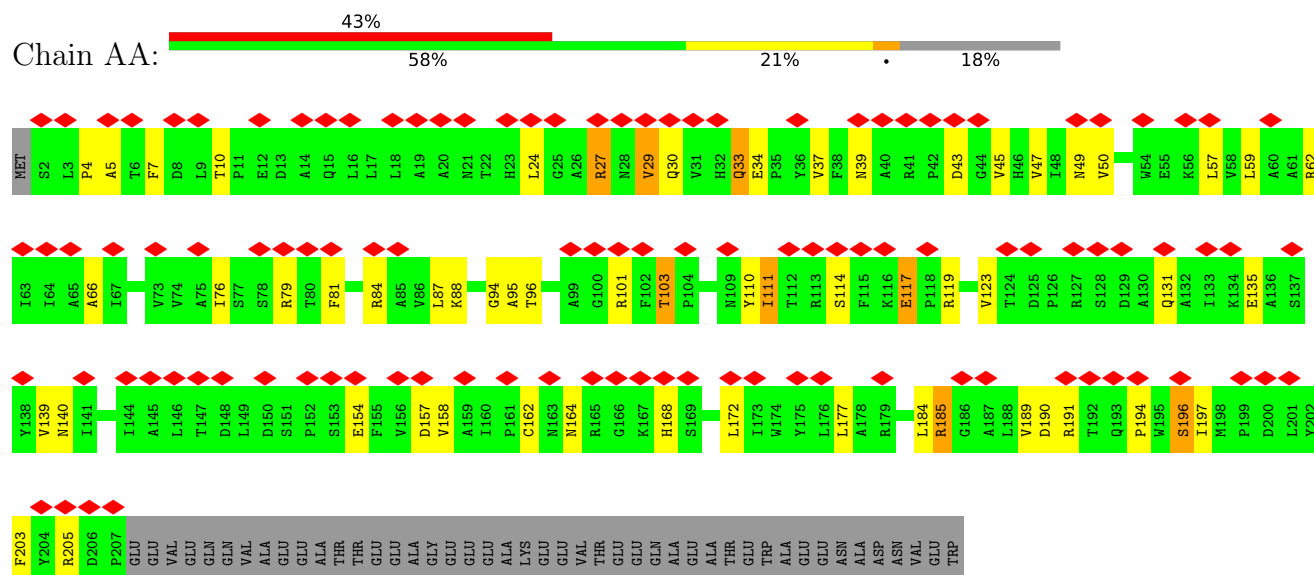
#### • Molecule 4: 40S RIBOSOMAL PROTEIN S29-A



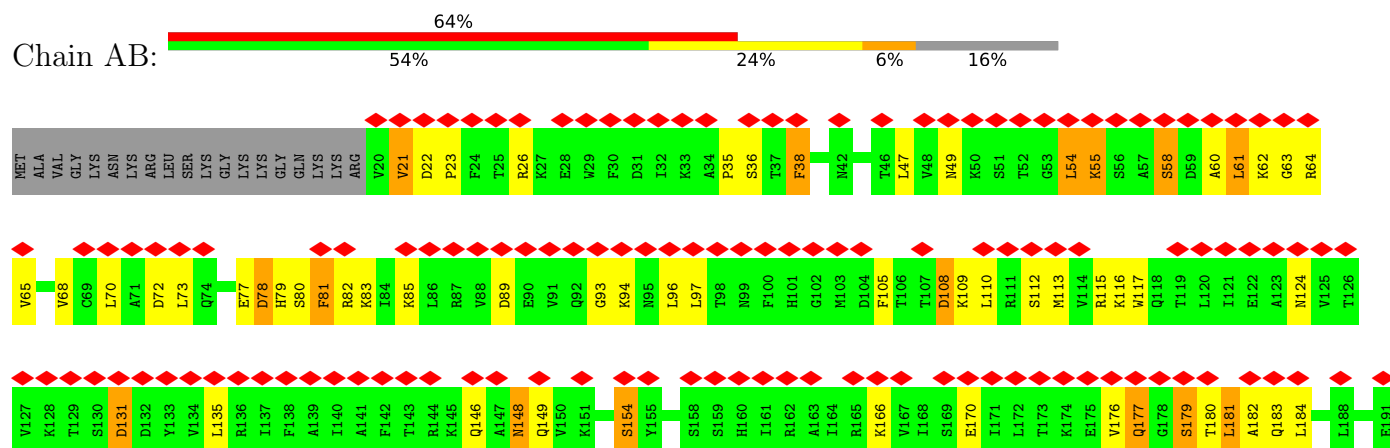


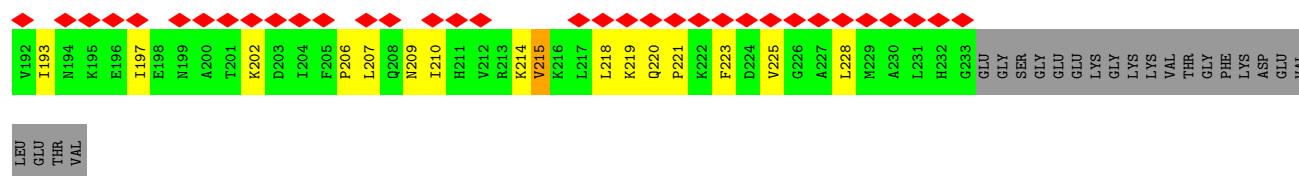


• Molecule 9: 40S RIBOSOMAL PROTEIN S0-A

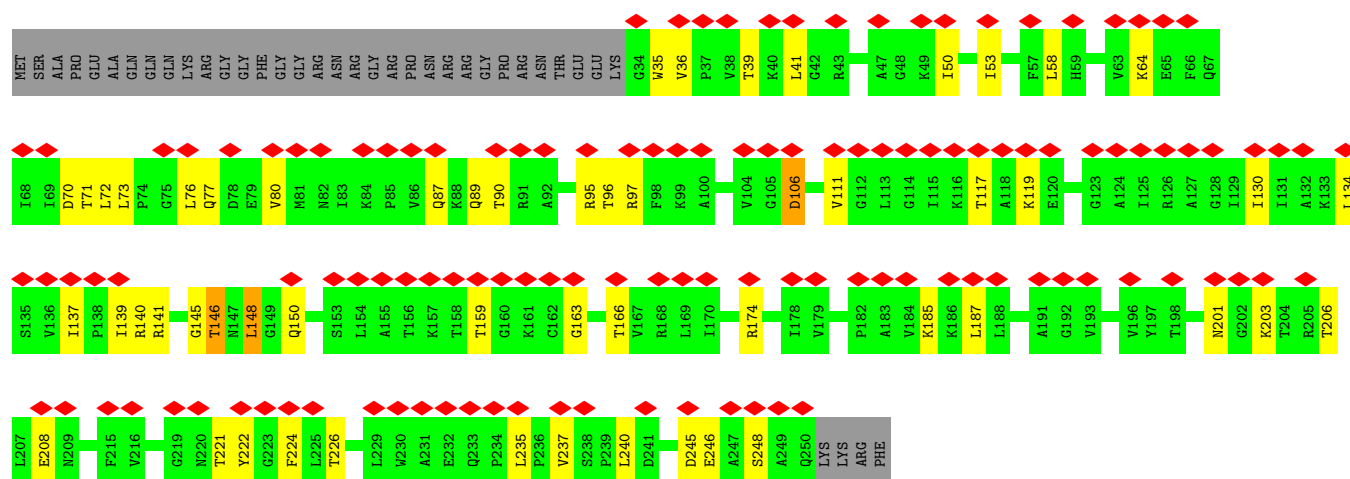


• Molecule 10: 40S RIBOSOMAL PROTEIN S1-A

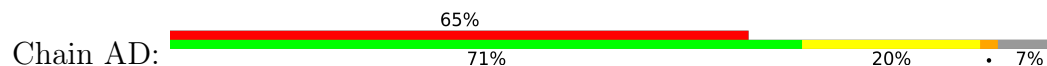




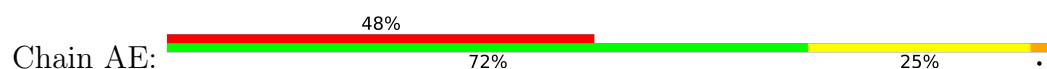
• Molecule 11: 40S RIBOSOMAL PROTEIN S2

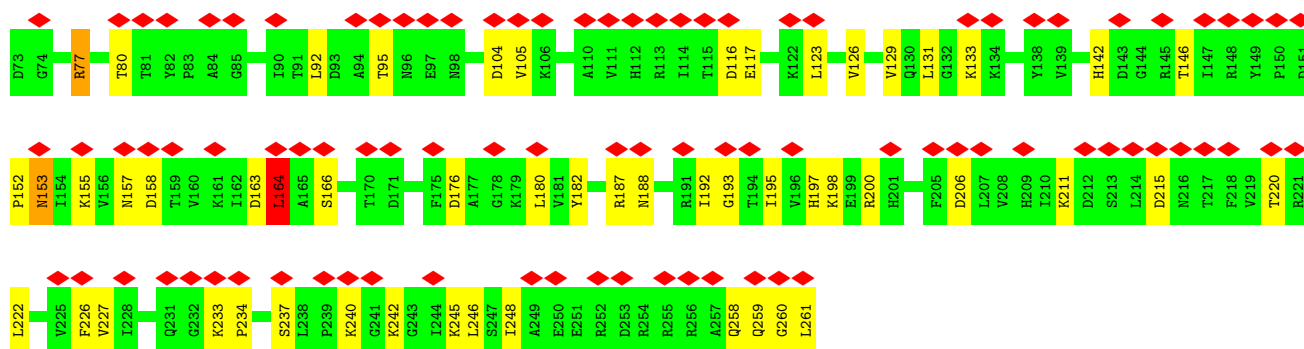


• Molecule 12: 40S RIBOSOMAL PROTEIN S3

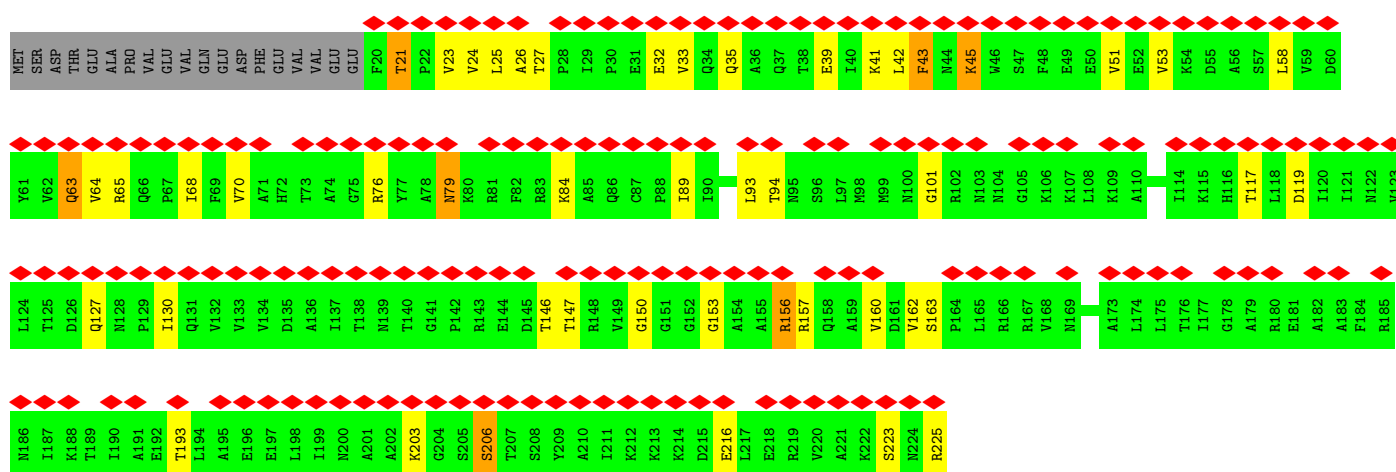
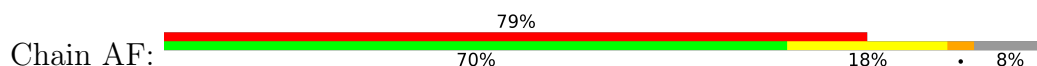


• Molecule 13: 40S RIBOSOMAL PROTEIN S4-A

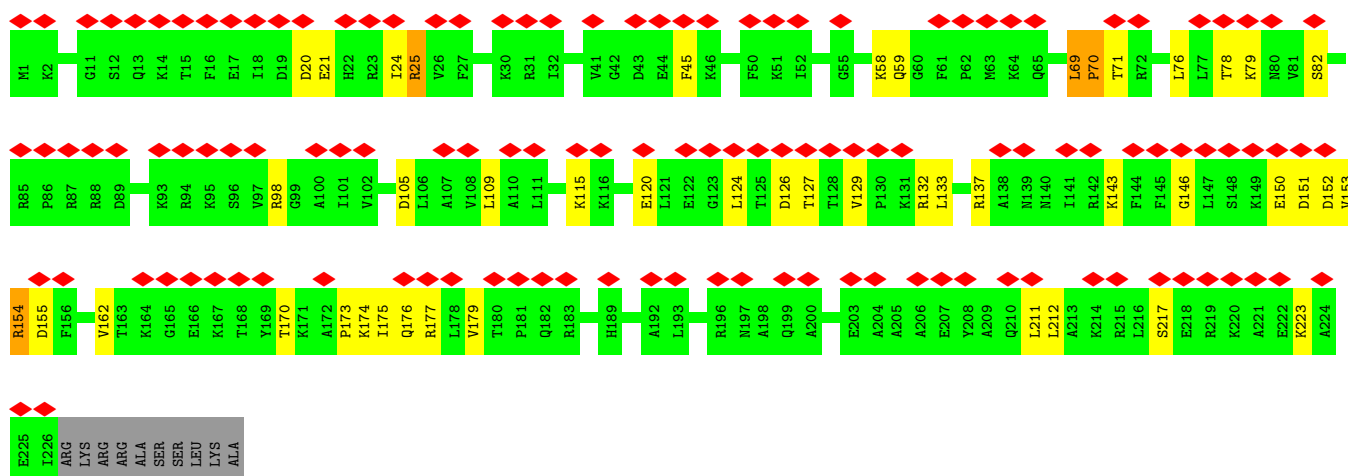




• Molecule 14: 40S RIBOSOMAL PROTEIN S5

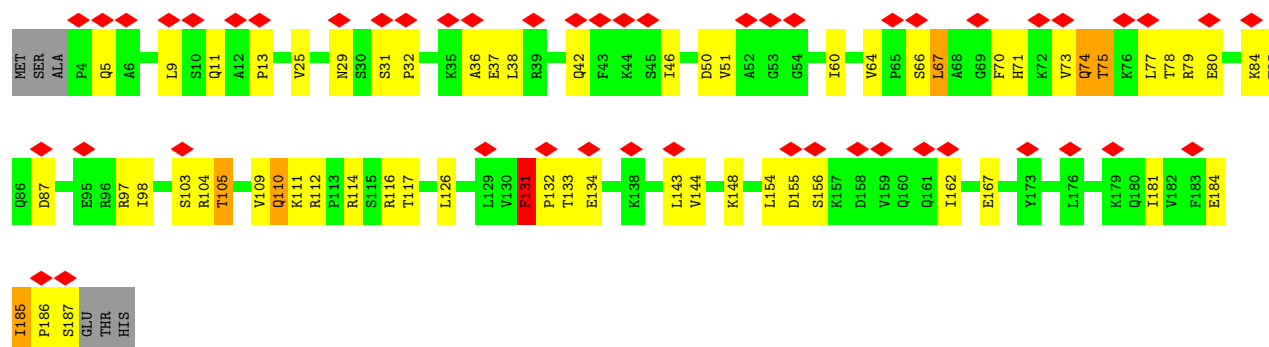


• Molecule 15: 40S RIBOSOMAL PROTEIN S6-A

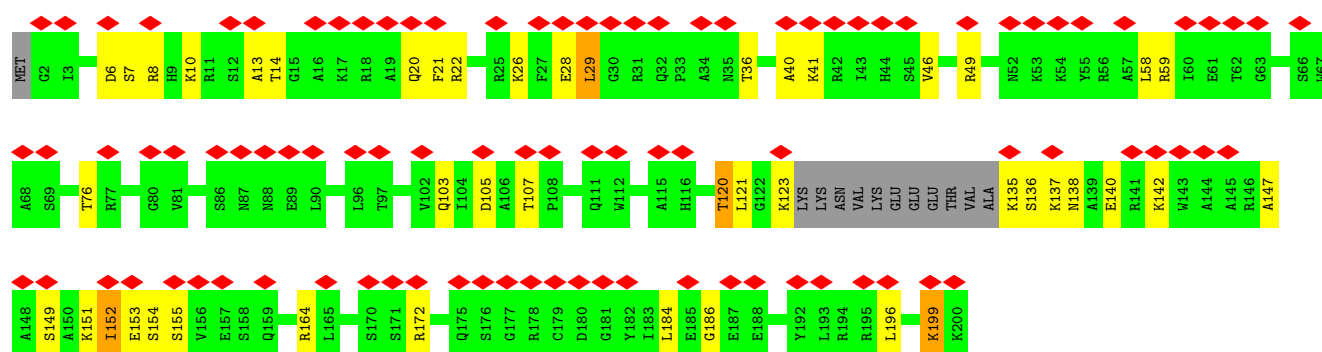
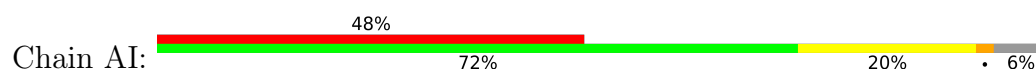


• Molecule 16: 40S RIBOSOMAL PROTEIN S7-A

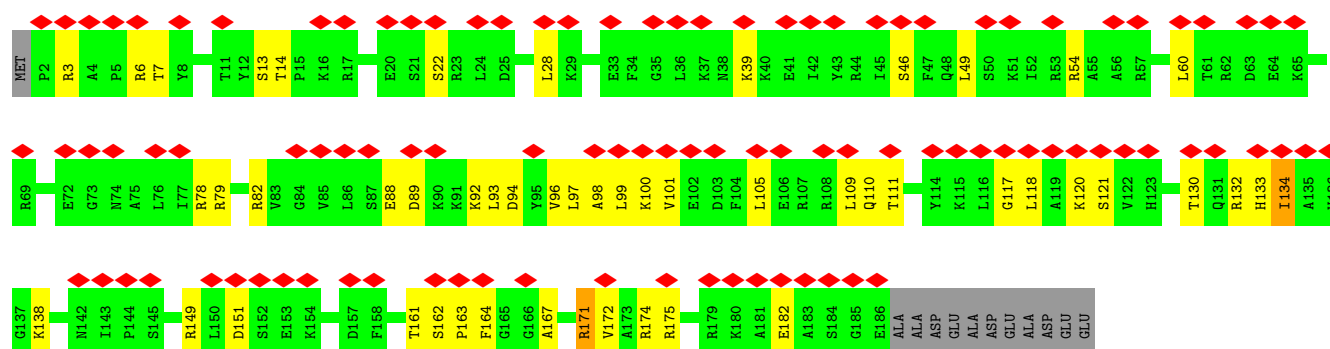




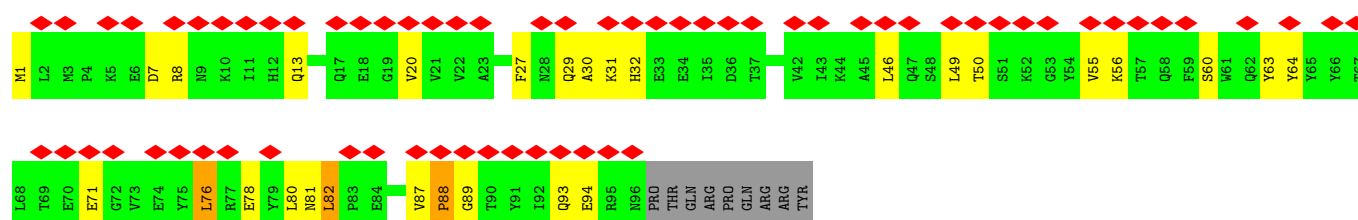
• Molecule 17: 40S RIBOSOMAL PROTEIN S8-A



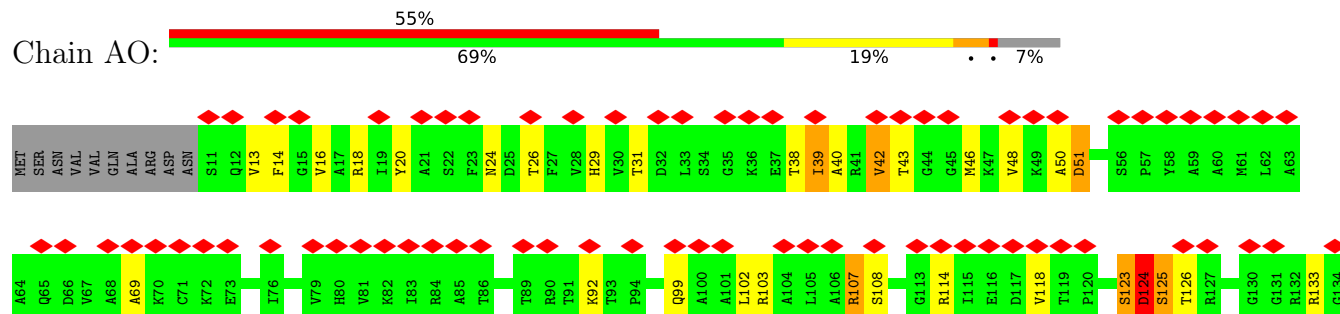
• Molecule 18: 40S RIBOSOMAL PROTEIN S9-A



• Molecule 19: 40S RIBOSOMAL PROTEIN S10-A

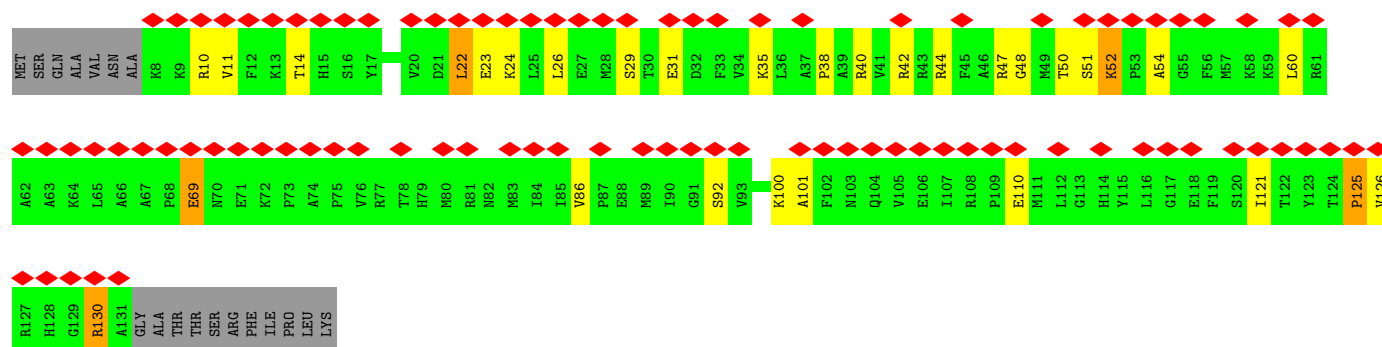




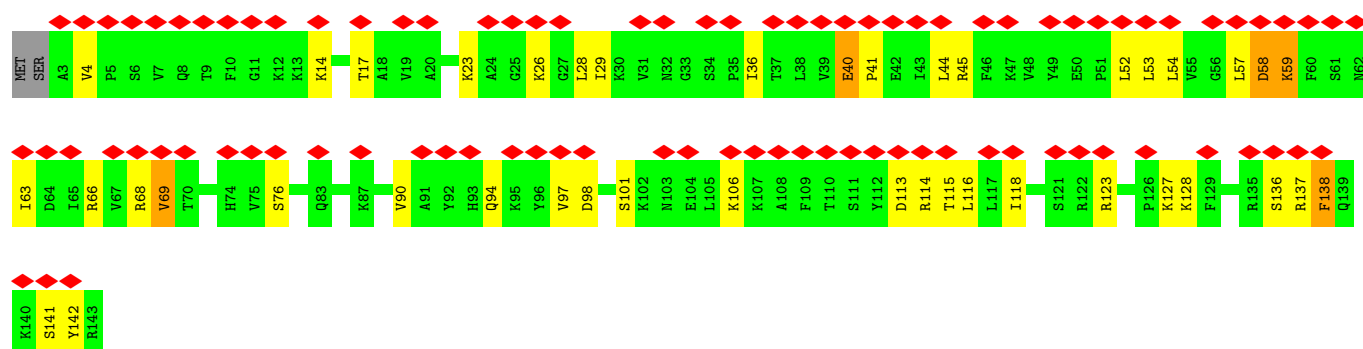
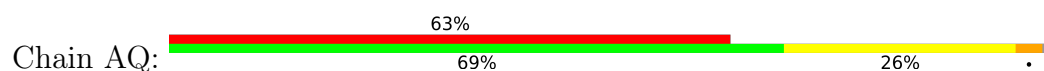




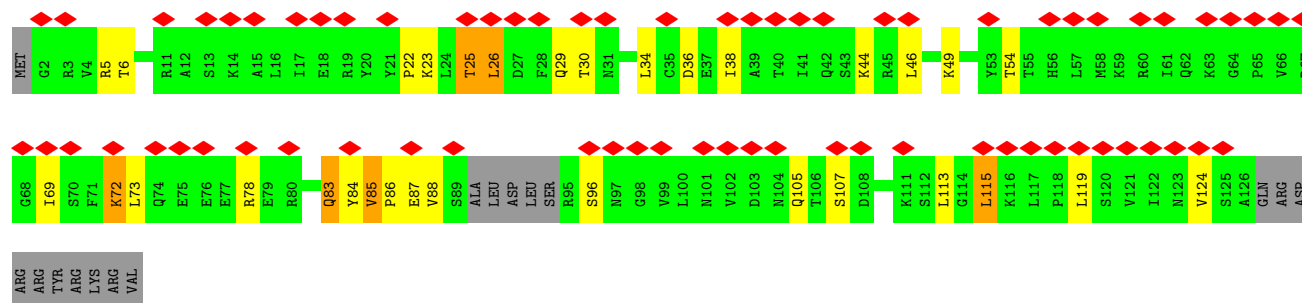
• Molecule 24: 40S RIBOSOMAL PROTEIN S15



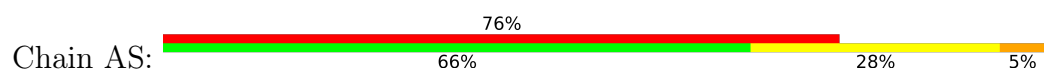
• Molecule 25: 40S RIBOSOMAL PROTEIN S16-A

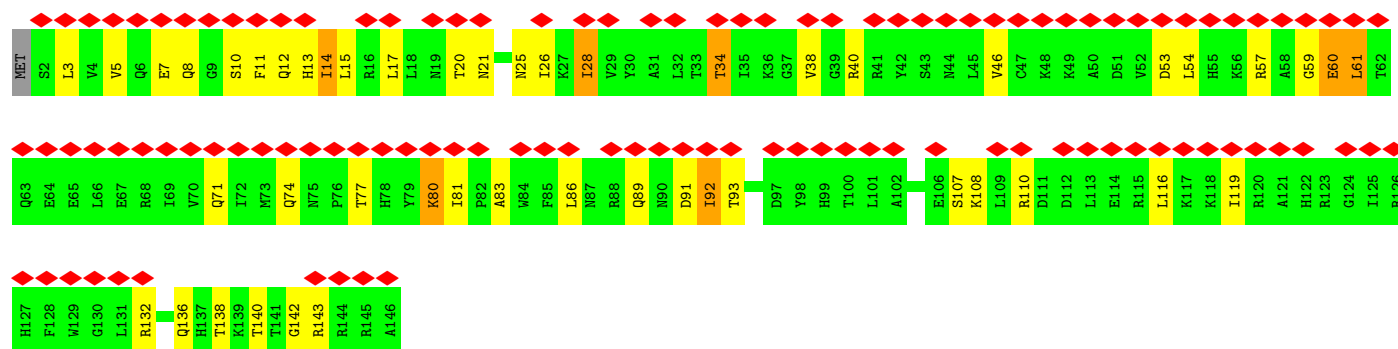


• Molecule 26: 40S RIBOSOMAL PROTEIN S17-A

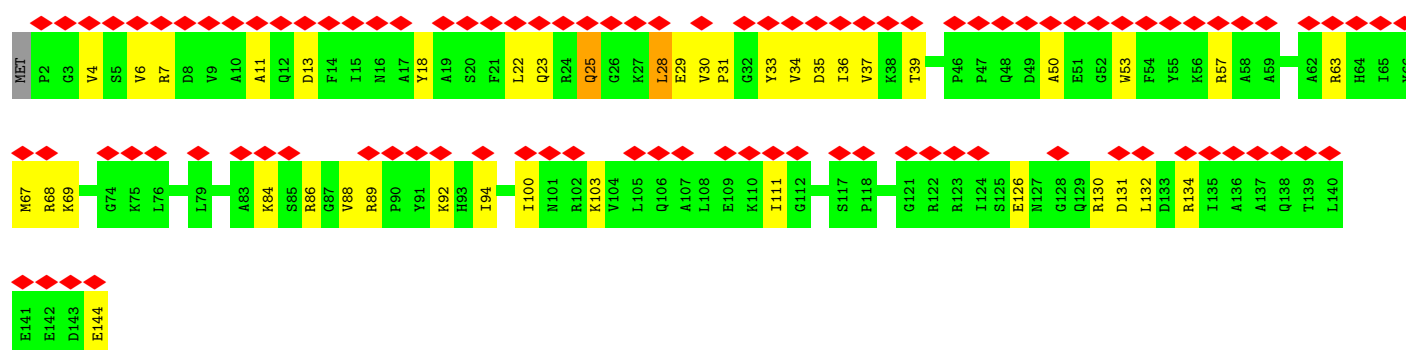


• Molecule 27: 40S RIBOSOMAL PROTEIN S18-A

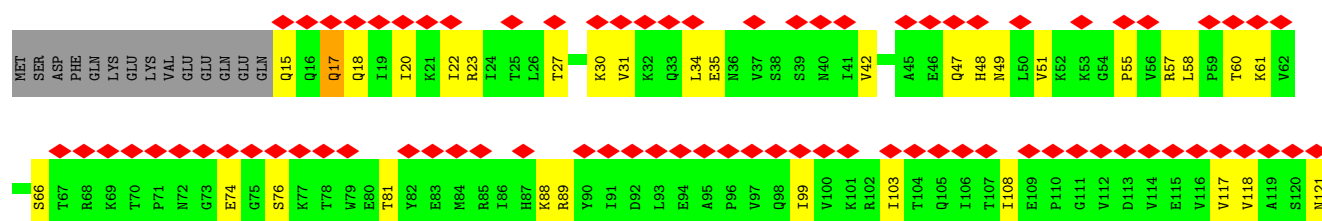




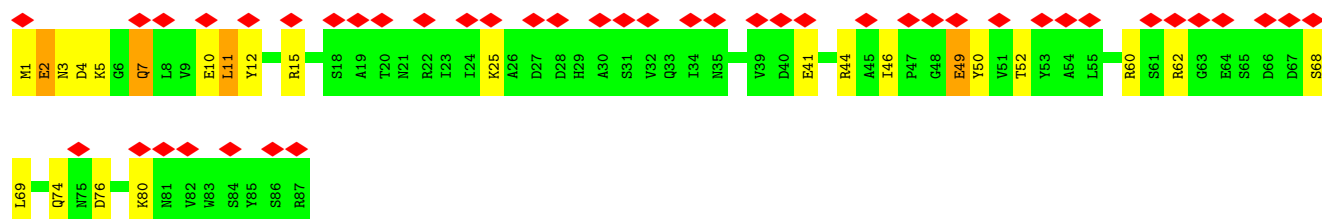
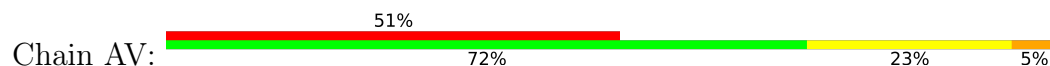
• Molecule 28: 40S RIBOSOMAL PROTEIN S19-A




• Molecule 29: 40S RIBOSOMAL PROTEIN S20

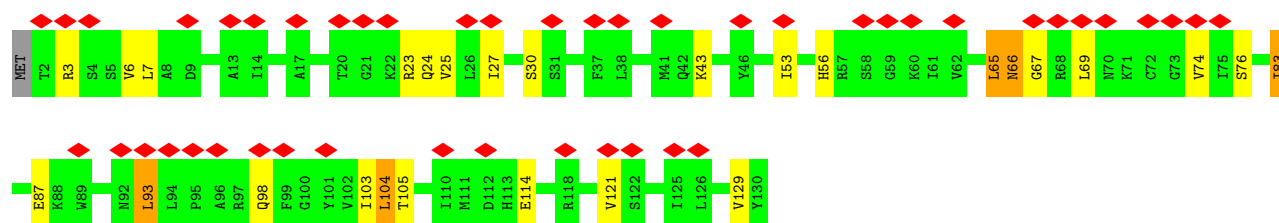


• Molecule 30: 40S RIBOSOMAL PROTEIN S21-A




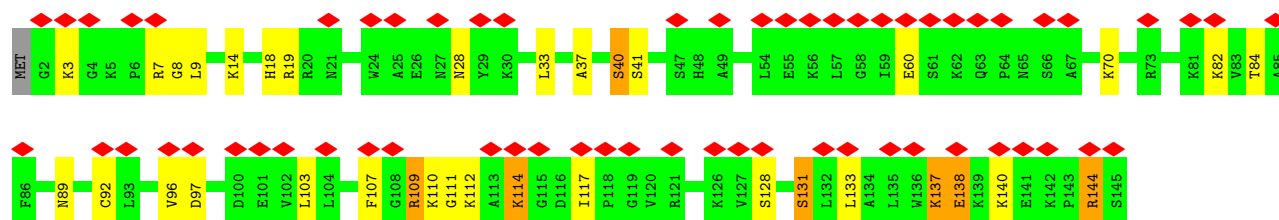
• Molecule 31: 40S RIBOSOMAL PROTEIN S22-A

Chain AW: 

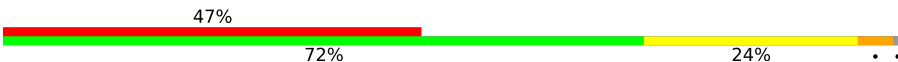


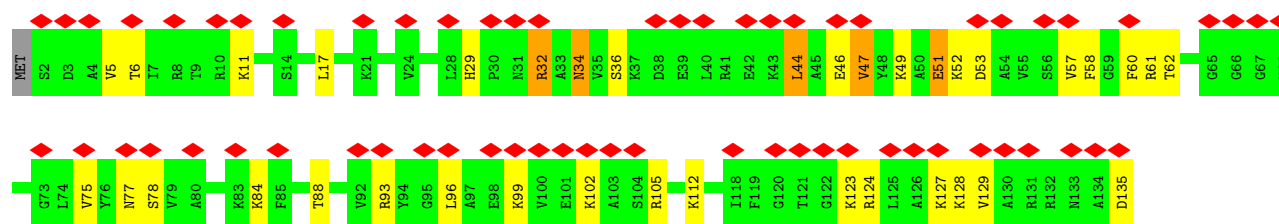
• Molecule 32: 40S RIBOSOMAL PROTEIN S23-A

Chain AX: 



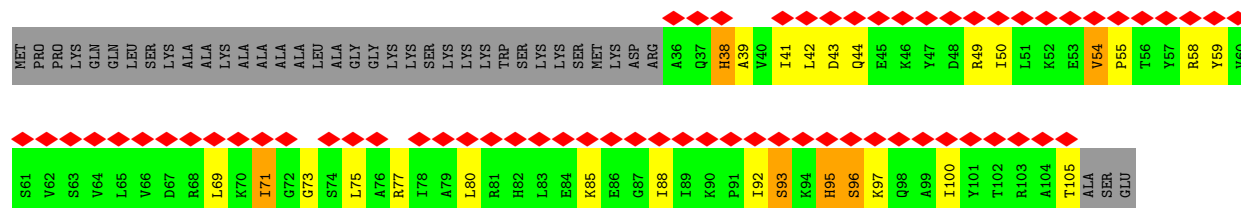
• Molecule 33: 40S RIBOSOMAL PROTEIN S24-A

Chain AY: 




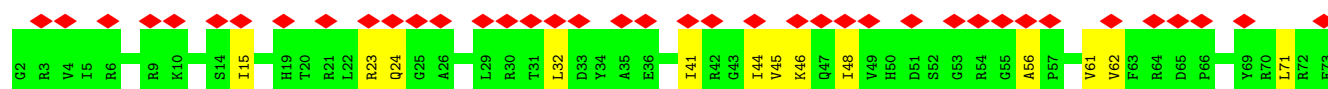
• Molecule 34: 40S RIBOSOMAL PROTEIN S25-A

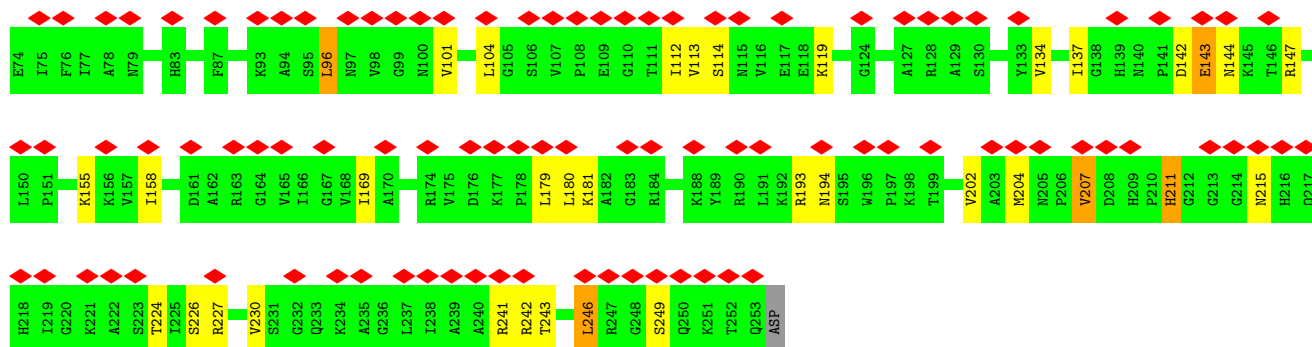
Chain AZ: 



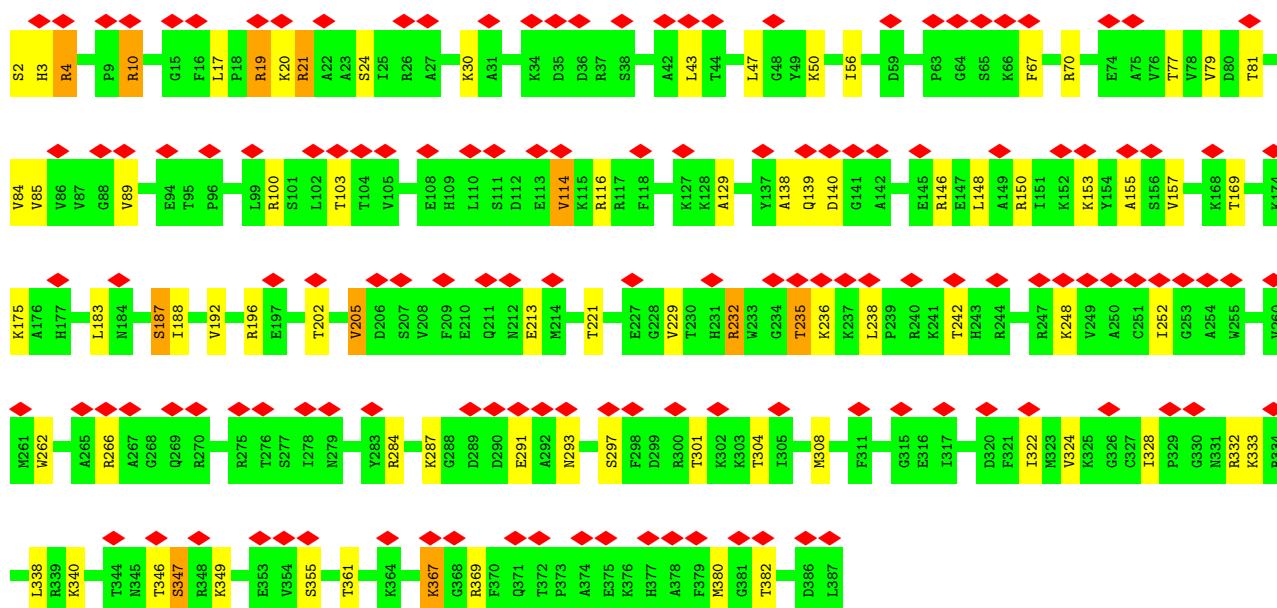
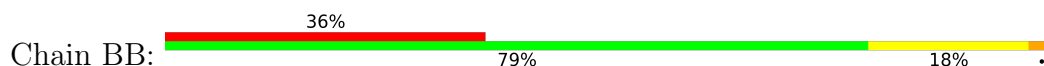
• Molecule 35: 60S RIBOSOMAL PROTEIN L2-B

Chain BA: 

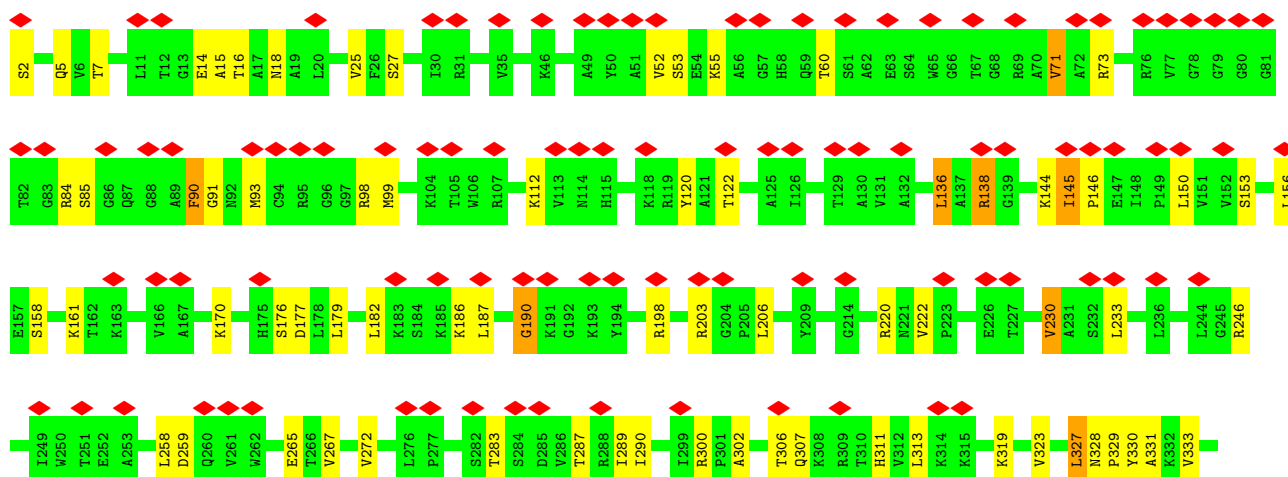
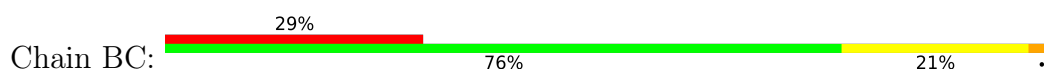


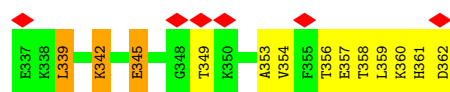


• Molecule 36: 60S RIBOSOMAL PROTEIN L3

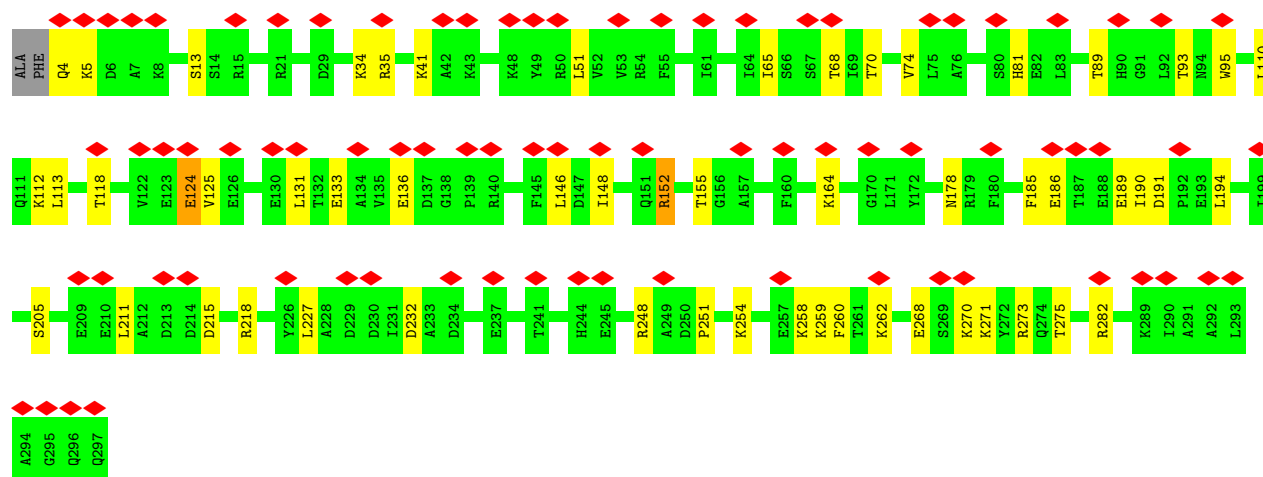
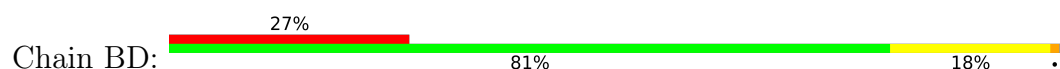


• Molecule 37: 60S RIBOSOMAL PROTEIN L4-A

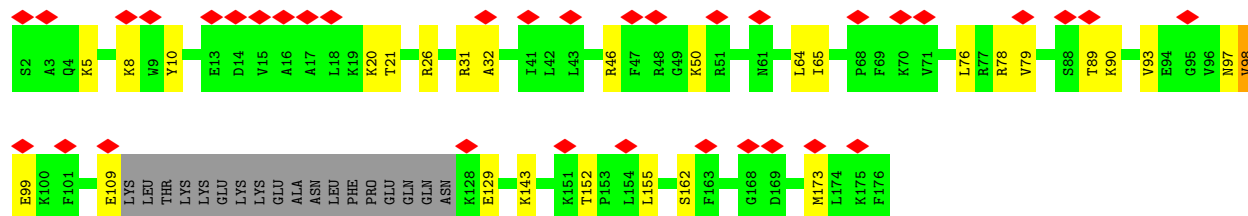
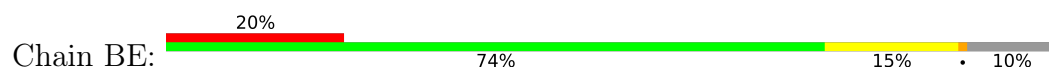




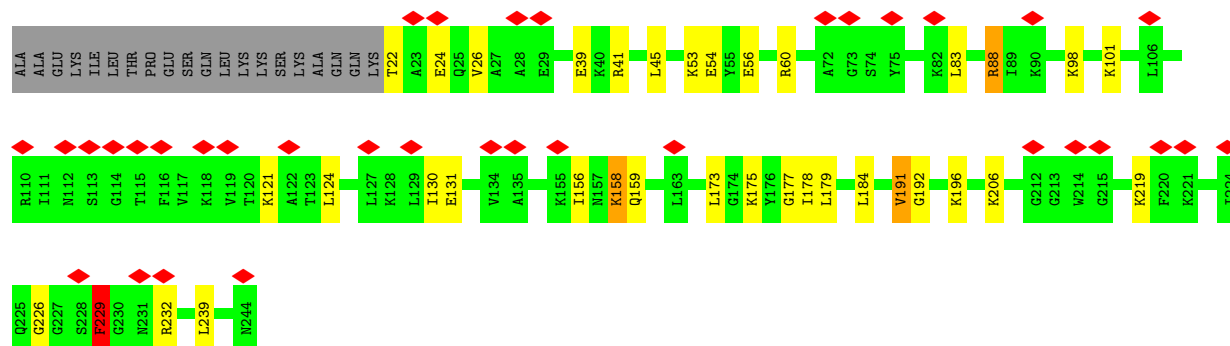
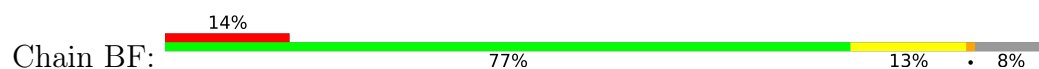
• Molecule 38: 60S RIBOSOMAL PROTEIN L5




• Molecule 39: 60S RIBOSOMAL PROTEIN L6-A

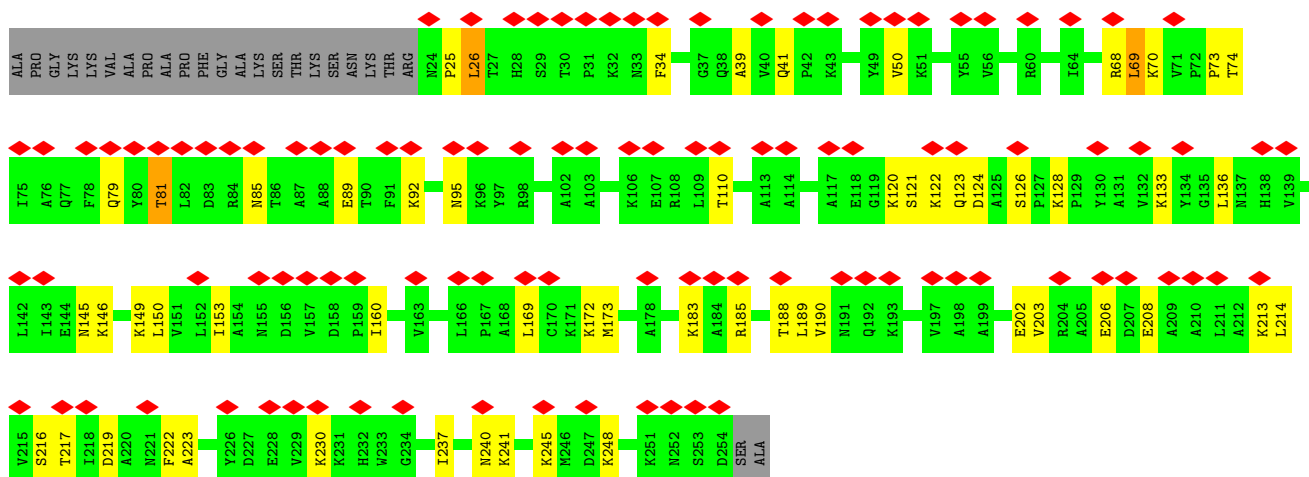


• Molecule 40: 60S RIBOSOMAL PROTEIN L7-A




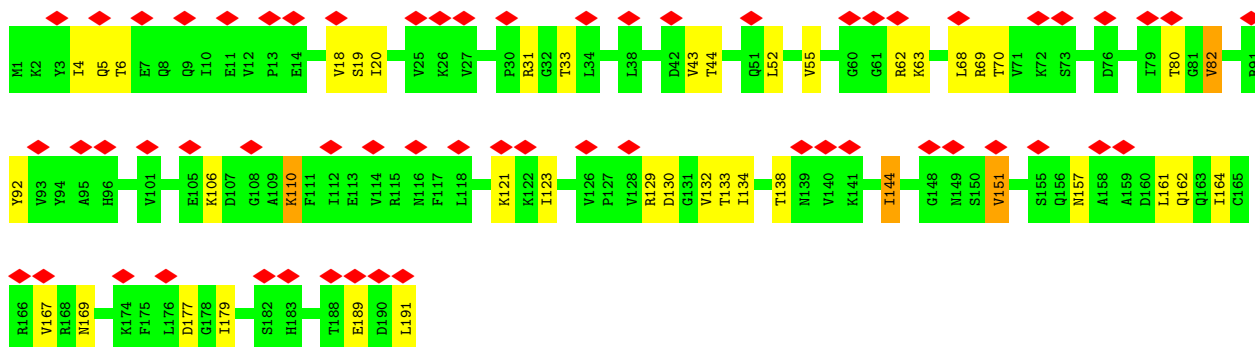
• Molecule 41: 60S RIBOSOMAL PROTEIN L8-A

Chain BG: 




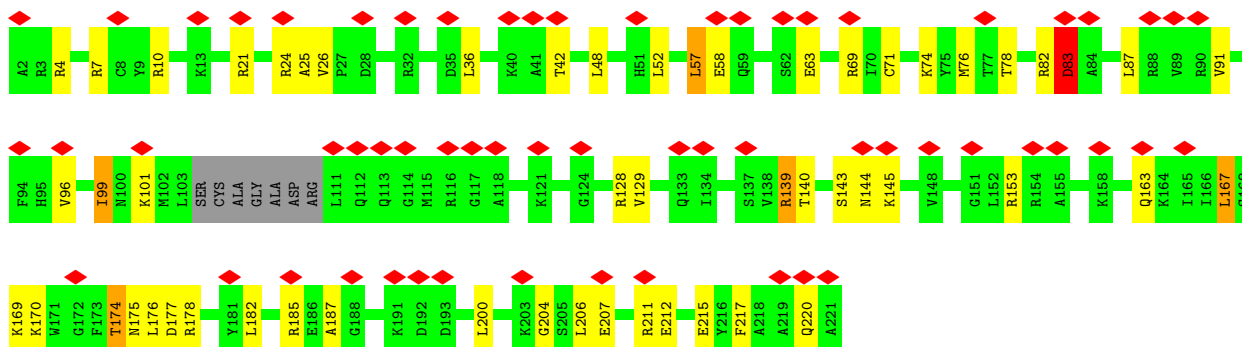
• Molecule 42: 60S RIBOSOMAL PROTEIN L9-A

Chain BH: 




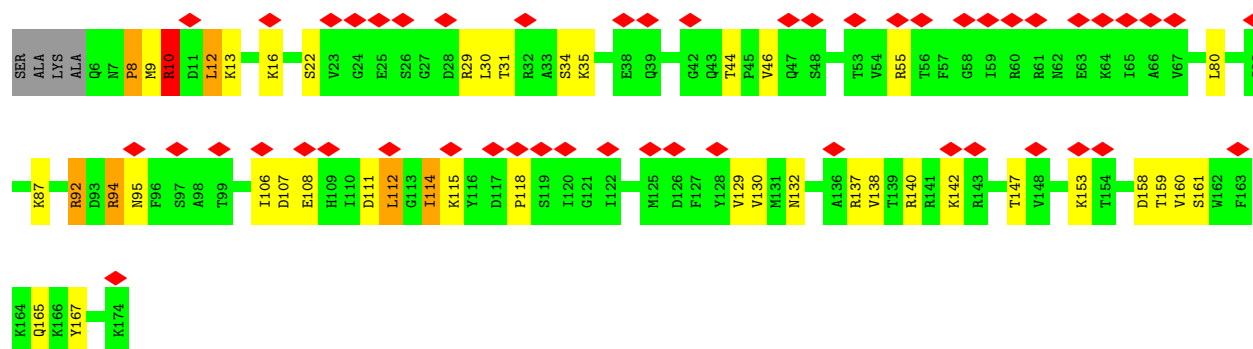
• Molecule 43: 60S RIBOSOMAL PROTEIN L10

Chain BI: 

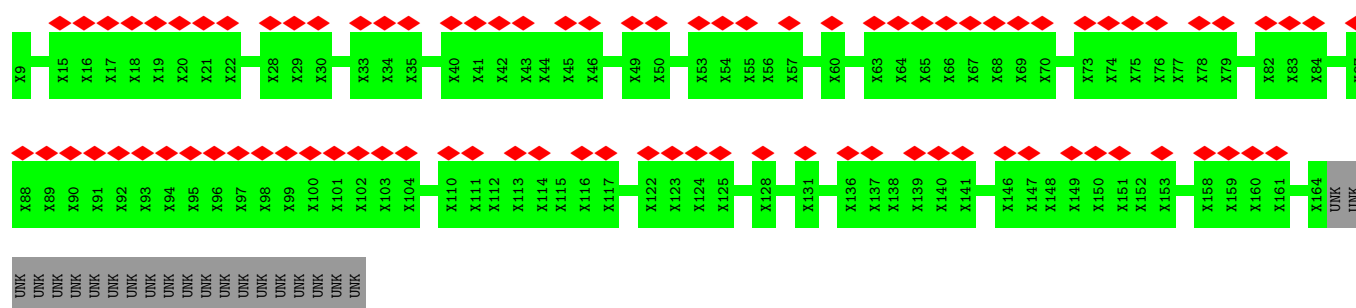


• Molecule 44: 60S RIBOSOMAL PROTEIN L11-A

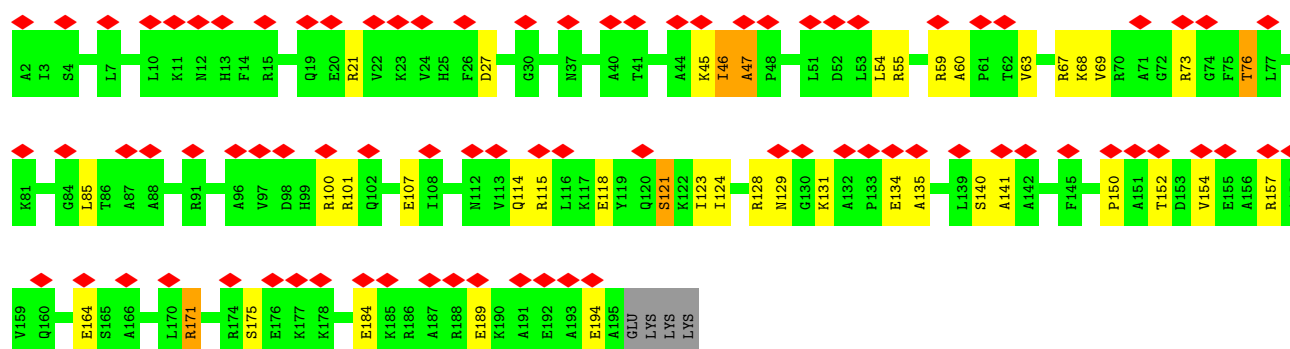
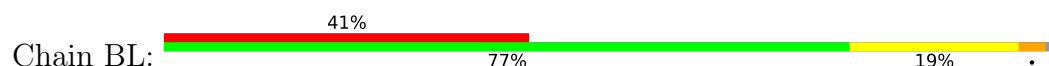
Chain BJ: 



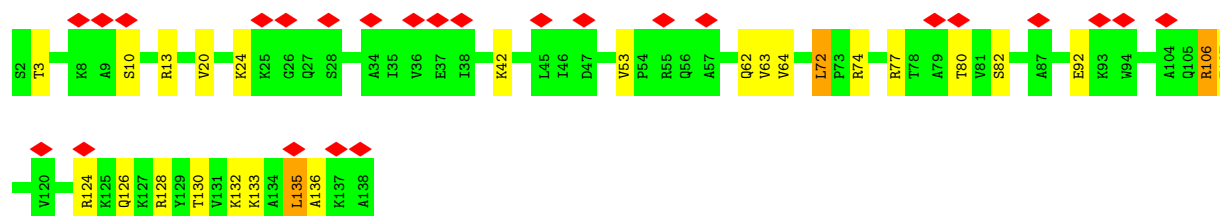
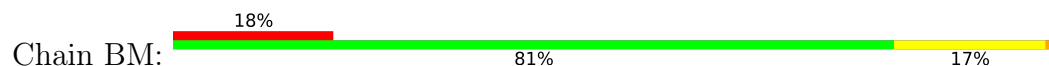
• Molecule 45: 60S RIBOSOMAL PROTEIN L11-A



• Molecule 46: 60S RIBOSOMAL PROTEIN L13-A

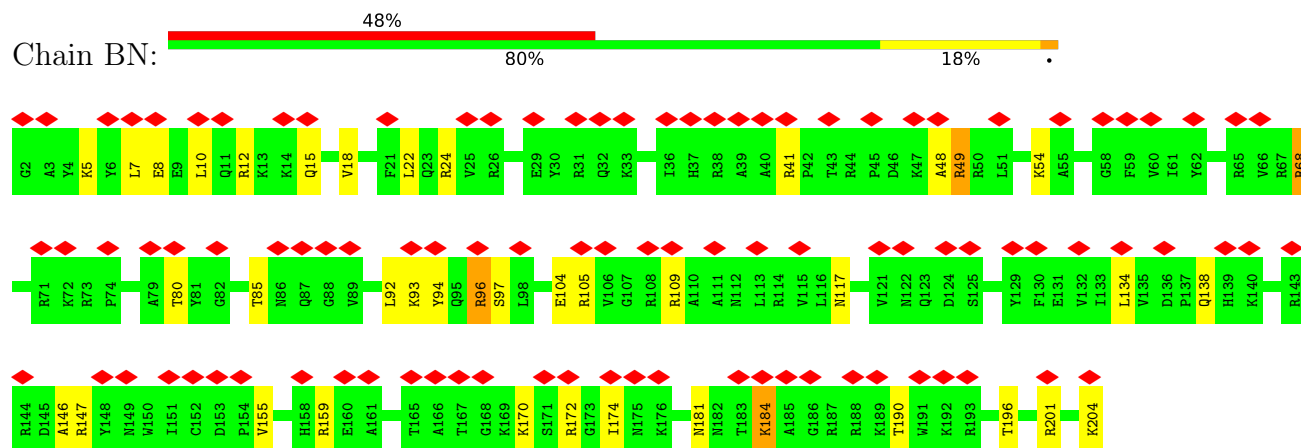


• Molecule 47: 60S RIBOSOMAL PROTEIN L14-B

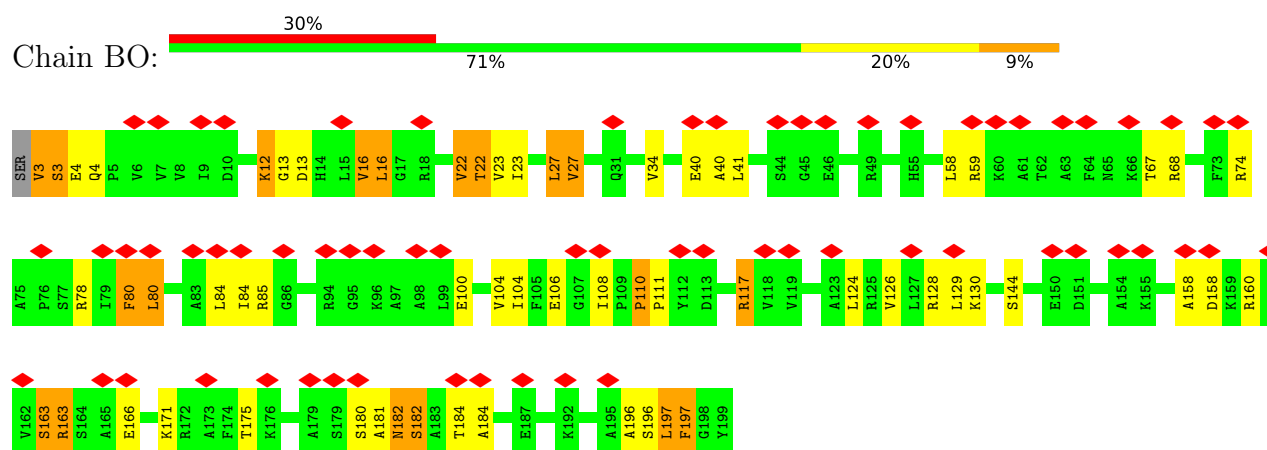




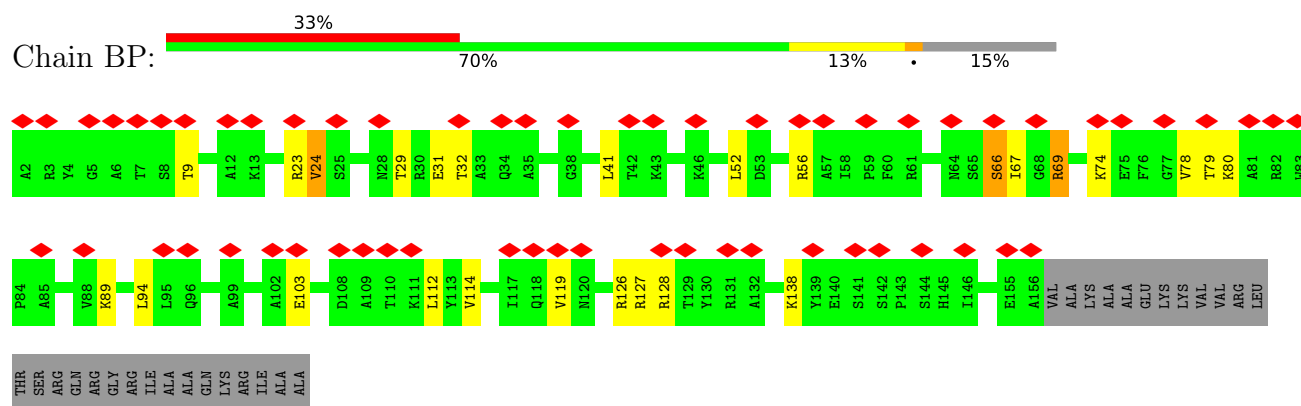
## • Molecule 48: 60S RIBOSOMAL PROTEIN L15-A



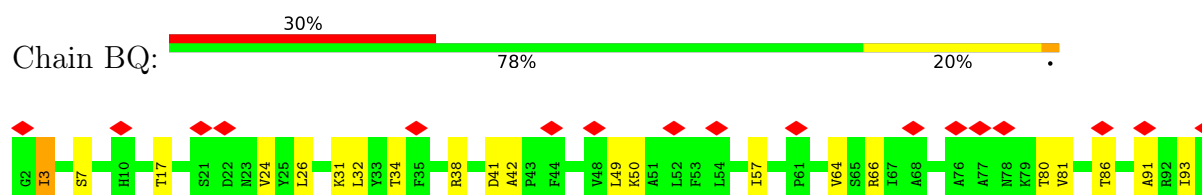
## • Molecule 49: 60S RIBOSOMAL PROTEIN L16-A

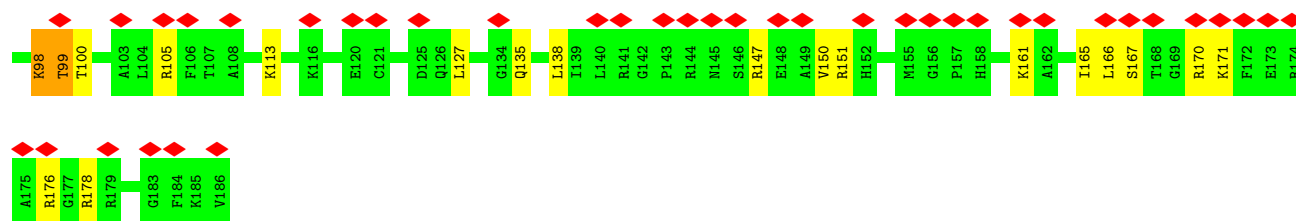


## • Molecule 50: 60S RIBOSOMAL PROTEIN L17-A

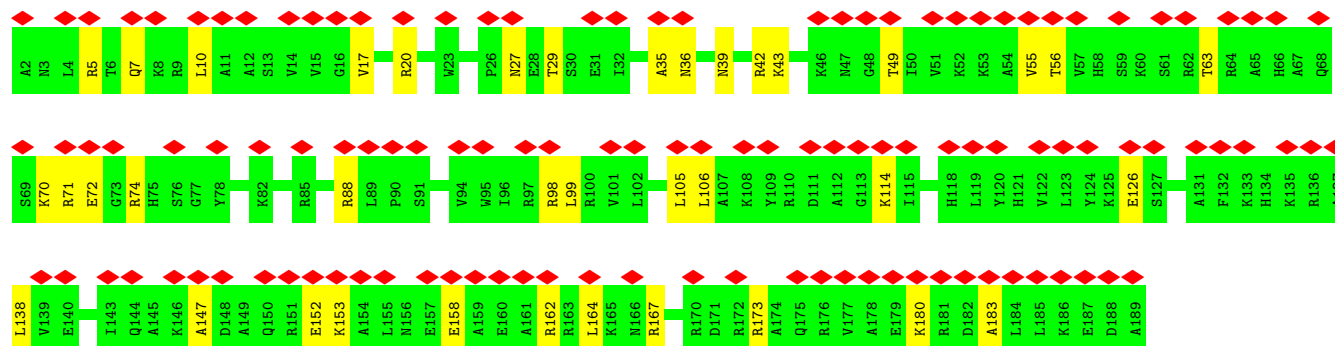
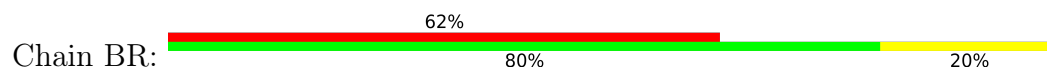


## • Molecule 51: 60S RIBOSOMAL PROTEIN L18-A

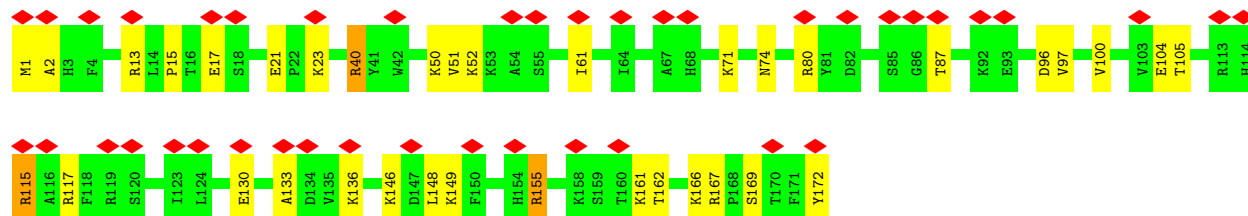
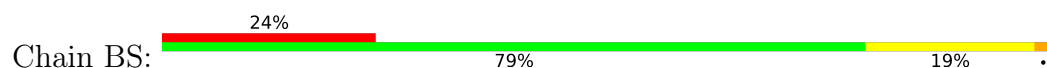




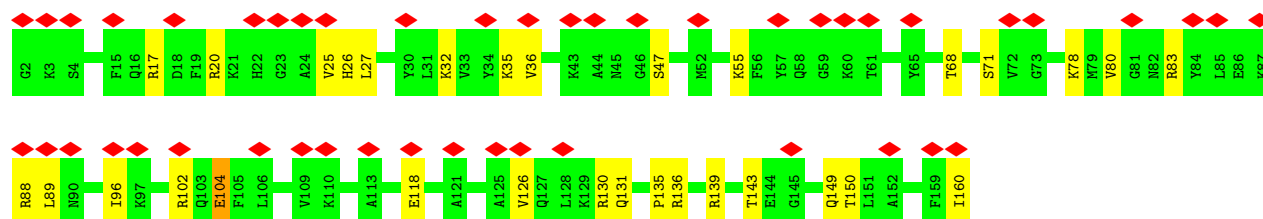
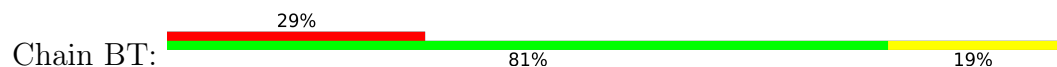
• Molecule 52: 60S RIBOSOMAL PROTEIN L19-B



• Molecule 53: 60S RIBOSOMAL PROTEIN L20-B

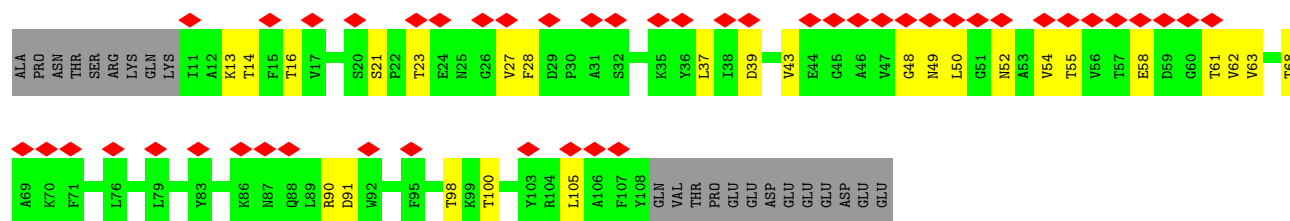


• Molecule 54: 60S RIBOSOMAL PROTEIN L21-A

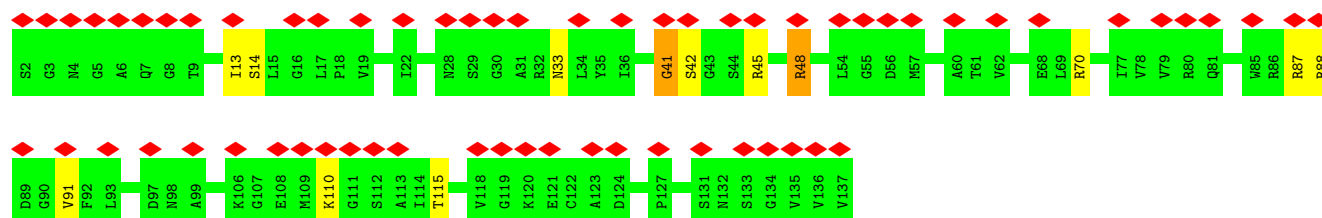


• Molecule 55: 60S RIBOSOMAL PROTEIN L22-A

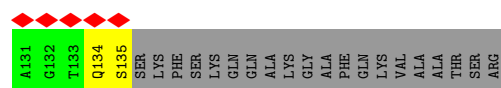
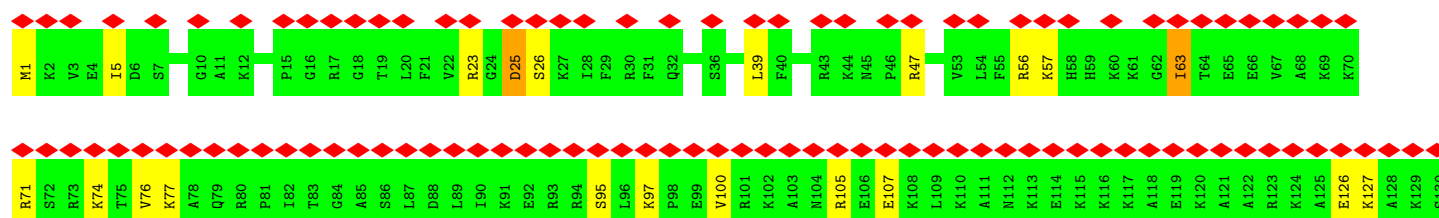
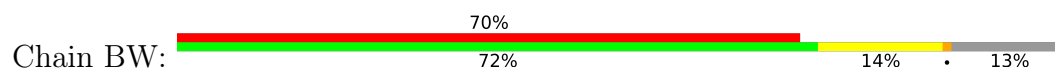




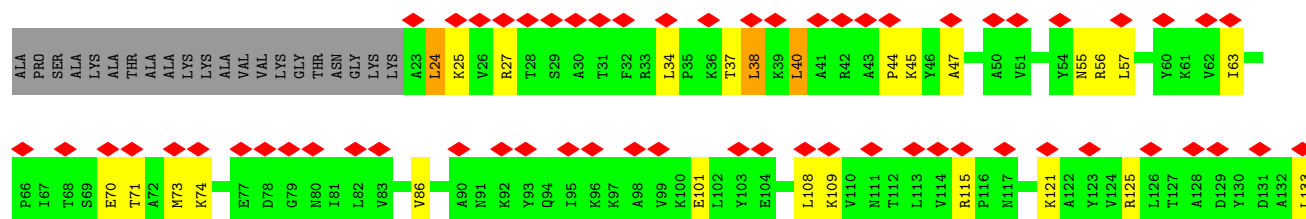
• Molecule 56: 60S RIBOSOMAL PROTEIN L23-A



• Molecule 57: 60S RIBOSOMAL PROTEIN L24-A

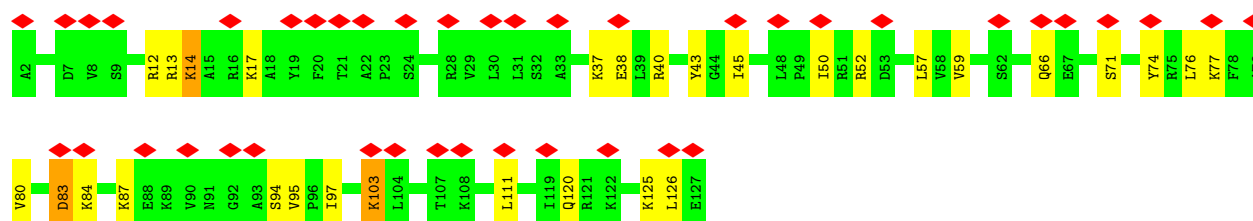
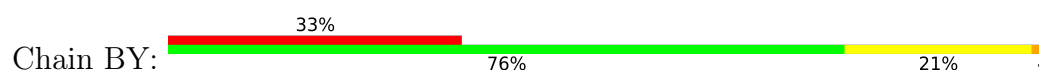


• Molecule 58: 60S RIBOSOMAL PROTEIN L25

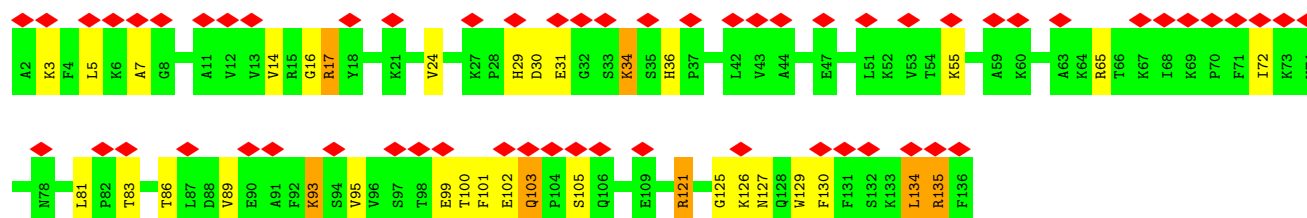
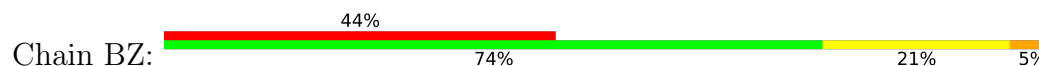


• Molecule 59: 60S RIBOSOMAL PROTEIN L26-A

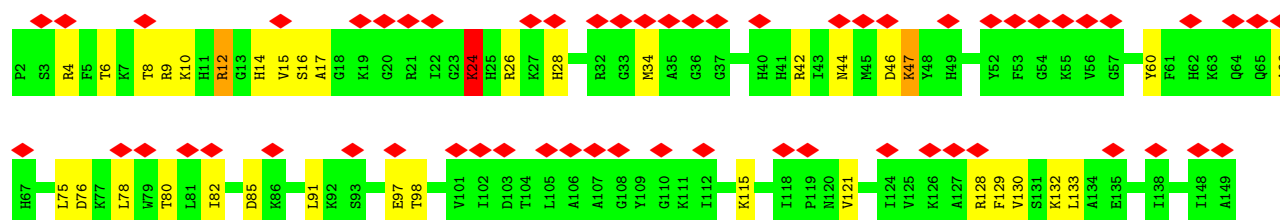
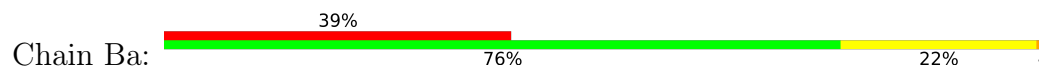




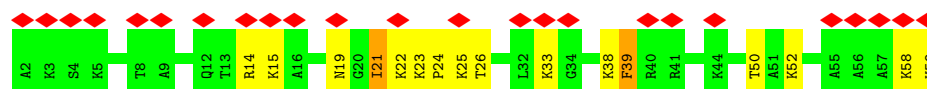
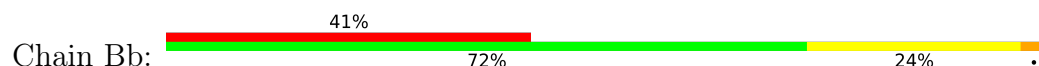
• Molecule 60: 60S RIBOSOMAL PROTEIN L27-A



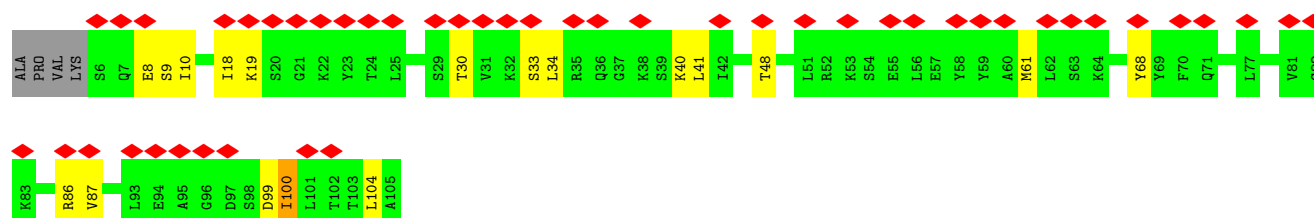
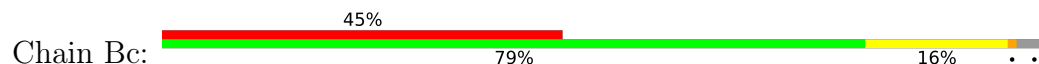
• Molecule 61: 60S RIBOSOMAL PROTEIN L28



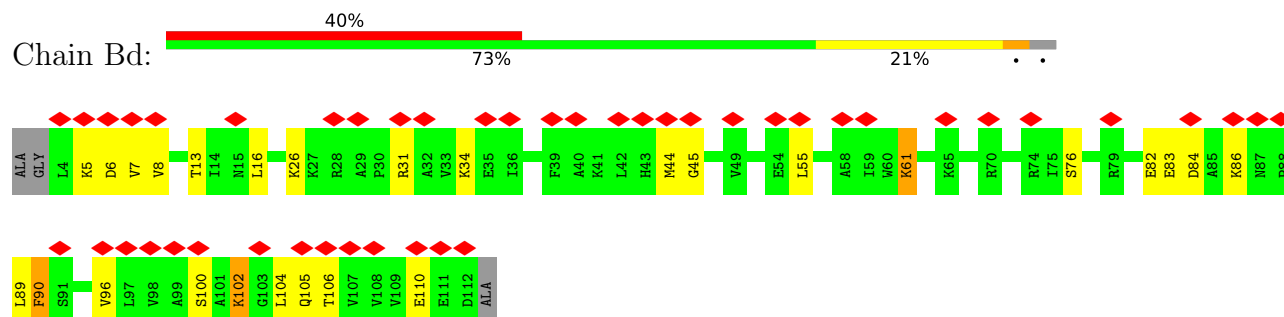
• Molecule 62: 60S RIBOSOMAL PROTEIN L29



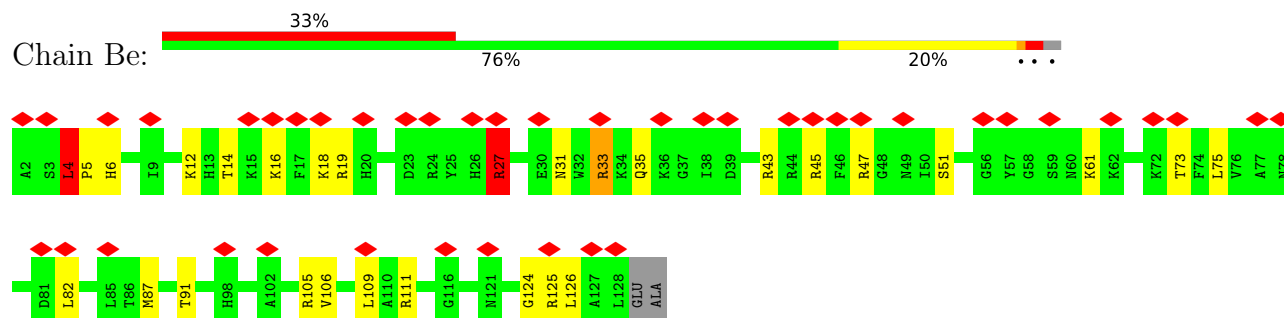
• Molecule 63: 60S RIBOSOMAL PROTEIN L30



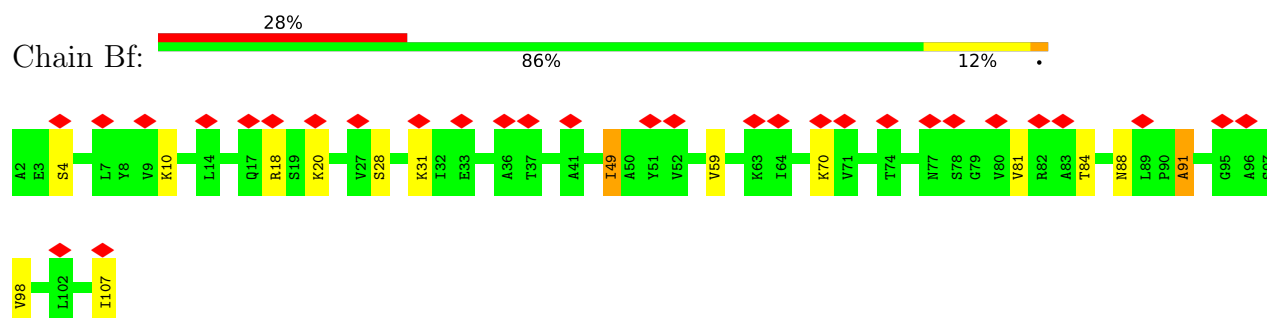
- Molecule 64: 60S RIBOSOMAL PROTEIN L31-A



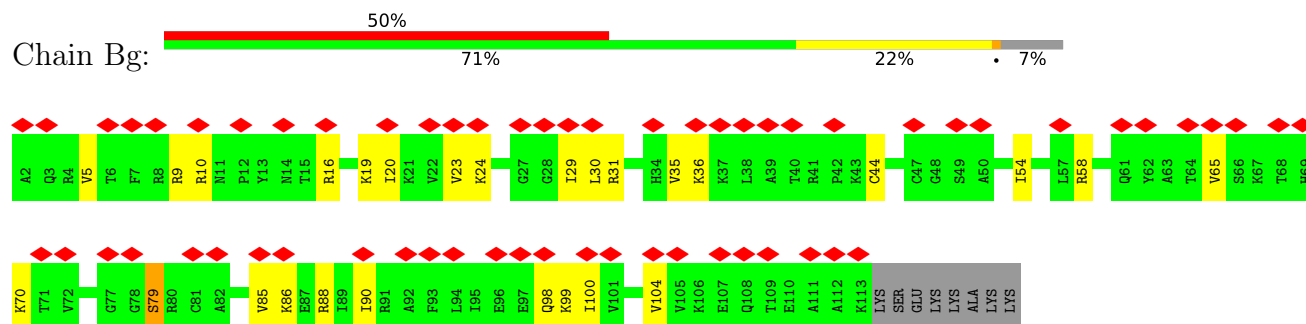
- Molecule 65: 60S RIBOSOMAL PROTEIN L32



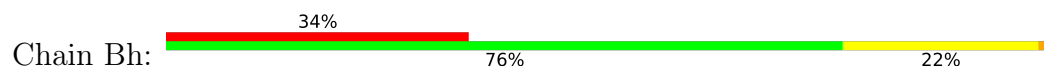
- Molecule 66: 60S RIBOSOMAL PROTEIN L33-A

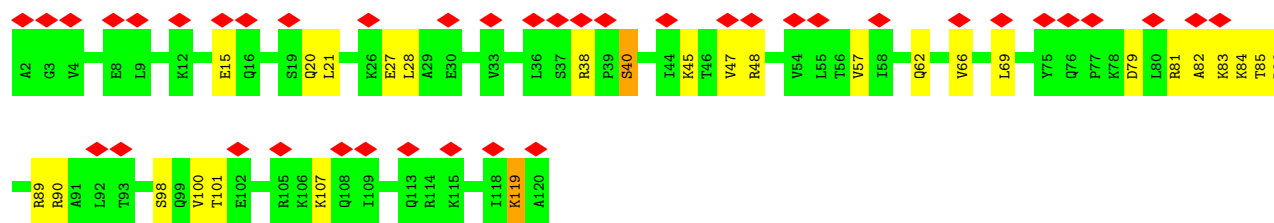


- Molecule 67: 60S RIBOSOMAL PROTEIN L34-A

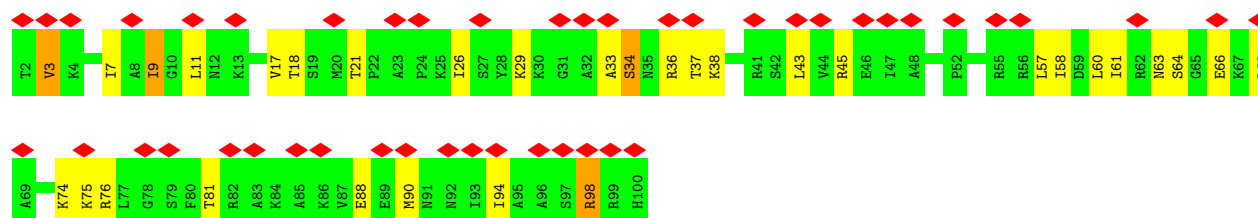


- Molecule 68: 60S RIBOSOMAL PROTEIN L35-B

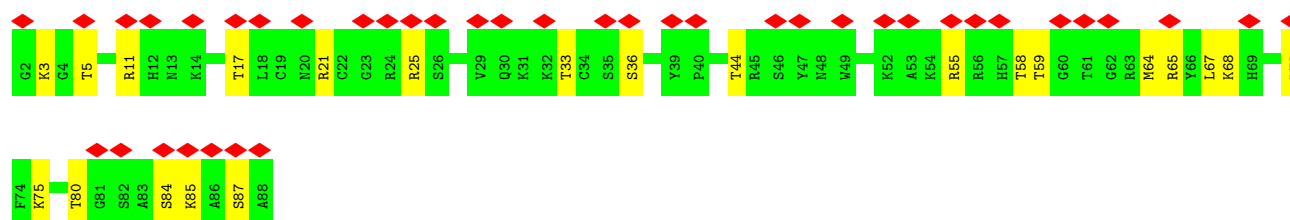
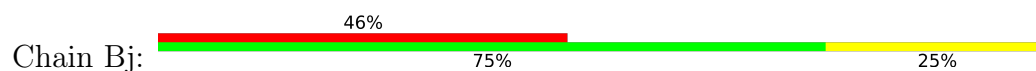




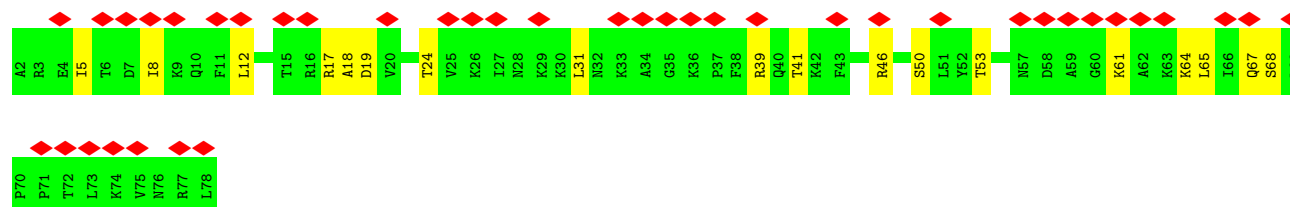
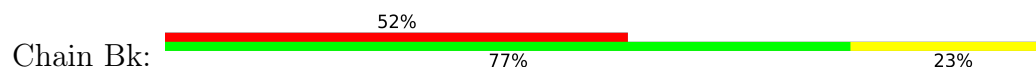
• Molecule 69: 60S RIBOSOMAL PROTEIN L36-A



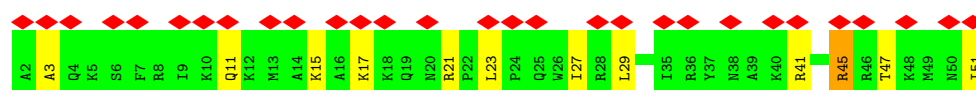
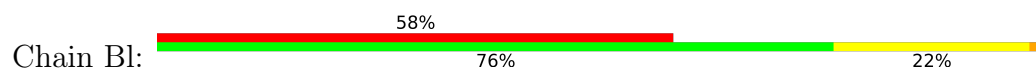
• Molecule 70: 60S RIBOSOMAL PROTEIN L37-A



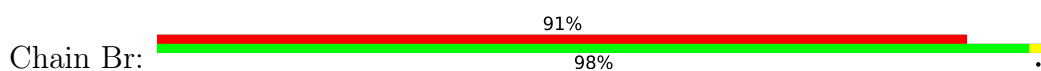
• Molecule 71: 60S RIBOSOMAL PROTEIN L38

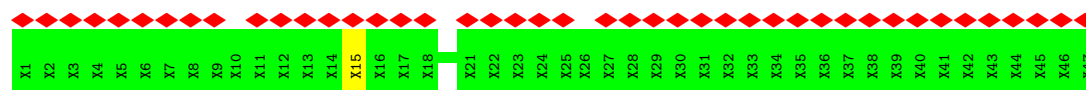


• Molecule 72: 60S RIBOSOMAL PROTEIN L39

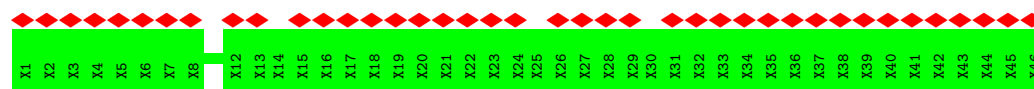
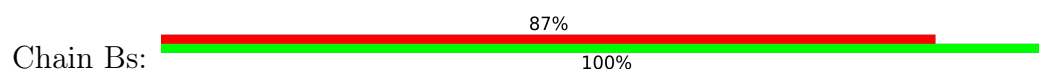


• Molecule 73: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

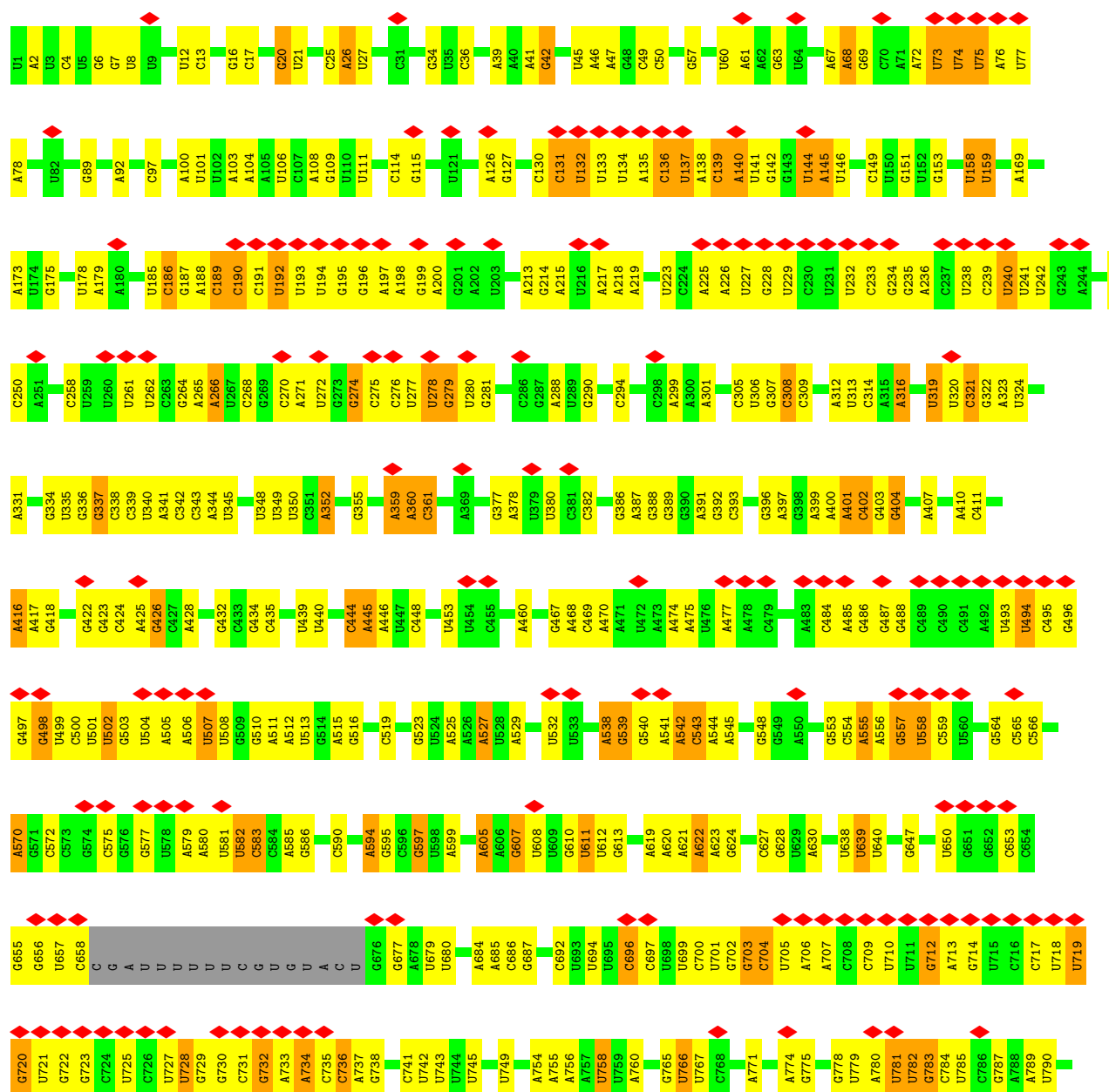




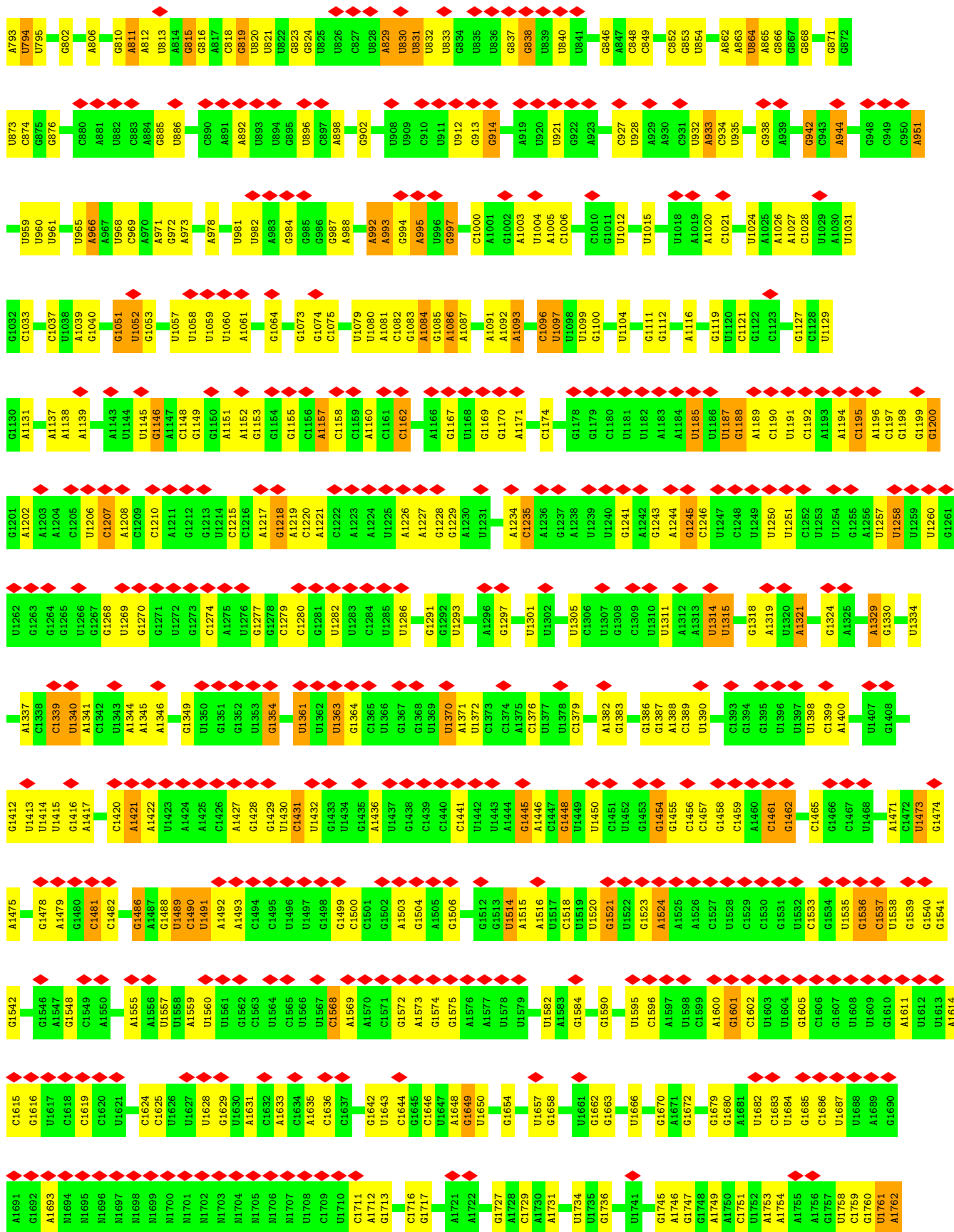
• Molecule 78: 60S ACIDIC RIBOSOMAL PROTEIN P2

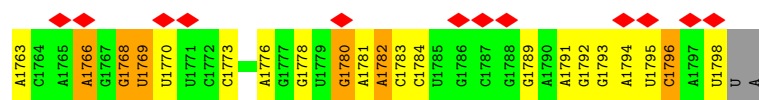


• Molecule 79: 18S RIBOSOMAL RNA

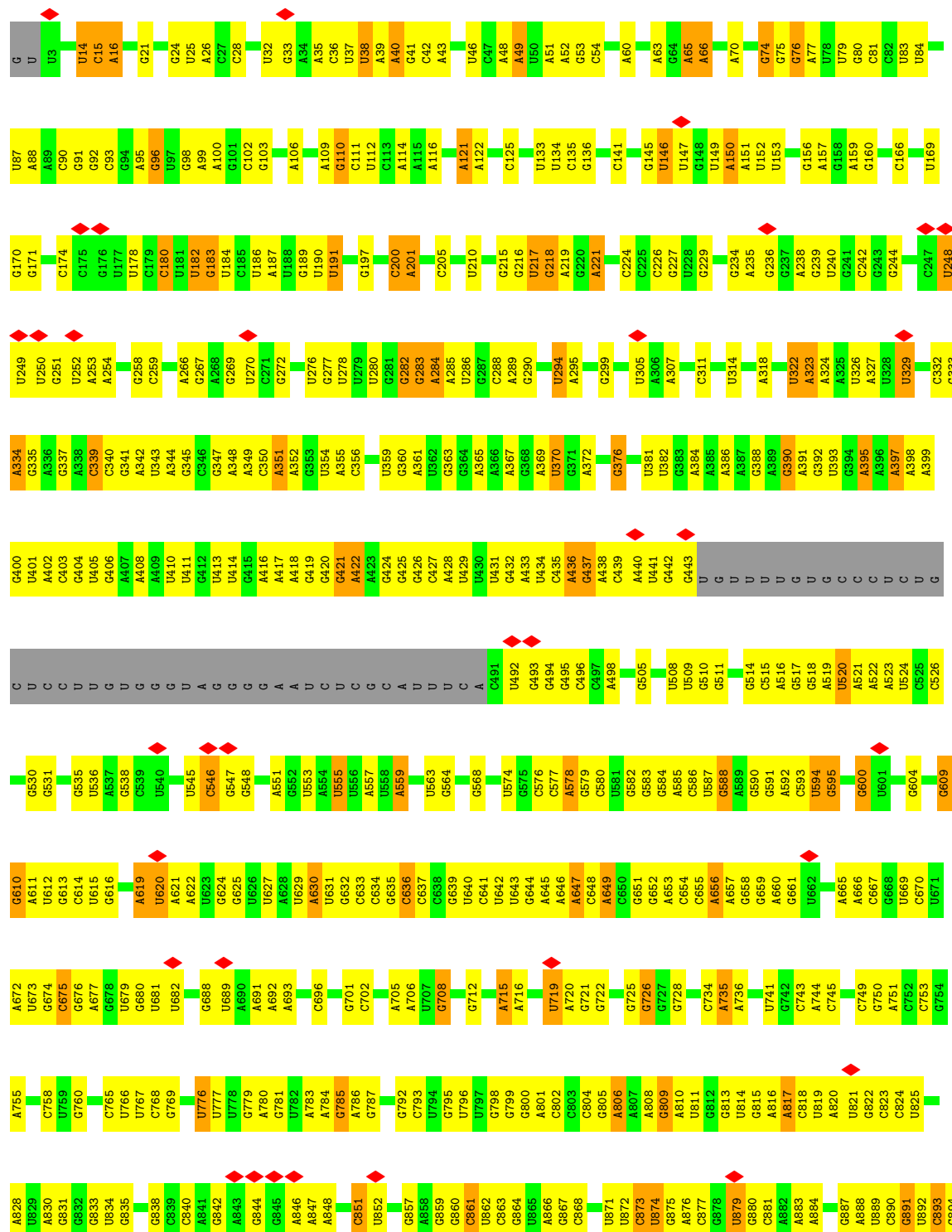


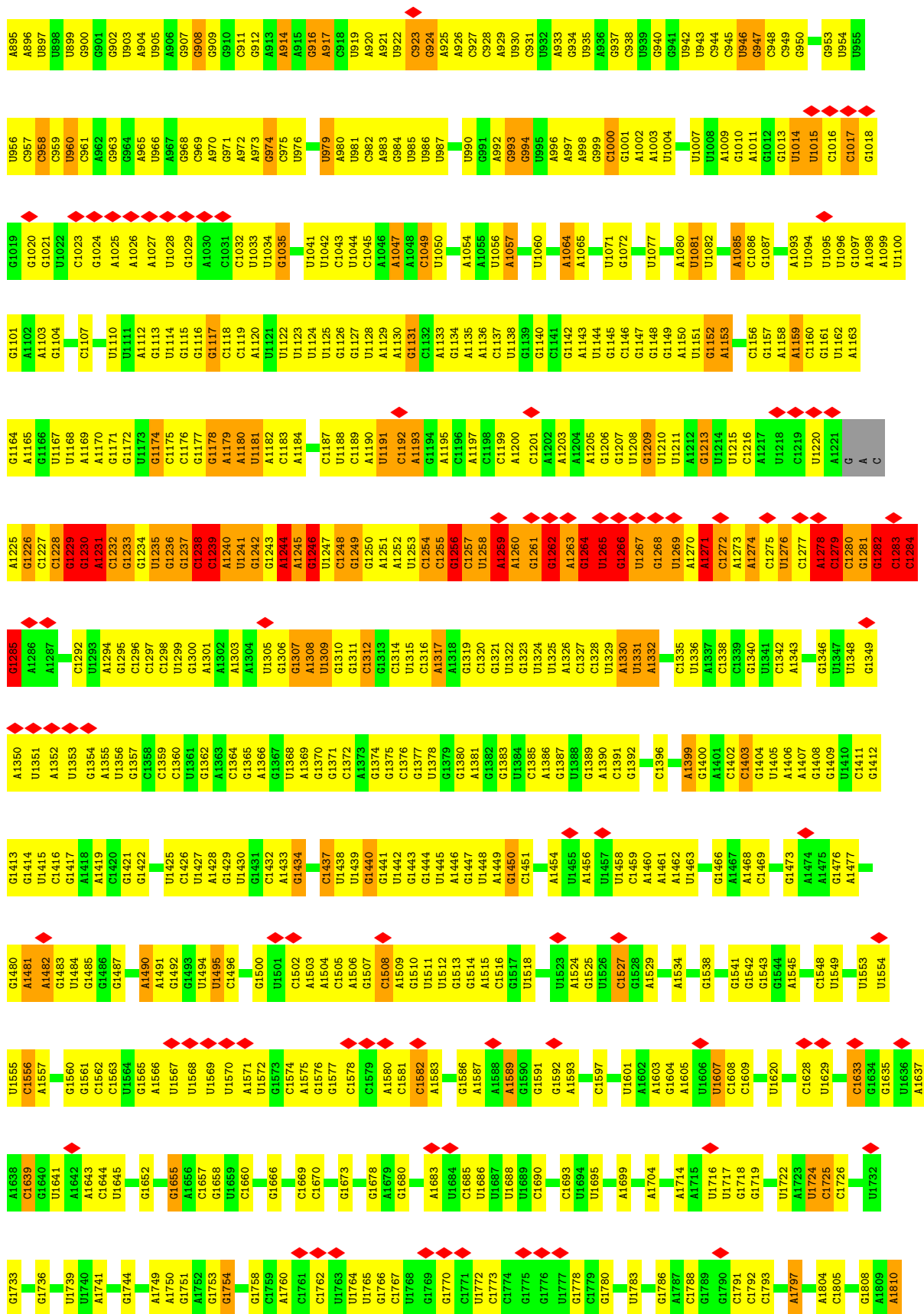




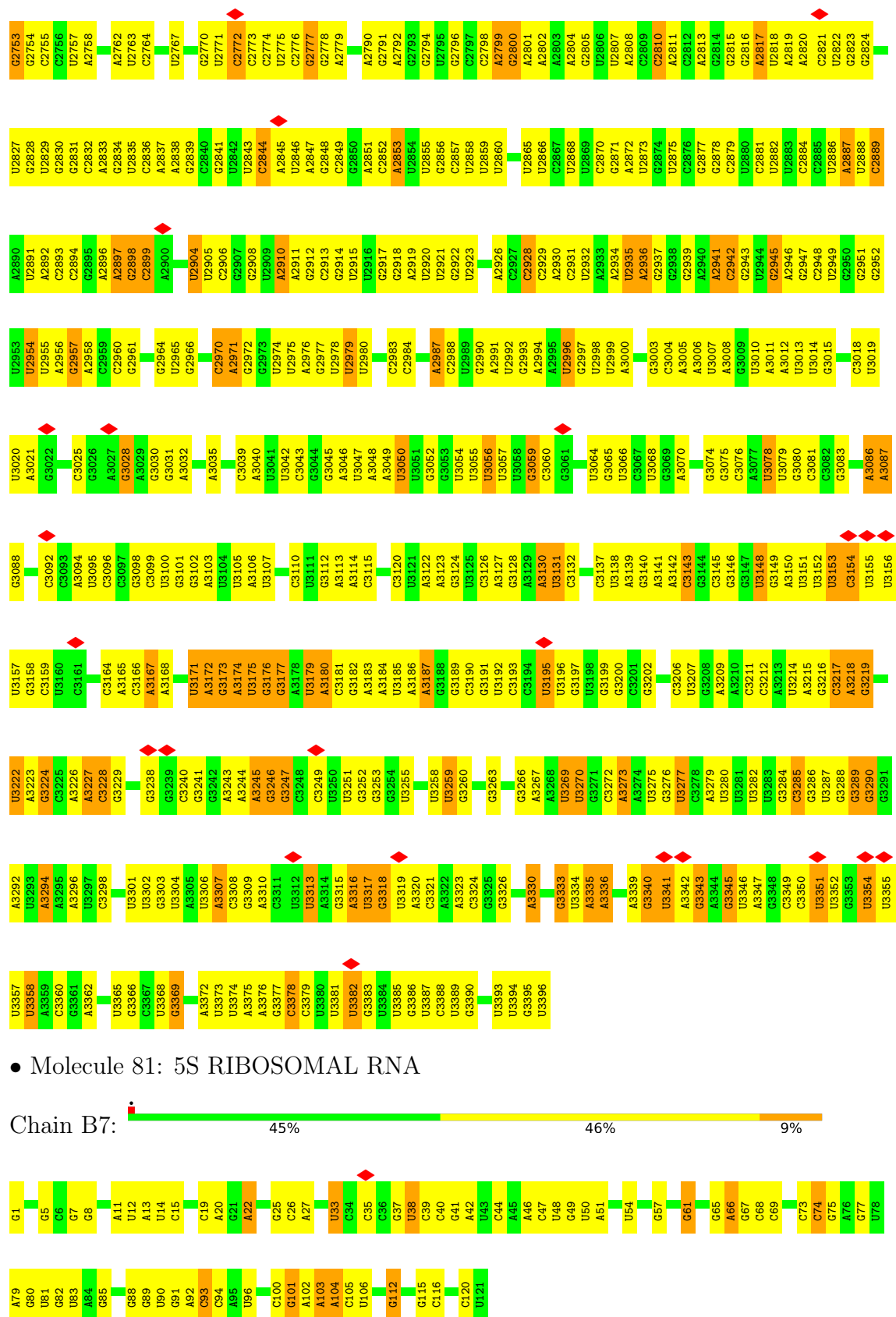


## ● Molecule 80: 25S RIBOSOMAL RNA



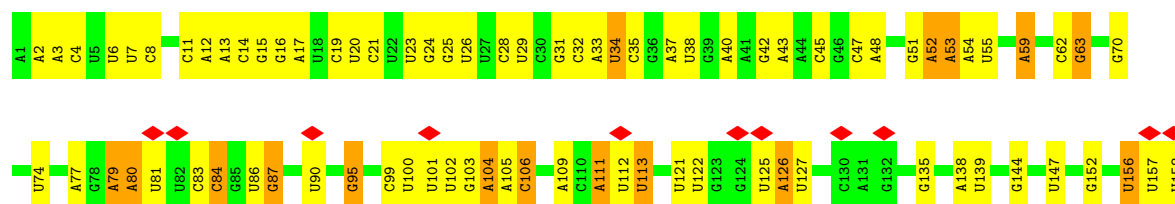




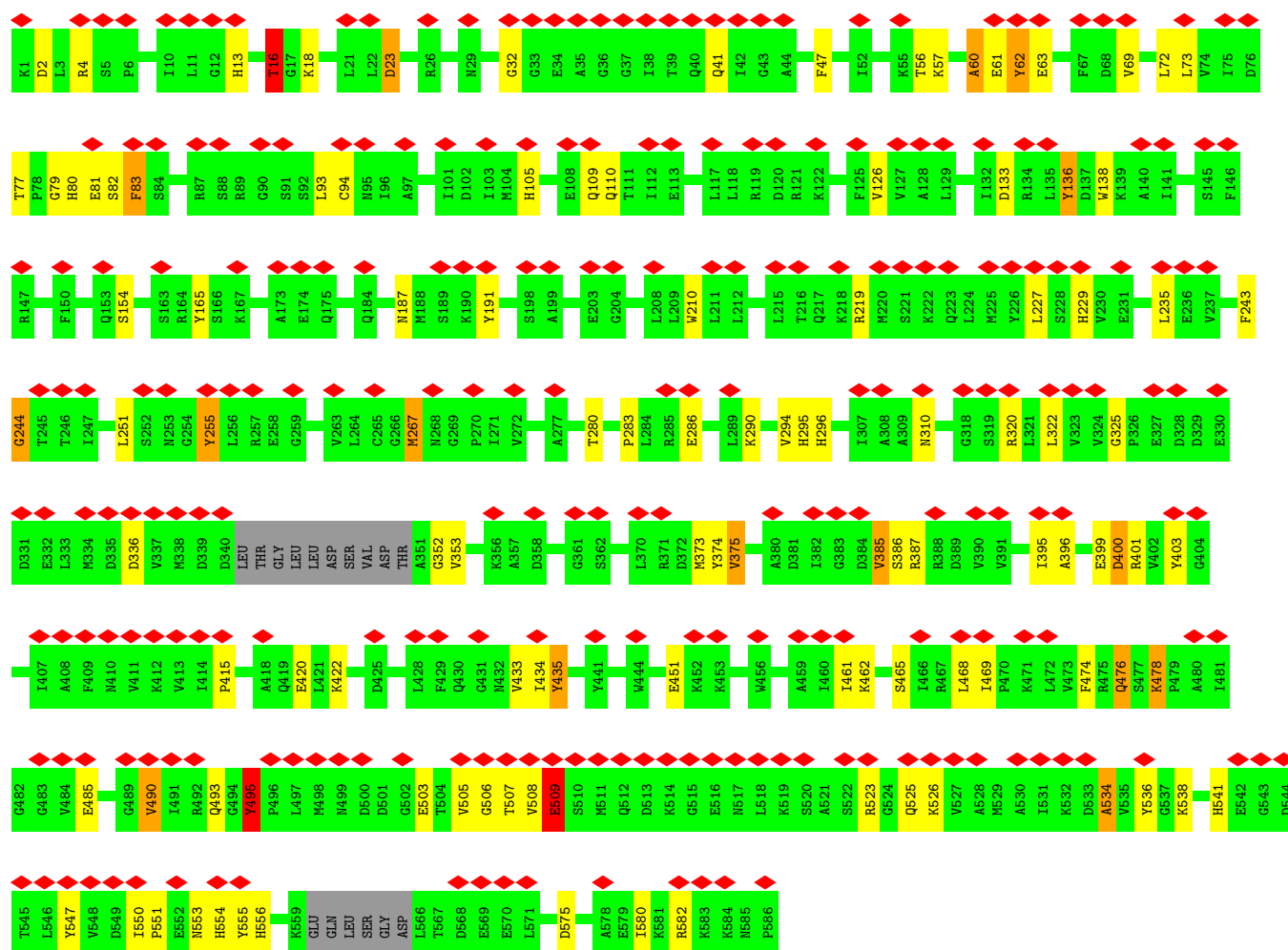
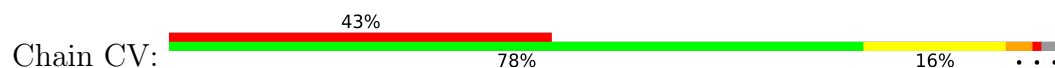


• Molecule 81: 5S RIBOSOMAL RNA

• Molecule 82: 5.8S RIBOSOMAL RNA



- Molecule 83: EUKARYOTIC TRANSLATION INITIATION FACTOR 5B, PROBABLE TRANSLATION INITIATION FACTOR IF-2



- Molecule 84: EUKARYOTIC RIBOSOMAL PI TRNA





- Molecule 85: 5'-R(\*AP\*UP\*GP)-3'



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5143	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	16	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	79096	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	0.643	Depositor
Minimum map value	-0.362	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	424.8, 424.8, 424.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.77, 1.77, 1.77	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OHX, ZN, HSO, GCP, MG

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	A0	0.54	0/782	0.77	0/1047
2	A1	0.53	0/620	0.81	1/838 (0.1%)
3	A2	0.43	0/499	0.72	0/670
4	A3	0.70	0/452	0.94	1/600 (0.2%)
5	A4	0.50	0/483	0.71	0/643
6	A5	0.53	0/404	0.99	1/542 (0.2%)
7	A6	0.49	0/2490	0.70	0/3389
8	A7	0.86	2/925 (0.2%)	0.87	2/1240 (0.2%)
9	AA	0.54	0/1617	0.80	0/2215
10	AB	0.45	0/1735	0.81	0/2335
11	AC	0.60	0/1665	0.77	0/2263
12	AD	0.59	0/1759	0.74	0/2368
13	AE	0.57	0/2109	0.86	1/2839 (0.0%)
14	AF	0.49	0/1629	0.72	0/2202
15	AG	0.55	0/1823	0.75	0/2439
16	AH	0.52	0/1506	0.77	0/2028
17	AI	0.68	0/1514	0.89	3/2021 (0.1%)
18	AJ	0.59	0/1519	0.81	0/2035
19	AK	0.55	0/789	0.83	3/1067 (0.3%)
20	AL	0.70	0/1239	0.81	0/1673
21	AM	0.49	0/898	0.76	0/1220
22	AN	0.61	0/1215	0.83	3/1638 (0.2%)
23	AO	0.48	0/901	0.82	1/1217 (0.1%)
24	AP	0.60	0/998	0.86	3/1341 (0.2%)
25	AQ	0.56	0/1125	0.85	3/1510 (0.2%)
26	AR	0.54	0/935	0.81	0/1254
27	AS	0.59	0/1211	0.80	0/1628
28	AT	0.57	0/1130	0.81	0/1517
29	AU	0.55	0/865	0.76	0/1169
30	AV	0.52	0/693	0.75	0/935
31	AW	0.65	0/1038	0.86	3/1395 (0.2%)
32	AX	0.72	0/1139	0.91	2/1518 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	AY	0.56	0/1087	0.77	1/1449 (0.1%)
34	AZ	0.50	0/571	0.85	1/768 (0.1%)
35	BA	0.87	1/1946 (0.1%)	1.05	4/2614 (0.2%)
36	BB	1.02	4/3146 (0.1%)	1.11	13/4228 (0.3%)
37	BC	0.87	0/2800	1.07	11/3790 (0.3%)
38	BD	0.89	1/2408 (0.0%)	0.96	3/3248 (0.1%)
39	BE	0.90	1/1269 (0.1%)	1.00	3/1705 (0.2%)
40	BF	0.99	1/1828 (0.1%)	1.04	6/2461 (0.2%)
41	BG	0.64	0/1795	0.81	1/2429 (0.0%)
42	BH	0.97	2/1539 (0.1%)	1.01	1/2073 (0.0%)
43	BI	0.92	1/1758 (0.1%)	1.08	12/2358 (0.5%)
44	BJ	0.81	1/1374 (0.1%)	0.99	4/1842 (0.2%)
46	BL	0.82	0/1573	1.04	6/2113 (0.3%)
47	BM	0.96	0/1074	1.01	4/1446 (0.3%)
48	BN	0.83	1/1757 (0.1%)	1.00	6/2354 (0.3%)
49	BO	0.98	11/3159 (0.3%)	1.02	25/4205 (0.6%)
50	BP	1.05	1/1250 (0.1%)	1.09	5/1683 (0.3%)
51	BQ	0.89	1/1465 (0.1%)	1.12	9/1965 (0.5%)
52	BR	0.78	1/1538 (0.1%)	0.87	2/2050 (0.1%)
53	BS	1.02	0/1481	1.09	7/1990 (0.4%)
54	BT	1.01	2/1300 (0.2%)	1.01	1/1743 (0.1%)
55	BU	0.56	0/794	0.77	0/1076
56	BV	0.98	0/1018	1.09	4/1369 (0.3%)
57	BW	0.80	0/1052	0.90	2/1398 (0.1%)
58	BX	0.72	0/974	0.86	0/1314
59	BY	0.79	1/1004 (0.1%)	0.98	2/1341 (0.1%)
60	BZ	0.55	0/1118	0.83	2/1497 (0.1%)
61	Ba	0.95	2/1204 (0.2%)	1.14	9/1612 (0.6%)
62	Bb	0.91	0/473	1.14	1/629 (0.2%)
63	Bc	0.61	0/775	0.77	0/1040
64	Bd	0.94	2/897 (0.2%)	0.95	1/1205 (0.1%)
65	Be	1.03	0/1041	1.27	12/1394 (0.9%)
66	Bf	1.12	0/868	1.09	3/1168 (0.3%)
67	Bg	0.72	0/890	0.92	0/1189
68	Bh	0.67	0/974	0.80	0/1297
69	Bi	0.67	0/777	0.85	0/1033
70	Bj	0.87	0/696	1.04	3/923 (0.3%)
71	Bk	0.50	0/614	0.70	0/822
72	Bl	0.90	0/443	1.02	1/588 (0.2%)
73	Bm	1.08	2/423 (0.5%)	1.13	1/562 (0.2%)
74	Bn	0.90	0/234	1.15	1/300 (0.3%)
75	Bo	0.83	0/860	0.89	1/1136 (0.1%)
76	Bq	1.09	0/1090	1.31	4/1474 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
79	B2	0.92	33/42128 (0.1%)	1.49	828/65642 (1.3%)
80	B5	1.49	661/75336 (0.9%)	1.92	3722/117449 (3.2%)
81	B7	1.38	12/2883 (0.4%)	1.80	119/4491 (2.6%)
82	B8	1.16	4/3746 (0.1%)	1.70	128/5832 (2.2%)
83	CV	1.87	8/4407 (0.2%)	1.47	47/5931 (0.8%)
84	CW	2.08	51/1801 (2.8%)	3.23	250/2803 (8.9%)
85	CX	2.12	4/69 (5.8%)	3.20	11/106 (10.4%)
All	All	1.14	811/222414 (0.4%)	1.53	5304/325931 (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
2	A1	0	1
6	A5	0	2
8	A7	0	1
10	AB	0	1
16	AH	0	1
20	AL	0	1
23	AO	0	1
26	AR	0	2
34	AZ	0	3
35	BA	0	2
37	BC	0	1
38	BD	0	1
39	BE	0	1
40	BF	0	2
49	BO	0	2
53	BS	0	1
56	BV	0	1
59	BY	0	1
60	BZ	0	1
61	Ba	0	3
62	Bb	0	1
76	Bq	0	7
77	Br	0	1
80	B5	0	35
83	CV	0	18
84	CW	0	32
85	CX	0	2
All	All	0	125

All (811) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	CV	63	GLU	N-CA	69.03	2.84	1.46
83	CV	210	TRP	CD2-CE3	34.76	1.92	1.40
83	CV	210	TRP	CD2-CE2	33.01	1.80	1.41
83	CV	210	TRP	CE2-CZ2	31.95	1.94	1.39
83	CV	210	TRP	CE3-CZ3	26.33	1.83	1.38
83	CV	210	TRP	CZ3-CH2	24.12	1.78	1.40
83	CV	210	TRP	CZ2-CH2	23.88	1.82	1.37
49	BO	197[B]	PHE	C-N	-21.97	0.93	1.33
49	BO	182[B]	SER	C-N	18.03	1.75	1.34
80	B5	1152	G	N9-C8	15.03	1.48	1.37
80	B5	1152	G	N9-C4	-14.81	1.26	1.38
8	A7	134	ASP	CG-OD1	13.93	1.57	1.25
80	B5	1226	G	N9-C4	-13.53	1.27	1.38
80	B5	1152	G	C2-N3	-13.37	1.22	1.32
8	A7	134	ASP	CG-OD2	12.60	1.54	1.25
49	BO	23[B]	ILE	C-N	-11.04	1.08	1.34
84	CW	19	G	P-O5'	-10.32	1.49	1.59
84	CW	38	A	N7-C5	-10.09	1.33	1.39
49	BO	3[B]	SER	C-N	9.61	1.56	1.34
80	B5	3216	G	N7-C5	-9.39	1.33	1.39
80	B5	1434	G	N7-C5	-9.19	1.33	1.39
80	B5	1254	C	P-O5'	-9.11	1.50	1.59
80	B5	2941	A	N9-C4	-9.06	1.32	1.37
80	B5	2914	G	P-OP2	-9.05	1.33	1.49
80	B5	1449	A	N9-C4	-8.94	1.32	1.37
80	B5	652	G	N1-C2	-8.82	1.30	1.37
80	B5	953	G	C5-C4	-8.76	1.32	1.38
80	B5	367	A	N9-C4	-8.68	1.32	1.37
80	B5	1227	C	C2-N3	8.65	1.42	1.35
80	B5	1450	G	C8-N7	-8.62	1.25	1.30
49	BO	80[B]	LEU	C-N	8.56	1.53	1.34
80	B5	3088	G	C6-O6	-8.41	1.16	1.24
80	B5	2278	C	C2-O2	-8.28	1.17	1.24
80	B5	2899	C	N3-C4	-8.24	1.28	1.33
80	B5	1227	C	C1'-N1	8.21	1.61	1.48
80	B5	1887	A	N9-C4	-8.21	1.32	1.37
80	B5	2191	U	C4-C5	-8.20	1.36	1.43
79	B2	553	G	C6-N1	8.16	1.45	1.39
80	B5	1178	G	P-OP2	-8.14	1.35	1.49
80	B5	2726	C	N3-C4	-8.10	1.28	1.33
80	B5	2393	G	C8-N7	-8.08	1.26	1.30
80	B5	3216	G	N9-C8	-8.03	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	1152	G	C5-C6	-8.03	1.34	1.42
80	B5	2817	A	P-OP1	-8.01	1.35	1.49
80	B5	1229	G	N7-C5	-7.99	1.34	1.39
35	BA	211	HIS	C-O	7.98	1.38	1.23
80	B5	2280	A	N9-C4	-7.96	1.33	1.37
80	B5	2314	U	N3-C4	7.95	1.45	1.38
80	B5	1152	G	N3-C4	-7.92	1.29	1.35
80	B5	1849	C	N3-C4	-7.91	1.28	1.33
80	B5	953	G	N7-C5	-7.87	1.34	1.39
80	B5	1311	G	C5-C4	-7.87	1.32	1.38
80	B5	917	A	N7-C5	-7.86	1.34	1.39
80	B5	2830	G	C6-N1	-7.86	1.34	1.39
80	B5	3245	A	N9-C4	-7.85	1.33	1.37
80	B5	3114	A	N9-C4	-7.83	1.33	1.37
80	B5	519	A	N7-C5	-7.79	1.34	1.39
80	B5	2945	G	P-O5'	-7.77	1.51	1.59
80	B5	2703	A	N7-C5	-7.72	1.34	1.39
80	B5	631	U	C2-N3	-7.69	1.32	1.37
84	CW	64	A	N7-C5	-7.67	1.34	1.39
80	B5	1902	G	C5-C4	-7.67	1.32	1.38
80	B5	2804	A	N9-C4	-7.65	1.33	1.37
80	B5	1434	G	N9-C8	-7.65	1.32	1.37
54	BT	104	GLU	CB-CG	7.64	1.66	1.52
84	CW	14	A	N7-C5	-7.64	1.34	1.39
80	B5	1301	A	N7-C5	-7.60	1.34	1.39
80	B5	41	G	P-OP1	-7.60	1.36	1.49
80	B5	1285	G	C6-N1	7.58	1.44	1.39
80	B5	345	G	N1-C2	-7.57	1.31	1.37
80	B5	3006	A	N3-C4	-7.57	1.30	1.34
49	BO	84[B]	ILE	C-N	7.55	1.51	1.34
80	B5	970	A	N9-C4	-7.54	1.33	1.37
80	B5	1276	U	C2-N3	7.54	1.43	1.37
80	B5	2314	U	C2-N3	7.52	1.43	1.37
80	B5	2272	G	C5-C4	-7.49	1.33	1.38
80	B5	1307	G	P-O5'	-7.49	1.52	1.59
51	BQ	171	LYS	CE-NZ	7.47	1.67	1.49
80	B5	2385	G	N9-C4	-7.43	1.32	1.38
80	B5	2335	G	N3-C4	-7.43	1.30	1.35
80	B5	2134	G	N1-C2	-7.42	1.31	1.37
80	B5	934	G	P-OP1	-7.40	1.36	1.49
80	B5	2948	C	N3-C4	-7.40	1.28	1.33
80	B5	2191	U	C4-O4	-7.39	1.17	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	1902	G	P-OP1	-7.39	1.36	1.49
80	B5	960	U	N1-C2	7.35	1.45	1.38
80	B5	953	G	N9-C8	-7.34	1.32	1.37
84	CW	15	G	N9-C4	-7.34	1.32	1.38
80	B5	1303	A	C5-C4	-7.32	1.33	1.38
80	B5	2943	G	N7-C5	-7.30	1.34	1.39
80	B5	3122	A	N3-C4	-7.30	1.30	1.34
80	B5	3245	A	C5-C6	-7.29	1.34	1.41
80	B5	1374	G	N1-C2	-7.27	1.31	1.37
80	B5	345	G	C6-N1	-7.27	1.34	1.39
80	B5	1515	A	C5-C6	-7.26	1.34	1.41
80	B5	1443	G	C2-N3	-7.24	1.26	1.32
80	B5	2919	A	C6-N1	-7.21	1.30	1.35
84	CW	42	C	O3'-P	-7.21	1.52	1.61
80	B5	644	G	N7-C5	-7.21	1.34	1.39
80	B5	2141	U	P-OP2	-7.19	1.36	1.49
81	B7	85	G	N1-C2	-7.19	1.31	1.37
80	B5	1849	C	C2-N3	-7.17	1.30	1.35
80	B5	2364	G	C6-N1	-7.16	1.34	1.39
80	B5	2689	A	N3-C4	-7.16	1.30	1.34
80	B5	2949	U	P-OP1	-7.16	1.36	1.49
80	B5	2364	G	N3-C4	-7.14	1.30	1.35
80	B5	1200	A	N3-C4	-7.12	1.30	1.34
80	B5	1430	U	P-OP1	-7.10	1.36	1.49
80	B5	2837	A	C5-C4	-7.10	1.33	1.38
84	CW	12	U	C2'-C1'	-7.10	1.45	1.53
79	B2	377	G	N9-C4	-7.09	1.32	1.38
81	B7	96	U	C2-O2	-7.07	1.16	1.22
80	B5	726	G	C5-C6	-7.03	1.35	1.42
82	B8	20	U	C4-O4	-7.03	1.18	1.23
80	B5	1233	G	C2'-C1'	-7.03	1.45	1.53
80	B5	1112	A	N7-C5	-7.01	1.35	1.39
80	B5	1887	A	N7-C5	-7.00	1.35	1.39
80	B5	2434	U	N3-C4	-6.99	1.32	1.38
80	B5	971	G	C5-C4	-6.98	1.33	1.38
84	CW	19	G	C6-N1	6.97	1.44	1.39
80	B5	420	G	N7-C5	-6.96	1.35	1.39
80	B5	2887	A	P-OP2	-6.96	1.37	1.49
80	B5	1042	U	C2-N3	-6.96	1.32	1.37
80	B5	2335	G	C6-N1	-6.94	1.34	1.39
80	B5	1159	A	N9-C4	-6.94	1.33	1.37
84	CW	72	C	C4'-C3'	6.94	1.60	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	3180	A	N3-C4	-6.91	1.30	1.34
80	B5	1110	U	C4-O4	-6.90	1.18	1.23
84	CW	67	C	C3'-O3'	6.90	1.51	1.42
80	B5	2361	A	N9-C4	6.90	1.42	1.37
79	B2	1456	C	N3-C4	-6.90	1.29	1.33
80	B5	2399	A	N9-C4	-6.88	1.33	1.37
80	B5	340	C	P-OP1	-6.86	1.37	1.49
80	B5	2336	U	C2-N3	-6.86	1.32	1.37
80	B5	2395	G	C5-C4	-6.84	1.33	1.38
80	B5	1184	A	N9-C4	-6.82	1.33	1.37
80	B5	1592	G	N1-C2	-6.79	1.32	1.37
80	B5	1901	A	N7-C5	-6.79	1.35	1.39
80	B5	2836	C	C4-C5	6.78	1.48	1.43
80	B5	1319	G	N7-C5	-6.77	1.35	1.39
80	B5	986	U	C4-C5	-6.76	1.37	1.43
80	B5	1178	G	C2-N3	-6.75	1.27	1.32
80	B5	1592	G	C6-N1	-6.75	1.34	1.39
80	B5	2636	A	C6-N1	-6.75	1.30	1.35
80	B5	334	A	C5-C4	-6.74	1.34	1.38
84	CW	16	U	P-O5'	-6.74	1.53	1.59
80	B5	429	U	C2-N3	-6.74	1.33	1.37
84	CW	5	G	C2-N3	6.73	1.38	1.32
80	B5	930	U	C4-O4	-6.73	1.18	1.23
80	B5	2138	A	N7-C5	-6.73	1.35	1.39
80	B5	1449	A	P-OP2	-6.73	1.37	1.49
79	B2	1455	G	C6-O6	6.72	1.30	1.24
80	B5	3316	A	N9-C4	-6.71	1.33	1.37
84	CW	37	A	C2'-C1'	-6.71	1.46	1.53
80	B5	1227	C	N3-C4	6.70	1.38	1.33
80	B5	847	A	N9-C4	-6.70	1.33	1.37
80	B5	2912	G	N7-C5	-6.69	1.35	1.39
80	B5	2853	A	N9-C4	-6.69	1.33	1.37
79	B2	992	A	C2-N3	-6.69	1.27	1.33
81	B7	85	G	C6-N1	-6.68	1.34	1.39
79	B2	553	G	C6-O6	6.66	1.30	1.24
80	B5	3006	A	N9-C4	-6.64	1.33	1.37
81	B7	81	U	C4-O4	-6.63	1.18	1.23
80	B5	1301	A	C5-C6	-6.62	1.35	1.41
80	B5	2918	G	N7-C5	-6.61	1.35	1.39
80	B5	2911	A	N7-C5	-6.61	1.35	1.39
80	B5	2693	C	C2-N3	-6.61	1.30	1.35
84	CW	7	A	O3'-P	-6.60	1.53	1.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	B2	1200	G	C6-N1	6.59	1.44	1.39
80	B5	1371	G	C6-N1	-6.58	1.34	1.39
80	B5	3137	C	N1-C6	6.58	1.41	1.37
49	BO	22[B]	THR	C-N	6.57	1.49	1.34
80	B5	1515	A	C6-N1	-6.57	1.30	1.35
85	CX	3	G	P-O5'	-6.56	1.53	1.59
49	BO	158[B]	ASP	C-N	6.56	1.49	1.34
80	B5	267	G	C8-N7	-6.56	1.27	1.30
80	B5	91	G	N3-C4	-6.56	1.30	1.35
80	B5	1429	G	C6-N1	-6.55	1.34	1.39
80	B5	3362	A	N3-C4	-6.55	1.30	1.34
80	B5	859	G	N1-C2	-6.53	1.32	1.37
80	B5	1833	G	N1-C2	-6.53	1.32	1.37
80	B5	1841	A	N7-C5	-6.53	1.35	1.39
80	B5	1849	C	N1-C6	-6.52	1.33	1.37
80	B5	1142	G	N7-C5	-6.52	1.35	1.39
80	B5	3106	A	N7-C5	-6.51	1.35	1.39
80	B5	1307	G	C3'-O3'	6.51	1.51	1.42
80	B5	3209	A	C5-C4	6.50	1.43	1.38
80	B5	942	U	P-OP1	-6.50	1.38	1.49
80	B5	813	G	N7-C5	-6.48	1.35	1.39
80	B5	1406	A	N3-C4	-6.46	1.30	1.34
80	B5	642	U	N3-C4	-6.44	1.32	1.38
80	B5	2323	G	C6-N1	-6.44	1.35	1.39
80	B5	1487	G	N1-C2	-6.43	1.32	1.37
80	B5	637	C	C2-O2	-6.43	1.18	1.24
80	B5	1117	G	C5-C4	-6.43	1.33	1.38
80	B5	2816	G	C5-C4	-6.43	1.33	1.38
80	B5	2147	A	C5-C6	-6.42	1.35	1.41
80	B5	2987	A	N7-C5	-6.41	1.35	1.39
79	B2	992	A	N9-C4	-6.40	1.34	1.37
80	B5	1490	A	N7-C5	-6.40	1.35	1.39
80	B5	1370	G	N1-C2	-6.40	1.32	1.37
79	B2	1754	A	N9-C4	-6.39	1.34	1.37
84	CW	58	A	N7-C5	-6.39	1.35	1.39
80	B5	3102	G	C6-N1	-6.38	1.35	1.39
80	B5	2123	G	C5-C4	-6.37	1.33	1.38
80	B5	2937	G	N9-C8	-6.37	1.33	1.37
84	CW	37	A	N7-C5	-6.36	1.35	1.39
80	B5	802	C	N1-C6	-6.36	1.33	1.37
84	CW	59	U	C2'-C1'	-6.35	1.46	1.53
80	B5	1143	A	N9-C4	-6.31	1.34	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	2905	U	C2-N3	-6.31	1.33	1.37
84	CW	67	C	C1'-N1	6.30	1.58	1.48
80	B5	2291	A	N3-C4	-6.29	1.31	1.34
80	B5	1902	G	N9-C8	-6.29	1.33	1.37
80	B5	2314	U	C4-O4	6.29	1.28	1.23
79	B2	1241	G	N9-C8	6.28	1.42	1.37
80	B5	2856	G	N9-C8	-6.28	1.33	1.37
80	B5	342	A	N9-C4	-6.28	1.34	1.37
80	B5	420	G	C5-C4	-6.28	1.33	1.38
80	B5	1259	A	N7-C5	-6.27	1.35	1.39
80	B5	1913	A	C5-C6	-6.26	1.35	1.41
80	B5	1258	U	P-O5'	-6.26	1.53	1.59
80	B5	3182	G	C6-N1	-6.26	1.35	1.39
80	B5	2754	G	P-OP1	-6.25	1.38	1.49
54	BT	32	LYS	CD-CE	6.25	1.66	1.51
80	B5	1487	G	C6-N1	-6.25	1.35	1.39
80	B5	1449	A	C5-C6	-6.23	1.35	1.41
80	B5	1226	G	N7-C5	-6.23	1.35	1.39
80	B5	872	U	C4-O4	-6.21	1.18	1.23
80	B5	1851	G	N9-C8	-6.21	1.33	1.37
80	B5	2194	G	C5-C4	-6.21	1.34	1.38
84	CW	6	G	N7-C5	-6.21	1.35	1.39
79	B2	49	C	P-OP2	-6.21	1.38	1.49
80	B5	953	G	N9-C4	-6.21	1.32	1.38
50	BP	66	SER	C-O	6.20	1.35	1.23
80	B5	434	U	C2-N3	-6.19	1.33	1.37
84	CW	11	C	P-O5'	-6.19	1.53	1.59
80	B5	1835	A	P-OP1	-6.19	1.38	1.49
80	B5	2881	C	C2-O2	-6.19	1.18	1.24
80	B5	1797	A	N7-C5	-6.18	1.35	1.39
80	B5	2858	U	N3-C4	-6.18	1.32	1.38
80	B5	1229	G	C5'-C4'	6.18	1.58	1.51
80	B5	884	A	C8-N7	6.18	1.35	1.31
80	B5	2128	C	N1-C6	-6.18	1.33	1.37
80	B5	363	G	C5-C4	-6.17	1.34	1.38
80	B5	795	G	C5-C4	-6.16	1.34	1.38
80	B5	421	G	C6-N1	-6.16	1.35	1.39
80	B5	1369	A	P-OP2	-6.16	1.38	1.49
81	B7	91	G	N9-C8	-6.16	1.33	1.37
36	BB	367	LYS	CE-NZ	6.16	1.64	1.49
61	Ba	24	LYS	CE-NZ	6.15	1.64	1.49
80	B5	1847	A	N9-C4	-6.15	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	2848	G	N7-C5	-6.15	1.35	1.39
80	B5	2737	C	N1-C6	-6.14	1.33	1.37
80	B5	3008	A	N9-C4	-6.14	1.34	1.37
80	B5	218	G	P-O5'	-6.14	1.53	1.59
80	B5	2823	G	N7-C5	-6.14	1.35	1.39
80	B5	876	A	N3-C4	-6.13	1.31	1.34
80	B5	1279	C	C2'-C1'	-6.13	1.46	1.53
80	B5	649	A	C5-C6	-6.13	1.35	1.41
80	B5	3308	C	N3-C4	-6.13	1.29	1.33
39	BE	90	LYS	CD-CE	6.12	1.66	1.51
80	B5	659	G	N7-C5	-6.12	1.35	1.39
80	B5	1169	A	N9-C4	-6.12	1.34	1.37
80	B5	2830	G	N3-C4	-6.11	1.31	1.35
80	B5	3172	A	C8-N7	-6.11	1.27	1.31
80	B5	2377	G	N9-C8	-6.11	1.33	1.37
80	B5	1268	G	N7-C5	-6.10	1.35	1.39
81	B7	96	U	C4-O4	-6.10	1.18	1.23
80	B5	2975	U	C4-O4	-6.09	1.18	1.23
84	CW	28	G	C2'-C1'	-6.09	1.46	1.53
80	B5	1490	A	C5-C6	-6.08	1.35	1.41
80	B5	2980	U	C2-O2	-6.06	1.16	1.22
80	B5	2915	U	C2-O2	-6.06	1.16	1.22
80	B5	2733	A	N9-C4	-6.05	1.34	1.37
80	B5	1152	G	C8-N7	6.04	1.34	1.30
80	B5	3102	G	N1-C2	-6.04	1.32	1.37
84	CW	25	C	C2'-C1'	-6.04	1.46	1.53
80	B5	2341	A	N3-C4	6.04	1.38	1.34
80	B5	859	G	C6-N1	-6.03	1.35	1.39
80	B5	3005	A	C6-N1	-6.03	1.31	1.35
84	CW	38	A	C8-N7	-6.03	1.27	1.31
80	B5	1454	A	C6-N6	-6.03	1.29	1.33
80	B5	2524	A	C5-C4	6.03	1.43	1.38
80	B5	2857	C	C4-N4	-6.02	1.28	1.33
80	B5	1149	G	C5-C4	-6.01	1.34	1.38
80	B5	3335	A	N9-C4	-6.01	1.34	1.37
36	BB	262	TRP	CB-CG	-6.01	1.39	1.50
80	B5	3006	A	N7-C5	-6.00	1.35	1.39
79	B2	1782	A	C6-N1	-6.00	1.31	1.35
80	B5	1256	G	O3'-P	-6.00	1.53	1.61
83	CV	63	GLU	CA-CB	6.00	1.67	1.53
80	B5	2372	A	N3-C4	-5.99	1.31	1.34
80	B5	2948	C	C4-N4	-5.98	1.28	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	1837	U	P-OP2	-5.98	1.38	1.49
80	B5	647	A	N3-C4	-5.97	1.31	1.34
80	B5	2214	A	P-OP2	-5.97	1.38	1.49
80	B5	1504	A	C6-N1	-5.97	1.31	1.35
81	B7	89	G	C5-C4	-5.97	1.34	1.38
80	B5	2730	G	N9-C4	-5.94	1.33	1.38
82	B8	111	A	N9-C4	-5.94	1.34	1.37
84	CW	45	U	P-O5'	-5.94	1.53	1.59
80	B5	1152	G	N1-C2	5.93	1.42	1.37
80	B5	1274	A	N7-C5	-5.92	1.35	1.39
80	B5	348	A	P-OP1	-5.92	1.38	1.49
80	B5	1233	G	C5'-C4'	5.92	1.58	1.51
80	B5	1174	G	C5-C4	-5.91	1.34	1.38
80	B5	744	A	N9-C4	-5.91	1.34	1.37
80	B5	2946	A	C6-N1	-5.90	1.31	1.35
80	B5	1138	U	C4-O4	-5.89	1.19	1.23
80	B5	1203	A	C5-C6	-5.89	1.35	1.41
80	B5	2704	A	N7-C5	-5.88	1.35	1.39
80	B5	857	G	C6-O6	-5.88	1.18	1.24
80	B5	931	C	C4-N4	-5.88	1.28	1.33
80	B5	345	G	C5-C4	-5.87	1.34	1.38
80	B5	1449	A	N7-C5	-5.87	1.35	1.39
80	B5	2706	G	C5-C4	-5.87	1.34	1.38
80	B5	784	A	C5-C6	-5.87	1.35	1.41
80	B5	416	A	N7-C5	-5.87	1.35	1.39
80	B5	2971	A	N9-C4	5.87	1.41	1.37
80	B5	3005	A	N7-C5	-5.86	1.35	1.39
80	B5	1332	A	C6-N1	-5.86	1.31	1.35
80	B5	2335	G	C5-C4	-5.86	1.34	1.38
80	B5	922	U	P-OP2	-5.86	1.39	1.49
80	B5	1429	G	N9-C8	-5.85	1.33	1.37
80	B5	2884	C	C2-O2	-5.84	1.19	1.24
80	B5	3095	U	C4-O4	-5.84	1.19	1.23
80	B5	1332	A	C5-C4	-5.84	1.34	1.38
80	B5	1266	G	C6-N1	5.84	1.43	1.39
80	B5	2960	C	C4-N4	-5.84	1.28	1.33
80	B5	2977	G	C6-N1	-5.84	1.35	1.39
80	B5	3000	A	N9-C4	-5.84	1.34	1.37
80	B5	3227	A	N3-C4	-5.84	1.31	1.34
80	B5	3010	U	C2-N3	-5.83	1.33	1.37
80	B5	1172	G	N1-C2	-5.82	1.33	1.37
80	B5	2188	A	N3-C4	-5.82	1.31	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	518	G	C5-C4	-5.82	1.34	1.38
79	B2	992	A	N9-C8	5.81	1.42	1.37
80	B5	2278	C	N1-C6	5.81	1.40	1.37
80	B5	1462	A	N9-C4	-5.80	1.34	1.37
80	B5	1156	C	C4-N4	-5.80	1.28	1.33
80	B5	1149	G	N9-C8	-5.79	1.33	1.37
80	B5	2367	A	N9-C4	5.79	1.41	1.37
80	B5	1281	G	O3'-P	-5.79	1.54	1.61
79	B2	1291	G	N3-C4	-5.79	1.31	1.35
80	B5	2915	U	C2-N3	-5.79	1.33	1.37
80	B5	1208	U	N3-C4	-5.78	1.33	1.38
80	B5	1213	G	N1-C2	-5.78	1.33	1.37
80	B5	1477	A	N3-C4	-5.78	1.31	1.34
80	B5	2401	A	N9-C4	5.78	1.41	1.37
84	CW	26	A	C2'-C1'	-5.78	1.47	1.53
80	B5	1273	A	N7-C5	-5.77	1.35	1.39
80	B5	805	G	N7-C5	5.77	1.42	1.39
80	B5	3245	A	N7-C5	-5.77	1.35	1.39
82	B8	54	A	N9-C4	-5.77	1.34	1.37
80	B5	1305	U	N1-C6	-5.77	1.32	1.38
80	B5	1308	A	N9-C8	-5.77	1.33	1.37
80	B5	3047	U	C2-N3	-5.77	1.33	1.37
80	B5	984	G	N7-C5	-5.77	1.35	1.39
80	B5	883	A	P-OP1	5.76	1.58	1.49
80	B5	2612	U	C2-N3	-5.76	1.33	1.37
79	B2	993	A	N7-C5	-5.76	1.35	1.39
80	B5	868	C	N1-C6	-5.76	1.33	1.37
80	B5	2732	G	C6-N1	-5.76	1.35	1.39
80	B5	369	A	C6-N6	-5.75	1.29	1.33
80	B5	1849	C	C4-C5	-5.75	1.38	1.43
80	B5	2646	C	N1-C6	-5.75	1.33	1.37
80	B5	577	C	N1-C6	-5.75	1.33	1.37
80	B5	100	A	N9-C4	-5.74	1.34	1.37
80	B5	1898	G	C5-C4	-5.74	1.34	1.38
80	B5	1365	G	C6-N1	-5.73	1.35	1.39
80	B5	2888	U	C4-C5	-5.73	1.38	1.43
80	B5	1903	U	C4-O4	5.73	1.28	1.23
80	B5	1127	G	C5-C4	-5.73	1.34	1.38
80	B5	2858	U	C2-N3	-5.72	1.33	1.37
80	B5	953	G	N3-C4	-5.72	1.31	1.35
79	B2	1560	U	N3-C4	-5.72	1.33	1.38
49	BO	40[B]	ALA	C-N	-5.72	1.20	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	1112	A	C6-N1	-5.72	1.31	1.35
80	B5	339	C	N3-C4	-5.71	1.29	1.33
80	B5	1450	G	C5-C4	-5.71	1.34	1.38
80	B5	2375	G	C6-N1	-5.71	1.35	1.39
80	B5	1230	G	C2'-C1'	-5.71	1.47	1.53
80	B5	2860	U	C4-O4	5.71	1.28	1.23
80	B5	2888	U	C2-N3	-5.71	1.33	1.37
80	B5	428	A	N7-C5	-5.71	1.35	1.39
80	B5	1145	G	N3-C4	-5.70	1.31	1.35
80	B5	1309	U	N1-C2	-5.70	1.33	1.38
80	B5	3013	U	C2-N3	-5.70	1.33	1.37
80	B5	326	U	C4-O4	-5.69	1.19	1.23
80	B5	3039	C	N1-C6	-5.69	1.33	1.37
84	CW	10	G	N7-C5	-5.69	1.35	1.39
80	B5	2892	A	C6-N1	-5.69	1.31	1.35
80	B5	2921	U	C4-O4	-5.69	1.19	1.23
80	B5	876	A	N1-C2	-5.68	1.29	1.34
80	B5	2957	G	C8-N7	-5.68	1.27	1.30
80	B5	2419	A	C6-N1	-5.68	1.31	1.35
84	CW	19	G	C2-N3	5.67	1.37	1.32
80	B5	1189	C	N1-C6	-5.66	1.33	1.37
81	B7	39	C	N3-C4	-5.66	1.29	1.33
80	B5	924	G	C2-N3	-5.66	1.28	1.32
80	B5	2412	G	N1-C2	-5.66	1.33	1.37
80	B5	1370	G	C6-N1	-5.66	1.35	1.39
79	B2	1746	A	N9-C4	-5.66	1.34	1.37
80	B5	2340	U	C4-O4	-5.66	1.19	1.23
80	B5	1284	C	N1-C2	-5.65	1.34	1.40
80	B5	2350	C	N1-C6	-5.65	1.33	1.37
84	CW	40	C	P-O5'	-5.65	1.54	1.59
80	B5	949	C	N3-C4	-5.64	1.29	1.33
80	B5	1910	A	C5-C4	-5.64	1.34	1.38
84	CW	48	C	O3'-P	-5.64	1.54	1.61
80	B5	652	G	C5-C4	-5.64	1.34	1.38
80	B5	2302	G	N1-C2	-5.63	1.33	1.37
80	B5	1043	C	N3-C4	-5.63	1.30	1.33
59	BY	38	GLU	CG-CD	5.62	1.60	1.51
80	B5	1338	C	N1-C6	-5.62	1.33	1.37
80	B5	1370	G	N9-C8	-5.62	1.33	1.37
80	B5	1413	G	C6-N1	-5.62	1.35	1.39
84	CW	23	A	N7-C5	-5.62	1.35	1.39
80	B5	2382	G	N7-C5	-5.62	1.35	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	200	C	N3-C4	-5.61	1.30	1.33
80	B5	657	A	N3-C4	-5.61	1.31	1.34
84	CW	41	C	P-O5'	-5.61	1.54	1.59
80	B5	2148	U	C4-O4	-5.60	1.19	1.23
80	B5	3088	G	C5-C6	-5.60	1.36	1.42
79	B2	1555	A	N3-C4	-5.60	1.31	1.34
80	B5	2391	G	C6-O6	-5.60	1.19	1.24
80	B5	2810	C	N1-C6	-5.60	1.33	1.37
80	B5	2904	U	C2-N3	-5.60	1.33	1.37
80	B5	2361	A	N7-C5	-5.60	1.35	1.39
80	B5	1320	C	C4-C5	-5.59	1.38	1.43
80	B5	2164	A	N7-C5	-5.59	1.35	1.39
80	B5	817	A	C4'-C3'	-5.59	1.47	1.52
80	B5	640	U	C2-N3	-5.59	1.33	1.37
84	CW	21	A	C2'-C1'	-5.59	1.47	1.53
80	B5	39	A	N3-C4	-5.58	1.31	1.34
80	B5	2134	G	C6-N1	-5.58	1.35	1.39
80	B5	2626	A	N9-C8	-5.58	1.33	1.37
80	B5	2323	G	N1-C2	-5.58	1.33	1.37
80	B5	2147	A	N7-C5	-5.58	1.35	1.39
49	BO	4[B]	GLN	C-N	-5.58	1.23	1.34
79	B2	577	G	C5-C6	-5.58	1.36	1.42
80	B5	1099	A	C6-N1	-5.57	1.31	1.35
80	B5	2823	G	C5-C4	-5.57	1.34	1.38
80	B5	987	U	C2-O2	-5.57	1.17	1.22
80	B5	3374	U	C4-O4	-5.57	1.19	1.23
80	B5	706	A	C5-C4	-5.56	1.34	1.38
84	CW	31	A	N7-C5	-5.56	1.35	1.39
80	B5	2941	A	N9-C8	-5.56	1.33	1.37
80	B5	3218	A	N9-C4	-5.56	1.34	1.37
80	B5	1433	A	N7-C5	-5.56	1.35	1.39
80	B5	657	A	N9-C4	-5.55	1.34	1.37
79	B2	865	A	C6-N1	-5.55	1.31	1.35
80	B5	1434	G	C5-C4	-5.55	1.34	1.38
80	B5	2647	A	N3-C4	-5.55	1.31	1.34
80	B5	1233	G	C2-N3	5.54	1.37	1.32
80	B5	2419	A	P-O5'	5.54	1.65	1.59
80	B5	2860	U	P-OP2	-5.54	1.39	1.49
80	B5	2987	A	C6-N1	-5.54	1.31	1.35
80	B5	3184	A	N9-C4	-5.54	1.34	1.37
80	B5	824	C	N3-C4	-5.54	1.30	1.33
80	B5	344	A	N9-C8	-5.54	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	1174	G	C8-N7	-5.54	1.27	1.30
80	B5	1195	A	N1-C2	-5.54	1.29	1.34
80	B5	2920	U	P-OP1	-5.53	1.39	1.49
80	B5	559	A	N7-C5	-5.53	1.35	1.39
80	B5	2301	U	C2-O2	-5.53	1.17	1.22
80	B5	49	A	C5-C4	-5.53	1.34	1.38
80	B5	2336	U	N3-C4	-5.53	1.33	1.38
80	B5	1911	A	C5-C6	-5.52	1.36	1.41
80	B5	2609	A	C5-C4	-5.52	1.34	1.38
80	B5	900	G	C6-N1	-5.52	1.35	1.39
80	B5	891	G	N9-C4	-5.51	1.33	1.38
80	B5	1432	C	N1-C6	-5.51	1.33	1.37
80	B5	2336	U	C2-O2	-5.51	1.17	1.22
84	CW	36	U	C1'-N1	5.51	1.57	1.48
80	B5	1226	G	N3-C4	-5.51	1.31	1.35
79	B2	553	G	N1-C2	5.50	1.42	1.37
85	CX	2	U	O3'-P	-5.50	1.54	1.61
80	B5	2122	G	C5-C4	-5.50	1.34	1.38
79	B2	1084	A	N3-C4	-5.50	1.31	1.34
36	BB	349	LYS	CD-CE	5.49	1.65	1.51
80	B5	1301	A	N9-C8	-5.49	1.33	1.37
80	B5	2932	U	C2-N3	-5.49	1.33	1.37
80	B5	1264	G	C6-N1	5.49	1.43	1.39
80	B5	420	G	N9-C8	-5.48	1.34	1.37
79	B2	377	G	C6-N1	5.48	1.43	1.39
80	B5	635	G	P-OP2	-5.48	1.39	1.49
80	B5	2908	G	C2-N3	-5.48	1.28	1.32
80	B5	3107	U	C2-N3	-5.48	1.33	1.37
80	B5	1285	G	N1-C2	5.47	1.42	1.37
80	B5	1320	C	C4-N4	-5.47	1.29	1.33
80	B5	3088	G	N7-C5	-5.47	1.35	1.39
80	B5	421	G	N1-C2	-5.47	1.33	1.37
80	B5	365	A	N7-C5	-5.47	1.35	1.39
84	CW	42	C	C2'-C1'	-5.47	1.47	1.53
80	B5	755	A	C6-N1	-5.46	1.31	1.35
80	B5	1319	G	N9-C8	-5.46	1.34	1.37
80	B5	2775	U	C2-N3	-5.46	1.33	1.37
80	B5	2912	G	N9-C8	-5.46	1.34	1.37
82	B8	25	G	N1-C2	-5.46	1.33	1.37
80	B5	3052	G	N1-C2	-5.46	1.33	1.37
80	B5	360	G	N9-C8	-5.46	1.34	1.37
80	B5	1443	G	N3-C4	-5.45	1.31	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	CW	5	G	N9-C4	5.45	1.42	1.38
84	CW	5	G	C6-N1	5.45	1.43	1.39
80	B5	1414	G	C6-N1	-5.45	1.35	1.39
80	B5	1901	A	N9-C8	-5.45	1.33	1.37
80	B5	2744	U	C2-N3	-5.45	1.33	1.37
80	B5	1147	G	N9-C8	-5.44	1.34	1.37
81	B7	88	G	N1-C2	-5.44	1.33	1.37
80	B5	1324	U	C2-N3	-5.44	1.33	1.37
80	B5	834	U	C4-O4	-5.43	1.19	1.23
80	B5	39	A	C5-C4	-5.43	1.34	1.38
80	B5	1492	G	C2-N3	5.43	1.37	1.32
80	B5	2824	G	N7-C5	-5.43	1.35	1.39
81	B7	5	G	N9-C8	-5.43	1.34	1.37
80	B5	95	A	C5-C4	-5.43	1.34	1.38
79	B2	542	A	N9-C4	-5.42	1.34	1.37
80	B5	899	U	C4-O4	-5.42	1.19	1.23
80	B5	3096	C	N1-C6	-5.42	1.33	1.37
80	B5	1177	G	N7-C5	-5.41	1.36	1.39
80	B5	2417	U	C4-O4	5.41	1.27	1.23
80	B5	3216	G	C5-C4	-5.41	1.34	1.38
80	B5	522	A	P-O5'	-5.41	1.54	1.59
80	B5	354	U	C2-N3	-5.41	1.33	1.37
80	B5	2198	A	N9-C4	-5.41	1.34	1.37
84	CW	21	A	N7-C5	-5.41	1.36	1.39
80	B5	1875	G	C6-N1	-5.40	1.35	1.39
80	B5	2611	U	P-OP1	-5.40	1.39	1.49
80	B5	3114	A	N3-C4	-5.40	1.31	1.34
80	B5	784	A	N7-C5	-5.40	1.36	1.39
80	B5	1135	A	N9-C8	-5.40	1.33	1.37
80	B5	1327	C	N3-C4	-5.40	1.30	1.33
80	B5	363	G	N3-C4	-5.39	1.31	1.35
80	B5	3307	A	C2-N3	-5.39	1.28	1.33
80	B5	889	U	C4-O4	-5.39	1.19	1.23
80	B5	1330	A	N3-C4	-5.39	1.31	1.34
80	B5	36	C	N1-C2	-5.39	1.34	1.40
79	B2	555	A	N9-C4	5.39	1.41	1.37
80	B5	1190	A	C6-N1	-5.39	1.31	1.35
80	B5	895	A	N3-C4	-5.38	1.31	1.34
84	CW	4	C	P-O5'	-5.38	1.54	1.59
80	B5	2342	U	C2-N3	-5.38	1.33	1.37
80	B5	2365	C	N3-C4	-5.38	1.30	1.33
80	B5	831	G	N7-C5	-5.38	1.36	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	2434	U	C2-N3	-5.38	1.33	1.37
79	B2	331	A	N9-C4	-5.37	1.34	1.37
80	B5	864	G	C5-C4	-5.37	1.34	1.38
80	B5	1338	C	C4-C5	-5.37	1.38	1.43
80	B5	2128	C	C4-N4	-5.37	1.29	1.33
80	B5	2395	G	C6-N1	-5.37	1.35	1.39
85	CX	3	G	C2-N3	5.37	1.37	1.32
80	B5	925	A	N7-C5	-5.37	1.36	1.39
80	B5	1908	A	C6-N1	-5.37	1.31	1.35
80	B5	1226	G	C5'-C4'	5.37	1.57	1.51
80	B5	1262	G	C2-N3	5.37	1.37	1.32
81	B7	66	A	P-OP2	-5.37	1.39	1.49
80	B5	417	A	N7-C5	-5.36	1.36	1.39
80	B5	2397	A	C5-C6	5.36	1.45	1.41
80	B5	52	A	N7-C5	-5.36	1.36	1.39
80	B5	2834	G	C2-N3	-5.36	1.28	1.32
80	B5	2376	G	C6-O6	-5.35	1.19	1.24
80	B5	3112	G	C5-C4	-5.35	1.34	1.38
80	B5	1130	A	N1-C2	-5.35	1.29	1.34
80	B5	1296	C	N3-C4	-5.35	1.30	1.33
80	B5	2717	U	C2-N3	-5.35	1.34	1.37
80	B5	2693	C	N1-C6	-5.35	1.33	1.37
80	B5	631	U	N3-C4	-5.35	1.33	1.38
80	B5	284	A	N9-C4	5.34	1.41	1.37
80	B5	2204	C	N3-C4	-5.34	1.30	1.33
80	B5	3273	A	N9-C4	-5.34	1.34	1.37
80	B5	3039	C	C4-C5	-5.34	1.38	1.43
80	B5	2937	G	C5-C4	-5.34	1.34	1.38
84	CW	72	C	C5'-C4'	5.34	1.57	1.51
80	B5	41	G	N9-C4	-5.34	1.33	1.38
80	B5	903	U	C2-N3	-5.33	1.34	1.37
80	B5	1895	A	N3-C4	-5.33	1.31	1.34
80	B5	508	U	C5-C6	-5.33	1.29	1.34
36	BB	287	LYS	CD-CE	5.33	1.64	1.51
80	B5	666	A	N3-C4	-5.33	1.31	1.34
80	B5	806	A	P-OP2	-5.32	1.40	1.49
80	B5	1845	G	C5-C4	-5.32	1.34	1.38
80	B5	2734	A	N3-C4	-5.32	1.31	1.34
80	B5	433	A	N9-C4	-5.31	1.34	1.37
80	B5	1404	G	N9-C8	-5.31	1.34	1.37
80	B5	2643	A	C6-N1	5.31	1.39	1.35
80	B5	1170	A	C8-N7	-5.31	1.27	1.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	BO	196[B]	SER	C-N	-5.31	1.21	1.34
80	B5	2632	G	C8-N7	5.31	1.34	1.30
80	B5	1443	G	N1-C2	-5.31	1.33	1.37
84	CW	6	G	N9-C4	-5.30	1.33	1.38
80	B5	994	G	C5-C4	-5.30	1.34	1.38
80	B5	1262	G	C2'-C1'	-5.30	1.47	1.53
80	B5	1415	U	C2-O2	-5.30	1.17	1.22
80	B5	818	C	P-OP1	-5.30	1.40	1.49
80	B5	2974	U	C2-N3	-5.30	1.34	1.37
43	BI	96	VAL	CB-CG2	-5.29	1.41	1.52
80	B5	505	G	N3-C4	-5.29	1.31	1.35
84	CW	59	U	C3'-C2'	-5.29	1.47	1.52
80	B5	290	G	C6-N1	-5.29	1.35	1.39
80	B5	2706	G	C8-N7	-5.29	1.27	1.30
80	B5	2697	A	N9-C4	5.29	1.41	1.37
80	B5	2730	G	N7-C5	-5.29	1.36	1.39
80	B5	934	G	C5-C4	-5.28	1.34	1.38
80	B5	1115	G	N7-C5	-5.28	1.36	1.39
80	B5	1116	G	N9-C8	-5.28	1.34	1.37
80	B5	1833	G	C6-N1	-5.28	1.35	1.39
80	B5	990	U	C2-N3	-5.28	1.34	1.37
80	B5	1362	G	C6-N1	-5.28	1.35	1.39
80	B5	1151	U	C4-O4	-5.28	1.19	1.23
80	B5	1888	U	N1-C6	-5.28	1.33	1.38
80	B5	1477	A	C6-N1	-5.28	1.31	1.35
80	B5	2163	C	N3-C4	-5.28	1.30	1.33
80	B5	2692	A	N7-C5	-5.28	1.36	1.39
84	CW	62	C	O3'-P	-5.28	1.54	1.61
80	B5	1266	G	C2-N3	5.27	1.36	1.32
61	Ba	15	VAL	C-O	5.27	1.33	1.23
80	B5	1131	G	N7-C5	-5.27	1.36	1.39
84	CW	33	U	P-O5'	-5.27	1.54	1.59
80	B5	2666	C	N1-C6	-5.27	1.33	1.37
80	B5	1278	A	C5'-C4'	5.27	1.57	1.51
80	B5	956	U	N3-C4	-5.26	1.33	1.38
80	B5	2619	G	C6-O6	-5.26	1.19	1.24
84	CW	50	U	P-O5'	-5.26	1.54	1.59
80	B5	2341	A	N9-C8	-5.26	1.33	1.37
79	B2	582	U	P-O5'	-5.26	1.54	1.59
80	B5	912	G	N3-C4	5.26	1.39	1.35
80	B5	1326	A	C5-C4	-5.26	1.35	1.38
80	B5	1086	C	C4-C5	-5.25	1.38	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	2172	A	N9-C4	-5.25	1.34	1.37
80	B5	1226	G	C5-C6	-5.25	1.37	1.42
80	B5	1840	U	C2-N3	-5.25	1.34	1.37
80	B5	2191	U	N3-C4	-5.25	1.33	1.38
80	B5	3032	A	N7-C5	-5.25	1.36	1.39
40	BF	131	GLU	CD-OE2	5.25	1.31	1.25
80	B5	1425	U	C2-N3	-5.25	1.34	1.37
80	B5	436	A	C5-C4	5.25	1.42	1.38
80	B5	1171	G	N7-C5	-5.24	1.36	1.39
79	B2	538	A	N3-C4	5.24	1.38	1.34
80	B5	2214	A	N9-C4	-5.24	1.34	1.37
79	B2	973	A	N7-C5	-5.24	1.36	1.39
80	B5	658	G	N3-C4	-5.24	1.31	1.35
80	B5	3070	A	C6-N1	-5.23	1.31	1.35
80	B5	1282	G	C2-N3	5.23	1.36	1.32
80	B5	1250	G	C6-N1	5.23	1.43	1.39
80	B5	1250	G	N1-C2	5.23	1.42	1.37
80	B5	798	G	C6-O6	-5.23	1.19	1.24
80	B5	1468	A	N7-C5	-5.22	1.36	1.39
80	B5	1902	G	C6-N1	-5.22	1.35	1.39
80	B5	2734	A	N9-C4	-5.22	1.34	1.37
80	B5	2318	U	N3-C4	-5.22	1.33	1.38
80	B5	3065	G	C6-N1	-5.21	1.35	1.39
80	B5	70	A	N7-C5	-5.21	1.36	1.39
80	B5	2617	U	C4-O4	-5.21	1.19	1.23
73	Bm	79	GLU	CD-OE1	5.21	1.31	1.25
80	B5	1851	G	C8-N7	-5.21	1.27	1.30
80	B5	693	A	N9-C4	-5.21	1.34	1.37
80	B5	3316	A	N3-C4	-5.21	1.31	1.34
80	B5	835	G	C5-C4	-5.21	1.34	1.38
84	CW	51	U	P-O5'	-5.21	1.54	1.59
85	CX	1	A	C2'-C1'	-5.21	1.47	1.53
80	B5	3000	A	C5-C4	-5.20	1.35	1.38
80	B5	1262	G	N7-C5	-5.20	1.36	1.39
80	B5	1338	C	C4-N4	-5.20	1.29	1.33
80	B5	1832	C	N1-C6	-5.20	1.34	1.37
80	B5	2375	G	P-OP2	-5.20	1.40	1.49
80	B5	1607	U	C3'-O3'	5.20	1.49	1.42
80	B5	2837	A	N3-C4	-5.20	1.31	1.34
80	B5	2922	G	C6-O6	-5.20	1.19	1.24
80	B5	1117	G	N7-C5	-5.19	1.36	1.39
80	B5	884	A	C5-C6	-5.19	1.36	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	1143	A	N3-C4	-5.19	1.31	1.34
80	B5	1209	G	C2-N3	-5.19	1.28	1.32
80	B5	1409	G	C6-N1	-5.19	1.35	1.39
80	B5	2272	G	C6-N1	-5.19	1.35	1.39
80	B5	652	G	N7-C5	-5.18	1.36	1.39
80	B5	2634	U	N3-C4	5.18	1.43	1.38
80	B5	3372	A	N9-C4	5.18	1.41	1.37
80	B5	999	G	C5-C4	-5.18	1.34	1.38
80	B5	282	G	C2-N3	-5.18	1.28	1.32
80	B5	1151	U	C2-N3	-5.18	1.34	1.37
80	B5	1208	U	C2-N3	-5.18	1.34	1.37
80	B5	1515	A	N7-C5	-5.18	1.36	1.39
80	B5	2620	G	N1-C2	-5.18	1.33	1.37
80	B5	3179	U	C4-O4	-5.17	1.19	1.23
80	B5	345	G	C6-O6	-5.17	1.19	1.24
80	B5	1228	C	P-O5'	-5.17	1.54	1.59
80	B5	917	A	N3-C4	-5.17	1.31	1.34
80	B5	645	A	C8-N7	-5.17	1.27	1.31
80	B5	2859	U	C2-N3	-5.17	1.34	1.37
38	BD	95	TRP	CG-CD1	5.16	1.44	1.36
44	BJ	8	PRO	CB-CG	5.16	1.75	1.50
80	B5	2859	U	N3-C4	-5.16	1.33	1.38
84	CW	70	G	N7-C5	-5.16	1.36	1.39
79	B2	352	A	N9-C8	-5.16	1.33	1.37
80	B5	404	G	N9-C8	-5.15	1.34	1.37
80	B5	3115	C	N3-C4	-5.15	1.30	1.33
80	B5	2858	U	C2-O2	-5.15	1.17	1.22
80	B5	658	G	N9-C4	-5.15	1.33	1.38
80	B5	2993	G	N7-C5	-5.15	1.36	1.39
80	B5	1838	G	C5-C4	-5.14	1.34	1.38
80	B5	2659	G	N1-C2	-5.14	1.33	1.37
80	B5	859	G	C2-N3	-5.14	1.28	1.32
80	B5	2936	A	C4'-C3'	-5.14	1.47	1.52
80	B5	649	A	N7-C5	-5.14	1.36	1.39
80	B5	1311	G	N7-C5	-5.14	1.36	1.39
79	B2	474	A	N9-C4	-5.13	1.34	1.37
80	B5	2327	U	N3-C4	-5.13	1.33	1.38
84	CW	53	G	C2'-C1'	-5.13	1.47	1.53
80	B5	1898	G	N9-C8	-5.13	1.34	1.37
80	B5	1056	U	C2-N3	5.13	1.41	1.37
42	BH	82	VAL	CB-CG2	-5.12	1.42	1.52
80	B5	1886	A	N3-C4	-5.12	1.31	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	Bm	79	GLU	CD-OE2	5.11	1.31	1.25
80	B5	2372	A	C6-N1	-5.11	1.31	1.35
80	B5	49	A	N3-C4	-5.11	1.31	1.34
80	B5	1902	G	C8-N7	-5.11	1.27	1.30
84	CW	9	A	N7-C5	-5.11	1.36	1.39
80	B5	627	U	C2-N3	-5.11	1.34	1.37
80	B5	1188	U	C5-C6	-5.11	1.29	1.34
80	B5	984	G	C6-N1	-5.11	1.35	1.39
80	B5	1117	G	C6-O6	-5.11	1.19	1.24
80	B5	2928	C	C4'-C3'	-5.11	1.47	1.52
80	B5	333	G	C6-N1	-5.10	1.35	1.39
80	B5	2993	G	N1-C2	-5.10	1.33	1.37
80	B5	1299	U	C4-O4	-5.10	1.19	1.23
80	B5	2291	A	N9-C4	-5.10	1.34	1.37
80	B5	2912	G	C5-C4	-5.10	1.34	1.38
80	B5	877	C	C4-N4	-5.09	1.29	1.33
80	B5	609	G	N3-C4	-5.09	1.31	1.35
80	B5	1049	C	C4-N4	-5.09	1.29	1.33
80	B5	585	A	N3-C4	-5.09	1.31	1.34
80	B5	1114	U	C2-N3	-5.09	1.34	1.37
64	Bd	61	LYS	CD-CE	5.09	1.64	1.51
79	B2	142	G	N9-C4	-5.09	1.33	1.38
80	B5	1244	A	N7-C5	-5.09	1.36	1.39
80	B5	867	G	C2-N3	-5.08	1.28	1.32
80	B5	1237	G	C2-N3	5.08	1.36	1.32
80	B5	2934	A	C6-N1	-5.08	1.31	1.35
80	B5	38	U	O3'-P	-5.08	1.55	1.61
80	B5	2243	A	N3-C4	-5.08	1.31	1.34
80	B5	3122	A	N7-C5	-5.08	1.36	1.39
80	B5	397	A	N3-C4	-5.08	1.31	1.34
80	B5	1238	C	N3-C4	5.08	1.37	1.33
80	B5	2372	A	C3'-O3'	5.08	1.49	1.42
80	B5	656	A	O3'-P	-5.08	1.55	1.61
80	B5	1150	A	C6-N1	-5.08	1.31	1.35
80	B5	2329	C	N3-C4	-5.08	1.30	1.33
80	B5	2717	U	C2-O2	-5.08	1.17	1.22
80	B5	1188	U	C2-N3	-5.08	1.34	1.37
80	B5	2414	G	C5-C4	-5.08	1.34	1.38
80	B5	2640	A	N3-C4	-5.08	1.31	1.34
80	B5	2743	A	C6-N6	-5.08	1.29	1.33
80	B5	103	G	C8-N7	5.07	1.33	1.30
80	B5	1179	A	P-OP2	-5.07	1.40	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	2302	G	C6-N1	-5.07	1.36	1.39
80	B5	1332	A	N3-C4	-5.07	1.31	1.34
80	B5	2652	U	N1-C2	-5.07	1.33	1.38
84	CW	15	G	N7-C5	-5.06	1.36	1.39
80	B5	891	G	N3-C4	-5.06	1.31	1.35
80	B5	1157	G	N9-C8	-5.06	1.34	1.37
80	B5	2141	U	P-OP1	-5.06	1.40	1.49
52	BR	72	GLU	CG-CD	5.06	1.59	1.51
80	B5	332	C	N1-C6	-5.06	1.34	1.37
80	B5	1265	U	P-O5'	-5.06	1.54	1.59
80	B5	2958	A	N9-C4	-5.06	1.34	1.37
80	B5	2620	G	C5-C4	-5.06	1.34	1.38
80	B5	1308	A	N7-C5	-5.05	1.36	1.39
80	B5	1371	G	C5-C4	-5.05	1.34	1.38
84	CW	3	C	C2'-C1'	-5.05	1.47	1.53
80	B5	1863	G	N1-C2	-5.04	1.33	1.37
80	B5	1145	G	C2-N3	-5.04	1.28	1.32
80	B5	2323	G	N3-C4	-5.04	1.31	1.35
80	B5	1295	G	C6-N1	-5.04	1.36	1.39
80	B5	2366	C	C2-N3	5.04	1.39	1.35
42	BH	110	LYS	CD-CE	5.04	1.63	1.51
48	BN	94	TYR	CE1-CZ	5.04	1.45	1.38
80	B5	2359	C	C2-N3	-5.04	1.31	1.35
79	B2	387	A	N7-C5	5.04	1.42	1.39
80	B5	755	A	N3-C4	-5.04	1.31	1.34
80	B5	1231	A	N7-C5	-5.03	1.36	1.39
81	B7	94	C	C4-C5	-5.03	1.39	1.43
80	B5	3245	A	N1-C2	5.03	1.38	1.34
80	B5	987	U	C4-C5	5.03	1.48	1.43
80	B5	1910	A	C6-N6	-5.03	1.29	1.33
80	B5	2147	A	C5-C4	-5.03	1.35	1.38
80	B5	2922	G	C5-C6	-5.03	1.37	1.42
80	B5	1123	U	N3-C4	-5.03	1.33	1.38
80	B5	2190	U	C2-O2	-5.02	1.17	1.22
80	B5	2371	G	N1-C2	-5.02	1.33	1.37
80	B5	2921	U	N3-C4	-5.02	1.33	1.38
80	B5	1791	C	N1-C6	-5.02	1.34	1.37
80	B5	1797	A	C5-C4	-5.02	1.35	1.38
80	B5	1851	G	C5-C4	-5.02	1.34	1.38
80	B5	2977	G	N1-C2	-5.02	1.33	1.37
80	B5	282	G	N3-C4	-5.02	1.31	1.35
80	B5	984	G	N9-C8	-5.01	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B5	2865	U	N1-C2	5.01	1.43	1.38
64	Bd	102	LYS	CD-CE	5.01	1.63	1.51
80	B5	1117	G	C8-N7	-5.01	1.27	1.30
80	B5	2303	A	N3-C4	-5.01	1.31	1.34
80	B5	2693	C	N3-C4	-5.01	1.30	1.33
80	B5	106	A	N9-C4	-5.01	1.34	1.37
80	B5	1427	U	C2-N3	-5.01	1.34	1.37
80	B5	2315	G	N9-C4	-5.01	1.33	1.38
80	B5	2327	U	C4-O4	-5.01	1.19	1.23
80	B5	2702	A	N7-C5	-5.01	1.36	1.39
80	B5	2882	U	C2-O2	-5.01	1.17	1.22
80	B5	726	G	N7-C5	-5.00	1.36	1.39
80	B5	875	G	P-OP1	-5.00	1.40	1.49

All (5304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	CW	36	U	P-O3'-C3'	-59.91	47.81	119.70
80	B5	1152	G	N3-C4-C5	33.59	145.40	128.60
80	B5	1256	G	P-O3'-C3'	32.78	159.04	119.70
80	B5	1152	G	N3-C4-N9	-31.65	107.01	126.00
80	B5	1152	G	N3-C2-N2	-26.89	101.08	119.90
80	B5	1152	G	C2-N3-C4	-23.94	99.93	111.90
84	CW	36	U	OP1-P-O3'	-22.58	55.52	105.20
80	B5	1238	C	P-O3'-C3'	22.24	146.38	119.70
80	B5	922	U	C5-C6-N1	-22.07	111.67	122.70
80	B5	922	U	C2-N3-C4	-21.57	114.06	127.00
80	B5	1152	G	C5-N7-C8	-19.99	94.31	104.30
80	B5	922	U	N1-C2-N3	19.42	126.55	114.90
80	B5	3245	A	C2-N3-C4	-18.99	101.10	110.60
80	B5	1152	G	C8-N9-C1'	18.97	151.67	127.00
84	CW	36	U	OP2-P-O3'	-18.96	63.48	105.20
80	B5	3245	A	C5-N7-C8	-18.62	94.59	103.90
79	B2	553	G	N1-C6-O6	18.57	131.04	119.90
79	B2	1200	G	N1-C6-O6	17.86	130.62	119.90
80	B5	1152	G	N1-C6-O6	17.22	130.23	119.90
84	CW	36	U	O3'-P-O5'	17.02	136.34	104.00
80	B5	1284	C	C6-N1-C2	-16.95	113.52	120.30
84	CW	5	G	C5-C6-O6	-16.95	118.43	128.60
80	B5	1152	G	C4-N9-C1'	-16.82	104.64	126.50
80	B5	1152	G	C4-C5-N7	16.65	117.46	110.80
84	CW	7	A	P-O3'-C3'	16.47	139.46	119.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1152	G	N1-C2-N2	16.24	130.82	116.20
80	B5	922	U	N1-C2-O2	-16.08	111.54	122.80
80	B5	3245	A	N7-C8-N9	15.79	121.70	113.80
80	B5	1226	G	C5'-C4'-C3'	15.75	141.20	116.00
80	B5	776	U	C5-C6-N1	-15.52	114.94	122.70
80	B5	2726	C	C6-N1-C2	-15.41	114.14	120.30
80	B5	1450	G	C5-N7-C8	15.27	111.94	104.30
80	B5	1274	A	N1-C6-N6	15.11	127.67	118.60
80	B5	3245	A	C4-C5-N7	15.02	118.21	110.70
79	B2	577	G	C4-C5-N7	15.00	116.80	110.80
84	CW	17	C	P-O3'-C3'	14.98	137.68	119.70
84	CW	21	A	N1-C6-N6	14.96	127.58	118.60
84	CW	19	G	P-O5'-C5'	14.92	144.78	120.90
80	B5	3245	A	N1-C6-N6	14.81	127.49	118.60
80	B5	3245	A	C6-C5-N7	-14.53	122.13	132.30
80	B5	1152	G	C5-C6-O6	-14.41	119.95	128.60
79	B2	1773	C	N3-C4-C5	-14.32	116.17	121.90
79	B2	1200	G	C5-C6-O6	-14.21	120.07	128.60
80	B5	2353	G	C5-C6-O6	-14.08	120.15	128.60
80	B5	2634	U	C5-C4-O4	-13.98	117.51	125.90
80	B5	2726	C	C5-C4-N4	13.97	129.98	120.20
80	B5	2634	U	C2-N3-C4	-13.96	118.63	127.00
85	CX	2	U	P-O3'-C3'	13.95	136.44	119.70
84	CW	76	A	N1-C6-N6	13.86	126.92	118.60
84	CW	5	G	N1-C6-O6	13.85	128.21	119.90
80	B5	776	U	N1-C2-N3	13.84	123.21	114.90
80	B5	1592	G	N1-C6-O6	-13.84	111.60	119.90
80	B5	1260	A	N1-C6-N6	13.69	126.81	118.60
84	CW	68	C	C5'-C4'-C3'	13.50	137.60	116.00
84	CW	38	A	N1-C6-N6	13.48	126.69	118.60
80	B5	776	U	C4-C5-C6	13.44	127.76	119.70
80	B5	1450	G	N7-C8-N9	-13.39	106.40	113.10
80	B5	1266	G	N1-C6-O6	13.39	127.93	119.90
79	B2	1560	U	C5-C4-O4	13.35	133.91	125.90
80	B5	2245	C	C6-N1-C2	-13.34	114.96	120.30
80	B5	2372	A	C8-N9-C4	-13.29	100.48	105.80
79	B2	1773	C	C6-N1-C2	-13.28	114.99	120.30
80	B5	922	U	C4-C5-C6	13.23	127.64	119.70
80	B5	1271	A	N1-C6-N6	13.20	126.52	118.60
80	B5	631	U	N3-C2-O2	-13.11	113.02	122.20
80	B5	1258	U	P-O5'-C5'	13.10	141.87	120.90
80	B5	2278	C	N1-C2-O2	-13.06	111.07	118.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1226	G	N1-C6-O6	13.04	127.72	119.90
80	B5	2303	A	C2-N3-C4	13.04	117.12	110.60
80	B5	1245	A	N1-C6-N6	12.95	126.37	118.60
80	B5	3214	U	C5-C4-O4	12.94	133.66	125.90
80	B5	2361	A	C2-N3-C4	12.88	117.04	110.60
85	CX	1	A	N1-C6-N6	12.86	126.31	118.60
80	B5	2726	C	N1-C2-N3	12.84	128.19	119.20
80	B5	1208	U	N3-C4-O4	-12.76	110.47	119.40
80	B5	2308	C	N1-C2-O2	-12.71	111.27	118.90
80	B5	1266	G	C5-C6-O6	-12.68	120.99	128.60
79	B2	577	G	C5-N7-C8	-12.67	97.97	104.30
80	B5	1208	U	C5-C4-O4	12.66	133.50	125.90
80	B5	3214	U	N3-C2-O2	-12.66	113.34	122.20
80	B5	2327	U	C5-C6-N1	-12.64	116.38	122.70
80	B5	1152	G	C4-C5-C6	-12.62	111.22	118.80
65	Be	43	ARG	NE-CZ-NH1	12.61	126.61	120.30
80	B5	1251	A	N1-C6-N6	12.60	126.16	118.60
80	B5	1258	U	P-O3'-C3'	12.58	134.79	119.70
84	CW	64	A	N1-C6-N6	12.56	126.14	118.60
79	B2	1541	G	N1-C6-O6	-12.56	112.37	119.90
84	CW	58	A	N1-C6-N6	12.56	126.13	118.60
80	B5	1371	G	N1-C6-O6	-12.54	112.38	119.90
80	B5	2758	A	C2-N3-C4	12.49	116.84	110.60
80	B5	1846	C	C5-C6-N1	-12.46	114.77	121.00
80	B5	1434	G	C5-N7-C8	12.35	110.48	104.30
80	B5	776	U	N3-C2-O2	-12.35	113.55	122.20
80	B5	1450	G	C4-C5-N7	-12.29	105.88	110.80
81	B7	120	C	C6-N1-C2	12.29	125.22	120.30
80	B5	1233	G	C5'-C4'-C3'	12.26	135.61	116.00
80	B5	591	G	C5-C6-O6	-12.25	121.25	128.60
80	B5	3245	A	N1-C2-N3	12.11	135.35	129.30
84	CW	48	C	O4'-C1'-N1	12.10	117.88	108.20
80	B5	1278	A	N1-C6-N6	12.06	125.83	118.60
80	B5	2340	U	N3-C4-O4	-11.99	111.00	119.40
80	B5	1268	G	N1-C6-O6	11.96	127.07	119.90
80	B5	2726	C	C4-C5-C6	11.96	123.38	117.40
80	B5	1285	G	N1-C6-O6	11.92	127.05	119.90
80	B5	1308	A	N7-C8-N9	11.92	119.76	113.80
80	B5	1252	A	N1-C6-N6	11.91	125.75	118.60
79	B2	1200	G	N3-C2-N2	-11.91	111.57	119.90
80	B5	1056	U	C4-C5-C6	11.90	126.84	119.70
80	B5	1225	A	N1-C6-N6	11.86	125.71	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	667	C	C6-N1-C2	11.84	125.04	120.30
80	B5	290	G	N1-C6-O6	-11.80	112.82	119.90
80	B5	966	U	N3-C2-O2	-11.76	113.97	122.20
80	B5	1231	A	N1-C6-N6	11.76	125.65	118.60
80	B5	2278	C	N1-C2-N3	11.73	127.41	119.20
84	CW	60	U	O4'-C1'-N1	11.69	117.55	108.20
79	B2	577	G	C5-C6-O6	-11.67	121.60	128.60
80	B5	2726	C	N3-C4-C5	-11.66	117.23	121.90
80	B5	2808	A	N9-C4-C5	-11.66	101.14	105.80
80	B5	1263	A	N1-C6-N6	11.64	125.59	118.60
84	CW	26	A	N1-C6-N6	11.61	125.57	118.60
84	CW	6	G	N1-C6-O6	11.61	126.86	119.90
84	CW	74	C	P-O3'-C3'	11.53	133.53	119.70
80	B5	1130	A	C2-N3-C4	11.52	116.36	110.60
80	B5	1389	G	C4-C5-N7	11.52	115.41	110.80
84	CW	53	G	C5-C6-O6	-11.45	121.73	128.60
79	B2	1782	A	N9-C4-C5	11.44	110.38	105.80
84	CW	37	A	N1-C6-N6	11.44	125.46	118.60
80	B5	1592	G	N3-C2-N2	11.42	127.90	119.90
80	B5	1226	G	O4'-C1'-N9	11.41	117.33	108.20
80	B5	1797	A	C5-N7-C8	11.41	109.60	103.90
80	B5	1232	C	O4'-C1'-N1	11.37	117.30	108.20
80	B5	2899	C	N3-C2-O2	-11.36	113.95	121.90
84	CW	67	C	P-O3'-C3'	-11.35	106.08	119.70
80	B5	2142	A	C5-C6-N1	11.34	123.37	117.70
79	B2	553	G	N3-C2-N2	-11.29	112.00	119.90
84	CW	58	A	P-O3'-C3'	-11.29	106.15	119.70
79	B2	1280	C	N3-C4-C5	-11.27	117.39	121.90
79	B2	393	C	C6-N1-C2	11.26	124.80	120.30
80	B5	414	U	C4-C5-C6	11.26	126.46	119.70
80	B5	1240	A	N1-C6-N6	11.26	125.36	118.60
79	B2	1600	A	C2-N3-C4	-11.25	104.98	110.60
80	B5	1273	A	N1-C6-N6	11.24	125.34	118.60
84	CW	31	A	N1-C6-N6	11.23	125.34	118.60
79	B2	639	U	N3-C2-O2	-11.22	114.35	122.20
80	B5	1229	G	O4'-C1'-N9	11.21	117.17	108.20
83	CV	63	GLU	CB-CA-C	-11.20	88.00	110.40
80	B5	1227	C	C6-N1-C2	-11.20	115.82	120.30
80	B5	1257	C	O4'-C1'-N1	11.19	117.15	108.20
80	B5	3377	G	C5-C6-O6	-11.18	121.89	128.60
80	B5	2744	U	N3-C2-O2	-11.17	114.38	122.20
80	B5	1249	G	N1-C6-O6	11.12	126.57	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1004	U	N1-C2-O2	11.11	130.58	122.80
79	B2	577	G	N1-C6-O6	11.08	126.55	119.90
80	B5	2278	C	N3-C4-N4	-11.06	110.26	118.00
80	B5	2836	C	C2-N3-C4	-11.06	114.37	119.90
80	B5	15	C	C6-N1-C2	-11.04	115.88	120.30
84	CW	47	U	P-O3'-C3'	11.03	132.94	119.70
80	B5	1270	A	N1-C6-N6	11.00	125.20	118.60
80	B5	3060	C	N1-C2-O2	-10.99	112.31	118.90
80	B5	776	U	C5-C4-O4	10.93	132.46	125.90
80	B5	3138	U	N1-C2-O2	-10.92	115.15	122.80
80	B5	41	G	N1-C6-O6	10.88	126.43	119.90
80	B5	947	G	N3-C4-C5	-10.88	123.16	128.60
80	B5	420	G	C6-N1-C2	-10.87	118.58	125.10
84	CW	73	A	N1-C6-N6	10.86	125.11	118.60
80	B5	931	C	C2-N3-C4	-10.85	114.47	119.90
80	B5	1119	C	N3-C4-C5	10.85	126.24	121.90
80	B5	2632	G	N1-C6-O6	-10.85	113.39	119.90
80	B5	41	G	C5-C6-O6	-10.83	122.10	128.60
80	B5	1403	C	C6-N1-C2	10.82	124.63	120.30
83	CV	63	GLU	N-CA-CB	10.82	130.08	110.60
80	B5	1259	A	N1-C6-N6	10.81	125.09	118.60
79	B2	144	U	N3-C2-O2	-10.81	114.63	122.20
79	B2	1782	A	C8-N9-C4	-10.79	101.48	105.80
80	B5	2726	C	N3-C2-O2	-10.79	114.34	121.90
80	B5	922	U	C2-N1-C1'	-10.78	104.77	117.70
80	B5	2343	C	N3-C4-C5	10.76	126.21	121.90
84	CW	53	G	N1-C6-O6	10.76	126.36	119.90
79	B2	1560	U	N3-C2-O2	-10.74	114.68	122.20
80	B5	2634	U	C5-C6-N1	-10.74	117.33	122.70
80	B5	2341	A	C8-N9-C4	10.74	110.09	105.80
79	B2	1455	G	C5-C6-N1	-10.73	106.14	111.50
84	CW	14	A	N1-C6-N6	10.72	125.03	118.60
80	B5	1147	G	C4-C5-N7	-10.68	106.53	110.80
80	B5	1228	C	C6-N1-C2	-10.67	116.03	120.30
80	B5	2288	G	C5-C6-N1	10.67	116.83	111.50
80	B5	2353	G	N1-C6-O6	10.67	126.30	119.90
80	B5	1434	G	N7-C8-N9	-10.65	107.77	113.10
80	B5	2290	C	C5-C6-N1	-10.65	115.68	121.00
80	B5	957	C	N3-C4-C5	10.64	126.16	121.90
80	B5	2631	U	C2-N3-C4	-10.64	120.62	127.00
80	B5	2899	C	N1-C2-N3	10.63	126.64	119.20
84	CW	16	U	C6-N1-C2	-10.61	114.63	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	CW	52	G	N1-C6-O6	10.59	126.25	119.90
80	B5	2905	U	C5-C6-N1	-10.59	117.41	122.70
84	CW	9	A	N1-C6-N6	10.58	124.95	118.60
80	B5	2234	G	C5-C6-O6	-10.57	122.26	128.60
84	CW	28	G	N1-C6-O6	10.55	126.23	119.90
79	B2	553	G	C5-C6-N1	-10.52	106.24	111.50
80	B5	546	C	C2-N1-C1'	10.52	130.37	118.80
80	B5	1592	G	N1-C2-N2	-10.52	106.73	116.20
80	B5	1907	C	C6-N1-C2	-10.51	116.09	120.30
80	B5	2314	U	C5-C4-O4	-10.51	119.59	125.90
80	B5	3172	A	C8-N9-C4	10.51	110.00	105.80
80	B5	1848	G	C5-C6-O6	-10.50	122.30	128.60
79	B2	577	G	C6-C5-N7	-10.50	124.10	130.40
80	B5	1911	A	C8-N9-C4	10.46	109.98	105.80
80	B5	2836	C	C5-C6-N1	-10.45	115.78	121.00
80	B5	965	A	C2-N3-C4	10.44	115.82	110.60
80	B5	2314	U	N3-C4-O4	10.43	126.70	119.40
80	B5	2512	C	C6-N1-C2	-10.42	116.13	120.30
79	B2	639	U	N1-C2-O2	10.41	130.09	122.80
80	B5	2211	U	C4-C5-C6	10.41	125.95	119.70
80	B5	930	U	N3-C4-C5	10.40	120.84	114.60
80	B5	819	U	C5-C6-N1	-10.39	117.50	122.70
84	CW	43	C	C5'-C4'-C3'	-10.39	99.37	116.00
79	B2	1782	A	C5-C6-N6	10.38	132.00	123.70
80	B5	3122	A	C8-N9-C4	-10.37	101.65	105.80
65	Be	27	ARG	NE-CZ-NH2	-10.35	115.12	120.30
80	B5	1301	A	N1-C6-N6	10.34	124.80	118.60
80	B5	1241	U	P-O3'-C3'	10.34	132.10	119.70
80	B5	1004	U	N3-C4-O4	-10.33	112.17	119.40
80	B5	1303	A	N1-C2-N3	-10.31	124.14	129.30
80	B5	2364	G	N1-C6-O6	-10.31	113.71	119.90
80	B5	1297	C	C2-N3-C4	-10.29	114.75	119.90
80	B5	2257	C	C6-N1-C2	-10.28	116.19	120.30
80	B5	1262	G	N1-C6-O6	10.28	126.07	119.90
80	B5	1429	G	N3-C2-N2	10.28	127.09	119.90
84	CW	75	C	O4'-C1'-N1	10.27	116.42	108.20
80	B5	1797	A	N7-C8-N9	-10.27	108.66	113.80
80	B5	2211	U	C5-C4-O4	10.26	132.05	125.90
80	B5	1391	C	N1-C2-O2	-10.25	112.75	118.90
84	CW	28	G	C5-C6-O6	-10.25	122.45	128.60
80	B5	847	A	C8-N9-C4	10.23	109.89	105.80
80	B5	1903	U	N3-C4-O4	10.21	126.55	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2148	U	N1-C2-O2	-10.20	115.66	122.80
80	B5	414	U	C5-C6-N1	-10.19	117.61	122.70
82	B8	8	C	C6-N1-C2	-10.19	116.23	120.30
84	CW	23	A	N1-C6-N6	10.18	124.71	118.60
80	B5	1513	G	C8-N9-C4	-10.18	102.33	106.40
80	B5	1240	A	P-O3'-C3'	10.15	131.89	119.70
80	B5	1284	C	C4'-C3'-C2'	10.14	112.74	102.60
80	B5	1481	A	C8-N9-C4	-10.13	101.75	105.80
80	B5	652	G	N1-C2-N2	-10.12	107.09	116.20
80	B5	1056	U	C6-N1-C2	-10.11	114.93	121.00
80	B5	1226	G	P-O3'-C3'	10.10	131.82	119.70
79	B2	507	U	N3-C2-O2	-10.10	115.13	122.20
80	B5	1285	G	C5-C6-O6	-10.09	122.54	128.60
80	B5	1440	G	N1-C6-O6	-10.09	113.85	119.90
84	CW	22	G	N1-C6-O6	10.08	125.95	119.90
80	B5	2632	G	C5-C6-O6	10.07	134.64	128.60
80	B5	3096	C	C4-C5-C6	10.06	122.43	117.40
80	B5	2343	C	C2-N3-C4	-10.04	114.88	119.90
80	B5	1124	U	C4-C5-C6	-10.03	113.68	119.70
83	CV	435	TYR	CA-CB-CG	10.03	132.45	113.40
84	CW	69	G	N1-C6-O6	10.02	125.91	119.90
80	B5	3006	A	C2-N3-C4	-10.02	105.59	110.60
82	B8	25	G	N1-C6-O6	-10.00	113.90	119.90
79	B2	542	A	N7-C8-N9	9.99	118.80	113.80
80	B5	1208	U	N3-C2-O2	-9.99	115.21	122.20
80	B5	1308	A	C8-N9-C4	-9.98	101.81	105.80
84	CW	17	C	O4'-C1'-N1	9.97	116.17	108.20
80	B5	420	G	C5-C6-O6	-9.95	122.63	128.60
80	B5	2905	U	C2-N3-C4	-9.95	121.03	127.00
80	B5	2366	C	C5-C6-N1	9.95	125.98	121.00
80	B5	2952	G	C5-C6-O6	-9.95	122.63	128.60
80	B5	2808	A	C8-N9-C4	9.94	109.78	105.80
80	B5	340	C	C2-N3-C4	-9.94	114.93	119.90
80	B5	2824	G	N3-C2-N2	-9.94	112.94	119.90
82	B8	32	C	N1-C2-O2	-9.94	112.94	118.90
80	B5	877	C	N3-C4-C5	9.93	125.87	121.90
80	B5	1484	U	C5-C6-N1	-9.93	117.74	122.70
80	B5	3362	A	C2-N3-C4	-9.91	105.64	110.60
79	B2	1096	C	C2-N1-C1'	9.90	129.69	118.80
80	B5	1246	G	P-O3'-C3'	9.89	131.57	119.70
80	B5	1284	C	O4'-C1'-N1	9.89	116.11	108.20
80	B5	1389	G	N9-C4-C5	-9.89	101.44	105.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	1486	G	C5-N7-C8	-9.89	99.36	104.30
80	B5	1655	G	C8-N9-C4	-9.89	102.44	106.40
80	B5	339	C	N3-C4-N4	-9.86	111.10	118.00
79	B2	1198	G	C8-N9-C4	-9.86	102.46	106.40
79	B2	1745	G	C5-C6-O6	-9.85	122.69	128.60
84	CW	44	G	N1-C6-O6	9.85	125.81	119.90
80	B5	1152	G	N7-C8-N9	9.84	118.02	113.10
80	B5	1655	G	N7-C8-N9	9.84	118.02	113.10
80	B5	2118	C	N3-C2-O2	-9.83	115.02	121.90
80	B5	1258	U	O4'-C1'-N1	9.82	116.06	108.20
79	B2	553	G	C5-C6-O6	-9.82	122.71	128.60
79	B2	1456	C	N3-C4-N4	-9.81	111.13	118.00
49	BO	182[B]	SER	O-C-N	-9.80	107.03	122.70
80	B5	947	G	C5-C6-N1	9.77	116.38	111.50
80	B5	1248	C	O4'-C1'-N1	9.76	116.01	108.20
80	B5	835	G	C5-C6-O6	-9.76	122.74	128.60
80	B5	1392	G	C8-N9-C4	9.76	110.30	106.40
80	B5	2134	G	N1-C6-O6	-9.76	114.05	119.90
80	B5	3096	C	C2-N3-C4	-9.76	115.02	119.90
80	B5	1064	A	N1-C6-N6	9.74	124.44	118.60
80	B5	1057	A	N1-C6-N6	9.74	124.44	118.60
80	B5	1147	G	C5-N7-C8	9.73	109.17	104.30
84	CW	52	G	C5-C6-O6	-9.73	122.76	128.60
80	B5	2948	C	N3-C4-N4	-9.73	111.19	118.00
80	B5	2917	G	C5-C6-O6	-9.73	122.76	128.60
80	B5	2278	C	C6-N1-C2	-9.72	116.41	120.30
84	CW	44	G	C5-C6-O6	-9.72	122.77	128.60
80	B5	815	G	N1-C6-O6	-9.71	114.07	119.90
80	B5	1260	A	O4'-C1'-N9	9.71	115.97	108.20
80	B5	645	A	C6-N1-C2	-9.71	112.77	118.60
80	B5	1448	U	C5-C6-N1	-9.71	117.84	122.70
80	B5	2361	A	N3-C4-C5	-9.71	120.00	126.80
80	B5	1152	G	C8-N9-C4	-9.71	102.52	106.40
80	B5	1888	U	C5-C6-N1	-9.70	117.85	122.70
80	B5	1229	G	N1-C6-O6	9.68	125.71	119.90
80	B5	1250	G	C5-C6-O6	-9.68	122.79	128.60
80	B5	3060	C	N3-C4-N4	9.68	124.77	118.00
80	B5	2757	U	N1-C2-N3	9.67	120.70	114.90
36	BB	10	ARG	NE-CZ-NH2	-9.66	115.47	120.30
84	CW	69	G	C5-C6-O6	-9.65	122.81	128.60
79	B2	553	G	C6-C5-N7	-9.64	124.61	130.40
79	B2	1280	C	N3-C4-N4	9.64	124.75	118.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1262	G	C5-C6-O6	-9.64	122.82	128.60
80	B5	1127	G	C5-C6-O6	-9.63	122.82	128.60
80	B5	2246	G	N9-C4-C5	9.63	109.25	105.40
80	B5	2211	U	N1-C2-N3	9.63	120.68	114.90
80	B5	591	G	N1-C6-O6	9.62	125.67	119.90
80	B5	1327	C	N3-C4-N4	-9.61	111.27	118.00
83	CV	495	TYR	CB-CG-CD2	-9.61	115.23	121.00
80	B5	2391	G	C8-N9-C4	-9.60	102.56	106.40
79	B2	1782	A	N1-C6-N6	-9.60	112.84	118.60
81	B7	49	G	N1-C6-O6	9.58	125.65	119.90
80	B5	518	G	C5-C6-O6	-9.57	122.86	128.60
80	B5	340	C	C5-C6-N1	-9.57	116.21	121.00
80	B5	2899	C	C5-C4-N4	9.56	126.89	120.20
80	B5	2424	A	N1-C6-N6	9.56	124.33	118.60
80	B5	776	U	C2-N3-C4	-9.55	121.27	127.00
84	CW	67	C	O3'-P-O5'	-9.54	85.88	104.00
80	B5	1056	U	N1-C2-N3	9.53	120.62	114.90
80	B5	2572	C	N1-C2-O2	9.53	124.62	118.90
80	B5	905	U	C5-C4-O4	-9.52	120.19	125.90
80	B5	1042	U	N3-C4-O4	-9.52	112.74	119.40
80	B5	1403	C	C5-C4-N4	-9.51	113.55	120.20
80	B5	2705	A	C5-C6-N1	9.51	122.45	117.70
80	B5	1848	G	N1-C6-O6	9.50	125.60	119.90
80	B5	1888	U	C4-C5-C6	9.49	125.39	119.70
84	CW	15	G	N1-C6-O6	9.49	125.59	119.90
83	CV	435	TYR	CB-CG-CD1	9.48	126.69	121.00
80	B5	708	G	C4-C5-N7	9.48	114.59	110.80
79	B2	1486	G	N7-C8-N9	9.48	117.84	113.10
82	B8	113	U	C5-C6-N1	9.48	127.44	122.70
80	B5	2202	C	C5-C4-N4	-9.46	113.58	120.20
84	CW	7	A	N1-C6-N6	9.46	124.27	118.60
80	B5	3362	A	N7-C8-N9	9.45	118.53	113.80
79	B2	139	C	C6-N1-C2	-9.45	116.52	120.30
80	B5	1858	A	C8-N9-C4	-9.45	102.02	105.80
79	B2	453	U	N3-C2-O2	-9.45	115.59	122.20
79	B2	1456	C	C5-C4-N4	9.45	126.81	120.20
80	B5	2978	U	N3-C2-O2	-9.44	115.59	122.20
80	B5	644	G	C2-N3-C4	9.44	116.62	111.90
80	B5	386	A	N1-C6-N6	9.42	124.25	118.60
80	B5	1902	G	C5-C6-O6	-9.42	122.95	128.60
80	B5	40	A	N1-C2-N3	9.42	134.01	129.30
80	B5	2830	G	N9-C4-C5	9.42	109.17	105.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1210	U	C5-C4-O4	9.41	131.55	125.90
79	B2	1282	U	N3-C2-O2	-9.41	115.61	122.20
80	B5	1449	A	C2-N3-C4	-9.41	105.89	110.60
80	B5	947	G	C2-N3-C4	9.41	116.61	111.90
80	B5	546	C	N1-C2-O2	9.41	124.55	118.90
79	B2	1258	U	N3-C2-O2	-9.39	115.62	122.20
80	B5	966	U	N1-C2-O2	9.39	129.37	122.80
80	B5	1447	G	C8-N9-C4	-9.39	102.64	106.40
80	B5	3218	A	C5-N7-C8	-9.38	99.21	103.90
80	B5	1437	C	C6-N1-C2	-9.38	116.55	120.30
80	B5	994	G	C5-C6-N1	9.37	116.18	111.50
80	B5	2899	C	C6-N1-C2	-9.37	116.55	120.30
79	B2	1654	G	C5-C6-N1	9.36	116.18	111.50
80	B5	282	G	C8-N9-C4	-9.36	102.66	106.40
80	B5	21	G	C2-N3-C4	-9.34	107.23	111.90
80	B5	1849	C	N1-C2-O2	9.34	124.50	118.90
80	B5	811	U	C5-C6-N1	-9.33	118.03	122.70
80	B5	1274	A	C5-C6-N6	-9.32	116.25	123.70
80	B5	3214	U	N3-C4-O4	-9.32	112.88	119.40
80	B5	3309	G	N3-C4-C5	-9.31	123.95	128.60
79	B2	1169	G	C8-N9-C4	-9.30	102.68	106.40
80	B5	1246	G	N1-C6-O6	9.28	125.47	119.90
80	B5	1284	C	N3-C4-C5	-9.28	118.19	121.90
80	B5	1879	A	N1-C6-N6	9.27	124.16	118.60
80	B5	2364	G	N9-C4-C5	9.27	109.11	105.40
82	B8	80	A	C8-N9-C4	-9.27	102.09	105.80
80	B5	3050	U	N3-C2-O2	-9.26	115.72	122.20
80	B5	3060	C	C5-C4-N4	-9.26	113.72	120.20
80	B5	3376	A	C8-N9-C4	-9.26	102.09	105.80
80	B5	721	G	N1-C6-O6	-9.26	114.34	119.90
80	B5	1371	G	C5-C6-N1	9.26	116.13	111.50
80	B5	1151	U	N3-C4-O4	-9.26	112.92	119.40
80	B5	1449	A	N1-C6-N6	9.25	124.15	118.60
84	CW	19	G	C5-C6-O6	-9.24	123.05	128.60
80	B5	2550	U	C5-C4-O4	9.23	131.44	125.90
80	B5	968	G	N3-C2-N2	9.23	126.36	119.90
36	BB	4	ARG	NE-CZ-NH1	9.22	124.91	120.30
80	B5	3377	G	C4-C5-N7	9.22	114.49	110.80
80	B5	2340	U	N3-C4-C5	9.22	120.13	114.60
80	B5	2693	C	N3-C2-O2	-9.21	115.45	121.90
80	B5	2142	A	C6-N1-C2	-9.20	113.08	118.60
80	B5	3186	A	C8-N9-C4	-9.19	102.12	105.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1156	C	N3-C4-C5	9.19	125.58	121.90
36	BB	2	SER	N-CA-C	-9.17	86.24	111.00
80	B5	1050	U	N3-C2-O2	-9.17	115.78	122.20
80	B5	1843	C	C6-N1-C2	-9.16	116.64	120.30
80	B5	1450	G	C8-N9-C4	9.15	110.06	106.40
80	B5	2354	C	N1-C2-O2	-9.15	113.41	118.90
84	CW	68	C	N3-C4-N4	9.15	124.40	118.00
80	B5	2246	G	C4-C5-N7	-9.14	107.14	110.80
80	B5	1064	A	N9-C4-C5	-9.14	102.14	105.80
80	B5	834	U	N3-C4-C5	9.13	120.08	114.60
80	B5	1101	G	N3-C2-N2	9.13	126.29	119.90
79	B2	142	G	N3-C2-N2	-9.12	113.52	119.90
80	B5	3362	A	C5-N7-C8	-9.12	99.34	103.90
80	B5	2365	C	N3-C4-N4	-9.12	111.62	118.00
80	B5	3266	G	C5-C6-O6	9.11	134.07	128.60
79	B2	558	U	N3-C2-O2	-9.11	115.82	122.20
80	B5	1133	A	C2-N3-C4	9.11	115.15	110.60
80	B5	3245	A	C8-N9-C4	-9.11	102.16	105.80
84	CW	75	C	C2-N1-C1'	9.10	128.81	118.80
79	B2	402	C	C6-N1-C2	9.09	123.94	120.30
80	B5	3308	C	C4-C5-C6	9.09	121.95	117.40
84	CW	46	G	N1-C6-O6	9.09	125.36	119.90
51	BQ	66	ARG	NE-CZ-NH2	-9.07	115.76	120.30
80	B5	2744	U	N1-C2-O2	9.07	129.15	122.80
80	B5	2942	C	N3-C4-N4	9.07	124.35	118.00
80	B5	1911	A	N9-C4-C5	-9.06	102.17	105.80
79	B2	794	U	N1-C2-O2	9.06	129.14	122.80
80	B5	1181	U	C5-C6-N1	-9.05	118.17	122.70
80	B5	2176	U	N3-C2-O2	-9.05	115.86	122.20
80	B5	369	A	C8-N9-C4	-9.04	102.19	105.80
79	B2	1596	C	N3-C2-O2	-9.03	115.58	121.90
80	B5	1234	G	N1-C6-O6	9.03	125.32	119.90
80	B5	1317	A	C5-C6-N6	-9.02	116.48	123.70
80	B5	1911	A	N1-C6-N6	9.02	124.01	118.60
79	B2	542	A	C5-N7-C8	-9.01	99.39	103.90
80	B5	1250	G	N1-C6-O6	9.01	125.31	119.90
80	B5	2830	G	N1-C2-N3	9.01	129.30	123.90
80	B5	2836	C	C4-C5-C6	9.01	121.90	117.40
80	B5	631	U	N1-C2-N3	9.00	120.30	114.90
80	B5	2728	G	N9-C4-C5	8.99	109.00	105.40
80	B5	2320	A	C5-C6-N6	8.98	130.88	123.70
80	B5	3212	C	C2-N3-C4	-8.97	115.42	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	802	C	C5-C6-N1	-8.96	116.52	121.00
82	B8	113	U	C2-N1-C1'	8.96	128.46	117.70
80	B5	2202	C	N1-C2-O2	-8.96	113.52	118.90
79	B2	969	C	C6-N1-C2	8.96	123.88	120.30
80	B5	3049	A	C5-C6-N1	-8.96	113.22	117.70
80	B5	1268	G	C5-C6-O6	-8.95	123.23	128.60
80	B5	881	C	N1-C2-O2	8.94	124.27	118.90
80	B5	726	G	C4-C5-N7	8.94	114.38	110.80
84	CW	70	G	N1-C6-O6	8.94	125.26	119.90
80	B5	2857	C	N3-C4-C5	8.93	125.47	121.90
80	B5	1113	G	C2-N3-C4	-8.93	107.43	111.90
80	B5	2393	G	C8-N9-C4	8.93	109.97	106.40
80	B5	2905	U	N3-C4-O4	-8.93	113.15	119.40
80	B5	1044	U	N3-C4-O4	-8.93	113.15	119.40
80	B5	2824	G	C6-N1-C2	-8.93	119.75	125.10
81	B7	101	G	N1-C6-O6	8.93	125.25	119.90
80	B5	1242	G	O4'-C1'-N9	8.92	115.34	108.20
80	B5	1487	G	N1-C6-O6	-8.92	114.55	119.90
80	B5	819	U	C4-C5-C6	8.92	125.05	119.70
19	AK	88	PRO	N-CA-CB	8.92	114.00	103.30
80	B5	1158	A	N1-C6-N6	8.92	123.95	118.60
80	B5	631	U	N3-C4-O4	-8.91	113.17	119.40
80	B5	1116	G	C4-C5-N7	-8.91	107.24	110.80
80	B5	2327	U	N3-C4-O4	-8.90	113.17	119.40
79	B2	1596	C	C6-N1-C2	-8.90	116.74	120.30
80	B5	2372	A	N7-C8-N9	8.90	118.25	113.80
80	B5	1429	G	N1-C2-N2	-8.90	108.19	116.20
80	B5	2327	U	C2-N3-C4	-8.89	121.67	127.00
80	B5	420	G	C5-C6-N1	8.89	115.94	111.50
56	BV	48	ARG	NE-CZ-NH1	8.88	124.74	120.30
80	B5	887	G	C5-C6-N1	-8.88	107.06	111.50
80	B5	3127	A	N1-C6-N6	-8.88	113.27	118.60
80	B5	802	C	C4-C5-C6	8.88	121.84	117.40
84	CW	19	G	N1-C6-O6	8.88	125.23	119.90
80	B5	2808	A	C2-N3-C4	-8.88	106.16	110.60
84	CW	65	G	N1-C6-O6	8.88	125.23	119.90
80	B5	3382	U	C2-N1-C1'	8.88	128.35	117.70
80	B5	1450	G	C6-C5-N7	8.87	135.72	130.40
80	B5	2382	G	C5-C6-O6	8.87	133.92	128.60
79	B2	1455	G	N3-C2-N2	-8.86	113.70	119.90
79	B2	1761	U	C5-C4-O4	8.86	131.21	125.90
79	B2	1745	G	N3-C4-N9	8.86	131.31	126.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	CW	57	G	N1-C6-O6	8.85	125.21	119.90
84	CW	71	G	N1-C6-O6	8.85	125.21	119.90
80	B5	1226	G	C5-C6-O6	-8.85	123.29	128.60
80	B5	2719	U	C2-N1-C1'	-8.85	107.09	117.70
84	CW	25	C	O4'-C1'-N1	8.85	115.28	108.20
80	B5	2833	A	N1-C6-N6	-8.84	113.29	118.60
80	B5	2647	A	N9-C4-C5	8.84	109.34	105.80
80	B5	2881	C	C2-N3-C4	-8.84	115.48	119.90
79	B2	507	U	N1-C2-O2	8.84	128.98	122.80
80	B5	3040	A	C8-N9-C4	8.82	109.33	105.80
80	B5	1931	U	C2-N1-C1'	-8.82	107.12	117.70
80	B5	1846	C	C2-N3-C4	-8.81	115.49	119.90
80	B5	437	G	C8-N9-C4	-8.81	102.88	106.40
80	B5	1264	G	N1-C6-O6	8.80	125.18	119.90
80	B5	1314	C	C2-N3-C4	-8.80	115.50	119.90
80	B5	947	G	C6-N1-C2	-8.80	119.82	125.10
79	B2	1654	G	C6-N1-C2	-8.80	119.82	125.10
83	CV	495	TYR	CB-CG-CD1	8.79	126.27	121.00
84	CW	42	C	C5'-C4'-C3'	-8.78	101.95	116.00
80	B5	1311	G	C2-N3-C4	8.78	116.29	111.90
84	CW	18	G	C5-C6-O6	-8.78	123.33	128.60
79	B2	1749	A	N1-C6-N6	8.77	123.86	118.60
80	B5	3047	U	C5-C6-N1	-8.77	118.32	122.70
80	B5	433	A	C2-N3-C4	-8.75	106.22	110.60
80	B5	2757	U	C4-C5-C6	8.75	124.95	119.70
79	B2	992	A	N3-C4-C5	8.75	132.93	126.80
80	B5	2271	A	N7-C8-N9	-8.74	109.43	113.80
80	B5	1412	G	C8-N9-C4	-8.74	102.91	106.40
80	B5	2858	U	N3-C2-O2	-8.74	116.08	122.20
81	B7	48	U	C2-N3-C4	-8.73	121.76	127.00
80	B5	1161	G	C5-C6-N1	8.73	115.86	111.50
80	B5	2434	U	C5-C6-N1	-8.72	118.34	122.70
80	B5	1907	C	N3-C4-C5	-8.72	118.41	121.90
79	B2	453	U	C2-N1-C1'	8.72	128.16	117.70
80	B5	2416	U	C6-N1-C2	-8.71	115.77	121.00
80	B5	1119	C	C2-N3-C4	-8.71	115.55	119.90
80	B5	2865	U	C5-C6-N1	8.71	127.06	122.70
80	B5	1327	C	N1-C2-O2	8.71	124.12	118.90
79	B2	1503	A	C2-N3-C4	-8.71	106.25	110.60
80	B5	1903	U	C4-C5-C6	8.70	124.92	119.70
80	B5	2832	C	C5-C6-N1	-8.70	116.65	121.00
80	B5	3123	A	C8-N9-C4	8.69	109.28	105.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2290	C	C2-N3-C4	-8.69	115.56	119.90
80	B5	1840	U	N3-C2-O2	-8.68	116.12	122.20
80	B5	821	U	C5-C6-N1	-8.68	118.36	122.70
80	B5	2730	G	N1-C6-O6	8.68	125.11	119.90
79	B2	558	U	N1-C2-O2	8.67	128.87	122.80
79	B2	794	U	N3-C2-O2	-8.66	116.14	122.20
80	B5	796	U	N3-C2-O2	-8.65	116.14	122.20
80	B5	2961	G	C8-N9-C4	-8.65	102.94	106.40
85	CX	1	A	O4'-C1'-N9	8.65	115.12	108.20
80	B5	834	U	C4-C5-C6	-8.65	114.51	119.70
82	B8	17	A	N1-C6-N6	8.65	123.79	118.60
80	B5	2190	U	C5-C4-O4	8.64	131.08	125.90
80	B5	2392	C	C2-N3-C4	-8.64	115.58	119.90
80	B5	2409	G	C8-N9-C4	-8.64	102.94	106.40
51	BQ	151	ARG	NE-CZ-NH1	-8.64	115.98	120.30
80	B5	3143	C	N1-C2-O2	-8.63	113.72	118.90
80	B5	3374	U	N3-C4-C5	8.63	119.78	114.60
80	B5	726	G	C6-C5-N7	-8.63	125.22	130.40
79	B2	92	A	C8-N9-C4	-8.63	102.35	105.80
80	B5	2687	G	N1-C6-O6	-8.63	114.72	119.90
80	B5	2728	G	N3-C2-N2	-8.63	113.86	119.90
80	B5	3040	A	N7-C8-N9	-8.63	109.48	113.80
79	B2	17	C	C6-N1-C2	-8.63	116.85	120.30
80	B5	2292	U	N3-C2-O2	-8.63	116.16	122.20
81	B7	92	A	N1-C6-N6	8.62	123.77	118.60
80	B5	1244	A	N1-C6-N6	8.62	123.77	118.60
80	B5	1249	G	C5-C6-O6	-8.61	123.43	128.60
80	B5	2391	G	N1-C6-O6	-8.62	114.73	119.90
80	B5	2638	C	N1-C2-O2	-8.62	113.73	118.90
79	B2	7	G	N1-C6-O6	-8.61	114.73	119.90
80	B5	2434	U	N3-C4-O4	-8.61	113.37	119.40
80	B5	644	G	C5-C6-N1	8.60	115.80	111.50
79	B2	1291	G	N7-C8-N9	8.59	117.40	113.10
80	B5	66	A	C8-N9-C4	8.59	109.24	105.80
80	B5	1149	G	C2-N3-C4	8.59	116.19	111.90
84	CW	19	G	O5'-C5'-C4'	-8.59	95.38	111.70
80	B5	726	G	C5-C6-O6	-8.59	123.45	128.60
80	B5	339	C	C5-C4-N4	8.58	126.21	120.20
79	B2	647	G	N3-C4-N9	-8.58	120.85	126.00
80	B5	1134	G	C5-C6-O6	-8.58	123.45	128.60
80	B5	938	C	C2-N3-C4	-8.58	115.61	119.90
80	B5	2988	C	N3-C2-O2	-8.57	115.90	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	3321	C	C5-C6-N1	-8.57	116.72	121.00
79	B2	1773	C	N3-C4-N4	8.57	124.00	118.00
80	B5	3010	U	N3-C2-O2	-8.56	116.20	122.20
80	B5	2385	G	N3-C4-C5	8.55	132.88	128.60
80	B5	2758	A	N1-C2-N3	-8.55	125.02	129.30
80	B5	2913	C	C4-C5-C6	8.55	121.68	117.40
80	B5	341	G	C5-C6-O6	-8.55	123.47	128.60
80	B5	326	U	C5-C4-O4	-8.55	120.77	125.90
79	B2	719	U	C2-N1-C1'	8.55	127.96	117.70
80	B5	345	G	C5-C6-N1	8.55	115.77	111.50
80	B5	2699	G	C5-C6-O6	-8.55	123.47	128.60
80	B5	946	U	N3-C2-O2	-8.54	116.22	122.20
80	B5	1050	U	N1-C2-O2	8.54	128.78	122.80
80	B5	1342	C	C5-C6-N1	-8.54	116.73	121.00
79	B2	1189	A	C8-N9-C4	8.53	109.21	105.80
80	B5	1284	C	C6-N1-C1'	-8.53	110.56	120.80
79	B2	1745	G	C5-C6-N1	8.52	115.76	111.50
80	B5	2524	A	C5-N7-C8	-8.52	99.64	103.90
80	B5	224	C	N1-C2-O2	8.51	124.00	118.90
80	B5	887	G	C5-C6-O6	8.50	133.70	128.60
80	B5	1156	C	C2-N3-C4	-8.50	115.65	119.90
79	B2	992	A	C5-C6-N1	-8.50	113.45	117.70
80	B5	2732	G	N1-C6-O6	-8.50	114.80	119.90
84	CW	10	G	N1-C6-O6	8.50	125.00	119.90
79	B2	992	A	N3-C4-N9	-8.49	120.61	127.40
80	B5	1237	G	C5-C6-O6	-8.49	123.51	128.60
80	B5	2301	U	C2-N3-C4	-8.49	121.91	127.00
80	B5	1085	A	N7-C8-N9	8.48	118.04	113.80
80	B5	2928	C	C4-C5-C6	8.48	121.64	117.40
80	B5	2988	C	C4-C5-C6	8.48	121.64	117.40
80	B5	2634	U	N1-C2-O2	-8.48	116.87	122.80
80	B5	2978	U	C5-C6-N1	-8.47	118.46	122.70
80	B5	3377	G	C5-C6-N1	8.47	115.74	111.50
80	B5	1942	U	N1-C2-O2	-8.47	116.87	122.80
80	B5	2952	G	N3-C2-N2	-8.47	113.97	119.90
83	CV	62	TYR	C-N-CA	8.47	142.87	121.70
79	B2	1387	G	N1-C6-O6	8.46	124.98	119.90
81	B7	48	U	C5-C4-O4	-8.46	120.82	125.90
82	B8	14	C	C5-C6-N1	-8.46	116.77	121.00
80	B5	999	G	N1-C6-O6	-8.46	114.83	119.90
80	B5	1143	A	C5-C6-N1	-8.45	113.47	117.70
79	B2	577	G	N7-C8-N9	8.45	117.33	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1402	C	N3-C2-O2	-8.45	115.99	121.90
80	B5	343	U	N3-C2-O2	-8.45	116.29	122.20
79	B2	1200	G	C6-C5-N7	-8.44	125.33	130.40
80	B5	1242	G	N1-C6-O6	8.44	124.96	119.90
80	B5	1409	G	N1-C6-O6	-8.43	114.84	119.90
80	B5	652	G	N3-C4-C5	-8.43	124.39	128.60
80	B5	2980	U	N1-C2-N3	8.43	119.96	114.90
80	B5	2683	U	N1-C2-O2	8.42	128.69	122.80
81	B7	96	U	C2-N3-C4	-8.42	121.95	127.00
80	B5	2345	A	N1-C6-N6	8.42	123.65	118.60
79	B2	1541	G	C5-C6-O6	8.41	133.65	128.60
80	B5	1064	A	C5-C6-N6	-8.41	116.97	123.70
82	B8	55	U	N1-C2-N3	8.41	119.95	114.90
79	B2	966	A	C8-N9-C4	8.41	109.16	105.80
84	CW	56	C	O4'-C1'-N1	8.40	114.92	108.20
84	CW	18	G	N1-C6-O6	8.40	124.94	119.90
79	B2	1486	G	C4-C5-N7	8.40	114.16	110.80
80	B5	817	A	C8-N9-C4	-8.40	102.44	105.80
80	B5	3050	U	C5-C4-O4	8.40	130.94	125.90
80	B5	1047	A	C2-N3-C4	8.39	114.80	110.60
80	B5	2307	G	N3-C4-C5	-8.39	124.41	128.60
80	B5	2913	C	C2-N3-C4	-8.39	115.71	119.90
80	B5	3102	G	N3-C2-N2	8.39	125.77	119.90
80	B5	986	U	C5-C4-O4	-8.38	120.87	125.90
80	B5	916	G	C5-C6-O6	8.38	133.63	128.60
84	CW	75	C	P-O3'-C3'	8.38	129.76	119.70
80	B5	616	G	C5-C6-N1	8.38	115.69	111.50
80	B5	3137	C	N3-C4-C5	8.37	125.25	121.90
79	B2	736	C	C2-N1-C1'	8.37	128.00	118.80
80	B5	2870	C	C6-N1-C2	-8.37	116.95	120.30
80	B5	811	U	C2-N3-C4	-8.36	121.98	127.00
80	B5	1480	G	N7-C8-N9	-8.36	108.92	113.10
80	B5	715	A	C2-N3-C4	8.36	114.78	110.60
80	B5	1898	G	C2-N3-C4	8.36	116.08	111.90
80	B5	580	C	C6-N1-C2	-8.35	116.96	120.30
84	CW	13	C	C5'-C4'-C3'	-8.35	102.64	116.00
84	CW	30	G	N1-C6-O6	8.35	124.91	119.90
43	BI	128	ARG	NE-CZ-NH2	-8.35	116.13	120.30
80	B5	1469	C	N3-C4-C5	-8.35	118.56	121.90
80	B5	3173	G	C5-C6-O6	-8.35	123.59	128.60
80	B5	1487	G	C5-C6-O6	8.35	133.61	128.60
80	B5	2320	A	C2-N3-C4	-8.35	106.43	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	926	A	C5-C6-N1	8.34	121.87	117.70
80	B5	2234	G	N9-C4-C5	-8.34	102.06	105.40
81	B7	96	U	N1-C2-N3	8.34	119.90	114.90
84	CW	38	A	C4-C5-C6	8.33	121.17	117.00
80	B5	945	C	N3-C4-C5	8.33	125.23	121.90
82	B8	80	A	N7-C8-N9	8.33	117.96	113.80
80	B5	1226	G	O4'-C4'-C3'	-8.32	95.68	104.00
79	B2	136	C	C2-N1-C1'	8.31	127.94	118.80
81	B7	93	C	C2-N3-C4	-8.31	115.74	119.90
79	B2	1387	G	C6-C5-N7	-8.31	125.42	130.40
49	BO	197[B]	PHE	C-N-CA	-8.31	104.86	122.30
80	B5	511	G	N1-C6-O6	-8.29	114.92	119.90
79	B2	1782	A	N1-C2-N3	8.29	133.44	129.30
80	B5	2371	G	N3-C2-N2	8.28	125.70	119.90
80	B5	1586	G	C5-C6-O6	-8.28	123.63	128.60
80	B5	2360	C	C4-C5-C6	8.27	121.54	117.40
80	B5	2683	U	N3-C2-O2	-8.27	116.41	122.20
84	CW	15	G	P-O5'-C5'	-8.26	107.68	120.90
79	B2	1280	C	N1-C2-O2	-8.26	113.94	118.90
80	B5	1494	U	C6-N1-C2	8.26	125.95	121.00
79	B2	542	A	C4-N9-C1'	8.26	141.16	126.30
80	B5	708	G	C5-N7-C8	-8.26	100.17	104.30
80	B5	818	C	N1-C2-O2	-8.26	113.94	118.90
80	B5	1604	G	C8-N9-C1'	-8.26	116.27	127.00
80	B5	1015	U	C5-C6-N1	8.25	126.83	122.70
80	B5	2621	G	N1-C6-O6	8.25	124.85	119.90
84	CW	51	U	P-O3'-C3'	-8.25	109.80	119.70
80	B5	1404	G	C8-N9-C4	8.25	109.70	106.40
80	B5	591	G	N9-C4-C5	-8.24	102.10	105.40
82	B8	55	U	C6-N1-C2	-8.24	116.05	121.00
79	B2	1096	C	N1-C2-O2	8.24	123.84	118.90
80	B5	2735	U	C5-C6-N1	8.24	126.82	122.70
80	B5	2820	A	C8-N9-C4	-8.23	102.51	105.80
80	B5	1110	U	N3-C4-C5	8.22	119.53	114.60
79	B2	319	U	N3-C2-O2	8.22	127.95	122.20
80	B5	922	U	C6-N1-C1'	8.22	132.71	121.20
80	B5	514	G	C5-C6-O6	-8.21	123.68	128.60
80	B5	715	A	N1-C6-N6	-8.20	113.68	118.60
80	B5	2859	U	N3-C4-O4	-8.20	113.66	119.40
79	B2	1129	U	N3-C4-C5	8.20	119.52	114.60
80	B5	1176	C	C5-C6-N1	-8.20	116.90	121.00
80	B5	1392	G	N7-C8-N9	-8.20	109.00	113.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	1291	G	N1-C2-N3	8.20	128.82	123.90
80	B5	1178	G	C8-N9-C4	-8.20	103.12	106.40
84	CW	24	G	N1-C6-O6	8.20	124.82	119.90
80	B5	2412	G	C8-N9-C4	-8.19	103.12	106.40
79	B2	1119	G	N1-C6-O6	-8.19	114.99	119.90
80	B5	280	U	C2-N3-C4	-8.19	122.09	127.00
80	B5	2665	U	N1-C2-N3	-8.19	109.99	114.90
80	B5	2190	U	N3-C4-O4	-8.18	113.67	119.40
80	B5	842	G	C5-C6-O6	-8.17	123.70	128.60
80	B5	1282	G	N1-C6-O6	8.17	124.80	119.90
53	BS	115	ARG	NE-CZ-NH1	8.17	124.38	120.30
80	B5	3317	U	C5-C4-O4	8.17	130.80	125.90
80	B5	2211	U	N3-C2-O2	-8.17	116.48	122.20
80	B5	2609	A	C5-N7-C8	8.17	107.98	103.90
81	B7	93	C	C5-C6-N1	-8.16	116.92	121.00
84	CW	24	G	C5-C6-O6	-8.16	123.70	128.60
80	B5	343	U	N1-C2-O2	8.16	128.51	122.80
80	B5	435	C	C5-C4-N4	-8.16	114.49	120.20
80	B5	968	G	N9-C4-C5	-8.16	102.14	105.40
80	B5	1193	A	N1-C2-N3	8.16	133.38	129.30
80	B5	2970	C	C4-C5-C6	8.16	121.48	117.40
80	B5	1054	A	C8-N9-C4	8.16	109.06	105.80
80	B5	2246	G	N1-C6-O6	-8.16	115.00	119.90
80	B5	726	G	N1-C6-O6	8.15	124.79	119.90
79	B2	308	C	C5-C6-N1	-8.15	116.92	121.00
80	B5	1230	G	O4'-C1'-N9	8.15	114.72	108.20
80	B5	949	C	C4-C5-C6	8.15	121.48	117.40
80	B5	805	G	C8-N9-C4	8.15	109.66	106.40
80	B5	2838	A	C5-C6-N6	-8.15	117.18	123.70
83	CV	136	TYR	CB-CG-CD1	8.15	125.89	121.00
80	B5	2175	U	C5-C6-N1	-8.15	118.62	122.70
80	B5	435	C	N3-C4-C5	8.15	125.16	121.90
80	B5	290	G	C5-C6-O6	8.14	133.48	128.60
80	B5	926	A	C5-C6-N6	-8.14	117.19	123.70
80	B5	1516	C	C2-N3-C4	-8.14	115.83	119.90
79	B2	992	A	C5-N7-C8	-8.13	99.83	103.90
81	B7	69	C	C6-N1-C2	8.13	123.55	120.30
82	B8	2	A	C8-N9-C4	-8.13	102.55	105.80
80	B5	769	G	C8-N9-C4	8.13	109.65	106.40
80	B5	2695	A	C8-N9-C4	-8.12	102.55	105.80
80	B5	916	G	N1-C6-O6	-8.12	115.03	119.90
80	B5	1445	U	C5-C4-O4	-8.12	121.03	125.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2913	C	N1-C2-N3	8.12	124.89	119.20
80	B5	15	C	C5-C6-N1	8.12	125.06	121.00
80	B5	3215	A	C2-N3-C4	-8.12	106.54	110.60
80	B5	1879	A	C8-N9-C4	-8.11	102.56	105.80
80	B5	2302	G	C5-C6-O6	8.11	133.47	128.60
80	B5	2202	C	N3-C2-O2	8.11	127.58	121.90
80	B5	2182	A	N1-C6-N6	-8.10	113.74	118.60
79	B2	1131	A	C8-N9-C4	8.10	109.04	105.80
80	B5	1281	G	N1-C6-O6	8.10	124.76	119.90
82	B8	74	U	C5-C4-O4	-8.10	121.04	125.90
80	B5	2440	G	C8-N9-C4	-8.10	103.16	106.40
84	CW	59	U	C4'-C3'-C2'	8.10	110.69	102.60
79	B2	1241	G	C5-N7-C8	-8.09	100.25	104.30
80	B5	3362	A	N1-C2-N3	8.09	133.35	129.30
80	B5	359	U	C2-N3-C4	-8.09	122.15	127.00
80	B5	945	C	C2-N3-C4	-8.09	115.86	119.90
80	B5	2290	C	C4-C5-C6	8.09	121.44	117.40
82	B8	113	U	N3-C4-O4	8.09	125.06	119.40
84	CW	67	C	C5'-C4'-C3'	8.09	128.94	116.00
80	B5	987	U	N1-C2-N3	8.09	119.75	114.90
80	B5	329	U	C5-C6-N1	-8.09	118.66	122.70
80	B5	1113	G	C8-N9-C4	8.09	109.64	106.40
80	B5	1512	U	N1-C2-N3	8.09	119.75	114.90
80	B5	2859	U	C5-C4-O4	8.09	130.75	125.90
80	B5	3215	A	N1-C6-N6	8.09	123.45	118.60
81	B7	81	U	N3-C4-C5	8.09	119.45	114.60
80	B5	637	C	N1-C2-O2	-8.08	114.05	118.90
80	B5	1449	A	C5-N7-C8	-8.08	99.86	103.90
82	B8	38	U	C5-C6-N1	-8.08	118.66	122.70
80	B5	3309	G	N3-C4-N9	8.08	130.85	126.00
81	B7	112	G	N1-C6-O6	-8.08	115.05	119.90
80	B5	2634	U	N3-C4-C5	8.07	119.44	114.60
79	B2	1436	A	N1-C6-N6	8.06	123.44	118.60
79	B2	1773	C	C5-C6-N1	8.06	125.03	121.00
80	B5	1858	A	N3-C4-C5	-8.06	121.16	126.80
79	B2	1200	G	N1-C2-N2	8.06	123.45	116.20
79	B2	1662	G	N1-C6-O6	-8.05	115.07	119.90
80	B5	2278	C	C5-C4-N4	8.05	125.84	120.20
49	BO	3[B]	SER	O-C-N	8.05	135.58	122.70
80	B5	631	U	C2-N3-C4	-8.05	122.17	127.00
80	B5	824	C	C6-N1-C2	-8.05	117.08	120.30
80	B5	1239	C	N3-C4-N4	8.05	123.63	118.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2281	A	C8-N9-C4	8.05	109.02	105.80
80	B5	3110	C	C4-C5-C6	8.04	121.42	117.40
80	B5	1390	A	N9-C4-C5	8.04	109.02	105.80
80	B5	1085	A	C5-N7-C8	-8.04	99.88	103.90
40	BF	88	ARG	NE-CZ-NH2	-8.03	116.28	120.30
84	CW	16	U	C2'-C3'-O3'	8.03	127.17	109.50
80	B5	345	G	N1-C6-O6	-8.03	115.08	119.90
76	Bq	12	PHE	CB-CG-CD1	8.03	126.42	120.80
80	B5	2278	C	C2-N3-C4	-8.03	115.89	119.90
80	B5	2288	G	C2-N3-C4	8.02	115.91	111.90
80	B5	41	G	C5-N7-C8	-8.02	100.29	104.30
80	B5	1317	A	N1-C6-N6	8.02	123.41	118.60
80	B5	3362	A	C8-N9-C4	-8.02	102.59	105.80
80	B5	2572	C	C2-N1-C1'	8.01	127.61	118.80
80	B5	3343	G	N3-C4-N9	8.01	130.81	126.00
80	B5	857	G	C5-C6-N1	8.01	115.50	111.50
80	B5	278	U	C5-C6-N1	8.01	126.70	122.70
80	B5	413	U	C2-N3-C4	-8.01	122.20	127.00
80	B5	2189	U	N1-C2-N3	8.01	119.70	114.90
80	B5	817	A	C2-N3-C4	8.00	114.60	110.60
80	B5	3122	A	N9-C4-C5	8.00	109.00	105.80
80	B5	945	C	C6-N1-C2	8.00	123.50	120.30
80	B5	1148	G	C2-N3-C4	8.00	115.90	111.90
80	B5	1592	G	C5-C6-N1	8.00	115.50	111.50
62	Bb	39	PHE	N-CA-CB	7.99	124.99	110.60
80	B5	1297	C	C5-C6-N1	-7.99	117.01	121.00
84	CW	22	G	C5-C6-O6	-7.98	123.81	128.60
80	B5	2317	A	C8-N9-C4	-7.98	102.61	105.80
80	B5	2777	G	C5-C6-O6	7.98	133.39	128.60
80	B5	1879	A	C6-C5-N7	-7.98	126.72	132.30
80	B5	355	A	C2-N3-C4	-7.98	106.61	110.60
80	B5	3343	G	N9-C4-C5	-7.97	102.21	105.40
79	B2	1432	U	C6-N1-C2	7.97	125.78	121.00
80	B5	2618	G	C5-C6-O6	-7.97	123.82	128.60
84	CW	12	U	O4'-C1'-N1	7.97	114.58	108.20
80	B5	3151	U	C6-N1-C2	7.97	125.78	121.00
79	B2	1490	C	C6-N1-C2	-7.96	117.11	120.30
80	B5	2366	C	N3-C4-N4	7.96	123.57	118.00
80	B5	1441	G	N1-C6-O6	-7.96	115.12	119.90
80	B5	2865	U	C5-C4-O4	-7.96	121.12	125.90
80	B5	2993	G	C5-C6-O6	-7.96	123.82	128.60
80	B5	784	A	N1-C6-N6	7.96	123.38	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2757	U	N3-C4-O4	7.96	124.97	119.40
80	B5	277	G	N1-C6-O6	-7.96	115.12	119.90
80	B5	2350	C	C5-C6-N1	-7.96	117.02	121.00
80	B5	3146	G	C5-C6-O6	7.96	133.37	128.60
80	B5	3377	G	N9-C4-C5	-7.96	102.22	105.40
80	B5	1939	G	C5-C6-O6	7.95	133.37	128.60
80	B5	2531	C	C2-N1-C1'	7.95	127.55	118.80
80	B5	2630	C	N3-C4-C5	7.95	125.08	121.90
79	B2	189	C	C2-N1-C1'	7.95	127.55	118.80
79	B2	316	A	C8-N9-C4	7.95	108.98	105.80
79	B2	349	U	N3-C2-O2	-7.95	116.64	122.20
80	B5	1261	G	N1-C6-O6	7.95	124.67	119.90
79	B2	1324	G	N3-C4-N9	-7.94	121.24	126.00
79	B2	145	A	C8-N9-C4	-7.93	102.63	105.80
80	B5	1481	A	N7-C8-N9	7.93	117.77	113.80
80	B5	2870	C	C6-N1-C1'	7.93	130.32	120.80
81	B7	85	G	N1-C6-O6	-7.93	115.14	119.90
84	CW	27	G	C5-C6-O6	-7.93	123.84	128.60
40	BF	88	ARG	NE-CZ-NH1	7.92	124.26	120.30
80	B5	1845	G	C5-C6-N1	7.92	115.46	111.50
65	Be	43	ARG	NE-CZ-NH2	-7.91	116.34	120.30
49	BO	27[B]	VAL	O-C-N	-7.91	110.05	122.70
80	B5	629	U	N3-C4-C5	7.90	119.34	114.60
80	B5	1793	C	N3-C4-C5	-7.90	118.74	121.90
80	B5	2836	C	N1-C2-N3	7.90	124.73	119.20
80	B5	813	G	C8-N9-C4	-7.90	103.24	106.40
80	B5	2130	G	N3-C2-N2	7.90	125.43	119.90
80	B5	2550	U	N1-C2-N3	7.90	119.64	114.90
80	B5	3102	G	N1-C6-O6	-7.90	115.16	119.90
84	CW	54	U	O4'-C1'-N1	7.89	114.51	108.20
80	B5	1484	U	C6-N1-C2	7.88	125.73	121.00
80	B5	1311	G	C5-C6-N1	7.88	115.44	111.50
79	B2	1481	C	C6-N1-C2	-7.88	117.15	120.30
81	B7	26	C	C4-C5-C6	7.88	121.34	117.40
80	B5	1480	G	C5-N7-C8	7.88	108.24	104.30
80	B5	3096	C	N1-C2-N3	7.87	124.71	119.20
80	B5	1237	G	N1-C6-O6	7.87	124.62	119.90
80	B5	1940	G	N3-C2-N2	7.87	125.41	119.90
80	B5	2891	U	C2-N3-C4	-7.87	122.28	127.00
80	B5	641	C	N1-C2-O2	-7.87	114.18	118.90
80	B5	960	U	C5-C6-N1	-7.87	118.77	122.70
80	B5	1227	C	N3-C4-N4	7.87	123.50	118.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	581	U	C2-N1-C1'	7.86	127.13	117.70
80	B5	1834	U	C2-N1-C1'	-7.86	108.27	117.70
37	BC	339	LEU	CA-CB-CG	7.86	133.37	115.30
80	B5	2703	A	C8-N9-C4	-7.86	102.66	105.80
80	B5	851	C	C6-N1-C2	-7.86	117.16	120.30
80	B5	2913	C	C5-C6-N1	-7.86	117.07	121.00
80	B5	226	C	C6-N1-C2	7.85	123.44	120.30
80	B5	1236	G	N1-C6-O6	7.85	124.61	119.90
79	B2	1611	A	N7-C8-N9	7.85	117.72	113.80
80	B5	1243	G	N1-C6-O6	7.85	124.61	119.90
80	B5	2288	G	C6-N1-C2	-7.85	120.39	125.10
84	CW	1	G	O4'-C1'-N9	7.85	114.48	108.20
79	B2	864	U	N3-C2-O2	-7.85	116.71	122.20
80	B5	2366	C	C2-N1-C1'	7.84	127.43	118.80
80	B5	530	G	N1-C6-O6	-7.84	115.20	119.90
80	B5	2882	U	N1-C2-N3	7.84	119.60	114.90
84	CW	48	C	O4'-C1'-C2'	-7.84	97.96	105.80
80	B5	934	G	C5-C6-O6	-7.83	123.90	128.60
80	B5	1246	G	C5-C6-O6	-7.83	123.90	128.60
80	B5	2400	G	C2-N3-C4	-7.83	107.98	111.90
80	B5	3187	A	N1-C6-N6	-7.83	113.90	118.60
80	B5	216	G	N1-C6-O6	7.83	124.60	119.90
80	B5	1440	G	C5-C6-O6	7.83	133.30	128.60
80	B5	3130	A	N1-C2-N3	7.83	133.21	129.30
79	B2	142	G	N3-C4-N9	-7.82	121.31	126.00
80	B5	2512	C	C5-C6-N1	7.82	124.91	121.00
84	CW	73	A	O4'-C1'-N9	7.82	114.46	108.20
80	B5	630	A	N1-C2-N3	7.82	133.21	129.30
80	B5	2905	U	N3-C4-C5	7.82	119.29	114.60
79	B2	1560	U	N3-C4-O4	-7.82	113.93	119.40
80	B5	2807	U	C5-C4-O4	-7.82	121.21	125.90
80	B5	2705	A	C5-C6-N6	-7.81	117.45	123.70
80	B5	2919	A	N1-C6-N6	-7.81	113.91	118.60
80	B5	2303	A	N9-C4-C5	7.81	108.92	105.80
84	CW	21	A	C5-C6-N6	-7.81	117.45	123.70
84	CW	69	G	O4'-C1'-N9	7.81	114.45	108.20
80	B5	1140	G	N1-C6-O6	-7.81	115.21	119.90
80	B5	1234	G	C5-C6-O6	-7.81	123.92	128.60
80	B5	343	U	N3-C4-O4	-7.81	113.94	119.40
80	B5	2134	G	C5-C6-N1	7.80	115.40	111.50
80	B5	3187	A	C5-N7-C8	7.80	107.80	103.90
84	CW	42	C	N3-C4-N4	7.80	123.46	118.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2393	G	N1-C6-O6	7.80	124.58	119.90
83	CV	435	TYR	CB-CG-CD2	-7.80	116.32	121.00
80	B5	1150	A	C2-N3-C4	-7.79	106.70	110.60
79	B2	555	A	C8-N9-C4	-7.79	102.68	105.80
80	B5	1370	G	N1-C6-O6	-7.79	115.23	119.90
80	B5	2246	G	C5-C6-O6	7.79	133.27	128.60
80	B5	2395	G	C5-N7-C8	7.79	108.19	104.30
80	B5	1480	G	C8-N9-C4	7.79	109.52	106.40
79	B2	1751	C	N3-C4-C5	7.78	125.01	121.90
80	B5	1392	G	N3-C4-N9	7.78	130.67	126.00
80	B5	2381	G	C8-N9-C4	-7.78	103.29	106.40
80	B5	2975	U	N3-C4-C5	7.78	119.27	114.60
80	B5	708	G	C5-C6-O6	-7.78	123.93	128.60
80	B5	1364	C	N1-C2-O2	-7.78	114.23	118.90
79	B2	334	G	C2-N3-C4	-7.77	108.01	111.90
80	B5	974	G	N3-C4-C5	-7.77	124.71	128.60
80	B5	2550	U	N3-C4-O4	-7.77	113.96	119.40
84	CW	29	G	N1-C6-O6	7.77	124.56	119.90
80	B5	3266	G	N9-C4-C5	7.76	108.51	105.40
80	B5	3206	C	N3-C2-O2	-7.76	116.47	121.90
80	B5	990	U	N1-C2-O2	7.76	128.23	122.80
83	CV	474	PHE	N-CA-C	7.76	131.94	111.00
79	B2	992	A	C6-N1-C2	7.75	123.25	118.60
80	B5	904	A	N1-C6-N6	-7.75	113.95	118.60
80	B5	2899	C	N3-C4-N4	-7.75	112.58	118.00
84	CW	67	C	O4'-C1'-N1	7.75	114.40	108.20
80	B5	1233	G	N3-C2-N2	7.75	125.32	119.90
43	BI	167	LEU	CA-CB-CG	7.74	133.11	115.30
80	B5	376	G	C5-C6-N1	7.74	115.37	111.50
84	CW	59	U	O4'-C1'-N1	7.74	114.39	108.20
65	Be	45	ARG	NE-CZ-NH2	-7.74	116.43	120.30
80	B5	1792	C	N1-C2-O2	-7.74	114.26	118.90
80	B5	2315	G	C8-N9-C4	7.74	109.50	106.40
80	B5	1295	G	N1-C6-O6	-7.74	115.26	119.90
80	B5	2303	A	C8-N9-C4	-7.74	102.70	105.80
80	B5	2757	U	C2-N3-C4	-7.74	122.36	127.00
79	B2	1486	G	C8-N9-C4	-7.73	103.31	106.40
80	B5	276	U	C5-C6-N1	-7.72	118.84	122.70
80	B5	546	C	C6-N1-C1'	-7.72	111.53	120.80
80	B5	1391	C	N3-C2-O2	7.72	127.31	121.90
79	B2	704	C	N1-C2-O2	7.72	123.53	118.90
80	B5	2643	A	C2-N3-C4	7.72	114.46	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	3050	U	N1-C2-O2	7.72	128.20	122.80
80	B5	2278	C	C6-N1-C1'	7.71	130.06	120.80
84	CW	72	C	O4'-C1'-N1	7.71	114.37	108.20
80	B5	2202	C	N3-C4-N4	7.71	123.40	118.00
80	B5	3308	C	N1-C2-N3	7.71	124.59	119.20
80	B5	2634	U	C6-N1-C2	7.71	125.62	121.00
80	B5	1390	A	C8-N9-C4	-7.70	102.72	105.80
80	B5	2346	C	C2-N3-C4	-7.70	116.05	119.90
80	B5	3377	G	N3-C4-N9	7.70	130.62	126.00
79	B2	1455	G	C4-C5-N7	-7.70	107.72	110.80
80	B5	859	G	C8-N9-C4	-7.70	103.32	106.40
80	B5	1402	C	C5-C6-N1	-7.70	117.15	121.00
84	CW	11	C	O4'-C1'-N1	7.70	114.36	108.20
80	B5	2234	G	C8-N9-C4	7.68	109.47	106.40
80	B5	2584	G	C4-N9-C1'	7.68	136.49	126.50
79	B2	1305	U	C5-C4-O4	7.68	130.51	125.90
80	B5	1889	G	N1-C6-O6	-7.68	115.29	119.90
80	B5	1281	G	O4'-C1'-N9	7.68	114.34	108.20
80	B5	3065	G	N1-C6-O6	-7.68	115.30	119.90
80	B5	3185	U	C2-N3-C4	-7.68	122.39	127.00
80	B5	2433	U	C6-N1-C2	7.67	125.60	121.00
80	B5	2698	G	C8-N9-C4	7.67	109.47	106.40
80	B5	3055	U	N3-C2-O2	-7.67	116.83	122.20
80	B5	630	A	C2-N3-C4	-7.66	106.77	110.60
80	B5	753	C	C2-N3-C4	-7.66	116.07	119.90
80	B5	2271	A	C8-N9-C4	7.66	108.86	105.80
80	B5	594	U	C6-N1-C2	-7.65	116.41	121.00
79	B2	1291	G	C8-N9-C4	-7.65	103.34	106.40
80	B5	1124	U	N1-C2-N3	-7.65	110.31	114.90
80	B5	1285	G	C6-N1-C2	-7.65	120.51	125.10
80	B5	3006	A	C5-C6-N1	-7.65	113.87	117.70
82	B8	144	G	N1-C6-O6	7.65	124.49	119.90
79	B2	704	C	C2-N1-C1'	7.65	127.22	118.80
80	B5	1604	G	C4-N9-C1'	7.65	136.45	126.50
80	B5	1833	G	N1-C6-O6	-7.65	115.31	119.90
82	B8	2	A	N9-C4-C5	7.64	108.86	105.80
80	B5	2611	U	C5-C6-N1	-7.64	118.88	122.70
80	B5	2372	A	N9-C4-C5	7.64	108.86	105.80
80	B5	3330	A	C5-C6-N1	7.64	121.52	117.70
80	B5	3378	C	N3-C4-C5	7.64	124.96	121.90
82	B8	11	C	N3-C2-O2	-7.64	116.56	121.90
80	B5	877	C	C4-C5-C6	-7.63	113.58	117.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2887	A	C5-C6-N1	-7.63	113.88	117.70
80	B5	2960	C	N3-C4-C5	7.63	124.95	121.90
46	BL	21	ARG	NE-CZ-NH1	-7.63	116.48	120.30
80	B5	1370	G	C5-C6-N1	7.62	115.31	111.50
84	CW	10	G	C5-C6-O6	-7.62	124.03	128.60
80	B5	519	A	N1-C6-N6	7.62	123.17	118.60
80	B5	665	A	N1-C6-N6	7.62	123.17	118.60
80	B5	2838	A	N1-C6-N6	7.62	123.17	118.60
79	B2	647	G	N9-C4-C5	7.61	108.44	105.40
80	B5	633	C	N1-C2-O2	-7.61	114.34	118.90
79	B2	553	G	C4-C5-C6	7.60	123.36	118.80
81	B7	39	C	C6-N1-C2	-7.60	117.26	120.30
80	B5	419	G	C5-C6-O6	-7.60	124.04	128.60
80	B5	1130	A	C5-C6-N1	7.60	121.50	117.70
81	B7	67	G	N3-C2-N2	-7.60	114.58	119.90
80	B5	1390	A	N1-C6-N6	-7.59	114.04	118.60
80	B5	1515	A	C2-N3-C4	-7.59	106.80	110.60
80	B5	1014	U	C2-N1-C1'	7.59	126.81	117.70
80	B5	1163	A	C5-N7-C8	7.59	107.69	103.90
80	B5	1342	C	C2-N3-C4	-7.59	116.11	119.90
80	B5	3154	C	N1-C2-O2	7.59	123.45	118.90
82	B8	6	U	C2-N3-C4	-7.59	122.45	127.00
80	B5	1305	U	C5-C4-O4	-7.58	121.35	125.90
80	B5	2693	C	N3-C4-C5	7.58	124.93	121.90
80	B5	1516	C	N1-C2-O2	-7.58	114.35	118.90
79	B2	1291	G	C2-N3-C4	-7.58	108.11	111.90
80	B5	1890	U	C4-C5-C6	7.58	124.25	119.70
80	B5	3088	G	C4-C5-N7	7.58	113.83	110.80
80	B5	3138	U	C2-N3-C4	-7.58	122.45	127.00
80	B5	3245	A	C5-C6-N1	-7.58	113.91	117.70
80	B5	2237	C	N3-C4-N4	-7.58	112.69	118.00
79	B2	1758	U	N3-C2-O2	-7.58	116.89	122.20
80	B5	324	A	C8-N9-C4	-7.58	102.77	105.80
81	B7	49	G	C5-C6-O6	-7.58	124.05	128.60
79	B2	978	A	C8-N9-C4	7.58	108.83	105.80
80	B5	1251	A	C5-C6-N6	-7.58	117.64	123.70
80	B5	1381	A	C8-N9-C4	7.58	108.83	105.80
80	B5	1396	C	N3-C4-C5	7.58	124.93	121.90
82	B8	144	G	N3-C2-N2	-7.58	114.60	119.90
80	B5	641	C	N3-C4-N4	-7.57	112.70	118.00
80	B5	851	C	C5-C6-N1	7.57	124.79	121.00
80	B5	1163	A	N1-C6-N6	-7.57	114.06	118.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1848	G	C4-C5-N7	7.57	113.83	110.80
80	B5	3172	A	N7-C8-N9	-7.57	110.02	113.80
80	B5	1256	G	P-O5'-C5'	7.57	133.01	120.90
80	B5	2138	A	C8-N9-C4	-7.57	102.77	105.80
80	B5	1910	A	C8-N9-C4	7.56	108.83	105.80
84	CW	65	G	C5-C6-O6	-7.56	124.06	128.60
80	B5	2849	C	N3-C4-C5	-7.56	118.88	121.90
56	BV	45	ARG	NE-CZ-NH1	-7.55	116.52	120.30
79	B2	323	A	C8-N9-C4	-7.55	102.78	105.80
80	B5	81	C	N3-C4-C5	7.55	124.92	121.90
80	B5	400	G	C5-C6-O6	-7.55	124.07	128.60
80	B5	1057	A	C5-C6-N6	-7.55	117.66	123.70
80	B5	1260	A	C5-C6-N6	-7.55	117.66	123.70
80	B5	121	A	C8-N9-C4	7.55	108.82	105.80
80	B5	929	A	C8-N9-C4	7.54	108.82	105.80
80	B5	289	A	C6-N1-C2	-7.54	114.08	118.60
80	B5	2289	U	N1-C2-O2	7.54	128.08	122.80
80	B5	2524	A	N7-C8-N9	7.54	117.57	113.80
80	B5	3007	U	C2-N3-C4	-7.54	122.48	127.00
80	B5	971	G	C5-N7-C8	7.54	108.07	104.30
80	B5	2625	C	C2-N3-C4	-7.54	116.13	119.90
82	B8	12	A	C5-N7-C8	-7.53	100.14	103.90
80	B5	928	C	C4-C5-C6	7.53	121.16	117.40
81	B7	41	G	C8-N9-C4	7.53	109.41	106.40
80	B5	1216	C	N1-C2-O2	-7.52	114.39	118.90
80	B5	1459	C	N3-C4-C5	7.52	124.91	121.90
80	B5	1176	C	C2-N3-C4	-7.52	116.14	119.90
80	B5	1340	G	C8-N9-C4	7.52	109.41	106.40
80	B5	3140	G	C4-C5-N7	7.52	113.81	110.80
80	B5	3192	U	C5-C6-N1	-7.52	118.94	122.70
80	B5	924	G	N1-C2-N2	7.52	122.97	116.20
80	B5	971	G	N7-C8-N9	-7.52	109.34	113.10
80	B5	3167	A	C8-N9-C4	-7.52	102.79	105.80
79	B2	871	G	N3-C4-C5	-7.52	124.84	128.60
81	B7	11	A	C8-N9-C4	7.52	108.81	105.80
80	B5	622	A	N1-C6-N6	7.51	123.11	118.60
80	B5	2395	G	N7-C8-N9	-7.51	109.34	113.10
79	B2	758	U	N3-C2-O2	-7.51	116.94	122.20
80	B5	2718	U	N1-C2-N3	7.51	119.41	114.90
84	CW	71	G	C5-C6-O6	-7.51	124.09	128.60
84	CW	1	G	N1-C6-O6	7.51	124.41	119.90
79	B2	594	A	C2-N3-C4	7.51	114.35	110.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1407	A	C6-N1-C2	7.51	123.10	118.60
80	B5	971	G	C2-N3-C4	7.50	115.65	111.90
80	B5	2342	U	N3-C4-O4	-7.50	114.15	119.40
80	B5	426	G	C8-N9-C4	7.50	109.40	106.40
79	B2	507	U	C2-N1-C1'	7.50	126.70	117.70
79	B2	1432	U	C5-C6-N1	-7.50	118.95	122.70
80	B5	436	A	N1-C6-N6	7.50	123.10	118.60
80	B5	42	C	C4-C5-C6	-7.49	113.65	117.40
79	B2	1280	C	C6-N1-C2	-7.48	117.31	120.30
80	B5	150	A	N1-C6-N6	7.48	123.09	118.60
80	B5	2791	G	C5-C6-O6	-7.48	124.11	128.60
80	B5	3096	C	C5-C6-N1	-7.48	117.26	121.00
80	B5	2234	G	C4-C5-N7	7.47	113.79	110.80
80	B5	3102	G	N1-C2-N2	-7.47	109.48	116.20
82	B8	144	G	C5-C6-O6	-7.47	124.12	128.60
80	B5	957	C	C2-N3-C4	-7.47	116.17	119.90
79	B2	1291	G	C5-N7-C8	-7.46	100.57	104.30
80	B5	2639	G	C5-C6-O6	-7.46	124.12	128.60
80	B5	2943	G	N3-C2-N2	7.46	125.12	119.90
80	B5	307	A	N1-C6-N6	-7.46	114.12	118.60
80	B5	1205	A	C8-N9-C4	-7.46	102.82	105.80
80	B5	2381	G	N9-C4-C5	7.46	108.38	105.40
80	B5	1372	C	N1-C2-O2	-7.46	114.42	118.90
82	B8	14	C	C4-C5-C6	7.45	121.13	117.40
80	B5	1227	C	C5-C6-N1	7.45	124.72	121.00
80	B5	1327	C	N3-C4-C5	7.45	124.88	121.90
80	B5	2743	A	C8-N9-C4	7.45	108.78	105.80
80	B5	3381	U	N3-C4-O4	-7.45	114.19	119.40
80	B5	2726	C	N3-C4-N4	-7.45	112.79	118.00
84	CW	49	C	O4'-C1'-N1	7.45	114.16	108.20
80	B5	3308	C	N1-C2-O2	-7.44	114.43	118.90
80	B5	2308	C	N3-C2-O2	7.44	127.11	121.90
80	B5	1879	A	N7-C8-N9	7.44	117.52	113.80
80	B5	2908	G	C8-N9-C4	-7.44	103.42	106.40
80	B5	645	A	C5-C6-N6	-7.44	117.75	123.70
80	B5	2996	U	N1-C2-O2	7.44	128.01	122.80
84	CW	64	A	C8-N9-C4	-7.44	102.82	105.80
80	B5	2810	C	N3-C2-O2	-7.44	116.69	121.90
79	B2	583	C	C6-N1-C2	-7.44	117.33	120.30
79	B2	1012	U	C2-N3-C4	7.44	131.46	127.00
79	B2	608	U	C2-N3-C4	-7.43	122.54	127.00
80	B5	74	G	N1-C6-O6	-7.43	115.44	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1484	U	C2-N3-C4	-7.43	122.54	127.00
80	B5	1855	U	C2-N3-C4	-7.43	122.54	127.00
82	B8	2	A	N1-C6-N6	-7.43	114.14	118.60
80	B5	1389	G	N3-C2-N2	7.43	125.10	119.90
80	B5	2743	A	N7-C8-N9	-7.43	110.09	113.80
84	CW	6	G	C5-C6-O6	-7.43	124.14	128.60
84	CW	40	C	O4'-C1'-N1	7.43	114.14	108.20
80	B5	1085	A	C2-N3-C4	-7.42	106.89	110.60
80	B5	2802	A	C2-N3-C4	7.42	114.31	110.60
84	CW	27	G	N1-C6-O6	7.42	124.35	119.90
80	B5	971	G	C4-C5-N7	-7.42	107.83	110.80
80	B5	3081	C	N3-C4-C5	7.42	124.87	121.90
80	B5	280	U	C5-C6-N1	-7.42	118.99	122.70
80	B5	2366	C	C5-C4-N4	-7.42	115.01	120.20
80	B5	2341	A	N7-C8-N9	-7.41	110.09	113.80
79	B2	89	G	C8-N9-C4	7.41	109.36	106.40
80	B5	2621	G	N3-C2-N2	-7.41	114.71	119.90
80	B5	1437	C	C5-C6-N1	7.41	124.70	121.00
80	B5	2630	C	C2-N3-C4	-7.41	116.20	119.90
80	B5	931	C	C5-C6-N1	-7.40	117.30	121.00
81	B7	96	U	N3-C2-O2	-7.40	117.02	122.20
80	B5	1586	G	N3-C4-N9	7.40	130.44	126.00
80	B5	2179	C	C6-N1-C2	7.40	123.26	120.30
80	B5	2541	U	C2-N1-C1'	7.40	126.58	117.70
84	CW	57	G	C5-C6-O6	-7.40	124.16	128.60
80	B5	2245	C	C5-C6-N1	7.39	124.70	121.00
53	BS	40	ARG	NE-CZ-NH1	7.39	124.00	120.30
79	B2	1761	U	C6-N1-C2	-7.39	116.56	121.00
80	B5	1227	C	N1-C2-O2	-7.39	114.46	118.90
80	B5	2991	A	N1-C6-N6	-7.39	114.17	118.60
80	B5	3025	C	N3-C4-N4	-7.39	112.83	118.00
80	B5	3151	U	N1-C2-N3	-7.39	110.47	114.90
80	B5	1014	U	C5-C4-O4	-7.39	121.47	125.90
80	B5	1317	A	C2-N3-C4	7.39	114.30	110.60
80	B5	1887	A	N1-C6-N6	7.39	123.03	118.60
80	B5	1192	C	C4-C5-C6	7.39	121.09	117.40
80	B5	1604	G	N3-C4-N9	7.39	130.43	126.00
25	AQ	40	GLU	C-N-CD	-7.39	104.35	120.60
80	B5	1449	A	C4-C5-N7	7.39	114.39	110.70
79	B2	831	U	C5-C6-N1	7.38	126.39	122.70
80	B5	1228	C	N3-C4-C5	-7.38	118.95	121.90
80	B5	1506	A	C8-N9-C4	-7.38	102.85	105.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	CW	42	C	C6-N1-C2	-7.38	117.35	120.30
80	B5	2142	A	C2-N3-C4	7.38	114.29	110.60
79	B2	1075	C	N1-C2-O2	-7.38	114.47	118.90
80	B5	931	C	N3-C4-C5	7.38	124.85	121.90
80	B5	3218	A	C4-C5-N7	7.38	114.39	110.70
84	CW	55	U	P-O3'-C3'	7.38	128.56	119.70
80	B5	1268	G	P-O5'-C5'	7.38	132.71	120.90
80	B5	2311	G	C8-N9-C4	7.38	109.35	106.40
79	B2	142	G	N3-C4-C5	7.37	132.29	128.60
80	B5	1117	G	C5-C6-N1	7.37	115.19	111.50
80	B5	2370	G	C6-N1-C2	-7.37	120.68	125.10
80	B5	3382	U	N1-C2-O2	7.37	127.96	122.80
82	B8	99	C	C6-N1-C2	7.37	123.25	120.30
79	B2	1241	G	N7-C8-N9	7.37	116.78	113.10
79	B2	1389	C	N1-C2-O2	7.37	123.32	118.90
82	B8	2	A	C5-C6-N6	7.37	129.59	123.70
80	B5	1144	U	N1-C2-N3	7.37	119.32	114.90
80	B5	2736	A	N1-C6-N6	-7.37	114.18	118.60
80	B5	1538	G	C8-N9-C4	7.36	109.34	106.40
80	B5	2350	C	C4-C5-C6	7.36	121.08	117.40
80	B5	2572	C	N3-C2-O2	-7.36	116.75	121.90
79	B2	1762	A	N1-C6-N6	7.36	123.02	118.60
80	B5	2884	C	C2-N3-C4	-7.36	116.22	119.90
80	B5	2320	A	C5-C6-N1	-7.36	114.02	117.70
80	B5	1280	C	O4'-C1'-N1	7.36	114.08	108.20
76	Bq	12	PHE	CB-CG-CD2	-7.35	115.66	120.80
80	B5	2851	A	N1-C2-N3	7.35	132.97	129.30
80	B5	2621	G	C5-C6-N1	-7.35	107.83	111.50
80	B5	2385	G	C4-N9-C1'	-7.34	116.95	126.50
80	B5	2611	U	N3-C2-O2	-7.34	117.06	122.20
80	B5	2307	G	N3-C4-N9	7.34	130.40	126.00
80	B5	1124	U	C5-C6-N1	7.34	126.37	122.70
80	B5	65	A	C8-N9-C4	-7.34	102.87	105.80
80	B5	2954	U	C6-N1-C1'	-7.34	110.93	121.20
80	B5	2699	G	C2-N3-C4	7.33	115.57	111.90
80	B5	3289	G	C8-N9-C4	-7.33	103.47	106.40
80	B5	1426	C	N3-C4-C5	7.33	124.83	121.90
81	B7	41	G	N9-C4-C5	-7.33	102.47	105.40
80	B5	98	G	C5-C6-N1	7.33	115.16	111.50
80	B5	2531	C	N1-C2-O2	7.33	123.30	118.90
80	B5	795	G	N7-C8-N9	-7.32	109.44	113.10
80	B5	2234	G	N1-C6-O6	7.32	124.29	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	CV	210	TRP	CG-CD1-NE1	7.32	117.42	110.10
80	B5	580	C	C4-C5-C6	7.32	121.06	117.40
80	B5	3290	G	C8-N9-C4	-7.32	103.47	106.40
80	B5	804	C	C4-C5-C6	7.32	121.06	117.40
79	B2	377	G	N3-C2-N2	-7.31	114.78	119.90
79	B2	355	G	C5-C6-N1	7.31	115.15	111.50
80	B5	969	C	C2-N3-C4	-7.31	116.25	119.90
80	B5	1846	C	C4-C5-C6	7.31	121.05	117.40
80	B5	2815	G	C8-N9-C4	7.31	109.32	106.40
80	B5	3369	G	C5-C6-O6	-7.31	124.22	128.60
80	B5	2245	C	N3-C2-O2	-7.31	116.79	121.90
54	BT	130	ARG	NE-CZ-NH2	-7.30	116.65	120.30
80	B5	2288	G	N3-C4-N9	7.30	130.38	126.00
79	B2	1096	C	C6-N1-C1'	-7.30	112.04	120.80
80	B5	1014	U	C6-N1-C1'	-7.30	110.98	121.20
80	B5	2836	C	N3-C4-N4	-7.30	112.89	118.00
80	B5	1364	C	C2-N3-C4	-7.30	116.25	119.90
80	B5	924	G	N1-C6-O6	7.30	124.28	119.90
80	B5	1921	A	N1-C6-N6	7.30	122.98	118.60
80	B5	1506	A	N7-C8-N9	7.30	117.45	113.80
80	B5	2892	A	C5-C6-N6	7.30	129.54	123.70
66	Bf	18	ARG	NE-CZ-NH1	-7.29	116.65	120.30
80	B5	1660	C	C6-N1-C2	-7.29	117.38	120.30
80	B5	834	U	C6-N1-C2	7.29	125.38	121.00
80	B5	1133	A	C5-C6-N1	7.29	121.35	117.70
83	CV	534	ALA	N-CA-CB	7.29	120.31	110.10
84	CW	70	G	C5-C6-O6	-7.29	124.22	128.60
80	B5	3255	U	C5-C4-O4	-7.29	121.53	125.90
80	B5	2662	G	C8-N9-C4	-7.29	103.49	106.40
85	CX	1	A	C5-C6-N6	-7.29	117.87	123.70
80	B5	3131	U	N3-C4-C5	7.27	118.96	114.60
80	B5	2584	G	C6-C5-N7	-7.27	126.04	130.40
84	CW	76	A	C5-C6-N6	-7.27	117.88	123.70
80	B5	39	A	C4-C5-C6	7.27	120.64	117.00
80	B5	2942	C	C4-C5-C6	7.27	121.03	117.40
81	B7	104	A	N1-C6-N6	7.27	122.96	118.60
80	B5	1430	U	C5-C6-N1	-7.27	119.06	122.70
80	B5	1283	C	N3-C4-C5	-7.27	118.99	121.90
80	B5	2616	C	C6-N1-C2	7.27	123.21	120.30
80	B5	639	G	N1-C6-O6	7.26	124.26	119.90
84	CW	21	A	P-O5'-C5'	7.26	132.52	120.90
80	B5	643	U	N3-C4-C5	7.26	118.96	114.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2758	A	C8-N9-C4	-7.26	102.89	105.80
80	B5	1189	C	N1-C2-O2	-7.26	114.54	118.90
82	B8	54	A	C2-N3-C4	-7.26	106.97	110.60
80	B5	2620	G	C5-C6-N1	7.26	115.13	111.50
79	B2	728	U	C2-N1-C1'	7.26	126.41	117.70
79	B2	1642	G	C2-N3-C4	7.26	115.53	111.90
80	B5	2372	A	P-O3'-C3'	7.26	128.41	119.70
36	BB	266	ARG	NE-CZ-NH2	-7.25	116.67	120.30
84	CW	46	G	C5-C6-O6	-7.25	124.25	128.60
80	B5	2911	A	C2-N3-C4	7.25	114.23	110.60
84	CW	14	A	C4-C5-C6	7.25	120.63	117.00
80	B5	1833	G	N3-C2-N2	7.25	124.97	119.90
79	B2	1745	G	C4-C5-N7	7.24	113.70	110.80
80	B5	643	U	C2-N3-C4	-7.24	122.65	127.00
80	B5	1227	C	C2-N1-C1'	7.24	126.77	118.80
79	B2	1654	G	C5-C6-O6	-7.24	124.25	128.60
80	B5	838	G	N1-C6-O6	-7.24	115.56	119.90
83	CV	63	GLU	N-CA-C	7.24	130.55	111.00
80	B5	1169	A	C5-C6-N1	-7.24	114.08	117.70
80	B5	1258	U	O4'-C4'-C3'	-7.24	96.76	104.00
79	B2	1329	A	N1-C6-N6	7.24	122.94	118.60
80	B5	578	A	N1-C6-N6	7.24	122.94	118.60
80	B5	2701	U	C5-C4-O4	-7.24	121.56	125.90
80	B5	3122	A	N7-C8-N9	7.23	117.42	113.80
80	B5	810	A	N1-C6-N6	-7.23	114.26	118.60
80	B5	2717	U	C5-C6-N1	-7.23	119.09	122.70
79	B2	1000	C	N3-C4-N4	-7.22	112.94	118.00
80	B5	1336	U	C5-C4-O4	-7.22	121.56	125.90
80	B5	1206	G	N9-C4-C5	7.22	108.29	105.40
81	B7	49	G	N3-C2-N2	-7.22	114.84	119.90
80	B5	46	U	N1-C2-O2	7.22	127.85	122.80
80	B5	283	G	C6-C5-N7	-7.22	126.07	130.40
80	B5	1724	U	C6-N1-C2	-7.22	116.67	121.00
80	B5	2370	G	C5-C6-O6	-7.22	124.27	128.60
80	B5	1140	G	N3-C2-N2	7.22	124.95	119.90
80	B5	1167	U	C5-C4-O4	-7.22	121.57	125.90
49	BO	16[B]	LEU	C-N-CA	7.21	137.45	122.30
80	B5	267	G	C8-N9-C4	7.21	109.29	106.40
80	B5	272	G	C8-N9-C4	7.21	109.29	106.40
80	B5	669	U	N1-C2-N3	7.21	119.23	114.90
80	B5	1049	C	N3-C4-C5	7.21	124.78	121.90
80	B5	1518	U	N3-C4-O4	-7.21	114.36	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	652	G	N3-C2-N2	7.20	124.94	119.90
80	B5	1406	A	C6-N1-C2	-7.20	114.28	118.60
79	B2	1611	A	C2-N3-C4	-7.20	107.00	110.60
80	B5	3052	G	N1-C6-O6	-7.20	115.58	119.90
80	B5	514	G	C4-C5-N7	7.20	113.68	110.80
80	B5	629	U	C2-N3-C4	-7.20	122.68	127.00
80	B5	1262	G	O4'-C1'-N9	7.20	113.96	108.20
80	B5	2363	A	C8-N9-C4	-7.20	102.92	105.80
80	B5	2754	G	N1-C2-N2	-7.20	109.72	116.20
80	B5	39	A	N1-C6-N6	7.20	122.92	118.60
80	B5	2410	U	C4-C5-C6	-7.20	115.38	119.70
80	B5	2964	G	C8-N9-C4	7.20	109.28	106.40
80	B5	37	U	C2-N3-C4	-7.19	122.68	127.00
80	B5	3060	C	N3-C2-O2	7.19	126.94	121.90
79	B2	1121	C	C4-C5-C6	7.19	121.00	117.40
80	B5	3245	A	N3-C4-C5	7.19	131.84	126.80
80	B5	2396	G	N9-C4-C5	7.19	108.28	105.40
80	B5	2305	G	N9-C4-C5	-7.19	102.53	105.40
80	B5	3040	A	C5-N7-C8	7.18	107.49	103.90
80	B5	577	C	C2-N3-C4	-7.18	116.31	119.90
80	B5	1902	G	C8-N9-C4	7.18	109.27	106.40
80	B5	2870	C	N3-C4-N4	-7.18	112.97	118.00
81	B7	44	C	N1-C2-O2	-7.18	114.59	118.90
80	B5	960	U	N1-C2-O2	7.18	127.83	122.80
80	B5	2908	G	N9-C4-C5	7.18	108.27	105.40
80	B5	2337	C	C6-N1-C2	7.18	123.17	120.30
80	B5	3379	C	C5-C6-N1	-7.18	117.41	121.00
80	B5	46	U	C5-C4-O4	7.17	130.21	125.90
80	B5	563	U	N1-C2-O2	7.17	127.82	122.80
80	B5	2148	U	C2-N3-C4	-7.17	122.69	127.00
80	B5	800	G	C8-N9-C4	7.17	109.27	106.40
84	CW	76	A	O4'-C1'-N9	7.17	113.94	108.20
80	B5	3005	A	N9-C4-C5	7.17	108.67	105.80
80	B5	1004	U	N3-C4-C5	7.17	118.90	114.60
80	B5	1158	A	C5-C6-N6	-7.17	117.97	123.70
80	B5	1887	A	C2-N3-C4	-7.17	107.02	110.60
80	B5	2631	U	N3-C4-C5	7.17	118.90	114.60
80	B5	2965	U	C4-C5-C6	7.17	124.00	119.70
82	B8	126	A	C8-N9-C4	-7.17	102.93	105.80
80	B5	2848	G	N3-C2-N2	-7.17	114.89	119.90
79	B2	1174	C	N1-C2-O2	7.16	123.20	118.90
80	B5	518	G	N9-C4-C5	-7.16	102.53	105.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	327	A	N7-C8-N9	-7.16	110.22	113.80
80	B5	1434	G	C4-C5-C6	7.16	123.10	118.80
80	B5	2383	C	N1-C2-O2	-7.16	114.60	118.90
80	B5	801	A	C5-C6-N1	-7.16	114.12	117.70
80	B5	1328	C	C4-C5-C6	7.16	120.98	117.40
80	B5	2917	G	C6-C5-N7	-7.16	126.10	130.40
80	B5	2169	G	C5-C6-N1	7.16	115.08	111.50
80	B5	2758	A	N9-C4-C5	7.16	108.66	105.80
82	B8	42	G	C8-N9-C4	7.16	109.26	106.40
80	B5	974	G	C4-N9-C1'	7.15	135.80	126.50
80	B5	434	U	N3-C4-C5	7.15	118.89	114.60
81	B7	11	A	N7-C8-N9	-7.15	110.22	113.80
80	B5	922	U	N3-C4-O4	-7.15	114.39	119.40
80	B5	1085	A	C8-N9-C4	-7.15	102.94	105.80
80	B5	1292	C	C6-N1-C2	7.15	123.16	120.30
80	B5	2824	G	N9-C4-C5	7.15	108.26	105.40
80	B5	1917	C	N1-C2-O2	-7.15	114.61	118.90
80	B5	594	U	N3-C2-O2	-7.14	117.20	122.20
80	B5	1226	G	O5'-C5'-C4'	7.14	125.27	111.70
80	B5	3192	U	N3-C4-O4	-7.14	114.40	119.40
80	B5	1144	U	C5-C6-N1	-7.14	119.13	122.70
80	B5	1591	G	N1-C6-O6	-7.14	115.61	119.90
80	B5	2993	G	C4-C5-N7	7.14	113.66	110.80
80	B5	1209	G	N3-C2-N2	-7.14	114.90	119.90
79	B2	992	A	C2-N3-C4	-7.14	107.03	110.60
80	B5	2732	G	C5-C6-O6	7.14	132.88	128.60
79	B2	1611	A	C5-N7-C8	-7.14	100.33	103.90
80	B5	2979	U	C6-N1-C2	7.14	125.28	121.00
80	B5	1118	C	N3-C4-C5	7.13	124.75	121.90
80	B5	2584	G	N3-C4-N9	7.13	130.28	126.00
80	B5	3076	C	N3-C4-C5	7.13	124.75	121.90
79	B2	577	G	N9-C4-C5	-7.13	102.55	105.40
80	B5	384	A	C8-N9-C4	7.13	108.65	105.80
80	B5	1403	C	C5-C6-N1	-7.12	117.44	121.00
79	B2	783	G	C4-C5-N7	7.12	113.65	110.80
84	CW	45	U	P-O5'-C5'	7.12	132.29	120.90
79	B2	61	A	N7-C8-N9	7.12	117.36	113.80
80	B5	2320	A	C4-C5-N7	-7.12	107.14	110.70
80	B5	3086	A	N7-C8-N9	-7.12	110.24	113.80
80	B5	1172	G	N1-C6-O6	-7.12	115.63	119.90
82	B8	139	U	N3-C4-O4	-7.12	114.42	119.40
80	B5	419	G	N9-C4-C5	-7.11	102.56	105.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	3052	G	C5-C6-O6	7.11	132.87	128.60
84	CW	66	U	O4'-C1'-N1	7.11	113.89	108.20
80	B5	437	G	N7-C8-N9	7.11	116.66	113.10
80	B5	3154	C	N3-C2-O2	-7.11	116.92	121.90
79	B2	1324	G	N3-C2-N2	-7.11	114.92	119.90
80	B5	1272	C	N3-C4-C5	-7.11	119.06	121.90
80	B5	1458	U	C2-N3-C4	-7.11	122.73	127.00
79	B2	1241	G	C4-C5-N7	7.11	113.64	110.80
80	B5	1264	G	C5-C6-O6	-7.11	124.34	128.60
80	B5	3214	U	N1-C2-N3	7.10	119.16	114.90
84	CW	75	C	C6-N1-C2	-7.10	117.46	120.30
80	B5	511	G	C5-C6-O6	7.10	132.86	128.60
80	B5	1858	A	C2-N3-C4	7.10	114.15	110.60
80	B5	641	C	C6-N1-C1'	7.10	129.32	120.80
44	BJ	112	LEU	CA-CB-CG	7.10	131.62	115.30
80	B5	622	A	N9-C4-C5	-7.10	102.96	105.80
79	B2	108	A	N1-C2-N3	7.09	132.85	129.30
80	B5	2305	G	N3-C2-N2	7.09	124.87	119.90
80	B5	3110	C	N1-C2-N3	7.09	124.17	119.20
80	B5	708	G	N7-C8-N9	7.09	116.65	113.10
80	B5	2244	A	N1-C6-N6	-7.09	114.34	118.60
80	B5	2242	A	N1-C6-N6	-7.09	114.34	118.60
80	B5	24	G	N1-C6-O6	7.09	124.15	119.90
80	B5	1283	C	C6-N1-C2	-7.09	117.47	120.30
80	B5	1243	G	C5-C6-O6	-7.09	124.35	128.60
80	B5	2618	G	C6-N1-C2	-7.09	120.85	125.10
80	B5	2693	C	C2-N3-C4	-7.09	116.36	119.90
80	B5	2127	U	N1-C2-N3	7.08	119.15	114.90
50	BP	69	ARG	NE-CZ-NH2	-7.08	116.76	120.30
80	B5	928	C	N1-C2-N3	7.08	124.16	119.20
80	B5	1229	G	C5-C6-O6	-7.08	124.35	128.60
80	B5	804	C	N3-C4-C5	-7.08	119.07	121.90
80	B5	1407	A	C5-C6-N1	-7.08	114.16	117.70
80	B5	872	U	N3-C4-C5	7.07	118.84	114.60
79	B2	1462	G	C8-N9-C4	7.07	109.23	106.40
80	B5	546	C	C5-C6-N1	7.07	124.53	121.00
80	B5	2300	G	N3-C2-N2	7.07	124.85	119.90
84	CW	16	U	C1'-O4'-C4'	7.07	115.55	109.90
80	B5	2169	G	C6-C5-N7	7.07	134.64	130.40
81	B7	101	G	C5-C6-O6	-7.07	124.36	128.60
80	B5	834	U	N3-C4-O4	-7.06	114.45	119.40
79	B2	1773	C	C2-N3-C4	7.06	123.43	119.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1340	G	N1-C2-N2	-7.06	109.84	116.20
80	B5	3317	U	C6-N1-C2	-7.06	116.76	121.00
80	B5	591	G	C4-C5-N7	7.06	113.62	110.80
79	B2	159	U	C6-N1-C2	7.06	125.23	121.00
84	CW	61	C	O4'-C1'-N1	7.06	113.84	108.20
80	B5	945	C	C5-C6-N1	-7.05	117.47	121.00
80	B5	1278	A	P-O3'-C3'	7.05	128.16	119.70
80	B5	2618	G	N3-C4-N9	7.05	130.23	126.00
79	B2	74	U	O4'-C1'-N1	7.05	113.84	108.20
79	B2	1456	C	N3-C2-O2	-7.05	116.97	121.90
80	B5	1255	C	N3-C4-N4	7.05	122.93	118.00
80	B5	1548	C	C2-N3-C4	-7.05	116.38	119.90
80	B5	3006	A	N1-C2-N3	7.05	132.82	129.30
79	B2	628	G	C2-N3-C4	-7.05	108.38	111.90
80	B5	2327	U	C6-N1-C2	7.05	125.23	121.00
79	B2	1749	A	C2-N3-C4	-7.05	107.08	110.60
80	B5	2988	C	C5-C6-N1	-7.05	117.48	121.00
84	CW	16	U	P-O3'-C3'	7.05	128.16	119.70
49	BO	4[B]	GLN	O-C-N	7.04	134.49	121.10
53	BS	115	ARG	NE-CZ-NH2	-7.04	116.78	120.30
80	B5	1232	C	C2'-C3'-O3'	7.04	125.00	109.50
80	B5	1370	G	N3-C2-N2	7.04	124.83	119.90
80	B5	2631	U	C5-C6-N1	-7.04	119.18	122.70
80	B5	1228	C	O4'-C1'-N1	7.04	113.83	108.20
79	B2	610	G	C8-N9-C1'	-7.04	117.85	127.00
80	B5	1229	G	C6-C5-N7	-7.04	126.17	130.40
80	B5	2344	U	C5-C6-N1	-7.04	119.18	122.70
80	B5	2942	C	N3-C4-C5	-7.04	119.08	121.90
80	B5	1314	C	C2-N1-C1'	7.04	126.54	118.80
82	B8	70	G	C8-N9-C4	7.04	109.22	106.40
80	B5	3182	G	N1-C6-O6	-7.04	115.68	119.90
82	B8	101	U	C6-N1-C2	-7.04	116.78	121.00
83	CV	478	LYS	CB-CA-C	7.04	124.48	110.40
79	B2	1274	C	C5-C6-N1	-7.04	117.48	121.00
80	B5	3086	A	C5-N7-C8	7.04	107.42	103.90
80	B5	930	U	N3-C4-O4	-7.03	114.48	119.40
80	B5	2882	U	C2-N3-C4	-7.03	122.78	127.00
83	CV	476	GLN	CA-CB-CG	7.03	128.87	113.40
80	B5	1417	G	N1-C6-O6	-7.03	115.68	119.90
80	B5	1925	U	C2-N3-C4	-7.03	122.78	127.00
80	B5	1939	G	N3-C2-N2	7.03	124.82	119.90
80	B5	3218	A	C2-N3-C4	-7.03	107.08	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	802	C	C2-N3-C4	-7.03	116.39	119.90
80	B5	2644	C	N1-C2-O2	-7.03	114.68	118.90
79	B2	1548	G	C2-N3-C4	7.03	115.41	111.90
80	B5	1110	U	C4-C5-C6	-7.03	115.48	119.70
80	B5	2943	G	N1-C6-O6	-7.03	115.68	119.90
79	B2	1533	C	C4-C5-C6	7.02	120.91	117.40
80	B5	1434	G	C4-C5-N7	-7.02	107.99	110.80
80	B5	2881	C	C5-C6-N1	-7.02	117.49	121.00
82	B8	139	U	C5-C6-N1	-7.02	119.19	122.70
80	B5	418	A	N1-C6-N6	7.02	122.81	118.60
80	B5	929	A	N7-C8-N9	-7.02	110.29	113.80
80	B5	2350	C	C2-N3-C4	-7.01	116.39	119.90
84	CW	61	C	N3-C4-N4	7.01	122.91	118.00
80	B5	436	A	C6-C5-N7	-7.01	127.39	132.30
80	B5	2190	U	N1-C2-N3	7.01	119.11	114.90
84	CW	62	C	N3-C4-N4	7.01	122.91	118.00
80	B5	3107	U	N3-C2-O2	-7.01	117.30	122.20
80	B5	3098	G	C5-C6-O6	7.00	132.80	128.60
80	B5	2293	C	N3-C4-C5	7.00	124.70	121.90
80	B5	2932	U	N1-C2-O2	7.00	127.70	122.80
79	B2	1654	G	N3-C4-C5	-7.00	125.10	128.60
80	B5	81	C	N3-C4-N4	-7.00	113.10	118.00
80	B5	2689	A	C6-N1-C2	-7.00	114.40	118.60
61	Ba	12	ARG	NE-CZ-NH2	-7.00	116.80	120.30
80	B5	32	U	N3-C4-C5	-7.00	110.40	114.60
80	B5	857	G	N9-C4-C5	-7.00	102.60	105.40
80	B5	1441	G	N7-C8-N9	-7.00	109.60	113.10
80	B5	2832	C	C2-N3-C4	-7.00	116.40	119.90
80	B5	343	U	C5-C4-O4	7.00	130.10	125.90
80	B5	2626	A	C5-C6-N6	7.00	129.30	123.70
80	B5	859	G	N1-C6-O6	-6.99	115.70	119.90
80	B5	1282	G	C5-C6-O6	-6.99	124.40	128.60
49	BO	104[B]	ILE	O-C-N	6.99	133.89	122.70
80	B5	1389	G	C5-C6-O6	-6.99	124.41	128.60
80	B5	2302	G	N1-C6-O6	-6.99	115.71	119.90
79	B2	321	C	C6-N1-C2	-6.99	117.51	120.30
79	B2	1600	A	C5-C6-N1	-6.99	114.21	117.70
80	B5	1673	G	N1-C6-O6	-6.98	115.71	119.90
80	B5	2189	U	C2-N3-C4	-6.98	122.81	127.00
80	B5	2149	A	C8-N9-C4	-6.98	103.01	105.80
80	B5	2167	A	C6-N1-C2	-6.98	114.41	118.60
80	B5	1592	G	C5-C6-O6	6.98	132.79	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2917	G	N3-C4-N9	6.98	130.19	126.00
80	B5	369	A	N7-C8-N9	6.98	117.29	113.80
80	B5	1236	G	O4'-C1'-N9	6.98	113.78	108.20
80	B5	2280	A	C2-N3-C4	-6.97	107.11	110.60
70	Bj	73	ARG	NE-CZ-NH2	-6.96	116.82	120.30
80	B5	1199	C	C4-C5-C6	6.96	120.88	117.40
80	B5	3020	U	N1-C2-O2	-6.96	117.93	122.80
22	AN	22	ALA	C-N-CD	-6.96	105.28	120.60
79	B2	1747	G	C2-N3-C4	-6.96	108.42	111.90
80	B5	1149	G	N9-C4-C5	6.96	108.19	105.40
84	CW	10	G	O4'-C1'-N9	6.96	113.77	108.20
80	B5	2426	U	N1-C2-O2	6.96	127.67	122.80
80	B5	2249	G	C3'-C2'-C1'	-6.95	95.94	101.50
79	B2	1057	U	C5-C6-N1	6.95	126.18	122.70
80	B5	2732	G	N3-C2-N2	6.95	124.77	119.90
80	B5	3099	C	C5-C6-N1	-6.95	117.53	121.00
80	B5	706	A	C8-N9-C4	6.95	108.58	105.80
80	B5	2362	C	N3-C4-C5	6.95	124.68	121.90
79	B2	360	A	N9-C4-C5	-6.95	103.02	105.80
80	B5	1879	A	C5-N7-C8	-6.94	100.43	103.90
80	B5	1513	G	N7-C8-N9	6.94	116.57	113.10
79	B2	1162	C	C6-N1-C2	-6.94	117.52	120.30
80	B5	857	G	C8-N9-C4	6.94	109.18	106.40
80	B5	2314	U	C5-C6-N1	6.94	126.17	122.70
80	B5	3362	A	C6-C5-N7	-6.94	127.44	132.30
80	B5	751	A	C2-N3-C4	-6.93	107.13	110.60
80	B5	784	A	C5-C6-N6	-6.93	118.15	123.70
80	B5	96	G	C5-C6-O6	6.93	132.76	128.60
80	B5	221	A	C8-N9-C4	6.93	108.57	105.80
80	B5	2917	G	C6-N1-C2	-6.93	120.94	125.10
80	B5	3321	C	C4-C5-C6	6.93	120.87	117.40
79	B2	981	U	N3-C2-O2	-6.93	117.35	122.20
80	B5	1883	A	N1-C6-N6	-6.93	114.44	118.60
80	B5	3019	U	C2-N3-C4	-6.93	122.84	127.00
80	B5	3374	U	N3-C4-O4	-6.93	114.55	119.40
82	B8	112	U	C2-N1-C1'	-6.93	109.39	117.70
80	B5	1834	U	N3-C4-O4	-6.93	114.55	119.40
80	B5	2290	C	C6-N1-C2	6.93	123.07	120.30
79	B2	1749	A	N9-C4-C5	-6.93	103.03	105.80
80	B5	1210	U	N3-C2-O2	-6.93	117.35	122.20
80	B5	833	G	C6-N1-C2	-6.92	120.94	125.10
80	B5	2978	U	N3-C4-O4	-6.92	114.56	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1152	G	N1-C2-N3	6.92	128.05	123.90
79	B2	542	A	C8-N9-C1'	-6.92	115.25	127.70
79	B2	736	C	C6-N1-C1'	-6.92	112.50	120.80
80	B5	942	U	C5-C4-O4	-6.92	121.75	125.90
80	B5	2524	A	C3'-C2'-C1'	-6.92	95.97	101.50
80	B5	3308	C	C6-N1-C2	-6.92	117.53	120.30
80	B5	1875	G	N1-C6-O6	-6.92	115.75	119.90
79	B2	360	A	C8-N9-C4	6.92	108.57	105.80
80	B5	835	G	C5-C6-N1	6.91	114.96	111.50
80	B5	3362	A	C5-C6-N1	-6.91	114.25	117.70
80	B5	2207	A	N1-C6-N6	6.91	122.75	118.60
81	B7	74	C	N1-C2-O2	-6.91	114.75	118.90
49	BO	3[B]	SER	CA-C-N	-6.91	102.00	117.20
80	B5	1238	C	O4'-C1'-N1	6.91	113.72	108.20
80	B5	1263	A	C4-C5-C6	6.91	120.45	117.00
80	B5	1833	G	C8-N9-C4	6.91	109.16	106.40
80	B5	1370	G	N1-C2-N2	-6.90	109.99	116.20
44	BJ	9	MET	N-CA-C	-6.90	92.37	111.00
80	B5	3101	G	C5-C6-O6	6.90	132.74	128.60
80	B5	3176	G	N1-C2-N3	6.90	128.04	123.90
79	B2	607	G	N1-C6-O6	6.90	124.04	119.90
80	B5	3081	C	C4-C5-C6	-6.90	113.95	117.40
79	B2	1146	G	C8-N9-C4	-6.90	103.64	106.40
80	B5	2184	U	C2-N3-C4	-6.90	122.86	127.00
79	B2	92	A	N9-C4-C5	6.89	108.56	105.80
79	B2	313	U	N3-C4-O4	-6.89	114.58	119.40
65	Be	33	ARG	NE-CZ-NH1	6.89	123.75	120.30
80	B5	3070	A	C2-N3-C4	-6.89	107.16	110.60
80	B5	3333	G	C5-C6-O6	-6.89	124.47	128.60
80	B5	933	A	N1-C2-N3	6.88	132.74	129.30
80	B5	864	G	C6-N1-C2	-6.88	120.97	125.10
80	B5	1609	C	N3-C4-N4	6.88	122.82	118.00
80	B5	1941	C	N3-C4-C5	6.88	124.65	121.90
79	B2	453	U	N1-C2-O2	6.88	127.62	122.80
79	B2	1361	U	N1-C2-O2	6.88	127.61	122.80
79	B2	1611	A	N1-C2-N3	6.88	132.74	129.30
80	B5	652	G	C6-N1-C2	-6.88	120.97	125.10
80	B5	1275	C	N3-C4-N4	6.88	122.81	118.00
80	B5	1903	U	N3-C4-C5	-6.88	110.47	114.60
80	B5	2824	G	C4-C5-N7	-6.87	108.05	110.80
80	B5	2987	A	C5-N7-C8	6.87	107.33	103.90
84	CW	20	U	O4'-C1'-N1	6.86	113.69	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2382	G	N1-C6-O6	-6.86	115.78	119.90
79	B2	1782	A	N7-C8-N9	6.86	117.23	113.80
80	B5	1261	G	C5-C6-O6	-6.86	124.48	128.60
84	CW	6	G	C6-C5-N7	-6.86	126.28	130.40
79	B2	305	C	C6-N1-C2	-6.86	117.56	120.30
80	B5	1589	A	C2-N3-C4	6.86	114.03	110.60
84	CW	75	C	C6-N1-C1'	-6.86	112.57	120.80
80	B5	815	G	C4-C5-N7	-6.86	108.06	110.80
80	B5	2524	A	C4-C5-N7	6.86	114.13	110.70
80	B5	2884	C	N1-C2-O2	-6.86	114.79	118.90
81	B7	112	G	C5-C6-O6	6.86	132.71	128.60
80	B5	693	A	N1-C6-N6	-6.85	114.49	118.60
80	B5	2412	G	N3-C4-C5	-6.85	125.17	128.60
80	B5	2830	G	C4-C5-N7	-6.85	108.06	110.80
80	B5	3172	A	C5-N7-C8	6.85	107.33	103.90
80	B5	1327	C	N3-C2-O2	-6.85	117.11	121.90
80	B5	1685	C	N3-C2-O2	-6.85	117.11	121.90
80	B5	2237	C	N1-C2-O2	6.85	123.01	118.90
37	BC	90	PHE	C-N-CA	-6.84	107.92	122.30
80	B5	1130	A	N1-C2-N3	-6.84	125.88	129.30
80	B5	1205	A	N7-C8-N9	6.84	117.22	113.80
84	CW	55	U	C2-N1-C1'	-6.84	109.49	117.70
80	B5	1940	G	N1-C6-O6	-6.84	115.79	119.90
79	B2	1318	G	N1-C6-O6	6.84	124.00	119.90
80	B5	327	A	C8-N9-C4	6.84	108.54	105.80
80	B5	2385	G	C2-N3-C4	-6.84	108.48	111.90
80	B5	1406	A	N1-C2-N3	6.84	132.72	129.30
80	B5	1868	G	C8-N9-C4	6.84	109.14	106.40
80	B5	3056	U	N1-C2-N3	6.84	119.00	114.90
80	B5	1481	A	P-O3'-C3'	6.83	127.90	119.70
79	B2	1206	U	N3-C4-O4	6.83	124.18	119.40
80	B5	1652	G	N7-C8-N9	-6.83	109.68	113.10
80	B5	3149	G	C2-N3-C4	-6.83	108.48	111.90
79	B2	1210	C	N3-C4-C5	-6.83	119.17	121.90
79	B2	934	C	C2-N1-C1'	6.83	126.31	118.80
80	B5	1124	U	N1-C2-O2	6.83	127.58	122.80
80	B5	2389	C	C2-N3-C4	-6.83	116.49	119.90
80	B5	2810	C	C4-C5-C6	6.83	120.81	117.40
79	B2	73	U	O4'-C1'-N1	6.83	113.66	108.20
80	B5	881	C	C2-N3-C4	6.83	123.31	119.90
80	B5	1245	A	C4-C5-C6	6.83	120.41	117.00
80	B5	1255	C	P-O5'-C5'	6.83	131.82	120.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	838	G	C5-C6-O6	6.82	132.69	128.60
80	B5	2821	C	C6-N1-C2	-6.82	117.57	120.30
81	B7	49	G	C8-N9-C4	6.82	109.13	106.40
79	B2	1190	C	C6-N1-C2	6.82	123.03	120.30
80	B5	622	A	C5-C6-N6	-6.82	118.24	123.70
80	B5	1113	G	N3-C4-C5	6.82	132.01	128.60
80	B5	1369	A	C8-N9-C4	6.82	108.53	105.80
80	B5	2729	U	C5-C6-N1	6.82	126.11	122.70
80	B5	2619	G	C5-C6-O6	-6.82	124.51	128.60
80	B5	3376	A	N7-C8-N9	6.81	117.21	113.80
80	B5	2932	U	N3-C2-O2	-6.81	117.43	122.20
81	B7	50	U	C5-C6-N1	6.81	126.11	122.70
80	B5	1449	A	C6-C5-N7	-6.81	127.53	132.30
80	B5	1843	C	N3-C2-O2	-6.81	117.14	121.90
79	B2	1319	A	N1-C6-N6	6.80	122.68	118.60
84	CW	2	C	N3-C4-C5	-6.80	119.18	121.90
80	B5	578	A	C5-C6-N6	-6.80	118.26	123.70
81	B7	11	A	C5-N7-C8	6.80	107.30	103.90
43	BI	48	LEU	CA-CB-CG	6.80	130.94	115.30
80	B5	48	A	C8-N9-C4	-6.80	103.08	105.80
80	B5	1902	G	C6-N1-C2	-6.80	121.02	125.10
80	B5	189	G	N1-C6-O6	-6.80	115.82	119.90
79	B2	1246	C	N3-C2-O2	-6.80	117.14	121.90
80	B5	419	G	N3-C4-N9	6.80	130.08	126.00
80	B5	749	C	C6-N1-C2	-6.79	117.58	120.30
80	B5	3105	U	N3-C2-O2	6.79	126.96	122.20
79	B2	240	U	C2-N1-C1'	6.79	125.85	117.70
80	B5	3088	G	N3-C2-N2	6.79	124.65	119.90
84	CW	64	A	C4-C5-C6	6.79	120.40	117.00
80	B5	887	G	C2-N3-C4	-6.79	108.50	111.90
80	B5	960	U	N3-C2-O2	-6.79	117.45	122.20
80	B5	1138	U	N3-C4-C5	6.79	118.67	114.60
80	B5	2692	A	N1-C6-N6	-6.79	114.53	118.60
80	B5	205	C	N3-C2-O2	-6.79	117.15	121.90
80	B5	2705	A	C2-N3-C4	6.79	113.99	110.60
79	B2	142	G	N1-C2-N2	6.79	122.31	116.20
80	B5	345	G	N1-C2-N2	-6.79	110.09	116.20
80	B5	2730	G	C2-N3-C4	-6.79	108.51	111.90
80	B5	1417	G	C5-C6-N1	6.78	114.89	111.50
80	B5	1603	A	C8-N9-C4	-6.78	103.09	105.80
80	B5	3313	U	C5-C4-O4	6.78	129.97	125.90
84	CW	18	G	C5'-C4'-C3'	-6.78	105.15	116.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2401	A	C2-N3-C4	6.78	113.99	110.60
80	B5	888	A	C5-C6-N1	-6.78	114.31	117.70
80	B5	3050	U	N3-C4-O4	-6.78	114.66	119.40
80	B5	1297	C	N1-C2-O2	-6.78	114.83	118.90
80	B5	2246	G	C8-N9-C4	-6.78	103.69	106.40
80	B5	3076	C	C2-N3-C4	-6.78	116.51	119.90
79	B2	89	G	N7-C8-N9	-6.78	109.71	113.10
80	B5	1941	C	C2-N3-C4	-6.78	116.51	119.90
80	B5	3375	A	C2-N3-C4	6.78	113.99	110.60
80	B5	587	U	N3-C4-C5	6.77	118.66	114.60
80	B5	1253	U	O4'-C1'-N1	6.77	113.62	108.20
80	B5	2647	A	N1-C6-N6	-6.77	114.54	118.60
80	B5	1448	U	C2-N3-C4	-6.77	122.94	127.00
80	B5	2422	C	N1-C2-O2	6.77	122.96	118.90
80	B5	400	G	C4-C5-N7	6.77	113.51	110.80
80	B5	652	G	N1-C2-N3	6.77	127.96	123.90
80	B5	1197	A	N1-C2-N3	6.77	132.68	129.30
80	B5	41	G	C4-C5-N7	6.76	113.51	110.80
80	B5	146	U	C5-C4-O4	6.76	129.96	125.90
80	B5	2685	C	C2-N3-C4	-6.76	116.52	119.90
80	B5	2920	U	C2-N3-C4	-6.76	122.94	127.00
4	A3	36	LEU	CA-CB-CG	6.76	130.85	115.30
84	CW	29	G	C5-C6-O6	-6.76	124.54	128.60
80	B5	95	A	C5-C6-N6	-6.76	118.29	123.70
80	B5	1556	C	C6-N1-C2	-6.76	117.60	120.30
82	B8	23	U	N1-C2-N3	6.76	118.95	114.90
80	B5	2693	C	N1-C2-O2	6.75	122.95	118.90
79	B2	1195	C	C6-N1-C2	-6.75	117.60	120.30
80	B5	644	G	N3-C4-C5	-6.75	125.22	128.60
80	B5	2317	A	N7-C8-N9	6.75	117.17	113.80
80	B5	2434	U	C5-C4-O4	6.75	129.95	125.90
79	B2	410	A	C8-N9-C4	6.75	108.50	105.80
80	B5	63	A	N1-C6-N6	6.75	122.65	118.60
80	B5	2359	C	C6-N1-C2	6.75	123.00	120.30
82	B8	38	U	C4-C5-C6	6.75	123.75	119.70
80	B5	776	U	N3-C4-O4	-6.75	114.68	119.40
80	B5	2135	U	C6-N1-C2	6.75	125.05	121.00
80	B5	2695	A	N7-C8-N9	6.75	117.17	113.80
80	B5	2400	G	N3-C4-C5	6.75	131.97	128.60
84	CW	76	A	C4-C5-C6	6.75	120.37	117.00
80	B5	1044	U	C5-C6-N1	-6.74	119.33	122.70
80	B5	1421	G	C2-N3-C4	-6.74	108.53	111.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1469	C	C6-N1-C2	-6.74	117.60	120.30
80	B5	1652	G	C5-N7-C8	6.74	107.67	104.30
79	B2	1521	G	N3-C4-C5	-6.74	125.23	128.60
80	B5	322	U	C5-C4-O4	-6.74	121.86	125.90
80	B5	564	G	C4-C5-N7	-6.74	108.10	110.80
80	B5	890	C	N3-C4-C5	6.74	124.59	121.90
80	B5	1056	U	N3-C4-O4	6.74	124.12	119.40
80	B5	2820	A	C6-N1-C2	-6.74	114.56	118.60
80	B5	3140	G	N1-C6-O6	6.74	123.94	119.90
80	B5	2584	G	C8-N9-C1'	-6.73	118.25	127.00
81	B7	22	A	N1-C6-N6	6.73	122.64	118.60
80	B5	215	G	C8-N9-C4	-6.73	103.71	106.40
80	B5	3309	G	C5-C6-O6	-6.73	124.56	128.60
80	B5	614	C	C6-N1-C2	6.73	122.99	120.30
80	B5	1389	G	C6-C5-N7	-6.73	126.36	130.40
79	B2	1006	C	C6-N1-C2	-6.73	117.61	120.30
80	B5	1134	G	C5-C6-N1	6.72	114.86	111.50
80	B5	3216	G	C6-C5-N7	-6.72	126.36	130.40
83	CV	244	GLY	N-CA-C	6.72	129.91	113.10
80	B5	1159	A	C4-C5-N7	6.72	114.06	110.70
79	B2	736	C	C5-C6-N1	6.72	124.36	121.00
80	B5	1375	G	C2-N3-C4	6.72	115.26	111.90
80	B5	3140	G	C5-C6-O6	-6.72	124.57	128.60
80	B5	615	U	C5-C4-O4	-6.72	121.87	125.90
80	B5	1274	A	C4-C5-C6	6.72	120.36	117.00
80	B5	1910	A	N7-C8-N9	-6.72	110.44	113.80
80	B5	2868	U	N3-C4-C5	6.72	118.63	114.60
80	B5	2899	C	C4-C5-C6	6.72	120.76	117.40
53	BS	40	ARG	CG-CD-NE	6.72	125.90	111.80
80	B5	2664	C	N3-C4-C5	6.72	124.59	121.90
80	B5	2743	A	C5-N7-C8	6.72	107.26	103.90
79	B2	539	G	N7-C8-N9	6.71	116.46	113.10
84	CW	60	U	C1'-O4'-C4'	-6.71	104.53	109.90
80	B5	2403	G	C5-N7-C8	6.71	107.66	104.30
82	B8	42	G	C4-N9-C1'	-6.71	117.77	126.50
79	B2	553	G	N1-C2-N2	6.71	122.24	116.20
80	B5	908	G	C4-N9-C1'	6.71	135.23	126.50
80	B5	2279	A	N1-C2-N3	6.71	132.66	129.30
80	B5	2767	U	C5-C4-O4	6.71	129.93	125.90
80	B5	2892	A	N9-C4-C5	6.71	108.48	105.80
80	B5	2145	A	N1-C6-N6	-6.71	114.58	118.60
79	B2	1762	A	C8-N9-C4	6.71	108.48	105.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1312	C	C6-N1-C2	-6.71	117.62	120.30
80	B5	2929	C	N1-C2-O2	-6.71	114.88	118.90
84	CW	53	G	P-O5'-C5'	-6.71	110.17	120.90
84	CW	60	U	P-O3'-C3'	-6.71	111.65	119.70
47	BM	72	LEU	CA-CB-CG	6.71	130.72	115.30
80	B5	1686	U	C5-C4-O4	-6.70	121.88	125.90
80	B5	2411	U	N3-C4-O4	-6.70	114.71	119.40
79	B2	1258	U	C5-C4-O4	6.70	129.92	125.90
80	B5	2341	A	N9-C4-C5	-6.70	103.12	105.80
80	B5	620	U	C5-C6-N1	6.70	126.05	122.70
80	B5	1392	G	N9-C4-C5	-6.70	102.72	105.40
80	B5	1911	A	C5-C6-N6	-6.70	118.34	123.70
80	B5	1496	C	C2-N1-C1'	6.70	126.17	118.80
84	CW	21	A	O4'-C1'-N9	6.70	113.56	108.20
79	B2	783	G	N9-C4-C5	-6.70	102.72	105.40
80	B5	1116	G	N9-C4-C5	6.70	108.08	105.40
80	B5	835	G	C6-N1-C2	-6.70	121.08	125.10
80	B5	1228	C	N3-C4-N4	6.70	122.69	118.00
80	B5	3336	A	N1-C2-N3	6.70	132.65	129.30
79	B2	192	U	C2-N1-C1'	6.69	125.73	117.70
80	B5	1159	A	N1-C2-N3	-6.69	125.95	129.30
82	B8	25	G	C5-C6-O6	6.69	132.62	128.60
84	CW	48	C	P-O3'-C3'	6.69	127.73	119.70
80	B5	2201	G	N1-C6-O6	-6.69	115.89	119.90
80	B5	355	A	N1-C2-N3	6.69	132.64	129.30
80	B5	649	A	C8-N9-C4	-6.69	103.12	105.80
35	BA	246	LEU	CA-CB-CG	6.69	130.68	115.30
80	B5	518	G	C4-C5-N7	6.69	113.47	110.80
80	B5	2407	C	C5-C4-N4	-6.69	115.52	120.20
80	B5	1206	G	C8-N9-C4	-6.68	103.73	106.40
81	B7	25	G	N1-C6-O6	6.68	123.91	119.90
80	B5	1229	G	C5'-C4'-C3'	6.68	126.69	116.00
80	B5	2231	C	C4-C5-C6	6.68	120.74	117.40
80	B5	3049	A	C6-N1-C2	6.68	122.61	118.60
79	B2	838	G	C8-N9-C4	6.68	109.07	106.40
80	B5	3039	C	C6-N1-C2	-6.68	117.63	120.30
80	B5	669	U	C2-N3-C4	-6.68	122.99	127.00
80	B5	413	U	C4-C5-C6	6.67	123.70	119.70
80	B5	2391	G	N7-C8-N9	6.67	116.44	113.10
83	CV	373	MET	CG-SD-CE	-6.67	89.52	100.20
46	BL	171	ARG	NE-CZ-NH2	-6.67	116.96	120.30
79	B2	266	A	N9-C4-C5	-6.67	103.13	105.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	930	U	C4-C5-C6	-6.67	115.70	119.70
80	B5	376	G	C2-N3-C4	6.67	115.23	111.90
80	B5	2908	G	C5-C6-O6	6.67	132.60	128.60
79	B2	1679	G	N3-C4-C5	-6.67	125.27	128.60
80	B5	413	U	C5-C6-N1	-6.67	119.37	122.70
80	B5	1359	C	C5-C4-N4	-6.67	115.53	120.20
80	B5	1392	G	C5-N7-C8	6.67	107.63	104.30
83	CV	210	TRP	CE2-CD2-CG	-6.67	101.97	107.30
80	B5	3266	G	N1-C6-O6	-6.66	115.90	119.90
80	B5	600	G	N7-C8-N9	6.66	116.43	113.10
80	B5	1042	U	N1-C2-O2	6.66	127.46	122.80
80	B5	1057	A	N9-C4-C5	-6.66	103.14	105.80
80	B5	2717	U	N1-C2-N3	6.66	118.90	114.90
79	B2	340	U	N1-C2-O2	6.66	127.46	122.80
80	B5	1844	C	N1-C2-O2	-6.66	114.91	118.90
80	B5	3138	U	N1-C2-N3	6.66	118.89	114.90
80	B5	1232	C	C1'-O4'-C4'	-6.65	104.58	109.90
80	B5	2889	C	N3-C2-O2	-6.65	117.24	121.90
79	B2	608	U	N1-C2-N3	6.65	118.89	114.90
80	B5	966	U	C2-N3-C4	-6.65	123.01	127.00
80	B5	2357	A	N1-C6-N6	6.65	122.59	118.60
80	B5	2811	A	C6-N1-C2	-6.65	114.61	118.60
80	B5	1307	G	C2-N3-C4	6.65	115.22	111.90
80	B5	436	A	N7-C8-N9	6.65	117.12	113.80
80	B5	1042	U	C5-C4-O4	6.65	129.89	125.90
80	B5	2309	A	N1-C2-N3	-6.65	125.98	129.30
80	B5	1235	U	O4'-C1'-N1	6.65	113.52	108.20
79	B2	566	C	N1-C2-O2	6.64	122.89	118.90
79	B2	1297	G	C8-N9-C4	6.64	109.06	106.40
80	B5	1409	G	C5-C6-O6	6.64	132.59	128.60
80	B5	2961	G	C5-C6-O6	6.64	132.59	128.60
79	B2	687	G	N3-C2-N2	-6.64	115.25	119.90
80	B5	986	U	N3-C4-O4	6.64	124.05	119.40
84	CW	15	G	P-O3'-C3'	6.64	127.67	119.70
80	B5	669	U	C4-C5-C6	6.64	123.68	119.70
80	B5	1342	C	C4-C5-C6	6.64	120.72	117.40
80	B5	2292	U	C2-N1-C1'	6.64	125.67	117.70
84	CW	21	A	C5'-C4'-C3'	6.64	126.62	116.00
80	B5	625	G	N9-C4-C5	6.64	108.06	105.40
80	B5	990	U	N3-C2-O2	-6.64	117.55	122.20
80	B5	2392	C	N1-C2-O2	-6.64	114.92	118.90
80	B5	644	G	C8-N9-C4	-6.64	103.75	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1439	U	C2-N3-C4	-6.64	123.02	127.00
80	B5	3335	A	C2-N3-C4	-6.64	107.28	110.60
80	B5	1233	G	N1-C6-O6	6.63	123.88	119.90
80	B5	3214	U	N1-C2-O2	6.63	127.44	122.80
80	B5	1260	A	P-O3'-C3'	6.63	127.66	119.70
80	B5	1882	G	C4-C5-N7	-6.63	108.15	110.80
80	B5	2169	G	C2-N3-C4	6.63	115.22	111.90
80	B5	1754	G	N1-C6-O6	-6.63	115.92	119.90
80	B5	1848	G	C6-C5-N7	-6.63	126.42	130.40
80	B5	3128	G	C5-C6-O6	-6.63	124.62	128.60
80	B5	1146	C	N3-C2-O2	-6.63	117.26	121.90
80	B5	2347	U	N3-C4-O4	-6.63	114.76	119.40
80	B5	2377	G	C2-N3-C4	6.62	115.21	111.90
80	B5	1007	U	C5-C6-N1	-6.62	119.39	122.70
80	B5	3244	A	C2-N3-C4	-6.62	107.29	110.60
80	B5	1262	G	C6-C5-N7	-6.62	126.43	130.40
80	B5	1516	C	C5-C6-N1	-6.62	117.69	121.00
80	B5	1931	U	N3-C4-O4	-6.62	114.77	119.40
84	CW	14	A	O4'-C1'-N9	6.62	113.50	108.20
84	CW	68	C	C5-C4-N4	-6.62	115.57	120.20
80	B5	2207	A	C6-C5-N7	-6.62	127.67	132.30
80	B5	267	G	N9-C4-C5	-6.62	102.75	105.40
80	B5	721	G	C5-C6-N1	6.62	114.81	111.50
79	B2	557	G	C4-N9-C1'	6.61	135.10	126.50
80	B5	145	G	N3-C4-N9	-6.61	122.03	126.00
80	B5	1049	C	C4-C5-C6	-6.61	114.09	117.40
80	B5	3007	U	N3-C4-C5	6.61	118.57	114.60
81	B7	57	G	C4-C5-N7	-6.61	108.16	110.80
80	B5	828	A	N3-C4-C5	-6.61	122.17	126.80
80	B5	3306	U	C5-C6-N1	-6.61	119.39	122.70
80	B5	2675	C	N1-C2-O2	-6.61	114.94	118.90
80	B5	361	A	N1-C6-N6	-6.61	114.64	118.60
80	B5	1890	U	C5-C6-N1	-6.61	119.40	122.70
80	B5	3185	U	C5-C6-N1	-6.61	119.40	122.70
80	B5	792	G	N1-C2-N3	6.60	127.86	123.90
80	B5	1236	G	C5-C6-O6	-6.60	124.64	128.60
80	B5	420	G	N3-C4-C5	-6.60	125.30	128.60
80	B5	934	G	C2-N3-C4	6.60	115.20	111.90
80	B5	2549	G	C6-C5-N7	-6.60	126.44	130.40
82	B8	24	G	N1-C6-O6	-6.60	115.94	119.90
80	B5	1722	U	N3-C2-O2	6.60	126.82	122.20
80	B5	1876	U	C5-C6-N1	6.60	126.00	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1448	U	N1-C2-O2	-6.60	118.18	122.80
80	B5	1245	A	C5-C6-N1	-6.60	114.40	117.70
83	CV	16	THR	N-CA-C	-6.60	93.19	111.00
82	B8	59	A	C2-N3-C4	6.60	113.90	110.60
37	BC	138	ARG	NE-CZ-NH2	-6.59	117.00	120.30
80	B5	1208	U	C5-C6-N1	-6.59	119.40	122.70
80	B5	1283	C	O4'-C1'-N1	6.59	113.47	108.20
80	B5	2851	A	C8-N9-C4	6.59	108.44	105.80
80	B5	3324	C	C6-N1-C2	6.59	122.94	120.30
80	B5	2719	U	C6-N1-C1'	6.59	130.43	121.20
80	B5	2954	U	C2-N1-C1'	6.59	125.61	117.70
80	B5	3153	U	N1-C2-O2	6.59	127.41	122.80
80	B5	880	G	C5-C6-O6	-6.59	124.65	128.60
80	B5	2617	U	N3-C4-O4	-6.59	114.79	119.40
80	B5	2984	C	C2-N3-C4	-6.59	116.61	119.90
80	B5	1242	G	C5-C6-O6	-6.59	124.65	128.60
17	AI	172	ARG	NE-CZ-NH1	6.58	123.59	120.30
80	B5	1225	A	C4-C5-C6	6.58	120.29	117.00
80	B5	1901	A	C4-C5-C6	6.58	120.29	117.00
80	B5	360	G	C8-N9-C4	6.58	109.03	106.40
80	B5	784	A	C6-C5-N7	-6.58	127.69	132.30
80	B5	1255	C	O4'-C1'-N1	6.58	113.47	108.20
80	B5	3303	G	N3-C2-N2	6.58	124.51	119.90
80	B5	3306	U	C6-N1-C2	6.58	124.95	121.00
80	B5	2114	C	C6-N1-C2	-6.58	117.67	120.30
80	B5	1229	G	N3-C2-N2	6.58	124.50	119.90
80	B5	3333	G	N1-C6-O6	6.58	123.85	119.90
79	B2	1462	G	N9-C4-C5	-6.58	102.77	105.40
80	B5	1151	U	C4-C5-C6	-6.58	115.75	119.70
80	B5	1365	G	C8-N9-C1'	-6.58	118.45	127.00
80	B5	2957	G	C8-N9-C4	6.58	109.03	106.40
80	B5	3025	C	C5-C4-N4	6.58	124.80	120.20
80	B5	640	U	N3-C2-O2	-6.57	117.60	122.20
81	B7	68	C	C2-N3-C4	-6.57	116.61	119.90
80	B5	2746	A	C8-N9-C4	6.57	108.43	105.80
80	B5	828	A	C2-N3-C4	6.57	113.89	110.60
80	B5	2147	A	N1-C6-N6	6.57	122.54	118.60
80	B5	1906	G	N1-C2-N3	6.57	127.84	123.90
80	B5	859	G	N9-C4-C5	6.57	108.03	105.40
80	B5	3122	A	C4-C5-C6	6.57	120.28	117.00
80	B5	925	A	C4-C5-C6	6.56	120.28	117.00
80	B5	2124	G	C8-N9-C4	6.56	109.03	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	B7	92	A	C5-N7-C8	-6.56	100.62	103.90
36	BB	21	ARG	NE-CZ-NH1	6.56	123.58	120.30
80	B5	3263	G	N3-C2-N2	6.56	124.49	119.90
80	B5	424	G	N3-C2-N2	6.56	124.49	119.90
80	B5	3115	C	N1-C2-O2	-6.56	114.96	118.90
79	B2	557	G	C8-N9-C1'	-6.56	118.48	127.00
80	B5	2626	A	C4-C5-N7	-6.56	107.42	110.70
79	B2	131	C	C6-N1-C2	-6.56	117.68	120.30
80	B5	370	U	C6-N1-C2	-6.56	117.07	121.00
80	B5	1131	G	C2-N3-C4	-6.56	108.62	111.90
79	B2	1274	C	N3-C4-N4	-6.55	113.41	118.00
80	B5	345	G	N3-C2-N2	6.55	124.49	119.90
80	B5	369	A	N9-C4-C5	6.55	108.42	105.80
80	B5	2866	U	N1-C2-O2	-6.55	118.21	122.80
80	B5	386	A	C6-C5-N7	-6.55	127.71	132.30
79	B2	965	U	C5-C6-N1	6.55	125.98	122.70
80	B5	332	C	C4-C5-C6	6.55	120.67	117.40
80	B5	2904	U	C5-C6-N1	-6.55	119.42	122.70
80	B5	3376	A	N9-C4-C5	6.55	108.42	105.80
80	B5	675	C	N3-C4-N4	6.55	122.58	118.00
80	B5	641	C	C2-N1-C1'	-6.55	111.60	118.80
80	B5	2258	U	N3-C2-O2	-6.55	117.62	122.20
80	B5	1408	G	N3-C4-N9	-6.55	122.07	126.00
80	B5	1518	U	N3-C4-C5	6.55	118.53	114.60
80	B5	3148	U	C5-C4-O4	-6.55	121.97	125.90
43	BI	10	ARG	NE-CZ-NH1	-6.54	117.03	120.30
80	B5	815	G	C5-C6-O6	6.54	132.53	128.60
80	B5	2626	A	C5-C6-N1	-6.54	114.43	117.70
80	B5	3270	U	N3-C4-O4	-6.54	114.82	119.40
79	B2	647	G	N3-C2-N2	-6.54	115.32	119.90
80	B5	1004	U	N3-C2-O2	-6.54	117.62	122.20
80	B5	1138	U	C2-N3-C4	-6.54	123.07	127.00
80	B5	1211	U	N3-C4-C5	6.54	118.53	114.60
80	B5	1259	A	C4-C5-C6	6.54	120.27	117.00
80	B5	226	C	N3-C4-C5	6.54	124.52	121.90
80	B5	1215	U	N3-C4-O4	6.54	123.98	119.40
80	B5	3310	A	N1-C6-N6	-6.54	114.68	118.60
79	B2	558	U	C2-N1-C1'	6.54	125.55	117.70
80	B5	692	A	N1-C2-N3	-6.54	126.03	129.30
66	Bf	49	ILE	CB-CA-C	-6.53	98.53	111.60
80	B5	1897	G	C5-C6-O6	-6.53	124.68	128.60
80	B5	3289	G	N7-C8-N9	6.53	116.37	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	BI	182	LEU	CA-CB-CG	-6.53	100.28	115.30
80	B5	2699	G	N1-C6-O6	6.53	123.82	119.90
80	B5	1240	A	C4-C5-C6	6.53	120.27	117.00
80	B5	2303	A	N3-C4-C5	-6.53	122.23	126.80
80	B5	2518	C	C5-C6-N1	-6.53	117.73	121.00
80	B5	783	A	N1-C6-N6	6.53	122.52	118.60
80	B5	217	U	C5-C6-N1	-6.53	119.44	122.70
80	B5	1151	U	N3-C4-C5	6.53	118.52	114.60
80	B5	2320	A	N1-C2-N3	6.53	132.56	129.30
80	B5	2884	C	N1-C2-N3	6.53	123.77	119.20
82	B8	54	A	C5-N7-C8	-6.53	100.64	103.90
80	B5	1284	C	C2'-C3'-O3'	6.52	124.14	113.70
79	B2	1282	U	C5-C4-O4	6.52	129.81	125.90
80	B5	2385	G	C8-N9-C4	6.52	109.01	106.40
80	B5	3190	C	C6-N1-C2	-6.52	117.69	120.30
80	B5	3341	U	C6-N1-C2	-6.52	117.09	121.00
80	B5	1408	G	N3-C4-C5	6.52	131.86	128.60
80	B5	2301	U	C5-C6-N1	-6.52	119.44	122.70
84	CW	50	U	O4'-C1'-N1	6.52	113.42	108.20
80	B5	299	G	C2-N3-C4	6.52	115.16	111.90
80	B5	584	G	C5-C6-O6	6.51	132.51	128.60
80	B5	1200	A	C4-C5-C6	6.51	120.26	117.00
79	B2	1473	U	N3-C2-O2	-6.51	117.64	122.20
82	B8	6	U	C5-C6-N1	-6.51	119.44	122.70
80	B5	2257	C	N3-C2-O2	-6.51	117.34	121.90
81	B7	20	A	C5-C6-N6	-6.51	118.50	123.70
79	B2	6	G	N1-C2-N3	6.50	127.80	123.90
80	B5	1256	G	N1-C6-O6	6.50	123.80	119.90
8	A7	134	ASP	OD1-CG-OD2	-6.50	110.94	123.30
80	B5	884	A	N3-C4-N9	-6.50	122.20	127.40
79	B2	136	C	N1-C2-O2	6.50	122.80	118.90
80	B5	3105	U	N1-C2-O2	-6.50	118.25	122.80
79	B2	355	G	C6-N1-C2	-6.50	121.20	125.10
80	B5	2336	U	N3-C4-O4	-6.50	114.85	119.40
81	B7	12	U	N3-C4-C5	6.50	118.50	114.60
80	B5	1256	G	C5-C6-O6	-6.50	124.70	128.60
84	CW	18	G	O3'-P-O5'	-6.50	91.65	104.00
79	B2	132	U	C2-N1-C1'	-6.50	109.90	117.70
80	B5	429	U	N3-C4-C5	6.50	118.50	114.60
80	B5	2320	A	C5-N7-C8	6.50	107.15	103.90
80	B5	290	G	N3-C2-N2	6.49	124.45	119.90
84	CW	75	C	N3-C4-N4	6.49	122.55	118.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2351	U	N3-C4-O4	-6.49	114.86	119.40
82	B8	11	C	C4-C5-C6	6.49	120.65	117.40
80	B5	1259	A	O4'-C1'-N9	6.49	113.39	108.20
80	B5	2314	U	C2-N1-C1'	6.49	125.49	117.70
80	B5	2833	A	C8-N9-C4	6.49	108.40	105.80
79	B2	1422	A	C8-N9-C4	6.49	108.40	105.80
80	B5	393	U	N3-C2-O2	-6.49	117.66	122.20
80	B5	2440	G	N7-C8-N9	6.49	116.34	113.10
80	B5	2849	C	C5-C6-N1	6.49	124.24	121.00
80	B5	1231	A	C4-C5-C6	6.49	120.24	117.00
79	B2	1455	G	N1-C6-O6	6.49	123.79	119.90
80	B5	2647	A	C8-N9-C4	-6.49	103.21	105.80
80	B5	3330	A	N1-C6-N6	-6.49	114.71	118.60
84	CW	5	G	C6-N1-C2	-6.49	121.21	125.10
84	CW	30	G	C5-C6-O6	-6.49	124.71	128.60
79	B2	1503	A	N1-C2-N3	6.48	132.54	129.30
80	B5	1434	G	C8-N9-C4	6.48	108.99	106.40
80	B5	1788	C	N3-C4-C5	-6.48	119.31	121.90
80	B5	3043	C	N3-C4-C5	6.48	124.49	121.90
80	B5	343	U	C5-C6-N1	-6.48	119.46	122.70
80	B5	370	U	N3-C2-O2	-6.48	117.67	122.20
80	B5	518	G	N1-C6-O6	6.48	123.79	119.90
80	B5	894	G	C5-C6-O6	-6.48	124.71	128.60
80	B5	1215	U	C5-C4-O4	-6.48	122.01	125.90
48	BN	68	ARG	NE-CZ-NH1	6.48	123.54	120.30
8	A7	134	ASP	CB-CG-OD2	-6.47	112.47	118.30
64	Bd	90	PHE	CB-CA-C	-6.47	97.45	110.40
80	B5	1402	C	C4-C5-C6	6.47	120.64	117.40
80	B5	3126	C	N3-C4-C5	6.47	124.49	121.90
80	B5	3306	U	N3-C4-C5	6.47	118.48	114.60
80	B5	2837	A	C2-N3-C4	6.47	113.84	110.60
80	B5	3186	A	N9-C4-C5	6.47	108.39	105.80
80	B5	963	G	C5-C6-O6	-6.47	124.72	128.60
80	B5	3004	C	C5-C4-N4	-6.47	115.67	120.20
79	B2	1536	G	N3-C4-N9	6.47	129.88	126.00
80	B5	1190	A	C5-C6-N6	6.47	128.88	123.70
80	B5	3175	U	N3-C4-C5	-6.47	110.72	114.60
80	B5	2433	U	N3-C4-C5	6.47	118.48	114.60
80	B5	2993	G	N9-C4-C5	-6.47	102.81	105.40
49	BO	27[B]	VAL	C-N-CA	6.46	137.86	121.70
79	B2	1024	U	N3-C2-O2	-6.46	117.68	122.20
80	B5	435	C	C2-N3-C4	-6.46	116.67	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	B7	1	G	C4-N9-C1'	6.46	134.90	126.50
80	B5	519	A	C5-C6-N6	-6.46	118.53	123.70
80	B5	2211	U	C5-C6-N1	-6.46	119.47	122.70
84	CW	67	C	C6-N1-C1'	-6.46	113.05	120.80
80	B5	1161	G	N7-C8-N9	-6.46	109.87	113.10
79	B2	1235	C	N1-C2-O2	-6.46	115.03	118.90
80	B5	651	G	C8-N9-C4	-6.46	103.82	106.40
80	B5	1392	G	C8-N9-C1'	-6.46	118.60	127.00
80	B5	2719	U	C5-C6-N1	-6.46	119.47	122.70
80	B5	950	G	N3-C2-N2	6.46	124.42	119.90
80	B5	916	G	C8-N9-C4	-6.46	103.82	106.40
80	B5	3167	A	N7-C8-N9	6.46	117.03	113.80
79	B2	554	C	C2-N1-C1'	6.45	125.90	118.80
80	B5	1215	U	N1-C2-O2	-6.45	118.28	122.80
79	B2	407	A	C4-C5-C6	6.45	120.22	117.00
79	B2	1169	G	N7-C8-N9	6.45	116.33	113.10
80	B5	2998	U	C5-C6-N1	-6.45	119.47	122.70
79	B2	830	U	N3-C2-O2	-6.45	117.69	122.20
80	B5	1399	A	C8-N9-C4	6.45	108.38	105.80
80	B5	940	G	C8-N9-C4	-6.45	103.82	106.40
80	B5	2146	C	C6-N1-C2	-6.45	117.72	120.30
80	B5	2891	U	C5-C6-N1	-6.44	119.48	122.70
80	B5	3006	A	N3-C4-N9	-6.44	122.25	127.40
83	CV	469	ILE	CB-CA-C	-6.44	98.71	111.60
80	B5	1283	C	C5'-C4'-C3'	6.44	126.31	116.00
80	B5	2345	A	C5-C6-N6	-6.44	118.55	123.70
80	B5	2375	G	C5-C6-N1	6.44	114.72	111.50
80	B5	2964	G	N7-C8-N9	-6.44	109.88	113.10
81	B7	38	U	C6-N1-C1'	-6.44	112.18	121.20
80	B5	1851	G	C4-C5-C6	6.44	122.66	118.80
80	B5	1298	C	N1-C2-O2	-6.44	115.04	118.90
80	B5	2817	A	C6-N1-C2	-6.44	114.74	118.60
79	B2	732	G	N9-C4-C5	-6.44	102.83	105.40
80	B5	2662	G	C3'-C2'-C1'	-6.44	96.35	101.50
80	B5	824	C	C4-C5-C6	6.43	120.62	117.40
80	B5	2431	C	N3-C4-C5	-6.43	119.33	121.90
83	CV	81	GLU	C-N-CA	6.43	137.79	121.70
79	B2	1200	G	C4-C5-C6	6.43	122.66	118.80
80	B5	947	G	N1-C6-O6	-6.43	116.04	119.90
80	B5	1496	C	C6-N1-C2	-6.43	117.73	120.30
80	B5	2246	G	N3-C4-C5	-6.43	125.38	128.60
82	B8	28	C	N3-C4-C5	6.43	124.47	121.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	266	A	C8-N9-C4	6.43	108.37	105.80
79	B2	628	G	N3-C2-N2	6.43	124.40	119.90
79	B2	1758	U	C6-N1-C2	-6.43	117.14	121.00
82	B8	111	A	C2-N3-C4	-6.43	107.39	110.60
80	B5	971	G	N1-C2-N2	6.43	121.98	116.20
80	B5	1271	A	C5-C6-N6	-6.43	118.56	123.70
80	B5	436	A	C4-N9-C1'	6.43	137.87	126.30
80	B5	2351	U	N3-C2-O2	-6.43	117.70	122.20
80	B5	2754	G	N3-C2-N2	6.43	124.40	119.90
79	B2	610	G	C4-N9-C1'	6.42	134.85	126.50
80	B5	1749	A	C8-N9-C4	6.42	108.37	105.80
80	B5	1843	C	C2-N1-C1'	6.42	125.87	118.80
79	B2	68	A	C8-N9-C4	-6.42	103.23	105.80
79	B2	1085	G	N3-C2-N2	6.42	124.39	119.90
80	B5	2288	G	N3-C4-C5	-6.42	125.39	128.60
84	CW	17	C	N3-C4-C5	-6.42	119.33	121.90
80	B5	1607	U	N1-C2-N3	6.42	118.75	114.90
80	B5	2800	G	N9-C4-C5	6.42	107.97	105.40
80	B5	2930	A	N1-C6-N6	-6.42	114.75	118.60
80	B5	1147	G	N7-C8-N9	-6.42	109.89	113.10
80	B5	2302	G	N1-C2-N2	-6.42	110.42	116.20
82	B8	29	U	C2-N3-C4	-6.42	123.15	127.00
84	CW	60	U	O4'-C1'-C2'	-6.42	99.38	105.80
80	B5	2894	C	N3-C4-C5	6.42	124.47	121.90
79	B2	404	G	C5-C6-O6	-6.41	124.75	128.60
80	B5	284	A	C2-N3-C4	6.41	113.81	110.60
80	B5	679	U	C5-C6-N1	-6.41	119.49	122.70
80	B5	1390	A	C5-C6-N6	6.41	128.83	123.70
80	B5	2288	G	C5-C6-O6	-6.41	124.75	128.60
79	B2	1027	A	N7-C8-N9	6.41	117.00	113.80
80	B5	833	G	N1-C2-N3	6.41	127.75	123.90
80	B5	1270	A	C4-C5-C6	6.41	120.21	117.00
80	B5	1907	C	N1-C2-O2	-6.41	115.05	118.90
80	B5	3187	A	C4-C5-N7	-6.41	107.50	110.70
79	B2	144	U	C6-N1-C2	-6.41	117.16	121.00
80	B5	3303	G	N1-C2-N2	-6.41	110.43	116.20
80	B5	1518	U	N1-C2-O2	6.41	127.28	122.80
84	CW	2	C	N3-C4-N4	6.41	122.48	118.00
79	B2	1185	U	C2-N1-C1'	6.40	125.39	117.70
80	B5	3354	U	N3-C2-O2	-6.40	117.72	122.20
38	BD	248	ARG	NE-CZ-NH2	-6.40	117.10	120.30
80	B5	1929	G	C8-N9-C4	6.40	108.96	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	943	U	C5-C6-N1	-6.40	119.50	122.70
80	B5	2396	G	N3-C4-C5	-6.40	125.40	128.60
80	B5	2857	C	C6-N1-C2	6.40	122.86	120.30
81	B7	40	C	N1-C2-O2	-6.40	115.06	118.90
80	B5	2817	A	N3-C4-C5	-6.40	122.32	126.80
80	B5	652	G	N3-C4-N9	6.40	129.84	126.00
80	B5	2123	G	C2-N3-C4	6.40	115.10	111.90
80	B5	667	C	N3-C4-C5	6.40	124.46	121.90
80	B5	1041	U	C6-N1-C2	6.40	124.84	121.00
80	B5	2631	U	N1-C2-N3	6.39	118.74	114.90
80	B5	2802	A	N1-C2-N3	-6.39	126.10	129.30
82	B8	19	C	C4-C5-C6	6.39	120.60	117.40
80	B5	2633	U	C5-C6-N1	-6.39	119.50	122.70
79	B2	1000	C	N1-C2-O2	6.39	122.73	118.90
80	B5	1902	G	N3-C4-N9	6.39	129.83	126.00
80	B5	2879	C	N1-C2-O2	6.39	122.73	118.90
80	B5	1321	G	C5-C6-N1	-6.39	108.31	111.50
32	AX	33	LEU	CA-CB-CG	-6.39	100.61	115.30
79	B2	1430	U	C5-C4-O4	6.39	129.73	125.90
80	B5	648	C	C6-N1-C2	-6.39	117.75	120.30
80	B5	2677	G	N3-C2-N2	-6.38	115.43	119.90
81	B7	93	C	C4-C5-C6	6.38	120.59	117.40
79	B2	1096	C	N3-C2-O2	-6.38	117.43	121.90
79	B2	75	U	N1-C2-O2	6.38	127.27	122.80
79	B2	942	G	N1-C6-O6	-6.38	116.07	119.90
80	B5	1793	C	C2-N3-C4	6.38	123.09	119.90
80	B5	2305	G	C4-C5-N7	6.38	113.35	110.80
80	B5	3245	A	C5-C6-N6	-6.38	118.60	123.70
84	CW	25	C	P-O3'-C3'	-6.38	112.05	119.70
80	B5	1879	A	C4-C5-N7	6.38	113.89	110.70
80	B5	2340	U	C2-N3-C4	-6.38	123.17	127.00
80	B5	2365	C	C5-C4-N4	6.38	124.66	120.20
80	B5	2611	U	C4-C5-C6	6.38	123.53	119.70
80	B5	2625	C	N3-C2-O2	-6.38	117.44	121.90
82	B8	29	U	N1-C2-N3	6.38	118.72	114.90
65	Be	45	ARG	NE-CZ-NH1	6.37	123.49	120.30
80	B5	75	G	C5-C6-O6	-6.37	124.78	128.60
80	B5	600	G	C8-N9-C4	-6.37	103.85	106.40
80	B5	1451	C	C5-C6-N1	-6.37	117.81	121.00
80	B5	1894	U	C2-N3-C4	-6.37	123.18	127.00
80	B5	2130	G	N1-C6-O6	-6.37	116.08	119.90
81	B7	92	A	C4-C5-N7	6.37	113.89	110.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	Ba	28	HIS	N-CA-C	6.37	128.19	111.00
80	B5	909	G	C4-C5-N7	-6.37	108.25	110.80
80	B5	2117	A	N1-C6-N6	-6.37	114.78	118.60
80	B5	2948	C	C5-C4-N4	6.37	124.66	120.20
81	B7	48	U	N3-C4-C5	6.37	118.42	114.60
80	B5	1840	U	C5-C6-N1	-6.37	119.52	122.70
80	B5	3189	G	N1-C2-N3	6.37	127.72	123.90
84	CW	26	A	C5-C6-N6	-6.37	118.61	123.70
84	CW	40	C	N3-C4-C5	-6.37	119.35	121.90
38	BD	152	ARG	NE-CZ-NH1	6.36	123.48	120.30
79	B2	1611	A	C8-N9-C4	-6.36	103.25	105.80
80	B5	676	G	C8-N9-C4	-6.36	103.86	106.40
80	B5	1413	G	N1-C6-O6	-6.36	116.08	119.90
80	B5	1858	A	N7-C8-N9	6.36	116.98	113.80
80	B5	2429	G	C8-N9-C4	-6.36	103.86	106.40
80	B5	3003	G	C5-C6-N1	6.36	114.68	111.50
49	BO	23[B]	ILE	O-C-N	6.36	132.88	122.70
80	B5	1115	G	C4-N9-C1'	6.36	134.77	126.50
79	B2	973	A	C2-N3-C4	-6.36	107.42	110.60
51	BQ	176	ARG	NE-CZ-NH2	-6.36	117.12	120.30
80	B5	1172	G	N3-C2-N2	6.36	124.35	119.90
80	B5	1300	G	C5-C6-O6	-6.36	124.78	128.60
80	B5	2408	U	N1-C2-N3	6.36	118.72	114.90
80	B5	2821	C	C5-C6-N1	6.36	124.18	121.00
79	B2	136	C	C6-N1-C1'	-6.36	113.17	120.80
80	B5	3309	G	C6-N1-C2	-6.36	121.29	125.10
80	B5	645	A	C5-C6-N1	6.35	120.88	117.70
80	B5	1403	C	N3-C4-N4	6.35	122.45	118.00
80	B5	1254	C	N3-C4-N4	6.35	122.45	118.00
80	B5	2416	U	C5-C6-N1	6.35	125.88	122.70
80	B5	2614	G	C8-N9-C1'	-6.35	118.74	127.00
79	B2	1745	G	N9-C4-C5	-6.35	102.86	105.40
82	B8	17	A	C4-C5-N7	6.35	113.88	110.70
80	B5	891	G	C5-C6-O6	6.35	132.41	128.60
80	B5	904	A	C8-N9-C4	-6.35	103.26	105.80
80	B5	1449	A	C5-C6-N1	-6.35	114.53	117.70
80	B5	1264	G	P-O3'-C3'	-6.34	112.09	119.70
80	B5	2777	G	C4-C5-N7	-6.34	108.26	110.80
80	B5	3174	A	C4-C5-N7	6.34	113.87	110.70
74	Bn	9	ARG	NE-CZ-NH2	-6.34	117.13	120.30
80	B5	248	U	N1-C2-O2	6.34	127.24	122.80
80	B5	1306	G	C6-N1-C2	-6.34	121.30	125.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1833	G	N7-C8-N9	-6.34	109.93	113.10
80	B5	1211	U	N3-C4-O4	-6.34	114.96	119.40
80	B5	2303	A	N1-C6-N6	-6.34	114.80	118.60
80	B5	2352	A	N1-C2-N3	6.34	132.47	129.30
80	B5	2753	G	N3-C2-N2	-6.34	115.46	119.90
81	B7	48	U	N1-C2-O2	-6.34	118.36	122.80
84	CW	51	U	O4'-C1'-N1	6.34	113.27	108.20
80	B5	1832	C	C2-N3-C4	-6.33	116.73	119.90
80	B5	2231	C	N3-C4-C5	-6.33	119.37	121.90
80	B5	2349	U	N3-C4-C5	6.33	118.40	114.60
82	B8	52	A	C8-N9-C4	-6.33	103.27	105.80
80	B5	1403	C	C6-N1-C1'	-6.33	113.20	120.80
80	B5	2361	A	C8-N9-C4	-6.33	103.27	105.80
84	CW	38	A	C5-C6-N6	-6.33	118.64	123.70
35	BA	204	MET	CG-SD-CE	-6.33	90.07	100.20
80	B5	1168	U	N3-C4-C5	6.33	118.40	114.60
84	CW	42	C	N3-C4-C5	-6.33	119.37	121.90
80	B5	1297	C	C4-C5-C6	6.33	120.56	117.40
79	B2	159	U	C2-N1-C1'	-6.33	110.11	117.70
80	B5	1188	U	C5-C4-O4	-6.33	122.10	125.90
80	B5	1211	U	C4-C5-C6	-6.33	115.91	119.70
80	B5	2211	U	N3-C4-C5	-6.33	110.81	114.60
80	B5	2277	C	C6-N1-C2	6.33	122.83	120.30
79	B2	213	A	C8-N9-C4	6.32	108.33	105.80
80	B5	2996	U	C2-N1-C1'	6.32	125.29	117.70
37	BC	327	LEU	CA-CB-CG	6.32	129.84	115.30
79	B2	1246	C	C5-C4-N4	6.32	124.63	120.20
79	B2	1465	C	N3-C4-C5	-6.32	119.37	121.90
80	B5	65	A	N7-C8-N9	6.32	116.96	113.80
80	B5	3309	G	C4-N9-C1'	6.32	134.72	126.50
36	BB	10	ARG	NE-CZ-NH1	6.32	123.46	120.30
79	B2	523	G	N3-C4-C5	-6.32	125.44	128.60
80	B5	42	C	C5-C6-N1	6.32	124.16	121.00
80	B5	938	C	C6-N1-C2	6.32	122.83	120.30
80	B5	950	G	C8-N9-C4	6.32	108.93	106.40
80	B5	2363	A	C2-N3-C4	6.32	113.76	110.60
80	B5	1277	C	N3-C4-N4	6.32	122.42	118.00
84	CW	42	C	C1'-O4'-C4'	-6.32	104.85	109.90
79	B2	377	G	N3-C4-C5	6.31	131.76	128.60
80	B5	793	C	N1-C2-O2	-6.31	115.11	118.90
80	B5	1496	C	C5-C6-N1	6.31	124.16	121.00
80	B5	1690	C	N1-C2-O2	-6.31	115.11	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2134	G	N3-C4-C5	-6.31	125.44	128.60
80	B5	2393	G	N9-C4-C5	-6.31	102.87	105.40
82	B8	84	C	C6-N1-C2	-6.31	117.77	120.30
46	BL	27	ASP	CB-CG-OD1	6.31	123.98	118.30
79	B2	557	G	C4-C5-C6	6.31	122.59	118.80
79	B2	1454	G	C5-C6-O6	6.31	132.39	128.60
80	B5	1416	C	N3-C2-O2	-6.31	117.48	121.90
80	B5	1468	A	C8-N9-C4	-6.31	103.28	105.80
80	B5	1753	G	N3-C4-C5	-6.31	125.44	128.60
80	B5	631	U	N3-C4-C5	6.31	118.39	114.60
80	B5	2728	G	C8-N9-C4	-6.31	103.88	106.40
80	B5	2886	U	N3-C2-O2	-6.31	117.78	122.20
80	B5	2261	G	C8-N9-C4	6.31	108.92	106.40
79	B2	1456	C	C6-N1-C2	-6.31	117.78	120.30
80	B5	3011	A	N1-C2-N3	-6.30	126.15	129.30
81	B7	46	A	C8-N9-C4	-6.30	103.28	105.80
80	B5	1254	C	C6-N1-C2	-6.30	117.78	120.30
80	B5	1130	A	N3-C4-C5	-6.30	122.39	126.80
80	B5	779	G	C8-N9-C4	-6.30	103.88	106.40
80	B5	1314	C	C6-N1-C1'	-6.30	113.24	120.80
80	B5	1340	G	N3-C2-N2	6.30	124.31	119.90
79	B2	627	C	N3-C4-N4	6.30	122.41	118.00
79	B2	1515	A	C8-N9-C4	-6.30	103.28	105.80
80	B5	2364	G	C5-C6-O6	6.30	132.38	128.60
80	B5	1254	C	P-O5'-C5'	6.30	130.97	120.90
80	B5	3218	A	N3-C4-C5	6.30	131.21	126.80
80	B5	32	U	N1-C2-O2	-6.29	118.39	122.80
80	B5	2808	A	N1-C2-N3	6.29	132.45	129.30
80	B5	3270	U	C5-C6-N1	-6.29	119.55	122.70
80	B5	903	U	N3-C2-O2	-6.29	117.80	122.20
80	B5	1511	U	C5-C6-N1	-6.29	119.55	122.70
81	B7	92	A	C6-C5-N7	-6.29	127.89	132.30
80	B5	582	G	C5-C6-O6	6.29	132.38	128.60
80	B5	1733	G	N1-C6-O6	6.29	123.67	119.90
80	B5	3317	U	C5-C6-N1	6.29	125.85	122.70
80	B5	3360	C	C6-N1-C2	-6.29	117.78	120.30
80	B5	1064	A	C4-C5-N7	6.29	113.84	110.70
80	B5	1449	A	N3-C4-C5	6.29	131.20	126.80
79	B2	494	U	N1-C2-O2	6.29	127.20	122.80
80	B5	2833	A	N7-C8-N9	-6.29	110.66	113.80
81	B7	15	C	N3-C4-C5	6.29	124.42	121.90
80	B5	656	A	C8-N9-C4	6.29	108.31	105.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	624	G	C8-N9-C4	6.29	108.91	106.40
80	B5	3174	A	C5-N7-C8	-6.29	100.76	103.90
84	CW	15	G	C5-C6-O6	-6.29	124.83	128.60
79	B2	1329	A	C5-C6-N6	-6.28	118.67	123.70
82	B8	38	U	C5-C4-O4	6.28	129.67	125.90
79	B2	590	C	C2-N1-C1'	6.28	125.71	118.80
79	B2	868	G	N1-C6-O6	6.28	123.67	119.90
80	B5	637	C	C2-N1-C1'	-6.28	111.89	118.80
80	B5	947	G	N3-C4-N9	6.28	129.77	126.00
80	B5	3266	G	C8-N9-C4	-6.28	103.89	106.40
80	B5	1148	G	C5-C6-O6	-6.28	124.83	128.60
80	B5	1200	A	N1-C2-N3	6.28	132.44	129.30
80	B5	1233	G	C5-C6-O6	-6.28	124.83	128.60
80	B5	3258	U	C6-N1-C2	6.28	124.77	121.00
80	B5	1407	A	C8-N9-C4	6.28	108.31	105.80
80	B5	2616	C	C5-C4-N4	-6.28	115.81	120.20
80	B5	625	G	C5-C6-O6	6.28	132.37	128.60
80	B5	1273	A	C4-C5-C6	6.28	120.14	117.00
80	B5	2420	C	C5-C4-N4	-6.28	115.81	120.20
80	B5	1254	C	O4'-C1'-N1	6.28	113.22	108.20
80	B5	2552	C	N3-C2-O2	-6.28	117.51	121.90
65	Be	47	ARG	NE-CZ-NH2	-6.27	117.16	120.30
80	B5	510	G	C5-C6-N1	6.27	114.64	111.50
80	B5	1123	U	C5-C6-N1	-6.27	119.56	122.70
80	B5	1260	A	P-O5'-C5'	-6.27	110.86	120.90
81	B7	25	G	N3-C2-N2	-6.27	115.51	119.90
79	B2	75	U	N3-C2-O2	-6.27	117.81	122.20
79	B2	189	C	N1-C2-O2	6.27	122.66	118.90
80	B5	276	U	C2-N3-C4	-6.27	123.24	127.00
80	B5	819	U	C6-N1-C2	6.27	124.76	121.00
84	CW	13	C	O4'-C1'-N1	6.27	113.22	108.20
80	B5	1227	C	N1-C1'-C2'	6.27	122.15	114.00
80	B5	1229	G	C8-N9-C4	-6.27	103.89	106.40
80	B5	2139	A	C5-N7-C8	6.27	107.03	103.90
80	B5	2572	C	C6-N1-C2	-6.27	117.79	120.30
80	B5	1888	U	C2-N3-C4	-6.27	123.24	127.00
80	B5	1940	G	N1-C2-N2	-6.27	110.56	116.20
80	B5	1500	G	C8-N9-C4	6.26	108.91	106.40
80	B5	2952	G	N1-C6-O6	6.26	123.66	119.90
84	CW	3	C	O4'-C1'-N1	6.26	113.21	108.20
79	B2	1363	U	N1-C2-O2	6.26	127.18	122.80
80	B5	1408	G	C2-N3-C4	-6.26	108.77	111.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1883	A	N9-C4-C5	6.26	108.30	105.80
80	B5	2164	A	C8-N9-C4	-6.26	103.30	105.80
80	B5	2133	U	N3-C4-C5	6.26	118.36	114.60
80	B5	2389	C	C5-C6-N1	-6.26	117.87	121.00
79	B2	404	G	C8-N9-C4	6.26	108.90	106.40
80	B5	904	A	N9-C4-C5	6.26	108.30	105.80
80	B5	1056	U	N3-C4-C5	-6.26	110.85	114.60
80	B5	1252	A	C5-C6-N6	-6.26	118.69	123.70
80	B5	1307	G	C8-N9-C4	-6.26	103.90	106.40
80	B5	2389	C	N3-C4-C5	6.26	124.40	121.90
80	B5	2524	A	C6-N1-C2	6.25	122.35	118.60
80	B5	3317	U	N3-C4-O4	-6.25	115.02	119.40
80	B5	146	U	N3-C4-O4	-6.25	115.02	119.40
80	B5	665	A	C2-N3-C4	-6.25	107.47	110.60
80	B5	1035	G	N3-C4-N9	6.25	129.75	126.00
80	B5	1931	U	C5-C6-N1	-6.25	119.57	122.70
83	CV	210	TRP	NE1-CE2-CZ2	6.25	137.28	130.40
79	B2	377	G	C5-C6-O6	-6.25	124.85	128.60
79	B2	543	C	N3-C2-O2	-6.25	117.53	121.90
79	B2	1198	G	N9-C4-C5	6.25	107.90	105.40
80	B5	1042	U	C5-C6-N1	-6.25	119.58	122.70
80	B5	1300	G	C4-C5-N7	6.25	113.30	110.80
80	B5	2516	U	C2-N3-C4	-6.25	123.25	127.00
80	B5	2735	U	C6-N1-C2	-6.25	117.25	121.00
79	B2	933	A	C8-N9-C4	-6.25	103.30	105.80
80	B5	892	U	N3-C4-C5	6.25	118.35	114.60
80	B5	974	G	N3-C4-N9	6.25	129.75	126.00
80	B5	1389	G	C5-N7-C8	-6.25	101.18	104.30
80	B5	2930	A	C8-N9-C4	-6.25	103.30	105.80
80	B5	112	U	C5-C4-O4	-6.24	122.15	125.90
80	B5	644	G	N1-C6-O6	-6.24	116.15	119.90
80	B5	2754	G	N1-C6-O6	-6.24	116.15	119.90
80	B5	1911	A	N7-C8-N9	-6.24	110.68	113.80
80	B5	691	A	C2-N3-C4	-6.24	107.48	110.60
82	B8	53	A	C2-N3-C4	6.24	113.72	110.60
80	B5	1115	G	N3-C4-C5	-6.24	125.48	128.60
80	B5	1149	G	N1-C2-N3	-6.24	120.16	123.90
19	AK	76	LEU	CA-CB-CG	6.24	129.65	115.30
79	B2	189	C	C6-N1-C1'	-6.24	113.31	120.80
80	B5	83	U	C5-C4-O4	-6.24	122.16	125.90
80	B5	590	G	C5-C6-N1	6.24	114.62	111.50
80	B5	1134	G	C6-N1-C2	-6.24	121.36	125.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1425	U	N3-C4-O4	-6.24	115.03	119.40
80	B5	2289	U	N3-C4-O4	-6.24	115.03	119.40
79	B2	810	G	C6-C5-N7	-6.23	126.66	130.40
79	B2	1670	G	C8-N9-C1'	-6.23	118.90	127.00
52	BR	88	ARG	NE-CZ-NH1	-6.23	117.18	120.30
79	B2	1297	G	N7-C8-N9	-6.23	109.98	113.10
80	B5	1383	G	N1-C6-O6	-6.23	116.16	119.90
80	B5	1506	A	C5-N7-C8	-6.23	100.78	103.90
79	B2	1000	C	C5-C6-N1	-6.23	117.88	121.00
80	B5	2133	U	N3-C4-O4	-6.23	115.04	119.40
80	B5	2169	G	N1-C6-O6	-6.23	116.16	119.90
80	B5	586	C	N3-C4-C5	6.23	124.39	121.90
80	B5	734	C	N1-C2-O2	6.23	122.64	118.90
84	CW	64	A	C5-C6-N6	-6.23	118.72	123.70
79	B2	1258	U	C4-C5-C6	6.23	123.44	119.70
80	B5	436	A	C5-N7-C8	-6.23	100.79	103.90
80	B5	2117	A	C6-N1-C2	-6.23	114.86	118.60
79	B2	852	C	C5-C6-N1	6.22	124.11	121.00
79	B2	1747	G	C8-N9-C4	6.22	108.89	106.40
80	B5	511	G	N3-C2-N2	6.22	124.26	119.90
79	B2	1746	A	C8-N9-C4	6.22	108.29	105.80
80	B5	726	G	C5-N7-C8	-6.22	101.19	104.30
80	B5	753	C	C5-C4-N4	-6.22	115.84	120.20
80	B5	1119	C	C5-C4-N4	-6.22	115.84	120.20
80	B5	2777	G	N9-C4-C5	6.22	107.89	105.40
80	B5	2978	U	C2-N3-C4	-6.22	123.27	127.00
80	B5	87	U	N3-C4-O4	-6.22	115.05	119.40
80	B5	670	C	N3-C4-C5	6.22	124.39	121.90
80	B5	425	G	N7-C8-N9	-6.22	109.99	113.10
80	B5	787	G	C2-N3-C4	-6.22	108.79	111.90
80	B5	1272	C	O4'-C1'-N1	6.22	113.17	108.20
81	B7	44	C	N3-C4-C5	-6.22	119.41	121.90
80	B5	1688	U	N1-C2-O2	6.21	127.15	122.80
80	B5	437	G	N3-C2-N2	-6.21	115.55	119.90
80	B5	911	C	N1-C2-O2	-6.21	115.17	118.90
80	B5	2228	A	C8-N9-C4	-6.21	103.31	105.80
79	B2	1654	G	C8-N9-C4	-6.21	103.92	106.40
80	B5	35	A	C2-N3-C4	-6.21	107.50	110.60
79	B2	736	C	N1-C2-O2	6.21	122.62	118.90
80	B5	822	G	N3-C4-N9	-6.21	122.28	126.00
80	B5	891	G	C8-N9-C4	6.21	108.88	106.40
80	B5	326	U	N3-C4-C5	6.21	118.32	114.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2808	A	N1-C6-N6	6.21	122.32	118.60
79	B2	942	G	C8-N9-C4	-6.20	103.92	106.40
80	B5	408	A	N1-C2-N3	6.20	132.40	129.30
80	B5	514	G	N1-C6-O6	6.20	123.62	119.90
80	B5	2392	C	N3-C4-C5	6.20	124.38	121.90
80	B5	2396	G	C8-N9-C4	-6.20	103.92	106.40
80	B5	3330	A	C2-N3-C4	6.20	113.70	110.60
49	BO	117[A]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
49	BO	117[B]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
79	B2	704	C	C6-N1-C1'	-6.20	113.36	120.80
79	B2	767	U	N3-C4-O4	-6.20	115.06	119.40
79	B2	1305	U	N1-C2-N3	6.20	118.62	114.90
80	B5	314	U	C5-C4-O4	6.20	129.62	125.90
80	B5	1283	C	N3-C4-N4	6.20	122.34	118.00
79	B2	1560	U	N1-C2-N3	6.20	118.62	114.90
80	B5	674	G	C8-N9-C4	-6.20	103.92	106.40
80	B5	1381	A	C2-N3-C4	-6.20	107.50	110.60
80	B5	2716	U	C6-N1-C2	-6.20	117.28	121.00
80	B5	3065	G	C5-C6-O6	6.20	132.32	128.60
80	B5	3298	C	N1-C2-O2	-6.20	115.18	118.90
79	B2	1595	U	C5-C4-O4	-6.20	122.18	125.90
84	CW	49	C	N3-C4-N4	6.20	122.34	118.00
84	CW	74	C	O4'-C1'-N1	6.20	113.16	108.20
49	BO	3[B]	SER	C-N-CA	-6.20	106.21	121.70
79	B2	1766	A	C8-N9-C4	6.20	108.28	105.80
80	B5	150	A	C5-C6-N6	-6.20	118.74	123.70
80	B5	1115	G	C8-N9-C4	-6.20	103.92	106.40
80	B5	1844	C	C2-N3-C4	-6.20	116.80	119.90
80	B5	3101	G	N1-C6-O6	-6.20	116.18	119.90
80	B5	600	G	C6-C5-N7	-6.19	126.68	130.40
80	B5	1162	U	C2-N3-C4	-6.19	123.28	127.00
80	B5	823	C	N3-C4-C5	6.19	124.38	121.90
80	B5	1064	A	C8-N9-C4	6.19	108.28	105.80
65	Be	4	LEU	C-N-CD	6.19	141.40	128.40
79	B2	186	C	C5-C6-N1	6.19	124.10	121.00
79	B2	719	U	C5-C6-N1	6.19	125.80	122.70
80	B5	436	A	C8-N9-C1'	-6.19	116.56	127.70
80	B5	2846	U	N1-C2-O2	-6.19	118.47	122.80
80	B5	3228	C	N3-C2-O2	-6.19	117.57	121.90
80	B5	3330	A	C6-N1-C2	-6.19	114.89	118.60
80	B5	42	C	C2-N3-C4	6.19	122.99	119.90
80	B5	2830	G	C6-N1-C2	-6.19	121.39	125.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	CW	27	G	O4'-C1'-N9	6.19	113.15	108.20
80	B5	1411	C	N1-C2-O2	-6.19	115.19	118.90
80	B5	2858	U	N1-C2-N3	6.18	118.61	114.90
80	B5	1009	A	C8-N9-C4	-6.18	103.33	105.80
80	B5	1114	U	N3-C4-C5	6.18	118.31	114.60
80	B5	3365	U	N1-C2-N3	6.18	118.61	114.90
31	AW	65	LEU	CA-CB-CG	6.18	129.51	115.30
80	B5	1206	G	N3-C4-C5	-6.18	125.51	128.60
80	B5	2645	G	C6-N1-C2	-6.18	121.39	125.10
80	B5	1525	G	C4-N9-C1'	6.18	134.53	126.50
80	B5	2128	C	N3-C2-O2	-6.18	117.58	121.90
80	B5	2775	U	C5-C4-O4	6.18	129.61	125.90
80	B5	1143	A	C6-N1-C2	6.17	122.31	118.60
80	B5	1303	A	C2-N3-C4	6.17	113.69	110.60
80	B5	2928	C	C6-N1-C2	-6.17	117.83	120.30
79	B2	340	U	N3-C2-O2	-6.17	117.88	122.20
79	B2	1670	G	C4-N9-C1'	6.17	134.53	126.50
80	B5	924	G	N3-C2-N2	-6.17	115.58	119.90
80	B5	1301	A	C5-C6-N6	-6.17	118.76	123.70
79	B2	61	A	C8-N9-C4	-6.17	103.33	105.80
79	B2	1436	A	N9-C4-C5	-6.17	103.33	105.80
80	B5	351	A	C5-C6-N6	-6.17	118.76	123.70
80	B5	494	G	N3-C4-C5	-6.17	125.52	128.60
80	B5	2824	G	N3-C4-C5	-6.17	125.52	128.60
80	B5	3216	G	C6-N1-C2	-6.17	121.40	125.10
79	B2	1218	G	N1-C6-O6	6.17	123.60	119.90
80	B5	1430	U	C6-N1-C2	6.17	124.70	121.00
80	B5	2930	A	N9-C4-C5	6.17	108.27	105.80
80	B5	3358	U	N3-C2-O2	-6.17	117.88	122.20
79	B2	1633	A	N9-C4-C5	6.17	108.27	105.80
80	B5	370	U	N1-C2-N3	6.17	118.60	114.90
80	B5	1228	C	C6-N1-C1'	-6.17	113.40	120.80
79	B2	621	A	C8-N9-C4	6.17	108.27	105.80
80	B5	424	G	N1-C6-O6	-6.16	116.20	119.90
80	B5	1161	G	C2-N3-C4	6.16	114.98	111.90
80	B5	1346	G	N3-C4-C5	6.16	131.68	128.60
80	B5	2301	U	N3-C4-C5	6.16	118.30	114.60
80	B5	994	G	N3-C2-N2	6.16	124.21	119.90
80	B5	1148	G	C5-C6-N1	6.16	114.58	111.50
80	B5	2615	G	C5-C6-O6	-6.16	124.90	128.60
80	B5	2650	U	N3-C4-O4	-6.16	115.09	119.40
80	B5	2757	U	N1-C2-O2	-6.16	118.49	122.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2198	A	C2-N3-C4	-6.16	107.52	110.60
80	B5	3052	G	N7-C8-N9	-6.16	110.02	113.10
84	CW	43	C	N3-C4-N4	6.16	122.31	118.00
79	B2	1628	U	N3-C2-O2	-6.16	117.89	122.20
80	B5	1810	A	C8-N9-C4	6.16	108.26	105.80
79	B2	1781	A	C5-C6-N6	6.16	128.63	123.70
80	B5	880	G	C5-C6-N1	6.16	114.58	111.50
79	B2	1514	U	N3-C2-O2	-6.16	117.89	122.20
80	B5	311	C	N3-C4-C5	6.16	124.36	121.90
80	B5	1872	C	C4-C5-C6	6.16	120.48	117.40
80	B5	3068	U	N1-C2-N3	6.16	118.59	114.90
79	B2	538	A	N1-C2-N3	-6.15	126.22	129.30
79	B2	932	U	C5-C4-O4	6.15	129.59	125.90
80	B5	3245	A	N9-C4-C5	-6.15	103.34	105.80
80	B5	1007	U	C2-N3-C4	-6.15	123.31	127.00
80	B5	2242	A	C5-C6-N6	6.15	128.62	123.70
80	B5	2381	G	N1-C6-O6	-6.15	116.21	119.90
80	B5	2939	G	N7-C8-N9	-6.15	110.02	113.10
83	CV	385	VAL	C-N-CA	6.15	137.08	121.70
84	CW	53	G	O4'-C1'-N9	6.15	113.12	108.20
79	B2	192	U	N3-C2-O2	-6.15	117.89	122.20
80	B5	933	A	C6-N1-C2	-6.15	114.91	118.60
80	B5	2603	G	C5-N7-C8	-6.15	101.22	104.30
80	B5	3308	C	C5-C6-N1	-6.15	117.92	121.00
84	CW	70	G	P-O3'-C3'	6.15	127.08	119.70
80	B5	2399	A	C8-N9-C4	6.15	108.26	105.80
84	CW	58	A	C5-C6-N6	-6.15	118.78	123.70
80	B5	3098	G	N1-C6-O6	-6.15	116.21	119.90
80	B5	909	G	C5-N7-C8	6.14	107.37	104.30
80	B5	3345	G	N3-C2-N2	-6.14	115.60	119.90
80	B5	359	U	C5-C4-O4	-6.14	122.22	125.90
80	B5	1270	A	O4'-C1'-N9	6.14	113.11	108.20
80	B5	1226	G	P-O5'-C5'	-6.14	111.08	120.90
79	B2	1490	C	C2-N1-C1'	6.14	125.55	118.80
79	B2	1121	C	C5-C6-N1	-6.14	117.93	121.00
80	B5	125	C	N3-C4-N4	-6.14	113.70	118.00
80	B5	785	G	C2-N3-C4	6.14	114.97	111.90
80	B5	1262	G	C8-N9-C4	-6.14	103.94	106.40
80	B5	3014	U	C5-C4-O4	-6.14	122.22	125.90
80	B5	3266	G	C4-C5-N7	-6.14	108.35	110.80
84	CW	63	G	N1-C6-O6	6.14	123.58	119.90
79	B2	874	C	C5-C6-N1	6.13	124.07	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	102	C	N3-C4-N4	6.13	122.29	118.00
80	B5	2764	C	N3-C4-C5	6.13	124.35	121.90
80	B5	3150	A	C2-N3-C4	-6.13	107.53	110.60
80	B5	3334	U	N3-C2-O2	-6.13	117.91	122.20
79	B2	36	C	N3-C4-N4	6.13	122.29	118.00
82	B8	79	A	N9-C4-C5	-6.13	103.35	105.80
84	CW	73	A	C4-C5-C6	6.13	120.07	117.00
79	B2	734	A	N1-C6-N6	6.13	122.28	118.60
80	B5	386	A	C4-C5-N7	6.13	113.77	110.70
80	B5	722	G	N9-C4-C5	6.13	107.85	105.40
80	B5	1124	U	N3-C4-C5	6.13	118.28	114.60
80	B5	1591	G	C5-C6-N1	6.13	114.56	111.50
80	B5	2415	C	N3-C4-C5	6.13	124.35	121.90
79	B2	781	U	C2-N1-C1'	6.12	125.05	117.70
80	B5	949	C	C5-C6-N1	-6.12	117.94	121.00
80	B5	2347	U	N3-C4-C5	6.12	118.28	114.60
80	B5	2353	G	C6-C5-N7	-6.12	126.72	130.40
80	B5	1772	U	N3-C2-O2	-6.12	117.91	122.20
80	B5	1929	G	N9-C4-C5	-6.12	102.95	105.40
80	B5	3138	U	C5-C4-O4	-6.12	122.23	125.90
84	CW	9	A	C4-C5-C6	6.12	120.06	117.00
80	B5	2865	U	N1-C2-N3	-6.12	111.23	114.90
80	B5	294	U	C5-C4-O4	-6.12	122.23	125.90
80	B5	3175	U	C6-N1-C2	-6.12	117.33	121.00
80	B5	2207	A	C5-N7-C8	-6.12	100.84	103.90
80	B5	2646	C	N1-C2-O2	-6.12	115.23	118.90
80	B5	32	U	C6-N1-C2	-6.12	117.33	121.00
80	B5	1666	G	C5-C6-O6	6.12	132.27	128.60
80	B5	2620	G	N1-C6-O6	-6.12	116.23	119.90
79	B2	335	U	N1-C2-O2	-6.11	118.52	122.80
80	B5	1389	G	N3-C4-N9	6.11	129.67	126.00
80	B5	2353	G	N3-C4-N9	6.11	129.67	126.00
80	B5	2368	A	N1-C6-N6	-6.11	114.93	118.60
80	B5	2930	A	C8-N9-C1'	6.11	138.70	127.70
80	B5	2728	G	C6-N1-C2	-6.11	121.44	125.10
80	B5	976	U	N3-C2-O2	-6.11	117.92	122.20
80	B5	1232	C	N3-C4-N4	6.11	122.28	118.00
80	B5	2954	U	C5-C4-O4	-6.11	122.24	125.90
84	CW	7	A	C4-C5-C6	6.11	120.05	117.00
79	B2	1387	G	C5-C6-O6	-6.10	124.94	128.60
80	B5	3148	U	N3-C4-C5	6.10	118.26	114.60
50	BP	127	ARG	NE-CZ-NH1	6.10	123.35	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1168	U	N3-C4-O4	-6.10	115.13	119.40
80	B5	1233	G	O4'-C1'-N9	6.10	113.08	108.20
80	B5	2176	U	N1-C2-N3	6.10	118.56	114.90
82	B8	14	C	C2-N3-C4	-6.10	116.85	119.90
83	CV	400	ASP	N-CA-CB	6.10	121.58	110.60
80	B5	999	G	C2-N3-C4	6.10	114.95	111.90
79	B2	865	A	N1-C6-N6	-6.10	114.94	118.60
80	B5	927	C	N3-C4-C5	6.10	124.34	121.90
80	B5	1719	G	N1-C6-O6	6.10	123.56	119.90
80	B5	2865	U	C2-N1-C1'	6.10	125.02	117.70
80	B5	2920	U	N1-C2-N3	6.10	118.56	114.90
83	CV	385	VAL	N-CA-C	6.10	127.47	111.00
84	CW	67	C	C4'-C3'-C2'	6.10	108.70	102.60
80	B5	1119	C	N1-C2-O2	-6.10	115.24	118.90
80	B5	673	U	C2-N3-C4	-6.09	123.34	127.00
80	B5	1582	C	C6-N1-C2	-6.09	117.86	120.30
36	BB	205	VAL	CB-CA-C	-6.09	99.83	111.40
48	BN	96	ARG	NE-CZ-NH1	6.09	123.34	120.30
80	B5	1147	G	C6-C5-N7	6.09	134.05	130.40
80	B5	3382	U	N3-C2-O2	-6.09	117.94	122.20
79	B2	1596	C	C2-N1-C1'	6.09	125.50	118.80
80	B5	917	A	C8-N9-C4	-6.09	103.36	105.80
79	B2	627	C	C5-C4-N4	-6.09	115.94	120.20
80	B5	2386	A	C5-C6-N6	-6.09	118.83	123.70
80	B5	3086	A	C8-N9-C4	6.09	108.23	105.80
84	CW	6	G	C5-C6-N1	-6.09	108.46	111.50
80	B5	367	A	N3-C4-N9	-6.08	122.53	127.40
80	B5	1044	U	N3-C4-C5	6.08	118.25	114.60
79	B2	144	U	N1-C2-N3	6.08	118.55	114.90
80	B5	2361	A	C5-N7-C8	6.08	106.94	103.90
80	B5	2730	G	N3-C4-N9	-6.08	122.35	126.00
80	B5	3000	A	C8-N9-C4	6.08	108.23	105.80
80	B5	1161	G	C8-N9-C4	6.08	108.83	106.40
80	B5	2911	A	N1-C2-N3	-6.08	126.26	129.30
80	B5	1184	A	C2-N3-C4	-6.08	107.56	110.60
80	B5	3110	C	C2-N3-C4	-6.08	116.86	119.90
80	B5	595	G	N1-C6-O6	-6.08	116.25	119.90
80	B5	1136	A	N1-C2-N3	-6.08	126.26	129.30
80	B5	1518	U	N3-C2-O2	-6.08	117.95	122.20
80	B5	3182	G	C5-C6-O6	6.08	132.25	128.60
80	B5	2371	G	C8-N9-C4	6.08	108.83	106.40
80	B5	1042	U	N3-C2-O2	-6.07	117.95	122.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2134	G	C2-N3-C4	6.07	114.94	111.90
79	B2	1346	A	N7-C8-N9	6.07	116.83	113.80
80	B5	818	C	N3-C4-C5	-6.07	119.47	121.90
80	B5	3120	C	N3-C4-C5	-6.07	119.47	121.90
80	B5	3216	G	C4-C5-C6	6.07	122.44	118.80
80	B5	2844	C	N1-C2-O2	6.07	122.54	118.90
80	B5	33	G	C6-N1-C2	-6.07	121.46	125.10
80	B5	933	A	C2-N3-C4	-6.07	107.57	110.60
80	B5	2980	U	C6-N1-C2	-6.07	117.36	121.00
49	BO	117[A]	ARG	CG-CD-NE	-6.07	99.06	111.80
49	BO	117[B]	ARG	CG-CD-NE	-6.07	99.06	111.80
80	B5	1902	G	N7-C8-N9	-6.07	110.07	113.10
80	B5	2128	C	C2-N3-C4	-6.07	116.87	119.90
80	B5	2791	G	N1-C6-O6	6.07	123.54	119.90
79	B2	377	G	N3-C4-N9	-6.06	122.36	126.00
81	B7	40	C	C4-C5-C6	6.06	120.43	117.40
84	CW	31	A	C5-C6-N6	-6.06	118.85	123.70
80	B5	66	A	N9-C4-C5	-6.06	103.38	105.80
80	B5	216	G	C6-C5-N7	-6.06	126.76	130.40
84	CW	67	C	C1'-O4'-C4'	6.06	114.75	109.90
80	B5	1284	C	N3-C4-N4	6.06	122.24	118.00
80	B5	1285	G	O4'-C1'-N9	6.06	113.05	108.20
80	B5	3140	G	C5-N7-C8	-6.06	101.27	104.30
82	B8	42	G	N7-C8-N9	-6.06	110.07	113.10
80	B5	1897	G	C5-C6-N1	6.06	114.53	111.50
80	B5	935	U	C5-C4-O4	-6.05	122.27	125.90
80	B5	1323	G	C8-N9-C4	-6.05	103.98	106.40
80	B5	1340	G	N7-C8-N9	-6.05	110.07	113.10
80	B5	1438	U	C2-N1-C1'	6.05	124.96	117.70
80	B5	2749	G	N1-C2-N3	-6.05	120.27	123.90
80	B5	3272	C	C6-N1-C2	6.05	122.72	120.30
80	B5	3382	U	C6-N1-C1'	-6.05	112.72	121.20
84	CW	38	A	C5-C6-N1	-6.05	114.67	117.70
79	B2	1246	C	N3-C4-N4	-6.05	113.76	118.00
80	B5	1858	A	C4-C5-C6	6.05	120.03	117.00
80	B5	3020	U	C5-C4-O4	-6.05	122.27	125.90
83	CV	83	PHE	CB-CG-CD2	-6.05	116.56	120.80
84	CW	74	C	C3'-C2'-C1'	6.05	106.34	101.50
79	B2	1473	U	C5-C4-O4	6.05	129.53	125.90
82	B8	15	G	C5-C6-N1	6.05	114.52	111.50
79	B2	557	G	C6-C5-N7	-6.05	126.77	130.40
80	B5	80	G	N1-C6-O6	-6.05	116.27	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1909	A	N1-C2-N3	-6.05	126.28	129.30
80	B5	3075	G	C4-C5-N7	-6.05	108.38	110.80
84	CW	58	A	C4-C5-C6	6.05	120.02	117.00
80	B5	655	C	C6-N1-C2	-6.04	117.88	120.30
80	B5	1371	G	C6-N1-C2	-6.04	121.47	125.10
83	CV	18	LYS	N-CA-C	-6.04	94.69	111.00
80	B5	1271	A	C4-C5-C6	6.04	120.02	117.00
80	B5	1278	A	C4-C5-C6	6.04	120.02	117.00
80	B5	386	A	N9-C4-C5	-6.04	103.38	105.80
80	B5	920	A	N7-C8-N9	-6.04	110.78	113.80
80	B5	1869	C	C2-N3-C4	-6.04	116.88	119.90
80	B5	2939	G	C5-N7-C8	6.04	107.32	104.30
80	B5	2346	C	N1-C2-O2	-6.04	115.28	118.90
80	B5	2359	C	C5-C6-N1	-6.04	117.98	121.00
79	B2	75	U	C2-N1-C1'	6.04	124.94	117.70
80	B5	341	G	N1-C6-O6	6.04	123.52	119.90
80	B5	641	C	C5-C4-N4	6.04	124.42	120.20
80	B5	2116	G	C6-C5-N7	-6.04	126.78	130.40
83	CV	396	ALA	N-CA-C	6.04	127.30	111.00
79	B2	1000	C	C5-C4-N4	6.03	124.42	120.20
80	B5	2632	G	N9-C4-C5	6.03	107.81	105.40
80	B5	2911	A	C8-N9-C4	-6.03	103.39	105.80
79	B2	1099	U	C5-C6-N1	6.03	125.72	122.70
80	B5	1110	U	N3-C4-O4	-6.03	115.18	119.40
80	B5	1117	G	C5-C6-O6	-6.03	124.98	128.60
80	B5	1368	U	C6-N1-C2	6.03	124.62	121.00
80	B5	2358	A	C8-N9-C4	6.03	108.21	105.80
80	B5	3318	G	N1-C6-O6	-6.03	116.28	119.90
79	B2	349	U	C4-C5-C6	6.03	123.32	119.70
80	B5	1047	A	C5-C6-N1	6.03	120.72	117.70
80	B5	1165	A	C8-N9-C4	6.03	108.21	105.80
80	B5	2364	G	N3-C4-C5	-6.03	125.58	128.60
80	B5	1910	A	C5-C6-N1	6.03	120.71	117.70
80	B5	2952	G	C6-N1-C2	-6.03	121.48	125.10
36	BB	232	ARG	NE-CZ-NH2	-6.02	117.29	120.30
79	B2	266	A	N1-C6-N6	6.02	122.22	118.60
79	B2	1450	U	C5-C4-O4	6.02	129.51	125.90
80	B5	282	G	N9-C4-C5	6.02	107.81	105.40
80	B5	3309	G	C5-C6-N1	6.02	114.51	111.50
79	B2	308	C	C2-N3-C4	-6.02	116.89	119.90
80	B5	2318	U	N3-C4-O4	-6.02	115.18	119.40
80	B5	2730	G	C5-N7-C8	-6.02	101.29	104.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2830	G	N3-C2-N2	-6.02	115.68	119.90
43	BI	7	ARG	NE-CZ-NH1	-6.02	117.29	120.30
79	B2	404	G	N9-C4-C5	-6.02	102.99	105.40
79	B2	1192	C	N3-C2-O2	6.02	126.11	121.90
79	B2	1749	A	C8-N9-C4	6.02	108.21	105.80
84	CW	51	U	P-O5'-C5'	6.02	130.53	120.90
48	BN	172	ARG	NE-CZ-NH2	6.02	123.31	120.30
79	B2	397	A	N1-C6-N6	-6.02	114.99	118.60
79	B2	538	A	C4-C5-C6	-6.02	113.99	117.00
80	B5	555	U	N3-C4-O4	6.02	123.61	119.40
80	B5	594	U	C5-C6-N1	6.02	125.71	122.70
80	B5	1652	G	C8-N9-C4	6.02	108.81	106.40
80	B5	2395	G	C4-C5-N7	-6.02	108.39	110.80
80	B5	2993	G	N3-C4-N9	6.02	129.61	126.00
80	B5	3222	U	N3-C2-O2	-6.02	117.99	122.20
79	B2	1057	U	C2-N1-C1'	6.01	124.92	117.70
79	B2	1119	G	C5-C6-O6	6.01	132.21	128.60
80	B5	1808	G	N1-C6-O6	6.01	123.51	119.90
80	B5	1227	C	P-O5'-C5'	-6.01	111.28	120.90
80	B5	2167	A	N9-C4-C5	6.01	108.20	105.80
84	CW	4	C	C6-N1-C2	-6.01	117.89	120.30
38	BD	248	ARG	NE-CZ-NH1	6.01	123.31	120.30
79	B2	781	U	N1-C2-O2	6.01	127.01	122.80
80	B5	822	G	N3-C2-N2	-6.01	115.69	119.90
80	B5	795	G	C2-N3-C4	6.01	114.91	111.90
80	B5	1000	C	C6-N1-C2	-6.01	117.90	120.30
80	B5	2837	A	N7-C8-N9	-6.01	110.80	113.80
80	B5	2917	G	N1-C6-O6	6.01	123.50	119.90
80	B5	3343	G	N1-C2-N2	-6.01	110.79	116.20
84	CW	68	C	C6-N1-C1'	-6.01	113.59	120.80
79	B2	1796	C	C4-C5-C6	6.01	120.40	117.40
80	B5	517	G	N1-C2-N3	6.00	127.50	123.90
80	B5	1190	A	N1-C6-N6	-6.00	115.00	118.60
80	B5	2108	C	N3-C4-N4	-6.00	113.80	118.00
80	B5	2421	U	N1-C2-N3	6.00	118.50	114.90
80	B5	3211	C	C4-C5-C6	6.00	120.40	117.40
79	B2	274	G	C4-N9-C1'	6.00	134.30	126.50
79	B2	445	A	C2-N3-C4	6.00	113.60	110.60
79	B2	1643	U	C5-C6-N1	-6.00	119.70	122.70
80	B5	811	U	C4-C5-C6	6.00	123.30	119.70
80	B5	1739	U	C5-C4-O4	6.00	129.50	125.90
49	BO	13[B]	ASP	C-N-CA	6.00	136.69	121.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	106	U	C6-N1-C2	-6.00	117.40	121.00
79	B2	377	G	N1-C6-O6	6.00	123.50	119.90
80	B5	994	G	C8-N9-C4	6.00	108.80	106.40
43	BI	83	ASP	CB-CG-OD1	-6.00	112.90	118.30
79	B2	557	G	N3-C4-N9	6.00	129.60	126.00
80	B5	679	U	C5-C4-O4	6.00	129.50	125.90
80	B5	968	G	C4-C5-N7	6.00	113.20	110.80
80	B5	1192	C	C2-N3-C4	-6.00	116.90	119.90
80	B5	2887	A	C6-N1-C2	6.00	122.20	118.60
84	CW	2	C	O4'-C1'-N1	6.00	113.00	108.20
80	B5	516	A	N1-C6-N6	6.00	122.20	118.60
80	B5	1469	C	C4-C5-C6	6.00	120.40	117.40
80	B5	3187	A	N7-C8-N9	-6.00	110.80	113.80
79	B2	151	G	N1-C6-O6	-5.99	116.30	119.90
84	CW	41	C	O4'-C1'-N1	5.99	113.00	108.20
80	B5	351	A	N1-C6-N6	5.99	122.19	118.60
80	B5	813	G	N9-C4-C5	5.99	107.80	105.40
80	B5	1301	A	N9-C4-C5	-5.99	103.40	105.80
80	B5	1438	U	N3-C2-O2	-5.99	118.01	122.20
80	B5	2617	U	N3-C4-C5	5.99	118.19	114.60
80	B5	3095	U	N3-C4-C5	5.99	118.19	114.60
80	B5	2526	C	N1-C2-O2	5.99	122.50	118.90
80	B5	341	G	N1-C2-N2	5.99	121.59	116.20
80	B5	1378	U	C6-N1-C2	5.99	124.59	121.00
80	B5	1548	C	N1-C2-O2	-5.99	115.31	118.90
80	B5	3192	U	C2-N3-C4	-5.99	123.41	127.00
80	B5	2381	G	C5-C6-O6	5.99	132.19	128.60
80	B5	1882	G	N9-C4-C5	5.98	107.79	105.40
43	BI	57	LEU	CA-CB-CG	5.98	129.06	115.30
79	B2	1521	G	N3-C4-N9	5.98	129.59	126.00
79	B2	1745	G	C6-N1-C2	-5.98	121.51	125.10
80	B5	3343	G	N3-C2-N2	5.98	124.09	119.90
79	B2	1188	G	C5-C6-O6	-5.98	125.01	128.60
37	BC	84	ARG	NE-CZ-NH2	-5.98	117.31	120.30
80	B5	283	G	N1-C6-O6	5.98	123.49	119.90
80	B5	2166	A	N1-C6-N6	5.98	122.19	118.60
81	B7	96	U	C2-N1-C1'	5.98	124.87	117.70
80	B5	392	G	C5-C6-O6	-5.98	125.01	128.60
80	B5	416	A	N9-C4-C5	5.98	108.19	105.80
80	B5	847	A	N7-C8-N9	-5.98	110.81	113.80
80	B5	912	G	N3-C4-N9	5.98	129.59	126.00
80	B5	3055	U	N1-C2-O2	5.98	126.98	122.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	B8	47	C	N1-C2-O2	5.98	122.49	118.90
79	B2	1121	C	N3-C4-C5	-5.98	119.51	121.90
79	B2	1600	A	C5-N7-C8	-5.98	100.91	103.90
79	B2	831	U	C6-N1-C2	-5.97	117.42	121.00
80	B5	701	G	C4-C5-N7	-5.97	108.41	110.80
80	B5	3298	C	C4-C5-C6	5.97	120.39	117.40
79	B2	1417	A	N1-C6-N6	5.97	122.18	118.60
80	B5	1305	U	N3-C4-O4	5.97	123.58	119.40
80	B5	1307	G	P-O3'-C3'	5.97	126.87	119.70
80	B5	2113	A	C8-N9-C4	5.97	108.19	105.80
80	B5	2130	G	N1-C2-N2	-5.97	110.83	116.20
80	B5	3112	G	N1-C6-O6	5.97	123.48	119.90
80	B5	226	C	C5-C4-N4	-5.97	116.02	120.20
80	B5	3003	G	C4-C5-C6	-5.97	115.22	118.80
80	B5	971	G	N1-C2-N3	-5.97	120.32	123.90
80	B5	3028	G	N3-C4-N9	5.97	129.58	126.00
80	B5	3341	U	C5-C6-N1	5.97	125.69	122.70
47	BM	135	LEU	CA-CB-CG	5.97	129.03	115.30
73	Bm	97	ARG	NE-CZ-NH2	-5.97	117.32	120.30
80	B5	2365	C	C5-C6-N1	-5.97	118.02	121.00
79	B2	542	A	C6-C5-N7	-5.97	128.12	132.30
79	B2	1455	G	N9-C4-C5	5.97	107.79	105.40
80	B5	359	U	C6-N1-C2	5.97	124.58	121.00
80	B5	619	A	N1-C6-N6	-5.97	115.02	118.60
80	B5	965	A	N3-C4-C5	-5.97	122.62	126.80
80	B5	1206	G	C4-C5-N7	-5.97	108.41	110.80
80	B5	1725	C	C5-C4-N4	5.97	124.38	120.20
80	B5	2833	A	C5-C6-N1	5.97	120.68	117.70
82	B8	63	G	N1-C6-O6	-5.97	116.32	119.90
80	B5	2915	U	N3-C2-O2	-5.96	118.03	122.20
84	CW	18	G	P-O5'-C5'	-5.96	111.36	120.90
79	B2	1753	A	C8-N9-C4	5.96	108.18	105.80
80	B5	2405	C	N3-C2-O2	-5.96	117.73	121.90
70	Bj	21	ARG	NE-CZ-NH2	-5.96	117.32	120.30
79	B2	719	U	N1-C2-O2	5.96	126.97	122.80
80	B5	667	C	C2-N1-C1'	-5.96	112.25	118.80
80	B5	884	A	C4-C5-C6	-5.96	114.02	117.00
80	B5	1280	C	N3-C4-N4	5.96	122.17	118.00
80	B5	2250	G	N1-C6-O6	-5.96	116.32	119.90
80	B5	2349	U	C4-C5-C6	-5.96	116.13	119.70
79	B2	360	A	N1-C6-N6	5.96	122.17	118.60
80	B5	2908	G	C5-C6-N1	-5.95	108.52	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1907	C	C5-C6-N1	5.95	123.98	121.00
82	B8	100	U	C5-C4-O4	-5.95	122.33	125.90
79	B2	416	A	C8-N9-C4	5.95	108.18	105.80
80	B5	83	U	C2-N1-C1'	5.95	124.84	117.70
80	B5	903	U	C5-C6-N1	-5.95	119.72	122.70
80	B5	987	U	N3-C2-O2	-5.95	118.03	122.20
80	B5	2792	A	C8-N9-C4	-5.95	103.42	105.80
79	B2	13	C	N3-C4-C5	5.95	124.28	121.90
79	B2	628	G	C5-C6-O6	5.95	132.17	128.60
79	B2	1387	G	C4-C5-N7	5.95	113.18	110.80
79	B2	1768	G	C4-N9-C1'	-5.95	118.77	126.50
80	B5	546	C	N3-C2-O2	-5.95	117.74	121.90
80	B5	2724	U	C5-C4-O4	5.95	129.47	125.90
80	B5	3240	C	N3-C4-N4	-5.95	113.84	118.00
80	B5	386	A	C5-C6-N6	-5.95	118.94	123.70
79	B2	382	C	C2-N3-C4	-5.95	116.93	119.90
80	B5	520	U	N1-C2-N3	5.95	118.47	114.90
80	B5	873	C	P-O3'-C3'	5.95	126.83	119.70
80	B5	1171	G	N7-C8-N9	5.95	116.07	113.10
80	B5	1753	G	C2-N3-C4	5.95	114.87	111.90
80	B5	2370	G	C5-C6-N1	5.95	114.47	111.50
80	B5	2753	G	N7-C8-N9	5.95	116.07	113.10
80	B5	2976	A	N7-C8-N9	-5.95	110.83	113.80
80	B5	3088	G	C5-N7-C8	-5.95	101.33	104.30
80	B5	3369	G	C6-N1-C2	-5.95	121.53	125.10
84	CW	37	A	O4'-C1'-N9	5.95	112.96	108.20
80	B5	2184	U	N3-C2-O2	-5.94	118.04	122.20
79	B2	1000	C	N3-C2-O2	-5.94	117.74	121.90
79	B2	1097	U	C2-N1-C1'	5.94	124.83	117.70
79	B2	1582	U	C6-N1-C2	5.94	124.57	121.00
80	B5	1678	G	C5-C6-N1	5.94	114.47	111.50
80	B5	2426	U	N3-C4-O4	-5.94	115.24	119.40
80	B5	2584	G	C4-C5-N7	5.94	113.18	110.80
80	B5	2617	U	C6-N1-C2	5.94	124.57	121.00
82	B8	12	A	N7-C8-N9	5.94	116.77	113.80
82	B8	24	G	N3-C2-N2	5.94	124.06	119.90
47	BM	106	ARG	NE-CZ-NH2	-5.94	117.33	120.30
80	B5	1122	U	N3-C2-O2	-5.94	118.04	122.20
80	B5	1311	G	N1-C2-N3	-5.94	120.34	123.90
80	B5	2167	A	N1-C6-N6	-5.94	115.03	118.60
80	B5	2409	G	N7-C8-N9	5.94	116.07	113.10
79	B2	192	U	N1-C2-O2	5.94	126.96	122.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	883	A	N7-C8-N9	-5.94	110.83	113.80
80	B5	974	G	C8-N9-C1'	-5.94	119.28	127.00
80	B5	1181	U	C6-N1-C2	5.94	124.56	121.00
80	B5	2114	C	N1-C2-N3	5.94	123.36	119.20
80	B5	2730	G	N3-C4-C5	5.94	131.57	128.60
79	B2	794	U	C2-N1-C1'	5.94	124.82	117.70
80	B5	39	A	N3-C4-N9	5.94	132.15	127.40
84	CW	37	A	C5-C6-N6	-5.93	118.95	123.70
33	AY	44	LEU	CA-CB-CG	5.93	128.94	115.30
80	B5	365	A	C5-C6-N6	-5.93	118.95	123.70
80	B5	749	C	N3-C4-C5	-5.93	119.53	121.90
80	B5	1035	G	C4-N9-C1'	5.93	134.21	126.50
51	BQ	99	THR	N-CA-C	5.93	127.01	111.00
80	B5	509	U	N1-C2-N3	5.93	118.46	114.90
80	B5	1495	U	N3-C4-C5	-5.93	111.04	114.60
40	BF	191	VAL	C-N-CA	-5.93	109.85	122.30
79	B2	393	C	N3-C4-C5	5.93	124.27	121.90
80	B5	708	G	C8-N9-C4	-5.93	104.03	106.40
80	B5	1128	U	C5-C6-N1	-5.93	119.73	122.70
80	B5	2943	G	N1-C2-N2	-5.93	110.86	116.20
80	B5	216	G	C5-C6-O6	-5.93	125.04	128.60
80	B5	337	G	N1-C6-O6	-5.93	116.34	119.90
80	B5	2411	U	N3-C4-C5	5.93	118.16	114.60
79	B2	1479	A	N1-C6-N6	5.93	122.16	118.60
79	B2	1542	G	C5-C6-O6	5.93	132.16	128.60
80	B5	2329	C	N3-C4-N4	-5.93	113.85	118.00
80	B5	2552	C	C5-C4-N4	5.93	124.35	120.20
36	BB	114	VAL	CB-CA-C	-5.92	100.14	111.40
79	B2	1314	U	N3-C2-O2	-5.92	118.05	122.20
80	B5	201	A	C2-N3-C4	-5.92	107.64	110.60
80	B5	283	G	C4-C5-N7	5.92	113.17	110.80
80	B5	2421	U	N1-C2-O2	-5.92	118.65	122.80
80	B5	2687	G	C5-C6-N1	5.92	114.46	111.50
79	B2	1157	A	C8-N9-C4	-5.92	103.43	105.80
79	B2	1274	C	C4-C5-C6	5.92	120.36	117.40
80	B5	994	G	C6-N1-C2	-5.92	121.55	125.10
79	B2	389	G	N3-C4-C5	-5.92	125.64	128.60
80	B5	874	U	N3-C4-O4	-5.92	115.26	119.40
80	B5	2323	G	N1-C6-O6	-5.92	116.35	119.90
80	B5	2643	A	N1-C2-N3	-5.92	126.34	129.30
80	B5	1227	C	C5-C4-N4	-5.92	116.06	120.20
80	B5	1231	A	C5-C6-N1	-5.92	114.74	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	3296	A	C8-N9-C4	5.92	108.17	105.80
81	B7	25	G	C5-C6-O6	-5.92	125.05	128.60
80	B5	1699	A	N1-C6-N6	5.92	122.15	118.60
79	B2	703	G	C8-N9-C4	-5.91	104.03	106.40
80	B5	3351	U	N3-C2-O2	-5.91	118.06	122.20
80	B5	590	G	C5-C6-O6	-5.91	125.05	128.60
80	B5	1772	U	C5-C4-O4	5.91	129.45	125.90
80	B5	2424	A	C5-C6-N6	-5.91	118.97	123.70
80	B5	2917	G	N3-C4-C5	-5.91	125.64	128.60
80	B5	3269	U	N3-C2-O2	-5.91	118.06	122.20
80	B5	2416	U	N3-C2-O2	-5.91	118.06	122.20
80	B5	2607	G	N1-C6-O6	-5.91	116.36	119.90
79	B2	554	C	N1-C2-O2	5.91	122.44	118.90
79	B2	1537	C	C5-C6-N1	5.91	123.95	121.00
80	B5	1043	C	C5-C6-N1	-5.91	118.05	121.00
80	B5	2347	U	C2-N3-C4	-5.91	123.46	127.00
80	B5	892	U	C2-N3-C4	-5.90	123.46	127.00
80	B5	1808	G	C8-N9-C4	5.90	108.76	106.40
80	B5	3075	G	C4-C5-C6	5.90	122.34	118.80
81	B7	92	A	N9-C4-C5	-5.90	103.44	105.80
85	CX	3	G	N1-C6-O6	5.90	123.44	119.90
80	B5	153	U	C5-C4-O4	5.90	129.44	125.90
80	B5	3075	G	C5-C6-N1	-5.90	108.55	111.50
79	B2	829	A	C8-N9-C4	-5.90	103.44	105.80
79	B2	1776	A	N9-C4-C5	5.90	108.16	105.80
80	B5	2148	U	N3-C2-O2	5.90	126.33	122.20
80	B5	2639	G	C6-C5-N7	-5.90	126.86	130.40
80	B5	3019	U	N3-C4-C5	5.90	118.14	114.60
82	B8	99	C	N3-C4-C5	5.90	124.26	121.90
80	B5	1178	G	C5-N7-C8	-5.89	101.35	104.30
80	B5	2931	C	C2-N3-C4	-5.89	116.95	119.90
80	B5	3013	U	N3-C2-O2	-5.89	118.07	122.20
82	B8	55	U	N3-C4-C5	-5.89	111.06	114.60
56	BV	33	ASN	CB-CA-C	-5.89	98.61	110.40
80	B5	345	G	C6-N1-C2	-5.89	121.56	125.10
80	B5	1834	U	C6-N1-C2	5.89	124.53	121.00
80	B5	3277	U	C6-N1-C2	-5.89	117.47	121.00
80	B5	3395	G	N3-C4-C5	5.89	131.55	128.60
81	B7	12	U	C5-C4-O4	-5.89	122.36	125.90
80	B5	2410	U	N3-C4-O4	-5.89	115.28	119.40
79	B2	1241	G	C8-N9-C4	-5.89	104.04	106.40
80	B5	419	G	C8-N9-C4	5.89	108.76	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2910	A	N1-C6-N6	-5.89	115.07	118.60
80	B5	2851	A	N7-C8-N9	-5.89	110.86	113.80
80	B5	680	G	N3-C2-N2	5.89	124.02	119.90
80	B5	1127	G	C5-C6-N1	5.89	114.44	111.50
80	B5	2744	U	C5-C6-N1	-5.89	119.76	122.70
79	B2	279	G	C8-N9-C4	-5.88	104.05	106.40
79	B2	344	A	N1-C6-N6	-5.88	115.07	118.60
79	B2	1601	G	C5-C6-N1	5.88	114.44	111.50
80	B5	1279	C	N3-C4-N4	5.88	122.12	118.00
80	B5	2792	A	C2-N3-C4	5.88	113.54	110.60
80	B5	1866	C	N3-C2-O2	5.88	126.02	121.90
79	B2	1027	A	C8-N9-C4	-5.88	103.45	105.80
80	B5	1226	G	N3-C4-C5	5.88	131.54	128.60
80	B5	1477	A	N1-C2-N3	5.88	132.24	129.30
80	B5	2893	C	C4-C5-C6	5.88	120.34	117.40
80	B5	1086	C	N1-C2-O2	5.88	122.43	118.90
80	B5	741	U	C2-N3-C4	5.88	130.53	127.00
80	B5	2965	U	N1-C2-O2	-5.88	118.69	122.80
80	B5	2988	C	N1-C2-N3	5.88	123.31	119.20
79	B2	1503	A	C5-N7-C8	-5.88	100.96	103.90
80	B5	416	A	C8-N9-C4	-5.88	103.45	105.80
80	B5	2366	C	C6-N1-C1'	-5.88	113.75	120.80
80	B5	2531	C	C6-N1-C1'	-5.88	113.75	120.80
80	B5	365	A	N1-C6-N6	5.87	122.12	118.60
80	B5	795	G	N1-C2-N3	-5.87	120.38	123.90
80	B5	3113	A	C5-C6-N1	5.87	120.64	117.70
79	B2	810	G	N1-C6-O6	5.87	123.42	119.90
80	B5	1369	A	N1-C6-N6	5.87	122.12	118.60
80	B5	2118	C	N1-C2-O2	5.87	122.42	118.90
80	B5	2849	C	C6-N1-C2	-5.87	117.95	120.30
80	B5	2992	U	N3-C2-O2	-5.87	118.09	122.20
79	B2	1291	G	N3-C2-N2	-5.87	115.79	119.90
80	B5	2961	G	N7-C8-N9	5.87	116.03	113.10
80	B5	426	G	N7-C8-N9	-5.87	110.17	113.10
80	B5	2770	G	C2-N3-C4	5.87	114.83	111.90
84	CW	23	A	C4-C5-C6	5.87	119.93	117.00
46	BL	46	ILE	CG1-CB-CG2	-5.87	98.49	111.40
80	B5	874	U	C5-C6-N1	-5.87	119.77	122.70
80	B5	1838	G	N7-C8-N9	-5.87	110.17	113.10
80	B5	2758	A	N3-C4-C5	-5.87	122.69	126.80
79	B2	169	A	C8-N9-C4	5.87	108.15	105.80
80	B5	795	G	C5-N7-C8	5.87	107.23	104.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	542	A	C4-C5-N7	5.86	113.63	110.70
80	B5	593	C	C2-N1-C1'	5.86	125.25	118.80
80	B5	2320	A	N1-C6-N6	-5.86	115.08	118.60
80	B5	2711	C	C4-C5-C6	5.86	120.33	117.40
80	B5	2745	G	C5-C6-O6	-5.86	125.08	128.60
80	B5	3064	U	N3-C2-O2	-5.86	118.10	122.20
84	CW	43	C	C5'-C4'-O4'	5.86	116.13	109.10
80	B5	1181	U	C2-N3-C4	-5.86	123.48	127.00
80	B5	1512	U	C5-C6-N1	-5.86	119.77	122.70
80	B5	3340	G	N1-C6-O6	-5.86	116.38	119.90
81	B7	5	G	C8-N9-C4	5.86	108.74	106.40
84	CW	18	G	C8-N9-C4	-5.86	104.06	106.40
80	B5	1116	G	C5-C6-O6	5.86	132.12	128.60
80	B5	2192	C	C4-C5-C6	5.86	120.33	117.40
79	B2	1536	G	C4-N9-C1'	5.86	134.11	126.50
80	B5	1175	C	N3-C4-C5	5.86	124.24	121.90
80	B5	1251	A	N9-C1'-C2'	-5.86	105.56	112.00
80	B5	1481	A	N3-C4-C5	-5.86	122.70	126.80
80	B5	2843	U	C2-N1-C1'	5.86	124.73	117.70
79	B2	1745	G	C6-C5-N7	-5.86	126.89	130.40
80	B5	908	G	C8-N9-C1'	-5.86	119.39	127.00
80	B5	1189	C	C6-N1-C2	5.86	122.64	120.30
80	B5	1278	A	C5-C6-N6	-5.86	119.02	123.70
80	B5	1317	A	N3-C4-N9	5.86	132.09	127.40
80	B5	1456	A	C8-N9-C4	5.86	108.14	105.80
79	B2	997	G	N9-C4-C5	-5.85	103.06	105.40
80	B5	1889	G	N3-C4-C5	-5.85	125.67	128.60
80	B5	2305	G	N1-C2-N2	-5.85	110.93	116.20
80	B5	3212	C	C5-C6-N1	-5.85	118.07	121.00
82	B8	33	A	C8-N9-C4	5.85	108.14	105.80
84	CW	18	G	N3-C2-N2	5.85	124.00	119.90
80	B5	2799	A	C2-N3-C4	-5.85	107.67	110.60
80	B5	3226	A	N1-C2-N3	-5.85	126.37	129.30
80	B5	3373	U	C5-C6-N1	-5.85	119.77	122.70
84	CW	62	C	O4'-C1'-N1	5.85	112.88	108.20
80	B5	432	G	C4-C5-N7	5.85	113.14	110.80
80	B5	2314	U	C6-N1-C1'	-5.85	113.01	121.20
82	B8	16	G	N1-C2-N3	5.85	127.41	123.90
84	CW	5	G	O4'-C1'-N9	5.85	112.88	108.20
79	B2	628	G	N1-C2-N2	-5.85	110.94	116.20
80	B5	376	G	N1-C6-O6	-5.85	116.39	119.90
80	B5	966	U	C2-N1-C1'	5.85	124.72	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1485	G	N3-C4-C5	-5.85	125.68	128.60
80	B5	3267	A	N1-C2-N3	5.85	132.22	129.30
80	B5	3326	G	N1-C6-O6	-5.85	116.39	119.90
80	B5	587	U	C5-C6-N1	-5.85	119.78	122.70
80	B5	2549	G	C4-N9-C1'	5.85	134.10	126.50
80	B5	3218	A	N7-C8-N9	5.85	116.72	113.80
80	B5	1158	A	C4-C5-N7	5.84	113.62	110.70
80	B5	2518	C	C2-N3-C4	-5.84	116.98	119.90
80	B5	3241	G	C4-C5-N7	5.84	113.14	110.80
79	B2	1798	U	C2-N1-C1'	5.84	124.71	117.70
80	B5	1437	C	C2-N1-C1'	5.84	125.23	118.80
80	B5	1586	G	N3-C4-C5	-5.84	125.68	128.60
80	B5	1892	G	N3-C2-N2	-5.84	115.81	119.90
80	B5	2706	G	C2-N3-C4	5.84	114.82	111.90
80	B5	182	U	C5-C6-N1	5.84	125.62	122.70
80	B5	591	G	N3-C4-N9	5.84	129.50	126.00
80	B5	1193	A	C2-N3-C4	-5.84	107.68	110.60
80	B5	1322	U	N3-C4-C5	5.84	118.11	114.60
80	B5	1323	G	N9-C4-C5	5.84	107.74	105.40
80	B5	2410	U	N3-C4-C5	5.84	118.11	114.60
80	B5	2835	U	N1-C2-N3	5.84	118.40	114.90
80	B5	25	U	N1-C2-O2	-5.84	118.71	122.80
80	B5	1136	A	C2-N3-C4	5.84	113.52	110.60
80	B5	1239	C	N3-C4-C5	-5.84	119.56	121.90
80	B5	2692	A	C5-C6-N6	5.84	128.37	123.70
79	B2	1633	A	N3-C4-C5	-5.84	122.71	126.80
79	B2	1370	U	N3-C2-O2	-5.84	118.11	122.20
79	B2	1666	U	C6-N1-C2	-5.84	117.50	121.00
80	B5	289	A	C5-C6-N1	5.84	120.62	117.70
80	B5	1225	A	C5-C6-N6	-5.83	119.03	123.70
80	B5	2381	G	C2-N3-C4	5.83	114.82	111.90
80	B5	2920	U	N1-C2-O2	-5.83	118.72	122.80
80	B5	3224	G	N1-C6-O6	-5.83	116.40	119.90
80	B5	1429	G	C2-N3-C4	-5.83	108.98	111.90
80	B5	3333	G	N9-C4-C5	-5.83	103.07	105.40
79	B2	294	C	C6-N1-C2	5.83	122.63	120.30
80	B5	432	G	C2-N3-C4	-5.83	108.98	111.90
80	B5	801	A	C6-N1-C2	5.83	122.10	118.60
80	B5	815	G	N9-C4-C5	5.83	107.73	105.40
80	B5	993	G	C8-N9-C4	-5.83	104.07	106.40
80	B5	2188	A	N7-C8-N9	-5.83	110.88	113.80
80	B5	894	G	N3-C4-N9	5.83	129.50	126.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2510	U	C2-N1-C1'	-5.83	110.70	117.70
80	B5	159	A	C8-N9-C4	5.83	108.13	105.80
80	B5	971	G	N9-C4-C5	5.83	107.73	105.40
80	B5	1939	G	N1-C2-N2	-5.83	110.95	116.20
80	B5	2248	C	C5-C6-N1	-5.83	118.09	121.00
80	B5	3095	U	C2-N3-C4	-5.83	123.50	127.00
80	B5	3388	C	N3-C2-O2	-5.83	117.82	121.90
80	B5	1846	C	N3-C2-O2	-5.83	117.82	121.90
79	B2	1416	G	C8-N9-C4	-5.83	104.07	106.40
80	B5	1369	A	N9-C4-C5	-5.83	103.47	105.80
80	B5	1902	G	C5-C6-N1	5.83	114.41	111.50
79	B2	1129	U	N3-C4-O4	-5.82	115.32	119.40
80	B5	2271	A	N1-C6-N6	-5.82	115.11	118.60
80	B5	3216	G	N1-C2-N3	5.82	127.39	123.90
80	B5	96	G	N1-C2-N3	5.82	127.39	123.90
80	B5	1512	U	C4-C5-C6	5.82	123.19	119.70
80	B5	2335	G	N9-C4-C5	5.82	107.73	105.40
83	CV	386	SER	N-CA-C	-5.82	95.29	111.00
80	B5	2292	U	C2-N3-C4	-5.82	123.51	127.00
46	BL	76	THR	N-CA-CB	5.81	121.34	110.30
79	B2	1614	A	C4-C5-C6	5.81	119.91	117.00
80	B5	518	G	C8-N9-C4	5.81	108.72	106.40
80	B5	1280	C	N3-C4-C5	-5.81	119.58	121.90
80	B5	2145	A	C5-C6-N1	5.81	120.61	117.70
79	B2	21	U	N3-C2-O2	-5.81	118.13	122.20
80	B5	706	A	C5-C6-N6	-5.81	119.05	123.70
80	B5	2346	C	C5-C4-N4	-5.81	116.13	120.20
80	B5	2426	U	N3-C2-O2	-5.81	118.13	122.20
80	B5	3112	G	C5-C6-O6	-5.81	125.11	128.60
80	B5	35	A	C8-N9-C4	5.81	108.12	105.80
80	B5	689	U	N3-C4-O4	-5.81	115.33	119.40
80	B5	968	G	C8-N9-C4	5.81	108.72	106.40
80	B5	1639	C	C6-N1-C2	-5.81	117.98	120.30
80	B5	2709	C	N3-C4-C5	5.81	124.22	121.90
80	B5	2838	A	C6-N1-C2	-5.81	115.11	118.60
80	B5	3141	A	C4-C5-C6	5.81	119.91	117.00
80	B5	1495	U	C2-N1-C1'	5.81	124.67	117.70
80	B5	3152	U	C6-N1-C2	5.81	124.48	121.00
81	B7	8	G	C8-N9-C4	-5.81	104.08	106.40
82	B8	104	A	N1-C6-N6	5.81	122.08	118.60
79	B2	581	U	C6-N1-C1'	-5.81	113.07	121.20
80	B5	1607	U	P-O3'-C3'	5.81	126.67	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	142	G	N1-C6-O6	5.80	123.38	119.90
79	B2	611	U	N1-C2-O2	-5.80	118.74	122.80
79	B2	1324	G	C8-N9-C1'	5.80	134.55	127.00
79	B2	1340	U	C5-C4-O4	5.80	129.38	125.90
80	B5	2306	C	C2-N1-C1'	5.80	125.19	118.80
80	B5	3076	C	N3-C2-O2	-5.80	117.84	121.90
80	B5	3215	A	C8-N9-C4	5.80	108.12	105.80
79	B2	460	A	N1-C6-N6	-5.80	115.12	118.60
80	B5	666	A	C2-N3-C4	-5.80	107.70	110.60
80	B5	1669	C	C6-N1-C2	5.80	122.62	120.30
80	B5	1607	U	C2-N3-C4	-5.80	123.52	127.00
80	B5	2207	A	N7-C8-N9	5.80	116.70	113.80
80	B5	2804	A	C8-N9-C4	5.80	108.12	105.80
80	B5	2827	U	N3-C2-O2	-5.80	118.14	122.20
80	B5	3100	U	N1-C2-O2	5.80	126.86	122.80
80	B5	3301	U	C6-N1-C2	5.80	124.48	121.00
79	B2	1274	C	C5-C4-N4	5.80	124.26	120.20
80	B5	1159	A	C6-N1-C2	5.80	122.08	118.60
80	B5	1438	U	C6-N1-C2	-5.80	117.52	121.00
82	B8	31	G	N7-C8-N9	-5.80	110.20	113.10
84	CW	46	G	O4'-C1'-N9	5.80	112.84	108.20
80	B5	1206	G	C2-N3-C4	5.79	114.80	111.90
36	BB	19	ARG	NE-CZ-NH2	-5.79	117.40	120.30
80	B5	1133	A	N1-C2-N3	-5.79	126.40	129.30
80	B5	224	C	N3-C2-O2	-5.79	117.85	121.90
80	B5	920	A	C8-N9-C4	5.79	108.12	105.80
80	B5	1129	A	C2-N3-C4	5.79	113.50	110.60
80	B5	1888	U	N1-C2-N3	5.79	118.38	114.90
80	B5	2370	G	N1-C2-N3	5.79	127.38	123.90
80	B5	2665	U	C2-N3-C4	5.79	130.47	127.00
53	BS	155	ARG	CG-CD-NE	5.79	123.96	111.80
79	B2	1602	C	C6-N1-C2	5.79	122.62	120.30
80	B5	979	U	N1-C2-O2	5.79	126.85	122.80
80	B5	1044	U	C2-N3-C4	-5.79	123.53	127.00
80	B5	1126	G	C2-N3-C4	-5.79	109.00	111.90
80	B5	1128	U	N1-C2-N3	5.79	118.37	114.90
80	B5	590	G	C5-N7-C8	-5.79	101.41	104.30
80	B5	1159	A	N3-C4-C5	5.79	130.85	126.80
80	B5	2147	A	C5-C6-N6	-5.79	119.07	123.70
80	B5	666	A	C8-N9-C4	5.79	108.11	105.80
79	B2	92	A	N1-C6-N6	-5.78	115.13	118.60
79	B2	339	C	N1-C2-O2	-5.78	115.43	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1856	C	C6-N1-C2	-5.78	117.99	120.30
80	B5	2906	C	N3-C4-C5	-5.78	119.59	121.90
81	B7	106	U	C5-C6-N1	-5.78	119.81	122.70
79	B2	934	C	C6-N1-C1'	-5.78	113.86	120.80
80	B5	2736	A	C5-C6-N6	5.78	128.32	123.70
80	B5	2978	U	N1-C2-N3	5.78	118.37	114.90
72	B1	45	ARG	NE-CZ-NH2	-5.78	117.41	120.30
80	B5	861	C	N1-C2-O2	-5.78	115.43	118.90
80	B5	1127	G	N9-C4-C5	-5.78	103.09	105.40
80	B5	2141	U	N3-C2-O2	-5.78	118.15	122.20
80	B5	2747	A	N9-C4-C5	5.78	108.11	105.80
80	B5	3130	A	C6-N1-C2	-5.78	115.13	118.60
80	B5	201	A	C5-C6-N1	-5.78	114.81	117.70
80	B5	1113	G	N7-C8-N9	-5.78	110.21	113.10
80	B5	1494	U	N3-C2-O2	5.78	126.25	122.20
80	B5	2361	A	N3-C4-N9	5.78	132.02	127.40
80	B5	2846	U	C5-C6-N1	-5.78	119.81	122.70
43	BI	21	ARG	NE-CZ-NH1	5.78	123.19	120.30
80	B5	1045	C	N1-C2-N3	5.78	123.25	119.20
80	B5	1210	U	N3-C4-O4	-5.78	115.36	119.40
49	BO	197[B]	PHE	O-C-N	5.78	133.02	123.20
80	B5	272	G	C2-N3-C4	-5.78	109.01	111.90
80	B5	524	U	N1-C2-O2	-5.78	118.76	122.80
80	B5	798	G	C5-C6-N1	5.78	114.39	111.50
80	B5	1490	A	C2-N3-C4	-5.78	107.71	110.60
80	B5	2129	U	N3-C4-C5	5.78	118.06	114.60
80	B5	2335	G	N1-C6-O6	-5.78	116.44	119.90
80	B5	2641	U	N1-C2-O2	-5.78	118.76	122.80
80	B5	3000	A	C5-C6-N6	-5.78	119.08	123.70
80	B5	3285	C	C2-N1-C1'	5.78	125.15	118.80
80	B5	1911	A	C2-N3-C4	-5.77	107.71	110.60
80	B5	2320	A	N3-C4-N9	-5.77	122.78	127.40
80	B5	3339	A	C5-C6-N6	-5.77	119.08	123.70
79	B2	1198	G	N7-C8-N9	5.77	115.99	113.10
79	B2	1291	G	N3-C4-N9	-5.77	122.54	126.00
80	B5	2971	A	C2-N3-C4	5.77	113.49	110.60
80	B5	1238	C	N3-C4-N4	5.77	122.04	118.00
80	B5	916	G	N3-C4-N9	-5.77	122.54	126.00
80	B5	1553	U	N3-C2-O2	5.77	126.24	122.20
80	B5	3088	G	N7-C8-N9	5.77	115.98	113.10
80	B5	526	C	C5-C4-N4	-5.77	116.16	120.20
80	B5	3212	C	N1-C2-O2	-5.76	115.44	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	332	C	C5-C6-N1	-5.76	118.12	121.00
80	B5	3197	G	N3-C4-N9	-5.76	122.54	126.00
80	B5	180	C	C6-N1-C2	-5.76	118.00	120.30
80	B5	798	G	C5-C6-O6	-5.76	125.14	128.60
80	B5	2329	C	C5-C4-N4	5.76	124.23	120.20
80	B5	2342	U	N3-C2-O2	-5.76	118.17	122.20
80	B5	2412	G	N9-C4-C5	5.76	107.70	105.40
84	CW	9	A	C5-C6-N1	-5.76	114.82	117.70
79	B2	971	A	C5-C6-N1	-5.76	114.82	117.70
80	B5	404	G	N3-C2-N2	-5.76	115.87	119.90
80	B5	911	C	C2-N3-C4	-5.76	117.02	119.90
80	B5	2516	U	C5-C4-O4	-5.76	122.44	125.90
80	B5	2920	U	C4-C5-C6	5.76	123.16	119.70
82	B8	17	A	C5-C6-N6	-5.76	119.09	123.70
80	B5	2692	A	C5-N7-C8	5.76	106.78	103.90
79	B2	864	U	N1-C2-N3	5.76	118.35	114.90
80	B5	1116	G	C4-C5-C6	5.76	122.25	118.80
80	B5	2817	A	C2-N3-C4	5.76	113.48	110.60
80	B5	2832	C	C6-N1-C2	5.76	122.60	120.30
80	B5	3375	A	N1-C2-N3	-5.76	126.42	129.30
84	CW	68	C	O4'-C1'-N1	5.76	112.81	108.20
80	B5	2338	C	N3-C4-C5	-5.75	119.60	121.90
80	B5	3099	C	C4-C5-C6	5.75	120.28	117.40
36	BB	266	ARG	NE-CZ-NH1	5.75	123.17	120.30
79	B2	377	G	N1-C2-N2	5.75	121.38	116.20
79	B2	1282	U	N1-C2-N3	5.75	118.35	114.90
80	B5	2305	G	C6-C5-N7	-5.75	126.95	130.40
80	B5	2733	A	C2-N3-C4	-5.75	107.72	110.60
80	B5	3131	U	C5-C4-O4	-5.75	122.45	125.90
84	CW	14	A	C5'-C4'-C3'	-5.75	106.80	116.00
80	B5	523	A	C5-C6-N6	5.75	128.30	123.70
80	B5	2142	A	N3-C4-N9	5.75	132.00	127.40
36	BB	21	ARG	NE-CZ-NH2	-5.75	117.43	120.30
79	B2	639	U	N3-C4-O4	-5.75	115.38	119.40
79	B2	1169	G	N3-C4-C5	-5.75	125.73	128.60
80	B5	2327	U	N3-C4-C5	5.75	118.05	114.60
80	B5	2337	C	C2-N3-C4	-5.75	117.03	119.90
80	B5	2899	C	C5-C6-N1	-5.75	118.13	121.00
80	B5	824	C	N3-C4-C5	-5.75	119.60	121.90
80	B5	1159	A	C5-N7-C8	-5.75	101.03	103.90
80	B5	88	A	C5-C6-N1	-5.74	114.83	117.70
80	B5	382	U	N1-C2-N3	5.74	118.35	114.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	427	C	C2-N3-C4	-5.74	117.03	119.90
80	B5	591	G	C8-N9-C4	5.74	108.70	106.40
82	B8	106	C	N3-C4-C5	5.74	124.20	121.90
80	B5	359	U	C5-C6-N1	-5.74	119.83	122.70
80	B5	760	G	C5-C6-O6	-5.74	125.16	128.60
80	B5	580	C	N3-C4-C5	-5.74	119.60	121.90
80	B5	2926	A	C2-N3-C4	5.74	113.47	110.60
79	B2	144	U	N1-C2-O2	5.74	126.82	122.80
80	B5	1035	G	C8-N9-C1'	-5.74	119.54	127.00
80	B5	2422	C	N3-C2-O2	-5.74	117.88	121.90
80	B5	2866	U	C2-N3-C4	-5.74	123.56	127.00
34	AZ	95	HIS	N-CA-C	5.74	126.49	111.00
79	B2	811	A	C8-N9-C4	-5.74	103.51	105.80
80	B5	326	U	C4-C5-C6	-5.74	116.26	119.70
80	B5	1208	U	N1-C2-N3	5.74	118.34	114.90
80	B5	1254	C	N3-C4-C5	-5.74	119.61	121.90
80	B5	1917	C	C2-N3-C4	-5.74	117.03	119.90
80	B5	2361	A	C5-C6-N1	5.74	120.57	117.70
80	B5	672	A	N1-C6-N6	5.73	122.04	118.60
80	B5	1116	G	N3-C4-C5	-5.73	125.73	128.60
80	B5	1652	G	C4-C5-N7	-5.73	108.51	110.80
80	B5	3006	A	N9-C4-C5	5.73	108.09	105.80
80	B5	3241	G	C5-C6-O6	-5.73	125.16	128.60
80	B5	1045	C	N1-C2-O2	-5.73	115.46	118.90
80	B5	2123	G	C5-C6-N1	5.73	114.36	111.50
80	B5	2619	G	C5-C6-N1	5.73	114.36	111.50
79	B2	1131	A	N7-C8-N9	-5.73	110.94	113.80
79	B2	1776	A	N1-C6-N6	-5.73	115.16	118.60
80	B5	665	A	N9-C4-C5	-5.73	103.51	105.80
80	B5	1443	G	C5-C6-N1	-5.73	108.64	111.50
80	B5	1883	A	C8-N9-C4	-5.73	103.51	105.80
80	B5	363	G	N9-C4-C5	5.73	107.69	105.40
80	B5	1849	C	N3-C2-O2	-5.73	117.89	121.90
80	B5	1904	C	N1-C2-O2	5.73	122.34	118.90
80	B5	2549	G	N1-C6-O6	5.73	123.33	119.90
80	B5	1060	U	C2-N3-C4	-5.72	123.56	127.00
80	B5	1297	C	C5-C4-N4	-5.72	116.19	120.20
83	CV	325	GLY	N-CA-C	-5.72	98.79	113.10
84	CW	53	G	N9-C1'-C2'	-5.72	105.70	112.00
79	B2	494	U	N3-C2-O2	-5.72	118.19	122.20
79	B2	732	G	C4-C5-N7	5.72	113.09	110.80
79	B2	1112	G	C6-N1-C2	-5.72	121.67	125.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1159	A	N9-C4-C5	-5.72	103.51	105.80
80	B5	2976	A	C8-N9-C4	5.72	108.09	105.80
80	B5	1931	U	C6-N1-C1'	5.72	129.21	121.20
80	B5	2892	A	N1-C6-N6	-5.72	115.17	118.60
51	BQ	50	LYS	CD-CE-NZ	5.72	124.85	111.70
79	B2	1489	U	N3-C2-O2	-5.72	118.20	122.20
80	B5	2197	C	C2-N1-C1'	-5.72	112.51	118.80
80	B5	2836	C	C5-C4-N4	5.72	124.20	120.20
80	B5	3047	U	C2-N3-C4	-5.72	123.57	127.00
80	B5	706	A	N1-C2-N3	-5.71	126.44	129.30
81	B7	46	A	N9-C4-C5	5.71	108.09	105.80
80	B5	1724	U	C2-N1-C1'	5.71	124.56	117.70
80	B5	3200	G	N3-C2-N2	-5.71	115.90	119.90
79	B2	527	A	C8-N9-C4	-5.71	103.52	105.80
80	B5	270	U	N3-C2-O2	-5.71	118.20	122.20
80	B5	880	G	C2-N3-C4	5.71	114.76	111.90
82	B8	26	U	C2-N1-C1'	5.71	124.55	117.70
83	CV	57	LYS	N-CA-C	-5.71	95.58	111.00
80	B5	2730	G	N3-C2-N2	-5.71	115.90	119.90
84	CW	75	C	N3-C4-C5	-5.71	119.62	121.90
80	B5	925	A	N1-C6-N6	5.71	122.03	118.60
80	B5	1268	G	N7-C8-N9	5.71	115.95	113.10
80	B5	2630	C	N1-C2-O2	-5.71	115.47	118.90
80	B5	2774	C	N1-C2-O2	-5.71	115.47	118.90
80	B5	2988	C	N3-C4-C5	-5.71	119.62	121.90
49	BO	163[B]	ARG	NE-CZ-NH2	-5.71	117.45	120.30
80	B5	2108	C	N3-C4-C5	5.71	124.18	121.90
80	B5	2188	A	N1-C2-N3	5.71	132.15	129.30
80	B5	1251	A	C4-C5-C6	5.71	119.85	117.00
79	B2	612	U	N3-C4-O4	-5.70	115.41	119.40
80	B5	2717	U	C2-N3-C4	-5.70	123.58	127.00
80	B5	2951	G	C5-C6-N1	5.70	114.35	111.50
80	B5	1143	A	C5-N7-C8	-5.70	101.05	103.90
80	B5	1282	G	N3-C2-N2	5.70	123.89	119.90
80	B5	2979	U	N3-C2-O2	5.70	126.19	122.20
79	B2	92	A	N3-C4-C5	-5.70	122.81	126.80
79	B2	831	U	C2-N1-C1'	5.70	124.54	117.70
79	B2	1324	G	N9-C4-C5	5.70	107.68	105.40
80	B5	411	U	N1-C2-N3	5.70	118.32	114.90
80	B5	2237	C	N3-C2-O2	-5.70	117.91	121.90
80	B5	2846	U	C2-N3-C4	-5.70	123.58	127.00
84	CW	68	C	P-O3'-C3'	-5.70	112.86	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	92	A	C6-N1-C2	-5.70	115.18	118.60
80	B5	1445	U	C2-N3-C4	-5.70	123.58	127.00
80	B5	1448	U	C4-C5-C6	5.70	123.12	119.70
80	B5	1524	A	N1-C2-N3	5.70	132.15	129.30
82	B8	7	U	C5-C6-N1	-5.70	119.85	122.70
84	CW	68	C	C6-N1-C2	-5.70	118.02	120.30
42	BH	151	VAL	CB-CA-C	-5.70	100.58	111.40
51	BQ	127	LEU	CA-CB-CG	5.70	128.40	115.30
80	B5	79	U	C5-C4-O4	-5.70	122.48	125.90
80	B5	355	A	N1-C6-N6	5.70	122.02	118.60
80	B5	637	C	C5-C6-N1	-5.70	118.15	121.00
80	B5	958	C	N3-C4-C5	5.70	124.18	121.90
83	CV	83	PHE	CB-CG-CD1	5.70	124.79	120.80
79	B2	1339	C	C6-N1-C2	-5.69	118.02	120.30
80	B5	563	U	N3-C2-O2	-5.69	118.21	122.20
80	B5	3020	U	N3-C2-O2	5.69	126.19	122.20
81	B7	38	U	C2-N1-C1'	5.69	124.53	117.70
79	B2	158	U	N3-C2-O2	-5.69	118.22	122.20
79	B2	1749	A	C4-C5-N7	5.69	113.55	110.70
80	B5	953	G	N3-C4-N9	-5.69	122.58	126.00
79	B2	355	G	N3-C4-C5	-5.69	125.75	128.60
79	B2	570	A	N3-C4-C5	-5.69	122.82	126.80
79	B2	741	C	N1-C2-O2	-5.69	115.49	118.90
79	B2	1781	A	C5-C6-N1	-5.69	114.85	117.70
80	B5	276	U	C4-C5-C6	5.69	123.11	119.70
80	B5	948	C	N3-C4-N4	5.69	121.98	118.00
80	B5	2363	A	N7-C8-N9	5.69	116.64	113.80
80	B5	3259	U	C5-C6-N1	5.69	125.55	122.70
82	B8	95	G	C4-N9-C1'	-5.69	119.10	126.50
80	B5	1840	U	N1-C2-O2	5.69	126.78	122.80
80	B5	2552	C	N3-C4-N4	-5.69	114.02	118.00
50	BP	24	VAL	CB-CA-C	-5.69	100.59	111.40
79	B2	1644	C	N1-C2-O2	-5.69	115.49	118.90
80	B5	2748	A	C5-C6-N6	-5.69	119.15	123.70
79	B2	507	U	C6-N1-C2	-5.69	117.59	121.00
79	B2	1361	U	N3-C2-O2	-5.69	118.22	122.20
80	B5	884	A	N1-C6-N6	-5.69	115.19	118.60
49	BO	23[B]	ILE	C-N-CA	-5.68	107.49	121.70
80	B5	1940	G	C8-N9-C4	5.68	108.67	106.40
80	B5	3102	G	C5-C6-O6	5.68	132.01	128.60
81	B7	103	A	C5-C6-N6	-5.68	119.15	123.70
80	B5	670	C	C2-N3-C4	-5.68	117.06	119.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	769	G	N7-C8-N9	-5.68	110.26	113.10
79	B2	1052	U	N3-C2-O2	-5.68	118.22	122.20
80	B5	334	A	C2-N3-C4	5.68	113.44	110.60
80	B5	1163	A	C4-C5-N7	-5.68	107.86	110.70
80	B5	1512	U	C2-N3-C4	-5.68	123.59	127.00
80	B5	65	A	P-O3'-C3'	5.68	126.51	119.70
80	B5	413	U	N1-C2-N3	5.68	118.31	114.90
80	B5	613	G	N1-C6-O6	-5.68	116.49	119.90
80	B5	1466	G	N3-C4-N9	-5.68	122.59	126.00
81	B7	47	C	C2-N3-C4	-5.68	117.06	119.90
80	B5	1371	G	N7-C8-N9	-5.67	110.26	113.10
80	B5	1726	C	C5-C6-N1	-5.67	118.16	121.00
80	B5	1832	C	C5-C4-N4	-5.67	116.23	120.20
80	B5	1845	G	N7-C8-N9	-5.67	110.26	113.10
80	B5	3290	G	N7-C8-N9	5.67	115.94	113.10
80	B5	3316	A	N1-C6-N6	5.67	122.00	118.60
82	B8	28	C	C4-C5-C6	-5.67	114.56	117.40
83	CV	255	TYR	N-CA-C	-5.67	95.68	111.00
80	B5	1458	U	N3-C4-C5	5.67	118.00	114.60
37	BC	136	LEU	CA-CB-CG	5.67	128.35	115.30
79	B2	539	G	C5-N7-C8	-5.67	101.46	104.30
80	B5	2320	A	N9-C4-C5	5.67	108.07	105.80
80	B5	2400	G	N1-C6-O6	5.67	123.30	119.90
85	CX	1	A	O4'-C4'-C3'	-5.67	98.33	104.00
82	B8	109	A	C8-N9-C4	-5.67	103.53	105.80
84	CW	26	A	C4-C5-C6	5.67	119.83	117.00
79	B2	498	G	N3-C4-C5	-5.67	125.77	128.60
79	B2	1354	G	N3-C4-C5	-5.67	125.77	128.60
80	B5	2744	U	C5-C4-O4	5.67	129.30	125.90
80	B5	842	G	N1-C6-O6	5.67	123.30	119.90
79	B2	323	A	N9-C4-C5	5.67	108.07	105.80
79	B2	1119	G	N9-C4-C5	5.67	107.67	105.40
79	B2	1761	U	N3-C4-C5	-5.67	111.20	114.60
80	B5	3010	U	N3-C4-O4	-5.67	115.44	119.40
80	B5	3298	C	C2-N3-C4	-5.66	117.07	119.90
84	CW	13	C	N3-C4-C5	-5.66	119.64	121.90
84	CW	14	A	P-O3'-C3'	-5.66	112.91	119.70
80	B5	636	C	C2-N3-C4	-5.66	117.07	119.90
80	B5	2392	C	C5-C6-N1	-5.66	118.17	121.00
79	B2	627	C	N1-C2-O2	-5.66	115.50	118.90
80	B5	825	U	N3-C4-O4	-5.66	115.44	119.40
80	B5	1525	G	C8-N9-C1'	-5.66	119.64	127.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1942	U	N1-C2-N3	5.66	118.30	114.90
81	B7	80	G	N3-C4-N9	5.66	129.40	126.00
82	B8	20	U	C5-C6-N1	-5.66	119.87	122.70
79	B2	1421	A	C8-N9-C4	5.66	108.06	105.80
80	B5	248	U	C2-N1-C1'	5.66	124.49	117.70
80	B5	1254	C	O5'-C5'-C4'	-5.66	100.95	111.70
80	B5	1307	G	N1-C6-O6	-5.66	116.50	119.90
80	B5	1364	C	C5-C6-N1	-5.66	118.17	121.00
80	B5	1371	G	C5-N7-C8	5.66	107.13	104.30
80	B5	1942	U	N3-C4-O4	5.66	123.36	119.40
79	B2	1458	G	C4-N9-C1'	5.66	133.85	126.50
80	B5	1485	G	C4-C5-N7	-5.66	108.54	110.80
83	CV	93	LEU	C-N-CA	5.66	135.84	121.70
79	B2	1075	C	N3-C2-O2	5.66	125.86	121.90
79	B2	1782	A	C4-C5-N7	-5.66	107.87	110.70
80	B5	53	G	N3-C2-N2	5.66	123.86	119.90
80	B5	905	U	N3-C4-O4	5.66	123.36	119.40
80	B5	3006	A	C8-N9-C4	-5.66	103.54	105.80
80	B5	1321	G	N1-C6-O6	5.65	123.29	119.90
80	B5	2148	U	C5-C4-O4	-5.65	122.51	125.90
80	B5	2616	C	N3-C4-C5	5.65	124.16	121.90
61	Ba	46	ASP	N-CA-C	-5.65	95.74	111.00
80	B5	1163	A	C5-C6-N1	5.65	120.53	117.70
80	B5	1331	U	C5-C4-O4	-5.65	122.51	125.90
80	B5	2293	C	N1-C2-O2	5.65	122.29	118.90
80	B5	2848	G	C4-C5-C6	5.65	122.19	118.80
80	B5	2955	U	N1-C2-N3	5.65	118.29	114.90
80	B5	998	A	N1-C2-N3	5.65	132.12	129.30
80	B5	1272	C	P-O5'-C5'	-5.65	111.86	120.90
80	B5	1415	U	C5-C6-N1	-5.65	119.88	122.70
80	B5	2293	C	C2-N1-C1'	5.65	125.02	118.80
81	B7	25	G	N1-C2-N2	5.65	121.28	116.20
82	B8	95	G	C8-N9-C1'	5.65	134.34	127.00
80	B5	1210	U	N1-C2-O2	5.65	126.75	122.80
81	B7	101	G	N9-C4-C5	-5.65	103.14	105.40
82	B8	113	U	C6-N1-C1'	-5.65	113.30	121.20
83	CV	478	LYS	CA-C-N	5.65	132.91	117.10
84	CW	14	A	C5-C6-N6	-5.65	119.18	123.70
79	B2	712	G	C8-N9-C4	-5.65	104.14	106.40
80	B5	217	U	C2-N3-C4	-5.65	123.61	127.00
80	B5	1183	C	N3-C4-C5	5.64	124.16	121.90
80	B5	2654	C	C2-N3-C4	-5.64	117.08	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	3313	U	N3-C4-O4	-5.64	115.45	119.40
82	B8	34	U	C5-C6-N1	-5.64	119.88	122.70
80	B5	2865	U	N1-C2-O2	5.64	126.75	122.80
80	B5	3123	A	N9-C4-C5	-5.64	103.54	105.80
80	B5	3197	G	N3-C2-N2	-5.64	115.95	119.90
80	B5	3200	G	C5-C6-O6	-5.64	125.22	128.60
80	B5	106	A	C8-N9-C4	5.64	108.06	105.80
80	B5	1244	A	O4'-C1'-N9	5.64	112.71	108.20
80	B5	2217	U	N3-C2-O2	-5.64	118.25	122.20
80	B5	2979	U	C5-C6-N1	-5.64	119.88	122.70
43	BI	139	ARG	NE-CZ-NH1	5.64	123.12	120.30
80	B5	1797	A	C4-C5-N7	-5.64	107.88	110.70
80	B5	2658	G	N7-C8-N9	-5.64	110.28	113.10
82	B8	100	U	C2-N1-C1'	5.64	124.47	117.70
80	B5	634	C	C2-N3-C4	-5.64	117.08	119.90
80	B5	950	G	N9-C4-C5	-5.64	103.14	105.40
80	B5	1909	A	C4-C5-C6	-5.64	114.18	117.00
80	B5	2116	G	C4-C5-C6	5.64	122.18	118.80
80	B5	2706	G	N3-C4-C5	-5.64	125.78	128.60
79	B2	1052	U	N1-C2-O2	5.64	126.75	122.80
79	B2	1445	G	N1-C6-O6	5.64	123.28	119.90
80	B5	114	A	N1-C6-N6	5.64	121.98	118.60
80	B5	3365	U	C6-N1-C2	-5.64	117.62	121.00
79	B2	966	A	N9-C4-C5	-5.63	103.55	105.80
80	B5	2830	G	N1-C6-O6	-5.63	116.52	119.90
80	B5	2870	C	C5-C4-N4	5.63	124.14	120.20
84	CW	67	C	O4'-C4'-C3'	-5.63	98.37	104.00
80	B5	1146	C	C2-N3-C4	-5.63	117.08	119.90
80	B5	1300	G	C6-C5-N7	-5.63	127.02	130.40
80	B5	2180	G	N3-C2-N2	5.63	123.84	119.90
80	B5	3336	A	C4-C5-C6	5.63	119.82	117.00
80	B5	347	G	C8-N9-C4	5.63	108.65	106.40
80	B5	2277	C	N1-C2-O2	5.63	122.28	118.90
80	B5	3350	C	C6-N1-C2	-5.63	118.05	120.30
39	BE	31	ARG	NE-CZ-NH2	-5.63	117.49	120.30
80	B5	946	U	N1-C2-O2	5.63	126.74	122.80
80	B5	1405	U	C2-N3-C4	-5.63	123.62	127.00
80	B5	1429	G	C6-C5-N7	-5.63	127.02	130.40
80	B5	1914	G	N1-C6-O6	-5.63	116.52	119.90
80	B5	2415	C	C6-N1-C2	5.63	122.55	120.30
80	B5	2719	U	N1-C2-O2	-5.63	118.86	122.80
40	BF	229	PHE	CB-CG-CD1	5.63	124.74	120.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	402	C	C2-N1-C1'	-5.63	112.61	118.80
79	B2	613	G	N1-C6-O6	-5.63	116.52	119.90
80	B5	335	G	N1-C6-O6	-5.63	116.52	119.90
80	B5	1773	C	C5-C6-N1	-5.63	118.19	121.00
80	B5	2828	G	N1-C6-O6	-5.63	116.52	119.90
81	B7	38	U	N3-C4-C5	5.63	117.98	114.60
79	B2	334	G	N3-C4-C5	5.62	131.41	128.60
79	B2	1642	G	N3-C4-C5	-5.62	125.79	128.60
80	B5	966	U	N3-C4-C5	5.62	117.97	114.60
80	B5	1226	G	N9-C1'-C2'	-5.62	105.81	112.00
80	B5	1843	C	C5-C6-N1	5.62	123.81	121.00
80	B5	2816	G	C4-N9-C1'	-5.62	119.19	126.50
81	B7	5	G	C5-C6-N1	-5.62	108.69	111.50
82	B8	15	G	C5-C6-O6	-5.62	125.23	128.60
80	B5	216	G	C4-C5-N7	5.62	113.05	110.80
80	B5	658	G	N1-C6-O6	5.62	123.27	119.90
80	B5	1434	G	C1'-O4'-C4'	-5.62	105.40	109.90
80	B5	1589	A	C5-C6-N1	5.62	120.51	117.70
80	B5	1744	G	C5-C6-N1	5.62	114.31	111.50
80	B5	1926	C	N1-C2-O2	-5.62	115.53	118.90
80	B5	3054	U	N3-C4-C5	-5.62	111.23	114.60
79	B2	852	C	C4-C5-C6	-5.62	114.59	117.40
79	B2	1277	G	N3-C4-N9	-5.62	122.63	126.00
80	B5	42	C	N1-C2-O2	5.62	122.27	118.90
80	B5	582	G	N1-C6-O6	-5.62	116.53	119.90
80	B5	911	C	C5-C6-N1	-5.62	118.19	121.00
80	B5	2249	G	C8-N9-C4	-5.62	104.15	106.40
80	B5	3140	G	C6-C5-N7	-5.62	127.03	130.40
80	B5	3285	C	N1-C2-O2	5.62	122.27	118.90
79	B2	951	A	C8-N9-C4	5.62	108.05	105.80
80	B5	1314	C	N3-C4-C5	5.62	124.15	121.90
79	B2	1153	G	N1-C6-O6	-5.62	116.53	119.90
80	B5	1510	G	N1-C2-N3	5.62	127.27	123.90
80	B5	145	G	N9-C4-C5	5.62	107.65	105.40
80	B5	1365	G	N1-C2-N3	5.62	127.27	123.90
80	B5	2341	A	C5-N7-C8	5.62	106.71	103.90
80	B5	3059	G	C8-N9-C4	5.62	108.65	106.40
80	B5	280	U	N3-C4-C5	5.61	117.97	114.60
80	B5	666	A	N7-C8-N9	-5.61	110.99	113.80
80	B5	935	U	C2-N3-C4	-5.61	123.63	127.00
80	B5	1207	G	N1-C6-O6	-5.61	116.53	119.90
80	B5	1380	G	C8-N9-C4	5.61	108.64	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1441	G	C5-C6-N1	5.61	114.31	111.50
80	B5	2326	A	C2-N3-C4	5.61	113.41	110.60
82	B8	12	A	C4-C5-C6	-5.61	114.19	117.00
79	B2	1600	A	C4-C5-N7	5.61	113.50	110.70
80	B5	282	G	C2'-C3'-O3'	5.61	122.68	113.70
80	B5	1603	A	N9-C4-C5	5.61	108.05	105.80
80	B5	1847	A	C2-N3-C4	-5.61	107.80	110.60
80	B5	2330	C	C4-C5-C6	5.61	120.21	117.40
80	B5	3350	C	C5-C6-N1	5.61	123.81	121.00
80	B5	2683	U	C2-N1-C1'	5.61	124.43	117.70
84	CW	40	C	P-O3'-C3'	-5.61	112.97	119.70
79	B2	1650	U	C5-C6-N1	-5.61	119.90	122.70
80	B5	625	G	C8-N9-C4	-5.61	104.16	106.40
80	B5	1206	G	C5-C6-O6	5.61	131.96	128.60
79	B2	74	U	C3'-C2'-C1'	-5.60	97.02	101.50
79	B2	144	U	C5-C4-O4	5.60	129.26	125.90
79	B2	453	U	C5-C4-O4	5.60	129.26	125.90
80	B5	546	C	C6-N1-C2	-5.60	118.06	120.30
80	B5	2642	A	C8-N9-C4	5.60	108.04	105.80
80	B5	2974	U	C5-C4-O4	5.60	129.26	125.90
80	B5	369	A	N1-C6-N6	-5.60	115.24	118.60
79	B2	115	G	N1-C6-O6	5.60	123.26	119.90
79	B2	1749	A	N3-C4-C5	5.60	130.72	126.80
80	B5	2182	A	C4-C5-C6	-5.60	114.20	117.00
79	B2	1280	C	C4-C5-C6	5.60	120.20	117.40
79	B2	1633	A	C4-C5-N7	-5.60	107.90	110.70
80	B5	24	G	C5-C6-O6	-5.60	125.24	128.60
80	B5	98	G	C8-N9-C4	5.60	108.64	106.40
80	B5	1229	G	O4'-C4'-C3'	-5.60	98.40	104.00
80	B5	1263	A	O4'-C1'-N9	5.60	112.68	108.20
82	B8	23	U	C4-C5-C6	5.60	123.06	119.70
82	B8	43	A	C8-N9-C4	-5.60	103.56	105.80
41	BG	69	LEU	CA-CB-CG	5.60	128.17	115.30
80	B5	909	G	N1-C6-O6	-5.60	116.54	119.90
80	B5	1360	C	C2-N3-C4	-5.60	117.10	119.90
80	B5	2584	G	C5-C6-O6	-5.60	125.24	128.60
80	B5	2975	U	N3-C4-O4	-5.60	115.48	119.40
79	B2	453	U	C6-N1-C1'	-5.59	113.37	121.20
80	B5	916	G	N9-C4-C5	5.59	107.64	105.40
80	B5	1365	G	C4-N9-C1'	5.59	133.77	126.50
80	B5	1370	G	N3-C4-N9	5.59	129.36	126.00
80	B5	2343	C	C5-C4-N4	-5.59	116.28	120.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	395	A	N7-C8-N9	5.59	116.60	113.80
47	BM	77	ARG	NE-CZ-NH1	-5.59	117.50	120.30
60	BZ	135	ARG	NE-CZ-NH1	5.59	123.09	120.30
79	B2	444	C	C2-N3-C4	5.59	122.69	119.90
79	B2	1536	G	C8-N9-C1'	-5.59	119.73	127.00
80	B5	347	G	N7-C8-N9	-5.59	110.31	113.10
80	B5	1245	A	C5-C6-N6	-5.59	119.23	123.70
80	B5	2904	U	C2-N3-C4	-5.59	123.65	127.00
80	B5	3003	G	C5-N7-C8	-5.59	101.51	104.30
65	Be	4	LEU	C-N-CA	-5.59	98.54	122.00
79	B2	279	G	N7-C8-N9	5.59	115.89	113.10
79	B2	810	G	C4-C5-N7	5.59	113.03	110.80
80	B5	405	U	C5-C4-O4	-5.59	122.55	125.90
80	B5	2191	U	C5-C6-N1	-5.59	119.91	122.70
80	B5	2307	G	N3-C2-N2	5.59	123.81	119.90
80	B5	3219	G	N3-C2-N2	5.59	123.81	119.90
79	B2	1129	U	C2-N3-C4	-5.58	123.65	127.00
79	B2	1279	C	C6-N1-C2	-5.58	118.07	120.30
80	B5	1171	G	C8-N9-C4	-5.58	104.17	106.40
80	B5	1192	C	C5-C6-N1	-5.58	118.21	121.00
80	B5	1869	C	C6-N1-C2	5.58	122.53	120.30
79	B2	542	A	C8-N9-C4	-5.58	103.57	105.80
79	B2	829	A	C2-N3-C4	5.58	113.39	110.60
80	B5	517	G	C4-C5-C6	5.58	122.15	118.80
80	B5	635	G	N1-C2-N2	5.58	121.22	116.20
80	B5	1315	U	C6-N1-C1'	-5.58	113.38	121.20
80	B5	2606	G	C4-C5-C6	5.58	122.15	118.80
80	B5	2631	U	N1-C2-O2	-5.58	118.89	122.80
80	B5	1338	C	C4-C5-C6	5.58	120.19	117.40
80	B5	1832	C	C6-N1-C2	5.58	122.53	120.30
80	B5	574	U	C5-C4-O4	-5.58	122.55	125.90
81	B7	79	A	N7-C8-N9	5.58	116.59	113.80
79	B2	1614	A	C6-C5-N7	-5.58	128.40	132.30
80	B5	1049	C	C5-C6-N1	5.58	123.79	121.00
80	B5	1271	A	C5-C6-N1	-5.58	114.91	117.70
80	B5	2434	U	C2-N3-C4	-5.58	123.65	127.00
80	B5	2889	C	N3-C4-N4	-5.58	114.10	118.00
80	B5	1381	A	N9-C4-C5	-5.58	103.57	105.80
80	B5	3287	U	N3-C2-O2	-5.58	118.30	122.20
82	B8	147	U	N3-C4-C5	5.58	117.95	114.60
25	AQ	69	VAL	CB-CA-C	-5.58	100.81	111.40
80	B5	819	U	N3-C4-O4	5.58	123.30	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	873	C	C4-C5-C6	5.58	120.19	117.40
80	B5	2975	U	C4-C5-C6	-5.58	116.36	119.70
80	B5	3252	G	C8-N9-C4	5.58	108.63	106.40
79	B2	401	A	N1-C6-N6	5.57	121.94	118.60
79	B2	1560	U	N1-C2-O2	5.57	126.70	122.80
79	B2	1636	C	N3-C4-N4	5.57	121.90	118.00
80	B5	340	C	N1-C2-N3	5.57	123.10	119.20
80	B5	911	C	C4-C5-C6	5.57	120.19	117.40
80	B5	1670	C	C5-C4-N4	-5.57	116.30	120.20
80	B5	2999	U	C5-C6-N1	-5.57	119.91	122.70
80	B5	903	U	N1-C2-O2	5.57	126.70	122.80
80	B5	957	C	C5-C6-N1	-5.57	118.22	121.00
80	B5	2309	A	C8-N9-C4	5.57	108.03	105.80
79	B2	1145	U	N1-C2-O2	-5.57	118.90	122.80
80	B5	666	A	N1-C2-N3	5.57	132.08	129.30
80	B5	2958	A	N1-C6-N6	-5.57	115.26	118.60
80	B5	3043	C	N3-C4-N4	-5.57	114.10	118.00
79	B2	696	C	C6-N1-C2	-5.57	118.07	120.30
79	B2	1462	G	C5-C6-O6	-5.57	125.26	128.60
80	B5	1906	G	C2-N3-C4	-5.57	109.12	111.90
80	B5	3173	G	C5-C6-N1	5.57	114.28	111.50
80	B5	3395	G	N1-C6-O6	5.57	123.24	119.90
82	B8	37	A	N1-C6-N6	-5.57	115.26	118.60
80	B5	2389	C	C5-C4-N4	-5.56	116.31	120.20
81	B7	1	G	C6-C5-N7	-5.56	127.06	130.40
82	B8	13	A	C5-N7-C8	-5.56	101.12	103.90
79	B2	397	A	C5-C6-N6	5.56	128.15	123.70
79	B2	972	G	C4-C5-N7	-5.56	108.58	110.80
80	B5	1086	C	C5-C6-N1	5.56	123.78	121.00
79	B2	380	U	N1-C2-O2	5.56	126.69	122.80
80	B5	1441	G	C5-N7-C8	5.56	107.08	104.30
80	B5	2257	C	N1-C2-O2	5.56	122.24	118.90
80	B5	2742	C	N3-C4-C5	5.56	124.12	121.90
80	B5	234	G	N1-C6-O6	5.56	123.24	119.90
80	B5	1183	C	C5-C6-N1	-5.56	118.22	121.00
80	B5	1403	C	C2-N3-C4	-5.56	117.12	119.90
79	B2	1027	A	C5-N7-C8	-5.56	101.12	103.90
80	B5	39	A	C5-N7-C8	5.56	106.68	103.90
80	B5	1256	G	OP2-P-O3'	5.56	117.43	105.20
84	CW	13	C	P-O3'-C3'	-5.56	113.03	119.70
61	Ba	17	ALA	C-N-CA	-5.56	110.63	122.30
80	B5	419	G	C4-C5-N7	5.56	113.02	110.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1115	G	C6-N1-C2	-5.56	121.77	125.10
79	B2	1127	G	N9-C4-C5	5.55	107.62	105.40
79	B2	1745	G	N3-C4-C5	-5.55	125.82	128.60
80	B5	1125	U	N3-C4-O4	-5.55	115.51	119.40
80	B5	1176	C	C4-C5-C6	5.55	120.18	117.40
79	B2	1456	C	N1-C2-N3	5.55	123.09	119.20
80	B5	39	A	C2-N3-C4	5.55	113.38	110.60
80	B5	728	G	N7-C8-N9	-5.55	110.32	113.10
79	B2	1024	U	N1-C2-O2	5.55	126.69	122.80
80	B5	953	G	N3-C4-C5	5.55	131.38	128.60
80	B5	1284	C	N3-C2-O2	5.55	125.79	121.90
80	B5	1724	U	N3-C2-O2	-5.55	118.31	122.20
80	B5	367	A	N3-C4-C5	5.55	130.69	126.80
80	B5	1905	G	N1-C6-O6	-5.55	116.57	119.90
80	B5	390	G	N9-C4-C5	-5.55	103.18	105.40
80	B5	1938	U	C5-C6-N1	-5.55	119.93	122.70
79	B2	42	G	C8-N9-C4	5.55	108.62	106.40
80	B5	1239	C	O4'-C1'-N1	5.55	112.64	108.20
80	B5	3055	U	C2-N1-C1'	5.55	124.36	117.70
49	BO	23[B]	ILE	CA-C-N	-5.54	105.00	117.20
79	B2	382	C	N3-C4-C5	5.54	124.12	121.90
80	B5	367	A	C5-C6-N6	5.54	128.14	123.70
80	B5	1601	U	N1-C2-N3	-5.54	111.57	114.90
80	B5	1754	G	N1-C2-N2	-5.54	111.21	116.20
80	B5	2607	G	C8-N9-C4	-5.54	104.18	106.40
80	B5	33	G	C5-C6-N1	5.54	114.27	111.50
80	B5	1872	C	N3-C2-O2	-5.54	118.02	121.90
80	B5	2522	G	N9-C4-C5	-5.54	103.18	105.40
75	Bo	41	ARG	NE-CZ-NH2	-5.54	117.53	120.30
80	B5	431	U	C2-N3-C4	-5.54	123.67	127.00
80	B5	648	C	C2-N1-C1'	5.54	124.89	118.80
80	B5	2320	A	N7-C8-N9	-5.54	111.03	113.80
80	B5	2400	G	C4-C5-N7	5.54	113.02	110.80
80	B5	2699	G	N3-C4-N9	5.54	129.32	126.00
80	B5	954	U	C6-N1-C2	-5.54	117.68	121.00
80	B5	1144	U	C2-N3-C4	-5.54	123.68	127.00
80	B5	796	U	N1-C2-O2	5.54	126.68	122.80
80	B5	1140	G	C5-C6-N1	5.54	114.27	111.50
80	B5	1773	C	C4-C5-C6	5.54	120.17	117.40
81	B7	69	C	N3-C4-C5	5.54	124.12	121.90
80	B5	21	G	N3-C4-C5	5.54	131.37	128.60
80	B5	25	U	N1-C2-N3	5.54	118.22	114.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2139	A	C5-C6-N6	5.54	128.13	123.70
82	B8	87	G	C5-C6-O6	-5.54	125.28	128.60
80	B5	1007	U	C6-N1-C2	5.53	124.32	121.00
80	B5	1189	C	N3-C2-O2	5.53	125.77	121.90
80	B5	1901	A	C6-C5-N7	-5.53	128.43	132.30
80	B5	1909	A	N1-C6-N6	-5.53	115.28	118.60
80	B5	2327	U	C2-N1-C1'	-5.53	111.06	117.70
84	CW	60	U	C5'-C4'-O4'	5.53	115.74	109.10
80	B5	46	U	C2-N3-C4	5.53	130.32	127.00
80	B5	1305	U	C6-N1-C2	5.53	124.32	121.00
80	B5	1380	G	C2-N3-C4	-5.53	109.13	111.90
80	B5	3052	G	C4-N9-C1'	-5.53	119.31	126.50
82	B8	112	U	C6-N1-C1'	5.53	128.94	121.20
79	B2	109	G	C5-C6-O6	-5.53	125.28	128.60
80	B5	745	C	N1-C2-O2	-5.53	115.58	118.90
80	B5	2658	G	N3-C2-N2	-5.53	116.03	119.90
80	B5	2870	C	C2-N1-C1'	-5.53	112.72	118.80
80	B5	3064	U	N1-C2-N3	5.53	118.22	114.90
84	CW	28	G	O4'-C1'-N9	5.53	112.62	108.20
80	B5	1041	U	C5-C6-N1	-5.53	119.94	122.70
80	B5	1658	G	N1-C6-O6	-5.53	116.58	119.90
80	B5	2717	U	N3-C2-O2	-5.53	118.33	122.20
79	B2	131	C	C5-C6-N1	5.53	123.76	121.00
80	B5	359	U	N3-C4-C5	5.53	117.92	114.60
80	B5	1306	G	C5-C6-N1	5.53	114.26	111.50
80	B5	1878	G	C4-N9-C1'	5.53	133.69	126.50
80	B5	3007	U	C5-C4-O4	-5.53	122.58	125.90
80	B5	2287	C	C6-N1-C2	-5.53	118.09	120.30
80	B5	2665	U	N1-C2-O2	5.53	126.67	122.80
80	B5	2777	G	C8-N9-C4	-5.53	104.19	106.40
80	B5	2996	U	C6-N1-C1'	-5.53	113.46	121.20
81	B7	100	C	N3-C4-C5	5.53	124.11	121.90
82	B8	104	A	N1-C2-N3	-5.53	126.54	129.30
80	B5	1305	U	C6-N1-C1'	-5.52	113.47	121.20
79	B2	36	C	C5-C4-N4	-5.52	116.33	120.20
79	B2	145	A	N9-C4-C5	5.52	108.01	105.80
80	B5	934	G	N1-C2-N2	5.52	121.17	116.20
80	B5	960	U	C4-C5-C6	5.52	123.01	119.70
80	B5	1797	A	C8-N9-C4	5.52	108.01	105.80
80	B5	1844	C	N1-C2-N3	5.52	123.07	119.20
80	B5	3336	A	C5-C6-N1	-5.52	114.94	117.70
80	B5	1178	G	N7-C8-N9	5.52	115.86	113.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	1796	C	C6-N1-C2	-5.52	118.09	120.30
80	B5	1444	G	C8-N9-C4	5.52	108.61	106.40
80	B5	1586	G	C6-N1-C2	-5.52	121.79	125.10
80	B5	2293	C	C5-C4-N4	-5.52	116.34	120.20
80	B5	2344	U	C2-N3-C4	-5.52	123.69	127.00
80	B5	2914	G	N1-C6-O6	-5.52	116.59	119.90
80	B5	3103	A	C5-C6-N1	5.52	120.46	117.70
80	B5	3318	G	C4-C5-N7	-5.52	108.59	110.80
81	B7	1	G	N3-C4-N9	5.52	129.31	126.00
79	B2	1455	G	C4-C5-C6	5.52	122.11	118.80
80	B5	2289	U	C5-C4-O4	5.52	129.21	125.90
79	B2	380	U	N3-C2-O2	-5.51	118.34	122.20
84	CW	21	A	C5-C6-N1	-5.51	114.94	117.70
65	Be	105	ARG	NE-CZ-NH2	-5.51	117.54	120.30
80	B5	814	U	N1-C2-N3	-5.51	111.59	114.90
80	B5	1887	A	N9-C4-C5	-5.51	103.59	105.80
80	B5	2729	U	C4-C5-C6	-5.51	116.39	119.70
80	B5	3326	G	C5-C6-O6	5.51	131.91	128.60
82	B8	19	C	N3-C4-C5	-5.51	119.70	121.90
61	Ba	9	ARG	NE-CZ-NH1	-5.51	117.55	120.30
79	B2	74	U	C1'-O4'-C4'	-5.51	105.49	109.90
80	B5	1491	A	C4-C5-C6	5.51	119.75	117.00
80	B5	3010	U	C5-C4-O4	5.51	129.21	125.90
80	B5	3387	U	N1-C2-O2	5.51	126.66	122.80
84	CW	4	C	N3-C4-C5	-5.51	119.70	121.90
80	B5	1365	G	N1-C2-N2	-5.51	111.24	116.20
80	B5	1841	A	C8-N9-C4	-5.51	103.60	105.80
80	B5	2346	C	N3-C4-C5	5.51	124.10	121.90
83	CV	375	VAL	N-CA-C	-5.51	96.13	111.00
79	B2	258	C	N3-C4-C5	5.51	124.10	121.90
79	B2	639	U	N3-C4-C5	5.51	117.90	114.60
80	B5	1447	G	N7-C8-N9	5.51	115.85	113.10
80	B5	3179	U	N3-C4-C5	5.51	117.90	114.60
81	B7	19	C	N3-C4-C5	5.51	124.10	121.90
79	B2	435	C	C2-N3-C4	5.50	122.65	119.90
79	B2	566	C	N3-C2-O2	-5.50	118.05	121.90
80	B5	2335	G	C6-N1-C2	-5.50	121.80	125.10
80	B5	363	G	C4-C5-N7	-5.50	108.60	110.80
80	B5	620	U	C2-N1-C1'	5.50	124.31	117.70
80	B5	715	A	C5-C6-N1	5.50	120.45	117.70
80	B5	2396	G	N1-C6-O6	-5.50	116.60	119.90
80	B5	2728	G	N1-C2-N2	5.50	121.15	116.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	42	G	N7-C8-N9	-5.50	110.35	113.10
80	B5	1670	C	C6-N1-C2	5.50	122.50	120.30
80	B5	1937	U	C5-C6-N1	-5.50	119.95	122.70
79	B2	703	G	N7-C8-N9	5.50	115.85	113.10
80	B5	54	C	N3-C4-N4	-5.50	114.15	118.00
80	B5	2605	G	C2-N3-C4	5.50	114.65	111.90
80	B5	3347	A	C8-N9-C4	5.50	108.00	105.80
80	B5	2119	A	C6-N1-C2	-5.50	115.30	118.60
80	B5	2430	A	N1-C2-N3	5.50	132.05	129.30
80	B5	3042	U	N1-C2-N3	5.50	118.20	114.90
79	B2	386	G	C4-C5-N7	-5.50	108.60	110.80
80	B5	1045	C	C2-N3-C4	-5.50	117.15	119.90
80	B5	2635	A	N1-C6-N6	-5.50	115.30	118.60
80	B5	3152	U	C5-C6-N1	-5.50	119.95	122.70
84	CW	37	A	C4-C5-C6	5.50	119.75	117.00
79	B2	1270	G	C2-N3-C4	5.49	114.65	111.90
79	B2	1503	A	N7-C8-N9	5.49	116.55	113.80
80	B5	266	A	N1-C2-N3	5.49	132.05	129.30
80	B5	1508	C	N1-C2-O2	5.49	122.20	118.90
80	B5	3341	U	N3-C2-O2	-5.49	118.36	122.20
82	B8	17	A	C5-N7-C8	-5.49	101.15	103.90
80	B5	631	U	N1-C2-O2	5.49	126.64	122.80
80	B5	1215	U	N3-C2-O2	5.49	126.04	122.20
80	B5	1660	C	N1-C2-O2	-5.49	115.61	118.90
80	B5	2549	G	C5-C6-N1	-5.49	108.75	111.50
80	B5	3008	A	C8-N9-C4	5.49	108.00	105.80
79	B2	264	G	N3-C4-N9	-5.49	122.71	126.00
80	B5	414	U	N3-C4-O4	5.49	123.24	119.40
80	B5	1343	A	C8-N9-C4	-5.49	103.60	105.80
80	B5	1505	C	C4-C5-C6	5.49	120.14	117.40
84	CW	43	C	P-O3'-C3'	5.49	126.29	119.70
79	B2	377	G	C4-N9-C1'	-5.49	119.36	126.50
79	B2	1207	C	C6-N1-C2	5.49	122.50	120.30
80	B5	436	A	C4-C5-N7	5.49	113.44	110.70
80	B5	590	G	C8-N9-C4	-5.49	104.20	106.40
80	B5	1427	U	N3-C4-O4	-5.49	115.56	119.40
80	B5	3112	G	C8-N9-C4	5.49	108.59	106.40
79	B2	342	C	C6-N1-C2	5.49	122.50	120.30
80	B5	844	G	N7-C8-N9	-5.49	110.36	113.10
80	B5	2665	U	C4-C5-C6	-5.49	116.41	119.70
80	B5	2966	G	C5-C6-N1	5.49	114.24	111.50
79	B2	42	G	N1-C6-O6	-5.49	116.61	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	743	C	C6-N1-C2	-5.49	118.11	120.30
80	B5	996	A	C5-C6-N1	5.49	120.44	117.70
80	B5	1127	G	N3-C4-N9	5.49	129.29	126.00
80	B5	2757	U	C5-C4-O4	-5.49	122.61	125.90
79	B2	1662	G	C8-N9-C4	-5.48	104.21	106.40
80	B5	1269	U	O4'-C1'-N1	5.48	112.59	108.20
80	B5	1451	C	C2-N3-C4	-5.48	117.16	119.90
80	B5	2904	U	N1-C2-N3	5.48	118.19	114.90
81	B7	8	G	N3-C2-N2	5.48	123.74	119.90
79	B2	938	G	N1-C2-N2	-5.48	111.27	116.20
80	B5	1263	A	C5-C6-N6	-5.48	119.31	123.70
80	B5	1828	A	C8-N9-C4	-5.48	103.61	105.80
80	B5	1869	C	N3-C4-C5	5.48	124.09	121.90
80	B5	2112	U	C6-N1-C2	-5.48	117.71	121.00
80	B5	3243	A	C4-C5-C6	5.48	119.74	117.00
81	B7	61	G	C8-N9-C4	5.48	108.59	106.40
80	B5	1283	C	O3'-P-O5'	5.48	114.41	104.00
80	B5	3302	U	N3-C4-C5	5.48	117.89	114.60
79	B2	838	G	N7-C8-N9	-5.48	110.36	113.10
80	B5	39	A	N7-C8-N9	-5.48	111.06	113.80
80	B5	422	A	C8-N9-C4	5.48	107.99	105.80
80	B5	519	A	C6-C5-N7	-5.48	128.47	132.30
80	B5	2172	A	N1-C6-N6	5.48	121.89	118.60
83	CV	136	TYR	CA-CB-CG	5.48	123.81	113.40
49	BO	197[B]	PHE	CA-C-N	-5.47	105.25	116.20
66	Bf	91	ALA	N-CA-CB	5.47	117.76	110.10
79	B2	393	C	C2-N3-C4	-5.47	117.16	119.90
80	B5	282	G	N7-C8-N9	5.47	115.84	113.10
80	B5	1191	U	C5-C6-N1	-5.47	119.96	122.70
80	B5	1295	G	C5-C6-O6	5.47	131.88	128.60
80	B5	2109	U	N3-C4-O4	-5.47	115.57	119.40
80	B5	2134	G	N3-C4-N9	5.47	129.28	126.00
80	B5	2257	C	C5-C6-N1	5.47	123.74	121.00
80	B5	2369	G	C8-N9-C4	5.47	108.59	106.40
80	B5	2948	C	N3-C4-C5	5.47	124.09	121.90
80	B5	3028	G	N3-C2-N2	5.47	123.73	119.90
80	B5	3215	A	C5-C6-N1	-5.47	114.96	117.70
80	B5	2177	G	C8-N9-C4	-5.47	104.21	106.40
80	B5	930	U	N1-C2-O2	5.47	126.63	122.80
79	B2	1486	G	C6-C5-N7	-5.47	127.12	130.40
80	B5	1152	G	N9-C4-C5	5.47	107.59	105.40
80	B5	1165	A	N7-C8-N9	-5.47	111.06	113.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2158	A	C6-N1-C2	-5.47	115.32	118.60
84	CW	17	C	N3-C4-N4	5.47	121.83	118.00
80	B5	2433	U	C5-C6-N1	-5.47	119.97	122.70
84	CW	13	C	N3-C4-N4	5.47	121.83	118.00
46	BL	47	ALA	C-N-CD	5.47	139.88	128.40
80	B5	810	A	C5-C6-N6	5.47	128.07	123.70
80	B5	1190	A	C5-N7-C8	5.47	106.63	103.90
80	B5	1538	G	N9-C4-C5	-5.47	103.21	105.40
80	B5	1792	C	C4-C5-C6	5.47	120.13	117.40
80	B5	2197	C	C6-N1-C1'	5.47	127.36	120.80
80	B5	2239	G	N3-C2-N2	5.47	123.73	119.90
80	B5	3346	U	C5-C6-N1	-5.47	119.97	122.70
79	B2	1097	U	C6-N1-C1'	-5.46	113.55	121.20
80	B5	2321	A	C5-C6-N1	5.46	120.43	117.70
80	B5	2549	G	N7-C8-N9	5.46	115.83	113.10
81	B7	33	U	N1-C2-O2	5.46	126.63	122.80
85	CX	2	U	O4'-C1'-N1	5.46	112.57	108.20
79	B2	268	C	C6-N1-C2	-5.46	118.11	120.30
79	B2	1666	U	C5-C6-N1	5.46	125.43	122.70
80	B5	909	G	N7-C8-N9	-5.46	110.37	113.10
80	B5	1399	A	N9-C4-C5	-5.46	103.61	105.80
80	B5	997	A	N7-C8-N9	5.46	116.53	113.80
80	B5	1931	U	C5-C4-O4	5.46	129.18	125.90
80	B5	3394	U	N3-C4-O4	-5.46	115.58	119.40
79	B2	790	U	N1-C2-N3	5.46	118.18	114.90
81	B7	8	G	N1-C2-N2	-5.46	111.29	116.20
80	B5	96	G	C4-C5-N7	-5.46	108.62	110.80
80	B5	408	A	C2-N3-C4	-5.46	107.87	110.60
80	B5	809	G	C5-N7-C8	5.46	107.03	104.30
80	B5	965	A	N1-C2-N3	-5.46	126.57	129.30
79	B2	599	A	C5-N7-C8	5.46	106.63	103.90
79	B2	1458	G	C8-N9-C1'	-5.46	119.91	127.00
80	B5	1170	A	C8-N9-C4	5.46	107.98	105.80
81	B7	37	G	N9-C4-C5	-5.46	103.22	105.40
80	B5	1240	A	C5-C6-N1	-5.46	114.97	117.70
80	B5	277	G	C5-C6-O6	5.45	131.87	128.60
80	B5	828	A	N1-C6-N6	-5.45	115.33	118.60
81	B7	1	G	C8-N9-C1'	-5.45	119.91	127.00
80	B5	1176	C	C6-N1-C2	5.45	122.48	120.30
37	BC	73	ARG	CB-CG-CD	-5.45	97.43	111.60
79	B2	42	G	C5-C6-N1	5.45	114.22	111.50
79	B2	1491	U	N3-C2-O2	-5.45	118.38	122.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1159	A	C4-C5-C6	-5.45	114.28	117.00
80	B5	1858	A	C4-N9-C1'	5.45	136.11	126.30
80	B5	2843	U	N3-C2-O2	-5.45	118.39	122.20
80	B5	3049	A	C8-N9-C4	5.45	107.98	105.80
80	B5	1925	U	N1-C2-N3	5.45	118.17	114.90
80	B5	2608	G	N1-C6-O6	-5.45	116.63	119.90
83	CV	509	GLU	N-CA-CB	5.45	120.41	110.60
80	B5	859	G	N3-C4-C5	-5.45	125.88	128.60
80	B5	1270	A	C3'-C2'-C1'	-5.45	97.14	101.50
80	B5	3083	G	N1-C2-N3	5.45	127.17	123.90
80	B5	2800	G	C4-C5-N7	-5.44	108.62	110.80
80	B5	2810	C	C6-N1-C2	-5.44	118.12	120.30
80	B5	3035	A	C8-N9-C4	5.44	107.98	105.80
79	B2	426	G	C4-N9-C1'	5.44	133.57	126.50
79	B2	1185	U	C6-N1-C1'	-5.44	113.58	121.20
80	B5	3115	C	N1-C2-N3	5.44	123.01	119.20
81	B7	90	U	C6-N1-C2	5.44	124.27	121.00
80	B5	285	A	C8-N9-C4	-5.44	103.62	105.80
80	B5	969	C	C5-C6-N1	-5.44	118.28	121.00
80	B5	1007	U	C5-C4-O4	-5.44	122.64	125.90
80	B5	2374	C	N3-C4-N4	-5.44	114.19	118.00
80	B5	2655	U	N3-C4-C5	5.44	117.86	114.60
80	B5	2998	U	C2-N3-C4	-5.44	123.74	127.00
53	BS	167	ARG	NE-CZ-NH2	-5.44	117.58	120.30
79	B2	396	G	C5-C6-O6	-5.44	125.34	128.60
79	B2	966	A	N7-C8-N9	-5.44	111.08	113.80
79	B2	1646	C	C6-N1-C2	-5.44	118.12	120.30
80	B5	1838	G	C4-C5-N7	-5.44	108.62	110.80
80	B5	1229	G	C4-C5-C6	5.44	122.06	118.80
61	Ba	28	HIS	CB-CA-C	-5.43	99.53	110.40
80	B5	41	G	C6-C5-N7	-5.43	127.14	130.40
80	B5	388	G	N3-C2-N2	-5.43	116.10	119.90
80	B5	2361	A	N9-C4-C5	5.43	107.97	105.80
80	B5	2754	G	N3-C4-N9	5.43	129.26	126.00
80	B5	3362	A	C4-C5-N7	5.43	113.42	110.70
82	B8	103	G	C5-C6-N1	5.43	114.22	111.50
80	B5	2174	G	N1-C2-N3	5.43	127.16	123.90
80	B5	2524	A	N3-C4-C5	5.43	130.60	126.80
80	B5	2744	U	N3-C4-O4	-5.43	115.60	119.40
80	B5	2894	C	C2-N3-C4	-5.43	117.18	119.90
80	B5	3113	A	C6-N1-C2	-5.43	115.34	118.60
79	B2	1754	A	N3-C4-C5	5.43	130.60	126.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	590	G	C2-N3-C4	5.43	114.61	111.90
80	B5	646	A	N1-C2-N3	5.43	132.01	129.30
61	Ba	4	ARG	NE-CZ-NH1	-5.43	117.59	120.30
80	B5	1285	G	C4'-C3'-C2'	-5.43	97.17	102.60
80	B5	2242	A	N9-C4-C5	5.43	107.97	105.80
80	B5	1244	A	P-O3'-C3'	5.43	126.21	119.70
80	B5	2319	U	C5-C6-N1	-5.43	119.99	122.70
80	B5	2379	U	N1-C2-N3	5.43	118.16	114.90
81	B7	105	C	C2-N3-C4	5.43	122.61	119.90
83	CV	60	ALA	N-CA-C	-5.43	96.35	111.00
79	B2	557	G	N1-C2-N2	-5.42	111.32	116.20
80	B5	322	U	C2-N3-C4	-5.42	123.75	127.00
80	B5	675	C	N1-C2-O2	-5.42	115.64	118.90
80	B5	1191	U	C4-C5-C6	5.42	122.95	119.70
80	B5	1273	A	C5-C6-N6	-5.42	119.36	123.70
80	B5	1433	A	C6-N1-C2	5.42	121.86	118.60
80	B5	3143	C	N3-C2-O2	5.42	125.70	121.90
79	B2	1170	G	C6-C5-N7	-5.42	127.15	130.40
79	B2	1330	G	C4-N9-C1'	-5.42	119.45	126.50
80	B5	283	G	C5-C6-O6	-5.42	125.35	128.60
80	B5	1164	G	C2-N3-C4	-5.42	109.19	111.90
80	B5	229	G	N1-C6-O6	5.42	123.15	119.90
80	B5	341	G	C5-N7-C8	-5.42	101.59	104.30
80	B5	600	G	C4-N9-C1'	5.42	133.55	126.50
80	B5	1268	G	C6-C5-N7	-5.42	127.15	130.40
80	B5	2891	U	N1-C2-N3	5.42	118.15	114.90
80	B5	3064	U	C2-N3-C4	-5.42	123.75	127.00
80	B5	498	A	N1-C6-N6	-5.42	115.35	118.60
80	B5	2808	A	C6-C5-N7	-5.42	128.51	132.30
36	BB	4	ARG	NE-CZ-NH2	-5.42	117.59	120.30
79	B2	1146	G	C4-N9-C1'	5.42	133.54	126.50
80	B5	266	A	C4-C5-C6	5.42	119.71	117.00
80	B5	514	G	N9-C4-C5	-5.42	103.23	105.40
80	B5	844	G	C8-N9-C4	5.42	108.57	106.40
80	B5	1209	G	N1-C2-N2	5.42	121.08	116.20
80	B5	2980	U	N3-C2-O2	-5.42	118.41	122.20
84	CW	7	A	P-O5'-C5'	-5.42	112.23	120.90
59	BY	14	LYS	CD-CE-NZ	5.42	124.16	111.70
79	B2	995	A	C8-N9-C4	5.42	107.97	105.80
79	B2	1642	G	N3-C4-N9	5.42	129.25	126.00
80	B5	1129	A	C5-C6-N1	5.42	120.41	117.70
80	B5	1187	C	N3-C4-N4	-5.42	114.21	118.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1227	C	C5'-C4'-C3'	-5.42	107.33	116.00
82	B8	126	A	N7-C8-N9	5.42	116.51	113.80
80	B5	3193	C	C4-C5-C6	5.42	120.11	117.40
80	B5	90	C	C6-N1-C2	-5.41	118.13	120.30
80	B5	706	A	N9-C4-C5	-5.41	103.64	105.80
80	B5	914	A	N1-C2-N3	5.41	132.01	129.30
80	B5	2385	G	C8-N9-C1'	5.41	134.04	127.00
80	B5	3015	G	N1-C6-O6	-5.41	116.65	119.90
79	B2	1679	G	C2-N3-C4	5.41	114.61	111.90
80	B5	879	U	C6-N1-C1'	-5.41	113.63	121.20
80	B5	1359	C	N3-C4-N4	5.41	121.79	118.00
80	B5	2377	G	N3-C4-C5	-5.41	125.89	128.60
80	B5	2393	G	C8-N9-C1'	-5.41	119.97	127.00
80	B5	3263	G	N1-C6-O6	-5.41	116.65	119.90
81	B7	82	G	N9-C4-C5	5.41	107.56	105.40
79	B2	992	A	C4-C5-N7	5.41	113.40	110.70
79	B2	1386	G	C4-C5-N7	-5.41	108.64	110.80
80	B5	591	G	C6-C5-N7	-5.41	127.16	130.40
80	B5	688	G	N3-C4-N9	-5.41	122.75	126.00
80	B5	1495	U	C6-N1-C2	-5.41	117.75	121.00
80	B5	3247	G	C5-C6-O6	5.41	131.85	128.60
80	B5	3323	A	N1-C2-N3	5.41	132.00	129.30
80	B5	799	G	C6-N1-C2	-5.41	121.86	125.10
79	B2	767	U	N3-C2-O2	-5.41	118.42	122.20
80	B5	961	C	C4-C5-C6	5.41	120.10	117.40
80	B5	2376	G	C8-N9-C1'	-5.41	119.97	127.00
79	B2	307	G	C8-N9-C4	5.40	108.56	106.40
79	B2	1504	G	C5-C6-O6	5.40	131.84	128.60
79	B2	1560	U	C6-N1-C2	-5.40	117.76	121.00
80	B5	1128	U	C2-N3-C4	-5.40	123.76	127.00
80	B5	2145	A	C6-N1-C2	-5.40	115.36	118.60
80	B5	3003	G	N3-C4-N9	-5.40	122.76	126.00
80	B5	3021	A	N1-C6-N6	-5.40	115.36	118.60
79	B2	529	A	C8-N9-C4	5.40	107.96	105.80
79	B2	864	U	C2-N1-C1'	5.40	124.18	117.70
79	B2	1389	C	N3-C2-O2	-5.40	118.12	121.90
80	B5	648	C	C4-C5-C6	5.40	120.10	117.40
80	B5	1396	C	C6-N1-C2	5.40	122.46	120.30
80	B5	1838	G	C6-N1-C2	-5.40	121.86	125.10
80	B5	2634	U	N3-C2-O2	5.40	125.98	122.20
82	B8	156	U	C5-C6-N1	5.40	125.40	122.70
80	B5	516	A	C5-C6-N6	-5.40	119.38	123.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	588	G	C5-C6-N1	5.40	114.20	111.50
80	B5	1257	C	N3-C4-C5	-5.40	119.74	121.90
80	B5	1534	A	C6-N1-C2	-5.40	115.36	118.60
80	B5	2123	G	N3-C4-C5	-5.40	125.90	128.60
80	B5	2955	U	C6-N1-C2	-5.40	117.76	121.00
82	B8	29	U	C5-C6-N1	-5.40	120.00	122.70
80	B5	2134	G	N3-C2-N2	5.40	123.68	119.90
80	B5	288	C	C6-N1-C2	5.40	122.46	120.30
80	B5	923	C	C5-C6-N1	-5.40	118.30	121.00
80	B5	1131	G	N1-C2-N3	5.40	127.14	123.90
80	B5	2355	G	C5-C6-O6	-5.40	125.36	128.60
80	B5	2928	C	N3-C4-C5	-5.40	119.74	121.90
80	B5	2429	G	N9-C4-C5	5.40	107.56	105.40
19	AK	63	TYR	N-CA-C	5.39	125.56	111.00
35	BA	207	VAL	CB-CA-C	-5.39	101.15	111.40
79	B2	396	G	N1-C6-O6	5.39	123.14	119.90
79	B2	407	A	C5-N7-C8	5.39	106.60	103.90
80	B5	98	G	N9-C4-C5	-5.39	103.24	105.40
80	B5	1017	C	C2-N1-C1'	5.39	124.73	118.80
80	B5	1889	G	C4-C5-N7	-5.39	108.64	110.80
80	B5	3366	G	N1-C6-O6	-5.39	116.66	119.90
79	B2	523	G	N1-C6-O6	-5.39	116.66	119.90
79	B2	1768	G	C8-N9-C1'	5.39	134.01	127.00
80	B5	1907	C	C6-N1-C1'	5.39	127.27	120.80
80	B5	2181	C	C6-N1-C2	-5.39	118.14	120.30
25	AQ	40	GLU	C-N-CA	5.39	144.64	122.00
80	B5	411	U	C2-N3-C4	-5.39	123.77	127.00
80	B5	616	G	C2-N3-C4	5.39	114.59	111.90
80	B5	1143	A	C2-N3-C4	-5.39	107.91	110.60
80	B5	1335	C	C6-N1-C2	-5.39	118.14	120.30
80	B5	2149	A	N9-C4-C5	5.39	107.96	105.80
80	B5	2386	A	C5-N7-C8	-5.39	101.20	103.90
80	B5	3374	U	C6-N1-C2	5.39	124.23	121.00
79	B2	1361	U	C2-N1-C1'	5.39	124.17	117.70
80	B5	811	U	N1-C2-N3	5.39	118.13	114.90
80	B5	2375	G	C4-C5-N7	5.39	112.96	110.80
79	B2	1524	A	N1-C2-N3	5.39	131.99	129.30
80	B5	227	G	C5-C6-O6	-5.39	125.37	128.60
80	B5	339	C	C6-N1-C2	-5.39	118.14	120.30
80	B5	1722	U	N1-C2-O2	-5.39	119.03	122.80
80	B5	555	U	N1-C2-O2	-5.39	119.03	122.80
80	B5	1126	G	C5-C6-N1	-5.39	108.81	111.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1178	G	C6-N1-C2	-5.39	121.87	125.10
80	B5	3350	C	N1-C2-O2	5.39	122.13	118.90
80	B5	852	U	N1-C2-N3	5.38	118.13	114.90
80	B5	2231	C	C2-N1-C1'	5.38	124.72	118.80
80	B5	3189	G	C6-N1-C2	-5.38	121.87	125.10
80	B5	3377	G	C6-N1-C2	-5.38	121.87	125.10
84	CW	41	C	C2-N1-C1'	5.38	124.72	118.80
79	B2	1334	U	N1-C2-N3	5.38	118.13	114.90
80	B5	641	C	C6-N1-C2	-5.38	118.15	120.30
80	B5	1409	G	N9-C4-C5	5.38	107.55	105.40
80	B5	2434	U	N3-C2-O2	-5.38	118.43	122.20
81	B7	93	C	N3-C4-C5	5.38	124.05	121.90
79	B2	720	G	P-O3'-C3'	5.38	126.16	119.70
80	B5	1724	U	N1-C2-N3	5.38	118.13	114.90
80	B5	1870	C	N1-C2-O2	-5.38	115.67	118.90
80	B5	2524	A	C5-C6-N1	-5.38	115.01	117.70
80	B5	2632	G	N1-C2-N3	-5.38	120.67	123.90
80	B5	2767	U	N3-C4-O4	-5.38	115.63	119.40
80	B5	3047	U	N3-C2-O2	-5.38	118.43	122.20
79	B2	336	G	C6-C5-N7	-5.38	127.17	130.40
80	B5	1081	U	C5-C6-N1	5.38	125.39	122.70
39	BE	173	MET	CB-CG-SD	-5.38	96.26	112.40
80	B5	2794	G	C5-C6-O6	-5.38	125.37	128.60
80	B5	3048	A	C6-N1-C2	-5.38	115.37	118.60
84	CW	12	U	C5-C6-N1	5.38	125.39	122.70
79	B2	1315	U	C5-C4-O4	-5.38	122.67	125.90
80	B5	14	U	N3-C4-C5	5.38	117.83	114.60
80	B5	806	A	C8-N9-C4	5.38	107.95	105.80
80	B5	1905	G	N9-C4-C5	5.38	107.55	105.40
80	B5	2614	G	C4-N9-C1'	5.38	133.49	126.50
85	CX	3	G	C5-C6-O6	-5.38	125.37	128.60
80	B5	2399	A	C5-C6-N6	-5.38	119.40	123.70
80	B5	3055	U	C6-N1-C1'	-5.38	113.67	121.20
79	B2	469	C	N3-C2-O2	5.37	125.66	121.90
80	B5	1150	A	C5-N7-C8	-5.37	101.21	103.90
80	B5	1243	G	O4'-C1'-N9	5.37	112.50	108.20
80	B5	1248	C	N3-C4-C5	-5.37	119.75	121.90
80	B5	3028	G	C8-N9-C1'	-5.37	120.02	127.00
84	CW	74	C	N3-C4-N4	5.37	121.76	118.00
80	B5	51	A	N1-C6-N6	5.37	121.82	118.60
80	B5	356	C	C5-C6-N1	-5.37	118.31	121.00
80	B5	2148	U	N3-C4-C5	5.37	117.82	114.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2755	C	N1-C2-O2	-5.37	115.68	118.90
80	B5	2763	U	C5-C4-O4	-5.37	122.68	125.90
80	B5	3052	G	C6-C5-N7	5.37	133.62	130.40
80	B5	3078	U	C2-N1-C1'	5.37	124.14	117.70
79	B2	393	C	C5-C6-N1	-5.37	118.31	121.00
80	B5	63	A	N9-C4-C5	-5.37	103.65	105.80
80	B5	2639	G	C6-N1-C2	-5.37	121.88	125.10
80	B5	2956	A	C5-C6-N1	-5.37	115.02	117.70
81	B7	105	C	N3-C4-C5	-5.37	119.75	121.90
79	B2	1422	A	N7-C8-N9	-5.37	111.12	113.80
80	B5	972	A	C4-C5-C6	5.37	119.68	117.00
80	B5	1312	C	C5-C4-N4	5.37	123.96	120.20
80	B5	1906	G	C6-N1-C2	-5.37	121.88	125.10
82	B8	3	A	C5-C6-N1	5.37	120.38	117.70
79	B2	1324	G	N1-C2-N2	5.37	121.03	116.20
80	B5	536	U	N3-C4-O4	-5.37	115.64	119.40
80	B5	848	A	N1-C2-N3	5.37	131.98	129.30
80	B5	3101	G	N1-C2-N2	-5.37	111.37	116.20
80	B5	365	A	C4-C5-N7	5.37	113.38	110.70
80	B5	2820	A	N9-C4-C5	5.37	107.95	105.80
81	B7	115	G	C8-N9-C4	-5.37	104.25	106.40
79	B2	719	U	C6-N1-C1'	-5.36	113.69	121.20
80	B5	1279	C	N3-C4-C5	-5.36	119.75	121.90
80	B5	2639	G	N1-C6-O6	5.36	123.12	119.90
79	B2	1679	G	N1-C6-O6	-5.36	116.68	119.90
80	B5	1161	G	C6-C5-N7	5.36	133.62	130.40
80	B5	1170	A	N9-C4-C5	-5.36	103.66	105.80
80	B5	2904	U	N3-C2-O2	-5.36	118.45	122.20
80	B5	3179	U	N1-C2-O2	5.36	126.55	122.80
79	B2	628	G	N3-C4-C5	5.36	131.28	128.60
79	B2	1192	C	N1-C2-O2	-5.36	115.68	118.90
80	B5	1110	U	N1-C2-N3	-5.36	111.68	114.90
80	B5	1846	C	C6-N1-C2	5.36	122.44	120.30
80	B5	2621	G	N1-C2-N2	5.36	121.03	116.20
80	B5	2915	U	N3-C4-O4	-5.36	115.65	119.40
81	B7	48	U	C5-C6-N1	-5.36	120.02	122.70
79	B2	1769	U	C5-C4-O4	5.36	129.12	125.90
80	B5	1374	G	N1-C2-N2	-5.36	111.38	116.20
80	B5	587	U	N3-C4-O4	-5.36	115.65	119.40
80	B5	905	U	C2-N3-C4	-5.36	123.79	127.00
80	B5	2837	A	C8-N9-C4	5.36	107.94	105.80
17	AI	29	LEU	CA-CB-CG	5.36	127.62	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	1524	A	N1-C6-N6	-5.36	115.39	118.60
79	B2	1762	A	N9-C4-C5	-5.36	103.66	105.80
80	B5	696	C	C2-N1-C1'	5.36	124.69	118.80
80	B5	2525	G	C8-N9-C4	5.36	108.54	106.40
79	B2	151	G	C5-C6-N1	5.35	114.18	111.50
80	B5	1300	G	N1-C6-O6	5.35	123.11	119.90
80	B5	1319	G	N1-C2-N2	-5.35	111.38	116.20
84	CW	11	C	N3-C4-N4	5.35	121.75	118.00
76	Bq	22	TYR	CB-CG-CD1	-5.35	117.79	121.00
79	B2	12	U	N3-C2-O2	-5.35	118.45	122.20
79	B2	932	U	C6-N1-C1'	5.35	128.69	121.20
80	B5	339	C	C6-N1-C1'	5.35	127.22	120.80
80	B5	1510	G	C2-N3-C4	-5.35	109.22	111.90
80	B5	2987	A	N7-C8-N9	-5.35	111.12	113.80
79	B2	393	C	C2-N1-C1'	-5.35	112.91	118.80
80	B5	1844	C	C6-N1-C2	-5.35	118.16	120.30
80	B5	91	G	N9-C4-C5	5.35	107.54	105.40
80	B5	363	G	C5-N7-C8	5.35	106.97	104.30
80	B5	1144	U	C4-C5-C6	5.35	122.91	119.70
80	B5	3019	U	C6-N1-C2	5.35	124.21	121.00
79	B2	1537	C	C5-C4-N4	-5.35	116.46	120.20
80	B5	372	A	N1-C6-N6	5.35	121.81	118.60
80	B5	404	G	C4-C5-N7	-5.35	108.66	110.80
80	B5	1321	G	C8-N9-C4	5.35	108.54	106.40
80	B5	2184	U	N3-C4-C5	5.35	117.81	114.60
80	B5	3005	A	C8-N9-C4	-5.35	103.66	105.80
80	B5	3043	C	N1-C2-O2	5.35	122.11	118.90
80	B5	3046	A	N1-C6-N6	-5.35	115.39	118.60
24	AP	60	LEU	CA-CB-CG	5.35	127.59	115.30
79	B2	1086	A	C5-C6-N1	5.35	120.37	117.70
80	B5	509	U	N3-C4-C5	5.35	117.81	114.60
80	B5	987	U	C5-C4-O4	5.34	129.11	125.90
80	B5	1846	C	N1-C2-N3	5.34	122.94	119.20
80	B5	3025	C	N3-C2-O2	-5.34	118.16	121.90
80	B5	76	G	N1-C6-O6	5.34	123.11	119.90
80	B5	141	C	C6-N1-C2	-5.34	118.16	120.30
80	B5	419	G	C5-C6-N1	5.34	114.17	111.50
80	B5	706	A	N1-C6-N6	5.34	121.81	118.60
80	B5	1011	A	C2-N3-C4	-5.34	107.93	110.60
80	B5	3141	A	N1-C2-N3	5.34	131.97	129.30
84	CW	38	A	C6-C5-N7	-5.34	128.56	132.30
80	B5	2300	G	C5-C6-N1	5.34	114.17	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2629	U	C2-N3-C4	-5.34	123.80	127.00
81	B7	35	C	N1-C2-O2	-5.34	115.70	118.90
80	B5	2636	A	N1-C6-N6	-5.34	115.40	118.60
82	B8	6	U	C5-C4-O4	-5.34	122.70	125.90
80	B5	1369	A	N1-C2-N3	-5.34	126.63	129.30
80	B5	1885	U	N1-C2-O2	-5.34	119.06	122.80
80	B5	2279	A	C2-N3-C4	-5.34	107.93	110.60
80	B5	2755	C	C4-C5-C6	5.34	120.07	117.40
80	B5	3368	U	C2-N1-C1'	-5.34	111.30	117.70
80	B5	3227	A	C2-N3-C4	-5.33	107.93	110.60
84	CW	23	A	C5-C6-N1	-5.33	115.03	117.70
2	A1	29	ARG	NE-CZ-NH1	5.33	122.97	120.30
79	B2	1145	U	N3-C2-O2	5.33	125.93	122.20
80	B5	564	G	C5-N7-C8	5.33	106.97	104.30
80	B5	924	G	C5-C6-O6	-5.33	125.40	128.60
80	B5	972	A	C5-N7-C8	5.33	106.57	103.90
80	B5	1378	U	N3-C4-C5	5.33	117.80	114.60
80	B5	1804	A	C8-N9-C4	5.33	107.93	105.80
80	B5	3031	G	C5-C6-O6	-5.33	125.40	128.60
80	B5	3336	A	C2-N3-C4	-5.33	107.93	110.60
82	B8	11	C	N1-C2-O2	5.33	122.10	118.90
83	CV	72	LEU	C-N-CA	5.33	135.03	121.70
80	B5	806	A	C6-N1-C2	5.33	121.80	118.60
80	B5	3173	G	C4-C5-N7	5.33	112.93	110.80
79	B2	554	C	C6-N1-C1'	-5.33	114.40	120.80
80	B5	494	G	N1-C6-O6	-5.33	116.70	119.90
80	B5	1203	A	N1-C6-N6	5.33	121.80	118.60
79	B2	214	G	C8-N9-C1'	5.33	133.93	127.00
79	B2	350	U	C5-C6-N1	-5.33	120.04	122.70
80	B5	327	A	N1-C2-N3	-5.33	126.64	129.30
81	B7	83	U	N3-C4-O4	-5.33	115.67	119.40
83	CV	507	THR	C-N-CA	5.33	135.02	121.70
79	B2	1370	U	C2-N1-C1'	5.33	124.09	117.70
80	B5	413	U	C5-C4-O4	-5.33	122.70	125.90
79	B2	392	G	C5-C6-O6	-5.33	125.41	128.60
79	B2	1481	C	C5-C6-N1	5.33	123.66	121.00
80	B5	496	C	N3-C2-O2	-5.33	118.17	121.90
80	B5	1808	G	C5-C6-O6	-5.33	125.41	128.60
80	B5	3138	U	N3-C2-O2	5.33	125.93	122.20
84	CW	4	C	N3-C4-N4	5.33	121.73	118.00
79	B2	313	U	C5-C4-O4	5.32	129.09	125.90
80	B5	800	G	N9-C4-C5	-5.32	103.27	105.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1192	C	N1-C2-N3	5.32	122.93	119.20
80	B5	1389	G	C8-N9-C4	5.32	108.53	106.40
80	B5	3246	G	N1-C6-O6	5.32	123.09	119.90
79	B2	1520	U	C5-C6-N1	-5.32	120.04	122.70
80	B5	1490	A	C6-C5-N7	-5.32	128.57	132.30
80	B5	1917	C	C4-C5-C6	5.32	120.06	117.40
79	B2	274	G	C8-N9-C4	-5.32	104.27	106.40
79	B2	811	A	C4-N9-C1'	5.32	135.88	126.30
79	B2	1052	U	C2-N1-C1'	5.32	124.08	117.70
79	B2	1778	G	N1-C6-O6	-5.32	116.71	119.90
80	B5	887	G	C4-C5-C6	5.32	121.99	118.80
82	B8	87	G	C4-C5-N7	5.32	112.93	110.80
80	B5	282	G	C5-C6-N1	-5.32	108.84	111.50
80	B5	1447	G	N9-C4-C5	5.32	107.53	105.40
79	B2	1119	G	N3-C4-C5	-5.32	125.94	128.60
80	B5	1283	C	P-O5'-C5'	-5.32	112.39	120.90
80	B5	1939	G	C8-N9-C1'	-5.32	120.09	127.00
80	B5	799	G	C5-C6-N1	5.32	114.16	111.50
80	B5	810	A	C4-C5-N7	-5.32	108.04	110.70
80	B5	1116	G	C5-C6-N1	-5.31	108.84	111.50
80	B5	1140	G	N3-C4-N9	5.31	129.19	126.00
80	B5	2342	U	N3-C4-C5	5.31	117.79	114.60
84	CW	29	G	O4'-C1'-N9	5.31	112.45	108.20
79	B2	319	U	N1-C2-N3	-5.31	111.71	114.90
79	B2	583	C	C2-N1-C1'	5.31	124.64	118.80
80	B5	831	G	C5-C6-O6	-5.31	125.41	128.60
80	B5	1929	G	C2-N3-C4	-5.31	109.24	111.90
80	B5	2323	G	C8-N9-C4	-5.31	104.28	106.40
80	B5	3045	G	N3-C4-C5	-5.31	125.94	128.60
82	B8	79	A	C4-C5-N7	5.31	113.36	110.70
82	B8	135	G	C4-C5-N7	-5.31	108.67	110.80
80	B5	2632	G	N3-C2-N2	5.31	123.62	119.90
79	B2	1542	G	N1-C6-O6	-5.31	116.72	119.90
80	B5	524	U	C2-N1-C1'	-5.31	111.33	117.70
80	B5	3245	A	C4-C5-C6	5.31	119.65	117.00
82	B8	95	G	N3-C4-N9	-5.31	122.81	126.00
59	BY	103	LYS	CD-CE-NZ	-5.31	99.49	111.70
79	B2	1736	G	C8-N9-C4	5.31	108.52	106.40
80	B5	496	C	N1-C2-O2	5.31	122.08	118.90
80	B5	802	C	N3-C2-O2	-5.31	118.18	121.90
80	B5	1167	U	N3-C2-O2	5.31	125.92	122.20
80	B5	1376	C	C6-N1-C2	5.31	122.42	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1458	U	C5-C4-O4	-5.31	122.72	125.90
80	B5	1483	G	N1-C6-O6	-5.31	116.72	119.90
80	B5	2369	G	N3-C2-N2	5.31	123.61	119.90
80	B5	3171	U	C6-N1-C2	5.31	124.19	121.00
79	B2	323	A	N7-C8-N9	5.31	116.45	113.80
79	B2	1148	C	C6-N1-C2	5.31	122.42	120.30
84	CW	41	C	C6-N1-C2	-5.31	118.18	120.30
79	B2	460	A	C4-C5-C6	-5.30	114.35	117.00
79	B2	1461	C	C6-N1-C2	5.30	122.42	120.30
80	B5	1054	A	N9-C4-C5	-5.30	103.68	105.80
80	B5	2836	C	N1-C2-O2	-5.30	115.72	118.90
79	B2	343	C	C6-N1-C2	-5.30	118.18	120.30
80	B5	1442	U	C2-N3-C4	-5.30	123.82	127.00
80	B5	2175	U	C2-N1-C1'	-5.30	111.34	117.70
80	B5	3112	G	N7-C8-N9	-5.30	110.45	113.10
48	BN	174	ILE	CG1-CB-CG2	-5.30	99.74	111.40
48	BN	201	ARG	NE-CZ-NH1	5.30	122.95	120.30
80	B5	35	A	N1-C2-N3	5.30	131.95	129.30
84	CW	58	A	C5-C6-N1	-5.30	115.05	117.70
80	B5	568	G	N1-C6-O6	-5.30	116.72	119.90
80	B5	815	G	N3-C4-C5	-5.30	125.95	128.60
80	B5	881	C	C5-C6-N1	5.30	123.65	121.00
80	B5	1137	C	N3-C4-C5	-5.30	119.78	121.90
80	B5	1307	G	N3-C2-N2	5.30	123.61	119.90
79	B2	68	A	N7-C8-N9	5.30	116.45	113.80
79	B2	1454	G	C4-C5-N7	-5.30	108.68	110.80
79	B2	1600	A	N1-C2-N3	5.30	131.95	129.30
80	B5	948	C	C4-C5-C6	5.30	120.05	117.40
80	B5	1325	U	N1-C2-N3	5.30	118.08	114.90
80	B5	1856	C	N3-C2-O2	-5.30	118.19	121.90
80	B5	2897	A	C5-N7-C8	5.30	106.55	103.90
80	B5	3294	A	N1-C2-N3	5.30	131.95	129.30
81	B7	100	C	C2-N3-C4	-5.30	117.25	119.90
80	B5	1586	G	C6-C5-N7	-5.29	127.22	130.40
80	B5	1741	A	N1-C2-N3	5.29	131.95	129.30
80	B5	2942	C	N1-C2-O2	-5.29	115.72	118.90
31	AW	93	LEU	CA-CB-CG	5.29	127.47	115.30
50	BP	127	ARG	NE-CZ-NH2	-5.29	117.65	120.30
79	B2	557	G	N3-C4-C5	-5.29	125.95	128.60
80	B5	632	G	C5-C6-N1	5.29	114.15	111.50
80	B5	2422	C	N3-C4-C5	5.29	124.02	121.90
81	B7	11	A	C5-C6-N1	-5.29	115.05	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BN	172	ARG	NE-CZ-NH1	-5.29	117.65	120.30
80	B5	186	U	N1-C2-O2	5.29	126.50	122.80
80	B5	637	C	C6-N1-C1'	5.29	127.15	120.80
80	B5	1080	A	N1-C2-N3	5.29	131.95	129.30
80	B5	1315	U	C6-N1-C2	5.29	124.17	121.00
80	B5	2303	A	C5-C6-N1	5.29	120.34	117.70
80	B5	2344	U	N1-C2-N3	5.29	118.08	114.90
80	B5	2893	C	N3-C2-O2	5.29	125.60	121.90
80	B5	2928	C	C2-N1-C1'	5.29	124.62	118.80
80	B5	2930	A	C5-C6-N1	5.29	120.34	117.70
81	B7	14	U	N1-C2-N3	5.29	118.07	114.90
79	B2	380	U	C6-N1-C2	-5.29	117.83	121.00
80	B5	2609	A	N7-C8-N9	-5.29	111.16	113.80
79	B2	137	U	N3-C2-O2	-5.29	118.50	122.20
80	B5	960	U	C6-N1-C1'	-5.29	113.80	121.20
80	B5	1007	U	N3-C4-C5	5.29	117.77	114.60
80	B5	1869	C	C5-C6-N1	-5.29	118.36	121.00
80	B5	2921	U	N1-C2-N3	5.29	118.07	114.90
80	B5	719	U	N3-C2-O2	-5.29	118.50	122.20
80	B5	998	A	C5-N7-C8	5.29	106.54	103.90
80	B5	1264	G	C5'-C4'-O4'	5.29	115.44	109.10
80	B5	1272	C	N3-C4-N4	5.29	121.70	118.00
80	B5	1274	A	C6-C5-N7	-5.29	128.60	132.30
80	B5	1375	G	C8-N9-C4	-5.29	104.29	106.40
80	B5	2163	C	N3-C4-C5	5.29	124.02	121.90
80	B5	1281	G	C5-C6-O6	-5.28	125.43	128.60
80	B5	2572	C	C6-N1-C1'	-5.28	114.46	120.80
80	B5	2664	C	C4-C5-C6	-5.28	114.76	117.40
80	B5	3307	A	C6-N1-C2	5.28	121.77	118.60
39	BE	26	ARG	NE-CZ-NH2	-5.28	117.66	120.30
79	B2	308	C	C6-N1-C2	5.28	122.41	120.30
80	B5	432	G	N3-C2-N2	5.28	123.60	119.90
80	B5	1114	U	C2-N3-C4	-5.28	123.83	127.00
80	B5	1220	U	C5-C6-N1	-5.28	120.06	122.70
80	B5	2167	A	C5-C6-N1	5.28	120.34	117.70
80	B5	2261	G	N7-C8-N9	-5.28	110.46	113.10
80	B5	3315	G	C4-C5-N7	-5.28	108.69	110.80
80	B5	975	C	N1-C2-N3	5.28	122.89	119.20
80	B5	1085	A	C4-C5-N7	5.28	113.34	110.70
80	B5	1283	C	C3'-C2'-C1'	5.28	105.72	101.50
80	B5	2359	C	N3-C4-N4	-5.28	114.30	118.00
80	B5	2549	G	C5-N7-C8	-5.28	101.66	104.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	B8	99	C	C5-C6-N1	-5.28	118.36	121.00
80	B5	637	C	C2-N3-C4	-5.28	117.26	119.90
80	B5	1628	C	C6-N1-C2	-5.28	118.19	120.30
80	B5	2625	C	N3-C4-C5	5.28	124.01	121.90
80	B5	147	U	C5-C4-O4	5.28	129.06	125.90
80	B5	354	U	C5-C6-N1	-5.28	120.06	122.70
80	B5	1788	C	C4-C5-C6	5.28	120.04	117.40
80	B5	2976	A	C5-C6-N1	5.28	120.34	117.70
83	CV	23	ASP	CB-CG-OD1	5.28	123.05	118.30
80	B5	689	U	N3-C4-C5	5.27	117.76	114.60
80	B5	1445	U	N1-C2-O2	-5.27	119.11	122.80
80	B5	2852	C	N1-C2-O2	-5.27	115.74	118.90
79	B2	1093	A	C8-N9-C4	5.27	107.91	105.80
80	B5	979	U	C2-N1-C1'	5.27	124.03	117.70
37	BC	98	ARG	NE-CZ-NH2	-5.27	117.66	120.30
80	B5	376	G	N3-C4-C5	-5.27	125.97	128.60
80	B5	1276	U	C2-N1-C1'	5.27	124.03	117.70
80	B5	2732	G	C5-N7-C8	5.27	106.94	104.30
80	B5	421	G	C5-C6-N1	5.27	114.14	111.50
80	B5	656	A	C5-N7-C8	5.27	106.53	103.90
80	B5	2658	G	C8-N9-C4	5.27	108.51	106.40
80	B5	2721	A	N3-C4-C5	-5.27	123.11	126.80
80	B5	2798	C	N3-C4-C5	-5.27	119.79	121.90
23	AO	107	ARG	NE-CZ-NH1	5.27	122.93	120.30
80	B5	1249	G	P-O5'-C5'	5.27	129.33	120.90
80	B5	1346	G	C8-N9-C4	5.27	108.51	106.40
80	B5	1786	G	N3-C4-C5	-5.27	125.97	128.60
80	B5	1833	G	N1-C2-N2	-5.27	111.46	116.20
80	B5	2211	U	C6-N1-C2	-5.27	117.84	121.00
80	B5	2403	G	N3-C4-N9	5.27	129.16	126.00
80	B5	2882	U	N3-C4-O4	-5.27	115.71	119.40
80	B5	2979	U	N1-C2-N3	-5.27	111.74	114.90
80	B5	3045	G	C4-C5-N7	-5.27	108.69	110.80
80	B5	3247	G	C4-C5-N7	-5.27	108.69	110.80
84	CW	39	U	O4'-C1'-N1	5.27	112.41	108.20
22	AN	22	ALA	C-N-CA	5.27	144.12	122.00
79	B2	190	C	C6-N1-C2	5.27	122.41	120.30
81	B7	50	U	C6-N1-C2	-5.27	117.84	121.00
79	B2	647	G	C8-N9-C4	-5.26	104.29	106.40
79	B2	1297	G	C4-N9-C1'	-5.26	119.66	126.50
80	B5	98	G	C4-C5-N7	5.26	112.91	110.80
80	B5	784	A	C4-C5-N7	5.26	113.33	110.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	929	A	C5-N7-C8	5.26	106.53	103.90
80	B5	1229	G	C4-N9-C1'	5.26	133.34	126.50
80	B5	1939	G	C4-N9-C1'	5.26	133.34	126.50
80	B5	2884	C	C5-C4-N4	-5.26	116.52	120.20
80	B5	2930	A	N1-C2-N3	-5.26	126.67	129.30
80	B5	2965	U	N3-C4-O4	5.26	123.08	119.40
84	CW	55	U	C5'-C4'-C3'	5.26	124.42	116.00
80	B5	1180	A	C2-N3-C4	-5.26	107.97	110.60
80	B5	1432	C	C2-N1-C1'	5.26	124.59	118.80
80	B5	2851	A	C2-N3-C4	-5.26	107.97	110.60
79	B2	527	A	N7-C8-N9	5.26	116.43	113.80
79	B2	1195	C	P-O3'-C3'	5.26	126.01	119.70
79	B2	1454	G	C5-N7-C8	5.26	106.93	104.30
79	B2	1541	G	N3-C4-C5	-5.26	125.97	128.60
79	B2	1761	U	N1-C2-N3	5.26	118.06	114.90
80	B5	323	A	N1-C2-N3	5.26	131.93	129.30
80	B5	582	G	C4-C5-N7	-5.26	108.69	110.80
80	B5	693	A	C5-C6-N6	5.26	127.91	123.70
80	B5	329	U	C6-N1-C2	5.26	124.16	121.00
80	B5	1050	U	C5-C4-O4	5.26	129.06	125.90
80	B5	1506	A	N9-C4-C5	5.26	107.90	105.80
80	B5	3309	G	C2-N3-C4	5.26	114.53	111.90
79	B2	605	A	C8-N9-C4	5.26	107.90	105.80
79	B2	1245	G	N3-C4-N9	-5.26	122.84	126.00
80	B5	3369	G	C5-C6-N1	5.26	114.13	111.50
79	B2	1600	A	N3-C4-C5	5.26	130.48	126.80
80	B5	218	G	N1-C6-O6	-5.26	116.75	119.90
80	B5	410	U	C5-C6-N1	-5.26	120.07	122.70
80	B5	2213	A	N7-C8-N9	-5.26	111.17	113.80
80	B5	2391	G	C5-C6-O6	5.26	131.75	128.60
81	B7	41	G	C5-C6-N1	5.26	114.13	111.50
82	B8	77	A	C2-N3-C4	-5.26	107.97	110.60
82	B8	121	U	N3-C2-O2	-5.26	118.52	122.20
80	B5	406	G	O4'-C1'-N9	5.25	112.40	108.20
80	B5	1153	A	C5-C6-N6	-5.25	119.50	123.70
80	B5	1901	A	C8-N9-C1'	-5.25	118.24	127.70
80	B5	2665	U	C5-C6-N1	5.25	125.33	122.70
80	B5	2279	A	N1-C6-N6	5.25	121.75	118.60
80	B5	2370	G	N3-C4-N9	5.25	129.15	126.00
80	B5	3048	A	C5-C6-N1	5.25	120.33	117.70
82	B8	147	U	C2-N3-C4	-5.25	123.85	127.00
44	BJ	10	ARG	NE-CZ-NH2	-5.25	117.67	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	BO	182[B]	SER	CA-C-N	5.25	128.75	117.20
79	B2	1614	A	N1-C6-N6	5.25	121.75	118.60
80	B5	333	G	C2-N3-C4	-5.25	109.27	111.90
80	B5	2721	A	C5-C6-N1	5.25	120.33	117.70
80	B5	3321	C	C6-N1-C2	5.25	122.40	120.30
84	CW	42	C	C3'-C2'-C1'	-5.25	97.30	101.50
80	B5	985	U	C6-N1-C2	5.25	124.15	121.00
80	B5	2772	C	P-O3'-C3'	5.25	126.00	119.70
80	B5	3177	G	C2-N3-C4	-5.25	109.28	111.90
80	B5	3385	U	C5-C6-N1	-5.25	120.08	122.70
37	BC	190	GLY	N-CA-C	5.25	126.22	113.10
79	B2	687	G	N3-C4-N9	-5.25	122.85	126.00
79	B2	969	C	N3-C4-C5	5.25	124.00	121.90
80	B5	1190	A	C4-N9-C1'	5.25	135.75	126.30
80	B5	2606	G	C6-C5-N7	-5.25	127.25	130.40
80	B5	3202	G	C5-C6-O6	5.25	131.75	128.60
79	B2	240	U	N1-C2-O2	5.25	126.47	122.80
79	B2	1086	A	N1-C6-N6	-5.25	115.45	118.60
80	B5	559	A	C8-N9-C4	-5.25	103.70	105.80
80	B5	1100	U	N3-C4-C5	5.25	117.75	114.60
80	B5	1516	C	C4-C5-C6	5.25	120.02	117.40
80	B5	1828	A	N7-C8-N9	5.25	116.42	113.80
80	B5	2374	C	C5-C4-N4	5.25	123.87	120.20
82	B8	12	A	C8-N9-C4	-5.25	103.70	105.80
80	B5	1604	G	N3-C4-C5	-5.25	125.98	128.60
80	B5	2524	A	C2-N3-C4	-5.25	107.98	110.60
80	B5	3028	G	N1-C2-N2	-5.25	111.48	116.20
81	B7	37	G	C8-N9-C4	5.25	108.50	106.40
79	B2	149	C	C6-N1-C2	5.24	122.40	120.30
79	B2	972	G	N1-C6-O6	-5.24	116.75	119.90
79	B2	1258	U	C5-C6-N1	-5.24	120.08	122.70
79	B2	1754	A	C4-C5-C6	-5.24	114.38	117.00
80	B5	911	C	C5-C4-N4	-5.24	116.53	120.20
80	B5	1158	A	N9-C4-C5	-5.24	103.70	105.80
80	B5	1178	G	C5-C6-O6	-5.24	125.45	128.60
80	B5	1724	U	P-O3'-C3'	5.24	125.99	119.70
81	B7	1	G	C4-C5-N7	5.24	112.90	110.80
80	B5	1243	G	N3-C2-N2	5.24	123.57	119.90
80	B5	2724	U	N3-C4-O4	-5.24	115.73	119.40
80	B5	3107	U	N3-C4-O4	-5.24	115.73	119.40
80	B5	3174	A	N1-C6-N6	5.24	121.75	118.60
80	B5	318	A	N1-C2-N3	-5.24	126.68	129.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1500	G	N7-C8-N9	-5.24	110.48	113.10
80	B5	2648	G	N9-C4-C5	-5.24	103.30	105.40
43	BI	99	ILE	CB-CA-C	-5.24	101.12	111.60
79	B2	608	U	C5-C6-N1	-5.24	120.08	122.70
80	B5	804	C	C2-N1-C1'	-5.24	113.04	118.80
80	B5	2321	A	C8-N9-C4	5.24	107.89	105.80
80	B5	2897	A	N7-C8-N9	-5.24	111.18	113.80
79	B2	582	U	C5-C6-N1	5.24	125.32	122.70
80	B5	1421	G	N3-C4-C5	5.24	131.22	128.60
80	B5	1833	G	C5-C6-O6	5.24	131.74	128.60
80	B5	2191	U	C4-C5-C6	5.24	122.84	119.70
79	B2	749	U	C5-C6-N1	5.24	125.32	122.70
80	B5	1324	U	N3-C2-O2	-5.24	118.53	122.20
80	B5	1693	C	N1-C2-O2	-5.24	115.76	118.90
80	B5	1834	U	C5-C6-N1	-5.24	120.08	122.70
80	B5	1876	U	C6-N1-C2	-5.24	117.86	121.00
80	B5	1925	U	N3-C4-C5	5.24	117.74	114.60
82	B8	34	U	C2-N3-C4	-5.24	123.86	127.00
79	B2	938	G	N3-C2-N2	5.23	123.56	119.90
79	B2	1796	C	C5-C4-N4	5.23	123.86	120.20
80	B5	1226	G	C5-C6-N1	-5.23	108.88	111.50
79	B2	1648	A	C5-C6-N1	5.23	120.32	117.70
80	B5	381	U	C5-C6-N1	-5.23	120.08	122.70
80	B5	682	U	C2-N3-C4	-5.23	123.86	127.00
80	B5	961	C	C5-C6-N1	-5.23	118.38	121.00
80	B5	1252	A	C4-C5-C6	5.23	119.62	117.00
80	B5	1265	U	N1-C2-N3	-5.23	111.76	114.90
80	B5	1927	G	C8-N9-C4	-5.23	104.31	106.40
80	B5	2349	U	N1-C2-O2	5.23	126.46	122.80
80	B5	3381	U	C5-C6-N1	-5.23	120.08	122.70
81	B7	88	G	N1-C6-O6	-5.23	116.76	119.90
79	B2	337	G	N3-C4-C5	-5.23	125.98	128.60
79	B2	1600	A	C6-C5-N7	-5.23	128.64	132.30
79	B2	1763	A	C5-N7-C8	-5.23	101.28	103.90
80	B5	227	G	N1-C6-O6	5.23	123.04	119.90
80	B5	299	G	C5-C6-N1	5.23	114.11	111.50
80	B5	661	G	C5-C6-O6	5.23	131.74	128.60
80	B5	857	G	N1-C2-N2	-5.23	111.49	116.20
80	B5	1545	A	C8-N9-C4	5.23	107.89	105.80
80	B5	2279	A	C5-N7-C8	-5.23	101.28	103.90
80	B5	2364	G	C4-C5-N7	-5.23	108.71	110.80
80	B5	2366	C	C2-N3-C4	5.23	122.52	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	3075	G	C5-N7-C8	5.23	106.92	104.30
79	B2	6	G	N3-C4-N9	5.23	129.14	126.00
79	B2	63	G	C5-C6-O6	5.23	131.74	128.60
79	B2	440	U	N1-C2-O2	5.23	126.46	122.80
79	B2	1648	A	N1-C6-N6	-5.23	115.46	118.60
80	B5	813	G	N3-C4-C5	-5.23	125.99	128.60
80	B5	1107	C	N3-C4-C5	5.23	123.99	121.90
80	B5	1317	A	N9-C4-C5	-5.23	103.71	105.80
84	CW	1	G	C1'-O4'-C4'	-5.23	105.72	109.90
81	B7	41	G	C4-C5-N7	5.23	112.89	110.80
51	BQ	178	ARG	NE-CZ-NH2	-5.22	117.69	120.30
79	B2	7	G	C5-C6-O6	5.22	131.74	128.60
80	B5	1403	C	N3-C4-C5	5.22	123.99	121.90
80	B5	1603	A	C5-C6-N1	-5.22	115.09	117.70
80	B5	2207	A	C4-C5-N7	5.22	113.31	110.70
84	CW	49	C	N3-C4-C5	-5.22	119.81	121.90
79	B2	971	A	C2-N3-C4	-5.22	107.99	110.60
79	B2	1258	U	N1-C2-N3	5.22	118.03	114.90
79	B2	1293	U	N3-C2-O2	-5.22	118.54	122.20
80	B5	861	C	N3-C4-N4	5.22	121.66	118.00
80	B5	928	C	C6-N1-C2	-5.22	118.21	120.30
80	B5	1013	G	C4-N9-C1'	5.22	133.29	126.50
80	B5	1714	A	C2-N3-C4	-5.22	107.99	110.60
80	B5	2144	A	N1-C6-N6	5.22	121.73	118.60
80	B5	2193	U	N1-C2-N3	5.22	118.03	114.90
80	B5	2716	U	C5-C4-O4	5.22	129.03	125.90
84	CW	73	A	C5-C6-N6	-5.22	119.52	123.70
79	B2	542	A	C5-C6-N1	-5.22	115.09	117.70
80	B5	595	G	C5-C6-O6	5.22	131.73	128.60
80	B5	2416	U	N1-C2-N3	5.22	118.03	114.90
80	B5	2506	U	C5-C6-N1	5.22	125.31	122.70
79	B2	1448	G	N1-C6-O6	-5.22	116.77	119.90
80	B5	1120	A	N1-C6-N6	-5.22	115.47	118.60
80	B5	1305	U	C5-C6-N1	-5.22	120.09	122.70
80	B5	3106	A	C8-N9-C4	-5.22	103.71	105.80
80	B5	1597	C	N3-C4-C5	-5.22	119.81	121.90
80	B5	1828	A	C2-N3-C4	-5.22	107.99	110.60
80	B5	2112	U	N1-C2-N3	5.22	118.03	114.90
80	B5	3259	U	C6-N1-C2	-5.22	117.87	121.00
81	B7	48	U	N3-C2-O2	5.22	125.85	122.20
80	B5	999	G	C5-C6-N1	5.22	114.11	111.50
80	B5	1149	G	C4-C5-N7	-5.22	108.71	110.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1485	G	N9-C4-C5	5.22	107.49	105.40
80	B5	1527	C	N1-C2-O2	5.22	122.03	118.90
84	CW	54	U	C5'-C4'-C3'	-5.22	107.65	116.00
61	Ba	15	VAL	N-CA-C	-5.21	96.92	111.00
79	B2	139	C	C4-C5-C6	5.21	120.01	117.40
79	B2	1170	G	C5-C6-O6	-5.21	125.47	128.60
79	B2	1611	A	C6-C5-N7	-5.21	128.65	132.30
80	B5	1872	C	N1-C2-N3	5.21	122.85	119.20
80	B5	2122	G	N7-C8-N9	-5.21	110.49	113.10
80	B5	3373	U	C2-N3-C4	-5.21	123.87	127.00
83	CV	60	ALA	N-CA-CB	5.21	117.40	110.10
80	B5	75	G	C5-C6-N1	5.21	114.11	111.50
80	B5	1312	C	C6-N1-C1'	5.21	127.06	120.80
80	B5	1845	G	C8-N9-C4	5.21	108.48	106.40
80	B5	2164	A	C4-C5-C6	5.21	119.61	117.00
80	B5	2693	C	N3-C4-N4	-5.21	114.35	118.00
80	B5	3339	A	N1-C6-N6	5.21	121.73	118.60
79	B2	387	A	N1-C6-N6	-5.21	115.47	118.60
79	B2	944	A	C2-N3-C4	-5.21	107.99	110.60
79	B2	1015	U	N1-C2-O2	5.21	126.45	122.80
80	B5	146	U	C5-C6-N1	-5.21	120.09	122.70
80	B5	284	A	C8-N9-C4	-5.21	103.72	105.80
80	B5	424	G	C5-C6-N1	5.21	114.11	111.50
80	B5	735	A	N7-C8-N9	5.21	116.41	113.80
80	B5	1792	C	C5-C6-N1	-5.21	118.39	121.00
80	B5	992	A	C8-N9-C4	5.21	107.88	105.80
80	B5	2804	A	C2-N3-C4	-5.21	108.00	110.60
80	B5	2877	G	C5-C6-O6	5.21	131.73	128.60
80	B5	3103	A	C6-N1-C2	-5.21	115.47	118.60
82	B8	113	U	C5-C4-O4	-5.21	122.77	125.90
80	B5	1208	U	N1-C2-O2	5.21	126.45	122.80
80	B5	1543	G	N1-C6-O6	-5.21	116.78	119.90
79	B2	445	A	N1-C2-N3	-5.21	126.70	129.30
80	B5	2686	A	N1-C6-N6	5.21	121.72	118.60
80	B5	3110	C	C5-C6-N1	-5.21	118.40	121.00
79	B2	266	A	C2-N3-C4	-5.21	108.00	110.60
84	CW	65	G	O4'-C1'-N9	5.21	112.36	108.20
35	BA	242	ARG	NE-CZ-NH2	-5.20	117.70	120.30
79	B2	192	U	C5-C6-N1	5.20	125.30	122.70
79	B2	1330	G	C8-N9-C1'	5.20	133.76	127.00
80	B5	267	G	N7-C8-N9	-5.20	110.50	113.10
80	B5	1263	A	C5-C6-N1	-5.20	115.10	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1277	C	P-O3'-C3'	5.20	125.94	119.70
80	B5	1327	C	C5-C4-N4	5.20	123.84	120.20
80	B5	1468	A	N7-C8-N9	5.20	116.40	113.80
80	B5	2550	U	N3-C2-O2	-5.20	118.56	122.20
80	B5	702	C	N3-C4-C5	5.20	123.98	121.90
80	B5	943	U	C5-C4-O4	-5.20	122.78	125.90
79	B2	1672	G	N3-C4-C5	-5.20	126.00	128.60
80	B5	83	U	C6-N1-C1'	-5.20	113.92	121.20
80	B5	197	G	C4-N9-C1'	5.20	133.26	126.50
80	B5	997	A	C8-N9-C4	-5.20	103.72	105.80
80	B5	2271	A	C6-C5-N7	5.20	135.94	132.30
80	B5	2724	U	N3-C2-O2	-5.20	118.56	122.20
80	B5	2942	C	C5-C4-N4	-5.20	116.56	120.20
80	B5	28	C	C6-N1-C2	5.20	122.38	120.30
80	B5	102	C	C4-C5-C6	5.20	120.00	117.40
80	B5	1513	G	N1-C6-O6	-5.20	116.78	119.90
80	B5	1733	G	C6-C5-N7	-5.20	127.28	130.40
80	B5	2526	C	C6-N1-C1'	-5.20	114.56	120.80
80	B5	2634	U	N3-C4-O4	5.20	123.04	119.40
81	B7	40	C	C2-N3-C4	-5.20	117.30	119.90
79	B2	1376	C	C6-N1-C2	5.20	122.38	120.30
80	B5	576	C	C2-N3-C4	-5.20	117.30	119.90
80	B5	610	G	C5-C6-N1	5.20	114.10	111.50
80	B5	1271	A	O4'-C1'-N9	5.20	112.36	108.20
80	B5	3387	U	N3-C2-O2	-5.20	118.56	122.20
82	B8	14	C	N1-C2-O2	-5.20	115.78	118.90
84	CW	31	A	C4-C5-C6	5.20	119.60	117.00
80	B5	307	A	N9-C4-C5	5.19	107.88	105.80
80	B5	580	C	N1-C2-N3	5.19	122.84	119.20
80	B5	1183	C	N3-C4-N4	-5.19	114.36	118.00
80	B5	3255	U	N3-C4-C5	5.19	117.72	114.60
80	B5	3302	U	C5-C6-N1	-5.19	120.10	122.70
49	BO	16[B]	LEU	O-C-N	-5.19	114.37	123.20
50	BP	23	ARG	NE-CZ-NH1	5.19	122.90	120.30
79	B2	987	G	C8-N9-C4	5.19	108.48	106.40
80	B5	1404	G	N1-C2-N2	-5.19	111.53	116.20
80	B5	2379	U	C5-C6-N1	-5.19	120.10	122.70
79	B2	139	C	P-O3'-C3'	5.19	125.93	119.70
79	B2	971	A	N1-C2-N3	5.19	131.90	129.30
79	B2	1462	G	N3-C4-N9	5.19	129.12	126.00
79	B2	1503	A	C5-C6-N1	-5.19	115.10	117.70
80	B5	84	U	N3-C4-O4	5.19	123.03	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	515	C	C5-C4-N4	-5.19	116.57	120.20
80	B5	613	G	C4-C5-N7	-5.19	108.72	110.80
80	B5	2406	C	C4-C5-C6	5.19	120.00	117.40
82	B8	95	G	N3-C4-C5	5.19	131.19	128.60
84	CW	19	G	C8-N9-C1'	5.19	133.75	127.00
79	B2	1116	A	N1-C6-N6	5.19	121.71	118.60
82	B8	32	C	N3-C2-O2	5.19	125.53	121.90
79	B2	361	C	C5-C6-N1	5.19	123.59	121.00
79	B2	1033	C	N3-C2-O2	-5.19	118.27	121.90
80	B5	102	C	N1-C2-O2	-5.19	115.79	118.90
80	B5	2228	A	N7-C8-N9	5.19	116.39	113.80
80	B5	2344	U	N1-C2-O2	-5.19	119.17	122.80
80	B5	2386	A	C4-C5-N7	5.19	113.29	110.70
80	B5	2830	G	C8-N9-C4	-5.19	104.33	106.40
79	B2	1148	C	N3-C4-C5	5.19	123.97	121.90
80	B5	1633	C	N3-C4-C5	-5.19	119.83	121.90
80	B5	2213	A	C5-N7-C8	5.19	106.49	103.90
49	BO	27[B]	VAL	CA-C-N	5.18	128.61	117.20
80	B5	340	C	N3-C2-O2	-5.18	118.27	121.90
80	B5	863	C	C5-C4-N4	5.18	123.83	120.20
80	B5	996	A	N7-C8-N9	-5.18	111.21	113.80
80	B5	1402	C	N1-C2-O2	5.18	122.01	118.90
80	B5	2148	U	N1-C2-N3	5.18	118.01	114.90
80	B5	2584	G	N7-C8-N9	5.18	115.69	113.10
82	B8	109	A	C5-C6-N1	5.18	120.29	117.70
79	B2	1188	G	C8-N9-C4	5.18	108.47	106.40
80	B5	46	U	N1-C2-N3	-5.18	111.79	114.90
80	B5	808	A	C6-N1-C2	5.18	121.71	118.60
80	B5	2340	U	N3-C2-O2	-5.18	118.57	122.20
80	B5	2351	U	N1-C2-O2	5.18	126.43	122.80
80	B5	3052	G	C5-N7-C8	5.18	106.89	104.30
84	CW	55	U	O4'-C1'-N1	5.18	112.35	108.20
37	BC	230	VAL	CB-CA-C	-5.18	101.56	111.40
80	B5	625	G	N3-C4-N9	-5.18	122.89	126.00
80	B5	943	U	C6-N1-C2	5.18	124.11	121.00
79	B2	712	G	N7-C8-N9	5.18	115.69	113.10
79	B2	1270	G	N1-C6-O6	-5.18	116.79	119.90
80	B5	1205	A	C2-N3-C4	5.18	113.19	110.60
80	B5	1603	A	C4-C5-C6	5.18	119.59	117.00
80	B5	2135	U	N3-C4-C5	5.18	117.71	114.60
80	B5	3098	G	N3-C2-N2	5.18	123.53	119.90
80	B5	3386	G	N1-C2-N3	5.18	127.01	123.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	CW	66	U	P-O5'-C5'	5.18	129.19	120.90
80	B5	1655	G	C5-N7-C8	-5.18	101.71	104.30
80	B5	2353	G	C4-C5-N7	5.18	112.87	110.80
49	BO	104[B]	ILE	CA-C-N	-5.18	105.81	117.20
79	B2	139	C	N1-C2-N3	5.18	122.82	119.20
79	B2	432	G	C5-C6-N1	5.18	114.09	111.50
79	B2	811	A	N3-C4-C5	-5.18	123.18	126.80
79	B2	1200	G	N7-C8-N9	5.18	115.69	113.10
80	B5	110	G	C5-C6-N1	5.18	114.09	111.50
80	B5	340	C	C4-C5-C6	5.18	119.99	117.40
80	B5	1476	G	N7-C8-N9	-5.18	110.51	113.10
80	B5	1704	A	C8-N9-C4	5.18	107.87	105.80
80	B5	2158	A	C5-C6-N1	5.18	120.29	117.70
80	B5	2833	A	C6-C5-N7	5.18	135.92	132.30
81	B7	90	U	C2-N3-C4	-5.18	123.89	127.00
79	B2	378	A	C4-C5-N7	5.17	113.29	110.70
80	B5	112	U	N3-C4-O4	5.17	123.02	119.40
80	B5	2280	A	C8-N9-C4	5.17	107.87	105.80
80	B5	2635	A	C8-N9-C4	-5.17	103.73	105.80
80	B5	2692	A	C4-C5-N7	-5.17	108.11	110.70
80	B5	437	G	C5-C6-O6	-5.17	125.50	128.60
80	B5	802	C	N1-C2-N3	5.17	122.82	119.20
80	B5	817	A	N9-C4-C5	5.17	107.87	105.80
80	B5	1805	C	C6-N1-C2	5.17	122.37	120.30
80	B5	3218	A	N3-C4-N9	-5.17	123.26	127.40
82	B8	24	G	C5-C6-O6	5.17	131.70	128.60
84	CW	14	A	C5-N7-C8	5.17	106.49	103.90
79	B2	49	C	C6-N1-C2	-5.17	118.23	120.30
79	B2	391	A	C4-C5-C6	-5.17	114.42	117.00
79	B2	783	G	C8-N9-C1'	-5.17	120.28	127.00
79	B2	994	G	C4-C5-N7	-5.17	108.73	110.80
79	B2	1781	A	C4-C5-N7	-5.17	108.11	110.70
80	B5	902	G	N7-C8-N9	-5.17	110.52	113.10
80	B5	1087	G	N1-C6-O6	5.17	123.00	119.90
80	B5	2604	U	N3-C4-C5	-5.17	111.50	114.60
80	B5	2706	G	N1-C6-O6	-5.17	116.80	119.90
80	B5	2790	A	C5-C6-N1	5.17	120.29	117.70
61	Ba	14	HIS	N-CA-C	-5.17	97.04	111.00
40	BF	232	ARG	NE-CZ-NH1	-5.17	117.72	120.30
79	B2	1363	U	N3-C2-O2	-5.17	118.58	122.20
80	B5	969	C	C6-N1-C2	5.17	122.37	120.30
80	B5	1316	C	C5-C6-N1	5.17	123.58	121.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2565	U	C6-N1-C2	-5.17	117.90	121.00
80	B5	3333	G	C4-C5-N7	5.17	112.87	110.80
82	B8	8	C	N1-C2-N3	5.17	122.82	119.20
84	CW	2	C	C3'-C2'-C1'	5.17	105.63	101.50
80	B5	39	A	N3-C4-C5	-5.17	123.18	126.80
80	B5	234	G	C5-C6-O6	-5.17	125.50	128.60
80	B5	852	U	N3-C2-O2	-5.17	118.58	122.20
80	B5	1004	U	N1-C2-N3	-5.17	111.80	114.90
80	B5	1226	G	C6-C5-N7	-5.17	127.30	130.40
80	B5	1257	C	C6-N1-C2	-5.17	118.23	120.30
80	B5	2145	A	N3-C4-C5	-5.17	123.18	126.80
84	CW	63	G	C3'-C2'-C1'	-5.17	97.37	101.50
79	B2	782	U	P-O3'-C3'	5.17	125.90	119.70
79	B2	815	G	C8-N9-C1'	5.17	133.71	127.00
79	B2	1784	C	N3-C4-C5	5.17	123.97	121.90
80	B5	2881	C	N1-C2-N3	5.17	122.82	119.20
80	B5	3094	A	C5-N7-C8	5.17	106.48	103.90
79	B2	1051	G	C8-N9-C1'	-5.16	120.29	127.00
79	B2	1354	G	C8-N9-C4	-5.16	104.33	106.40
79	B2	1431	C	C6-N1-C2	5.16	122.36	120.30
80	B5	926	A	C4-C5-C6	-5.16	114.42	117.00
80	B5	3318	G	C5-C6-O6	5.16	131.70	128.60
81	B7	120	C	C5-C6-N1	-5.16	118.42	121.00
82	B8	31	G	C5-N7-C8	5.16	106.88	104.30
80	B5	3335	A	C5-N7-C8	-5.16	101.32	103.90
79	B2	142	G	C5-C6-N1	-5.16	108.92	111.50
80	B5	341	G	C4-C5-N7	5.16	112.86	110.80
80	B5	1445	U	C6-N1-C2	5.16	124.10	121.00
80	B5	2290	C	N1-C2-O2	-5.16	115.80	118.90
80	B5	2810	C	C2-N3-C4	-5.16	117.32	119.90
80	B5	2858	U	C2-N1-C1'	5.16	123.89	117.70
80	B5	2941	A	C8-N9-C4	5.16	107.86	105.80
84	CW	15	G	O4'-C1'-N9	5.16	112.33	108.20
79	B2	7	G	N9-C4-C5	5.16	107.46	105.40
80	B5	3107	U	N1-C2-O2	5.16	126.41	122.80
82	B8	45	C	C4-C5-C6	5.16	119.98	117.40
79	B2	1761	U	N3-C2-O2	-5.16	118.59	122.20
80	B5	1137	C	N3-C4-N4	5.16	121.61	118.00
80	B5	1637	A	N1-C6-N6	-5.16	115.51	118.60
80	B5	1832	C	C5-C6-N1	-5.16	118.42	121.00
80	B5	1938	U	C6-N1-C2	5.16	124.09	121.00
80	B5	583	G	C8-N9-C4	5.16	108.46	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	635	G	N3-C4-C5	5.16	131.18	128.60
80	B5	1238	C	C4'-C3'-C2'	-5.16	97.44	102.60
79	B2	572	C	N3-C2-O2	-5.15	118.29	121.90
80	B5	2614	G	C2-N3-C4	-5.15	109.32	111.90
84	CW	4	C	O4'-C1'-N1	5.15	112.32	108.20
76	Bq	87	VAL	N-CA-C	-5.15	97.09	111.00
80	B5	726	G	N7-C8-N9	5.15	115.68	113.10
80	B5	893	C	N3-C2-O2	5.15	125.51	121.90
80	B5	903	U	N3-C4-C5	5.15	117.69	114.60
80	B5	1231	A	C5-C6-N6	-5.15	119.58	123.70
80	B5	2142	A	C5-C6-N6	-5.15	119.58	123.70
80	B5	2600	C	C2-N1-C1'	5.15	124.47	118.80
80	B5	2960	C	C2-N3-C4	-5.15	117.32	119.90
79	B2	766	U	N1-C2-O2	5.15	126.41	122.80
80	B5	1205	A	C5-N7-C8	-5.15	101.32	103.90
80	B5	1695	U	N3-C2-O2	-5.15	118.59	122.20
80	B5	2139	A	N1-C6-N6	-5.15	115.51	118.60
80	B5	2899	C	C2-N3-C4	-5.15	117.33	119.90
81	B7	79	A	C8-N9-C4	-5.15	103.74	105.80
81	B7	89	G	C5-C6-N1	5.15	114.08	111.50
80	B5	66	A	N7-C8-N9	-5.15	111.23	113.80
80	B5	1272	C	C2-N3-C4	5.15	122.47	119.90
80	B5	2831	G	C2-N3-C4	5.15	114.47	111.90
80	B5	2841	G	N3-C2-N2	5.15	123.50	119.90
80	B5	3130	A	C4-C5-C6	5.15	119.57	117.00
52	BR	42	ARG	NE-CZ-NH2	-5.15	117.73	120.30
80	B5	1138	U	N3-C4-O4	-5.15	115.80	119.40
80	B5	2375	G	C5-N7-C8	-5.15	101.73	104.30
80	B5	2934	A	N1-C6-N6	-5.15	115.51	118.60
80	B5	3180	A	C6-N1-C2	-5.15	115.51	118.60
85	CX	2	U	C2-N3-C4	-5.15	123.91	127.00
79	B2	140	A	C4-N9-C1'	5.15	135.56	126.30
80	B5	3241	G	N1-C6-O6	5.15	122.99	119.90
81	B7	75	G	N3-C2-N2	-5.15	116.30	119.90
79	B2	1245	G	C4-N9-C1'	-5.14	119.81	126.50
80	B5	860	G	N3-C4-C5	-5.14	126.03	128.60
80	B5	979	U	N1-C2-N3	-5.14	111.81	114.90
80	B5	1658	G	C5-C6-O6	5.14	131.69	128.60
80	B5	2549	G	C8-N9-C1'	-5.14	120.31	127.00
80	B5	3019	U	C5-C6-N1	-5.14	120.13	122.70
79	B2	564	G	C5-C6-O6	5.14	131.69	128.60
79	B2	1536	G	N3-C4-C5	-5.14	126.03	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	80	G	C5-C6-O6	5.14	131.69	128.60
80	B5	367	A	C2-N3-C4	-5.14	108.03	110.60
80	B5	809	G	C8-N9-C4	5.14	108.46	106.40
80	B5	1278	A	C5-C6-N1	-5.14	115.13	117.70
80	B5	1466	G	N1-C6-O6	-5.14	116.81	119.90
80	B5	1822	C	C6-N1-C2	5.14	122.36	120.30
80	B5	2169	G	N9-C4-C5	5.14	107.46	105.40
80	B5	3100	U	N3-C2-O2	-5.14	118.60	122.20
85	CX	1	A	C4-C5-C6	5.14	119.57	117.00
79	B2	26	A	C8-N9-C4	-5.14	103.74	105.80
80	B5	1259	A	C5-C6-N1	-5.14	115.13	117.70
81	B7	77	G	C6-C5-N7	-5.14	127.31	130.40
82	B8	51	G	N3-C2-N2	-5.14	116.30	119.90
79	B2	422	G	C8-N9-C4	-5.14	104.34	106.40
80	B5	2352	A	C5-N7-C8	5.14	106.47	103.90
80	B5	3101	G	N3-C2-N2	5.14	123.50	119.90
79	B2	638	U	C2-N3-C4	-5.14	123.92	127.00
80	B5	434	U	N1-C2-O2	5.14	126.40	122.80
79	B2	992	A	N7-C8-N9	5.14	116.37	113.80
79	B2	1200	G	C8-N9-C4	-5.14	104.34	106.40
79	B2	1751	C	C2-N3-C4	-5.14	117.33	119.90
80	B5	433	A	C8-N9-C4	5.14	107.86	105.80
80	B5	436	A	N1-C2-N3	5.14	131.87	129.30
80	B5	1114	U	C5-C4-O4	-5.14	122.82	125.90
80	B5	1142	G	N3-C2-N2	5.14	123.50	119.90
80	B5	1310	G	C5-C6-N1	5.14	114.07	111.50
80	B5	1377	G	C8-N9-C4	-5.14	104.34	106.40
80	B5	3294	A	C5-C6-N6	5.14	127.81	123.70
79	B2	312	A	C8-N9-C4	-5.13	103.75	105.80
79	B2	502	U	C5-C6-N1	5.13	125.27	122.70
79	B2	577	G	C2-N3-C4	-5.13	109.33	111.90
80	B5	1851	G	C4-N9-C1'	5.13	133.18	126.50
80	B5	2118	C	C5-C4-N4	5.13	123.79	120.20
80	B5	2848	G	C4-N9-C1'	5.13	133.18	126.50
80	B5	928	C	C2-N3-C4	-5.13	117.33	119.90
80	B5	2737	C	N1-C2-O2	-5.13	115.82	118.90
79	B2	555	A	N9-C4-C5	5.13	107.85	105.80
79	B2	1000	C	C6-N1-C2	5.13	122.35	120.30
80	B5	894	G	C4-C5-N7	5.13	112.85	110.80
80	B5	1445	U	N3-C2-O2	5.13	125.79	122.20
80	B5	1813	A	C8-N9-C4	-5.13	103.75	105.80
80	B5	2309	A	N1-C6-N6	5.13	121.68	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2855	U	N3-C4-C5	5.13	117.68	114.60
60	BZ	121	ARG	NE-CZ-NH1	5.13	122.86	120.30
79	B2	20	G	N1-C2-N2	-5.13	111.58	116.20
79	B2	294	C	N1-C2-N3	-5.13	115.61	119.20
79	B2	1189	A	N7-C8-N9	-5.13	111.23	113.80
80	B5	2272	G	O4'-C1'-N9	5.13	112.30	108.20
81	B7	35	C	N3-C4-C5	5.13	123.95	121.90
79	B2	886	U	N3-C2-O2	-5.13	118.61	122.20
80	B5	1412	G	N3-C2-N2	-5.13	116.31	119.90
80	B5	1726	C	C6-N1-C2	5.13	122.35	120.30
80	B5	2246	G	C6-C5-N7	5.13	133.48	130.40
79	B2	810	G	C4-N9-C1'	5.13	133.16	126.50
79	B2	927	C	C6-N1-C2	-5.13	118.25	120.30
79	B2	1245	G	N3-C4-C5	5.13	131.16	128.60
79	B2	1441	C	C6-N1-C2	5.13	122.35	120.30
80	B5	149	U	N3-C2-O2	-5.13	118.61	122.20
80	B5	2245	C	N1-C2-N3	5.13	122.79	119.20
80	B5	968	G	C6-N1-C2	5.12	128.18	125.10
80	B5	2866	U	N1-C2-N3	5.12	117.97	114.90
79	B2	1187	U	N3-C2-O2	-5.12	118.61	122.20
80	B5	1250	G	O4'-C1'-N9	5.12	112.30	108.20
80	B5	2518	C	C4-C5-C6	5.12	119.96	117.40
80	B5	2731	U	N1-C2-N3	5.12	117.97	114.90
80	B5	2988	C	C5-C4-N4	5.12	123.79	120.20
80	B5	3074	G	N1-C2-N2	-5.12	111.59	116.20
80	B5	3186	A	N7-C8-N9	5.12	116.36	113.80
84	CW	25	C	N3-C4-N4	5.12	121.59	118.00
84	CW	64	A	C5-C6-N1	-5.12	115.14	117.70
79	B2	586	G	N1-C6-O6	-5.12	116.83	119.90
79	B2	866	G	C8-N9-C4	5.12	108.45	106.40
79	B2	1782	A	C5-C6-N1	-5.12	115.14	117.70
80	B5	114	A	C5-C6-N1	-5.12	115.14	117.70
80	B5	672	A	C5-C6-N6	-5.12	119.60	123.70
80	B5	2280	A	C5-N7-C8	-5.12	101.34	103.90
80	B5	284	A	N1-C6-N6	-5.12	115.53	118.60
80	B5	872	U	N3-C4-O4	-5.12	115.82	119.40
80	B5	1607	U	N3-C4-O4	-5.12	115.82	119.40
80	B5	2124	G	N7-C8-N9	-5.12	110.54	113.10
80	B5	2167	A	N3-C4-C5	-5.12	123.22	126.80
80	B5	3215	A	N9-C4-C5	-5.12	103.75	105.80
80	B5	1270	A	C5-C6-N6	-5.12	119.61	123.70
37	BC	60	THR	CB-CA-C	-5.12	97.79	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	1321	A	N1-C6-N6	-5.12	115.53	118.60
80	B5	2128	C	C6-N1-C2	-5.12	118.25	120.30
82	B8	40	A	N7-C8-N9	5.12	116.36	113.80
79	B2	494	U	C2-N1-C1'	5.11	123.84	117.70
80	B5	919	U	C5-C4-O4	-5.11	122.83	125.90
80	B5	934	G	C8-N9-C1'	-5.11	120.35	127.00
80	B5	2138	A	C5-C6-N1	-5.11	115.14	117.70
80	B5	2820	A	N3-C4-C5	-5.11	123.22	126.80
80	B5	2731	U	C5-C6-N1	-5.11	120.14	122.70
84	CW	40	C	N3-C4-N4	5.11	121.58	118.00
79	B2	359	A	C4-C5-C6	-5.11	114.44	117.00
79	B2	972	G	C5-N7-C8	5.11	106.86	104.30
80	B5	183	G	C3'-C2'-C1'	-5.11	97.41	101.50
80	B5	1482	A	C8-N9-C4	-5.11	103.76	105.80
80	B5	1942	U	C4-C5-C6	5.11	122.77	119.70
80	B5	2884	C	N3-C4-N4	5.11	121.58	118.00
80	B5	2965	U	C5-C6-N1	-5.11	120.14	122.70
84	CW	6	G	C4-N9-C1'	5.11	133.14	126.50
56	BV	87	ARG	NE-CZ-NH2	-5.11	117.75	120.30
79	B2	173	A	C2-N3-C4	-5.11	108.05	110.60
79	B2	1096	C	C6-N1-C2	-5.11	118.26	120.30
80	B5	418	A	C4-C5-C6	5.11	119.55	117.00
80	B5	523	A	N1-C6-N6	-5.11	115.53	118.60
80	B5	1100	U	C5-C4-O4	-5.11	122.83	125.90
80	B5	2978	U	C5-C4-O4	5.11	128.97	125.90
79	B2	1171	A	N1-C6-N6	-5.11	115.54	118.60
80	B5	887	G	N1-C2-N2	-5.11	111.60	116.20
80	B5	943	U	C2-N3-C4	-5.11	123.94	127.00
80	B5	3310	A	C5-N7-C8	5.11	106.45	103.90
80	B5	341	G	N3-C2-N2	-5.11	116.33	119.90
80	B5	1261	G	P-O3'-C3'	-5.11	113.57	119.70
80	B5	2392	C	C2-N1-C1'	-5.11	113.18	118.80
81	B7	51	A	C2-N3-C4	5.11	113.15	110.60
80	B5	1227	C	C2'-C3'-O3'	5.10	121.87	113.70
80	B5	1518	U	C4-C5-C6	-5.10	116.64	119.70
80	B5	3124	G	C4-C5-N7	-5.10	108.76	110.80
79	B2	704	C	C5-C6-N1	5.10	123.55	121.00
80	B5	884	A	C8-N9-C1'	5.10	136.88	127.70
80	B5	1872	C	C2-N3-C4	-5.10	117.35	119.90
80	B5	3056	U	N1-C2-O2	-5.10	119.23	122.80
80	B5	813	G	C4-N9-C1'	5.10	133.13	126.50
80	B5	2278	C	P-O3'-C3'	5.10	125.82	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2745	G	C5-C6-N1	5.10	114.05	111.50
57	BW	39	LEU	CA-CB-CG	5.10	127.03	115.30
80	B5	868	C	C6-N1-C2	5.10	122.34	120.30
80	B5	880	G	C6-N1-C2	-5.10	122.04	125.10
80	B5	1147	G	C5-C6-O6	5.10	131.66	128.60
80	B5	2136	C	C2-N3-C4	-5.10	117.35	119.90
80	B5	2271	A	C5-C6-N6	5.10	127.78	123.70
80	B5	2378	C	C2-N3-C4	5.10	122.45	119.90
80	B5	2393	G	N7-C8-N9	-5.10	110.55	113.10
80	B5	2560	C	N1-C2-O2	5.10	121.96	118.90
82	B8	109	A	C5-N7-C8	-5.10	101.35	103.90
83	CV	468	LEU	N-CA-C	5.10	124.77	111.00
79	B2	111	U	C6-N1-C2	-5.10	117.94	121.00
79	B2	719	U	N3-C2-O2	-5.10	118.63	122.20
79	B2	871	G	N3-C4-N9	5.10	129.06	126.00
79	B2	1643	U	C2-N3-C4	-5.10	123.94	127.00
80	B5	95	A	C5-C6-N1	5.10	120.25	117.70
80	B5	2317	A	C5-N7-C8	-5.10	101.35	103.90
80	B5	3173	G	C6-N1-C2	-5.10	122.04	125.10
81	B7	41	G	C5-C6-O6	-5.10	125.54	128.60
83	CV	434	ILE	N-CA-C	5.10	124.77	111.00
80	B5	1412	G	N9-C4-C5	5.10	107.44	105.40
80	B5	1932	A	N1-C2-N3	5.10	131.85	129.30
82	B8	100	U	C6-N1-C1'	-5.10	114.07	121.20
65	Be	33	ARG	NE-CZ-NH2	-5.09	117.75	120.30
80	B5	1902	G	N9-C4-C5	-5.09	103.36	105.40
81	B7	13	A	C8-N9-C4	-5.09	103.76	105.80
31	AW	104	LEU	CA-CB-CG	5.09	127.01	115.30
80	B5	530	G	N9-C4-C5	5.09	107.44	105.40
80	B5	2848	G	C8-N9-C4	-5.09	104.36	106.40
80	B5	1261	G	O4'-C1'-N9	5.09	112.27	108.20
80	B5	2639	G	C4-C5-C6	5.09	121.86	118.80
80	B5	2695	A	C5-N7-C8	-5.09	101.36	103.90
80	B5	3378	C	N3-C4-N4	-5.09	114.44	118.00
80	B5	2593	A	P-O3'-C3'	5.09	125.81	119.70
80	B5	2691	A	N1-C2-N3	5.09	131.84	129.30
80	B5	3309	G	C8-N9-C4	-5.09	104.36	106.40
84	CW	29	G	C8-N9-C1'	5.09	133.62	127.00
79	B2	278	U	C6-N1-C2	-5.09	117.95	121.00
80	B5	1851	G	C8-N9-C1'	-5.09	120.39	127.00
80	B5	3173	G	N3-C4-N9	5.09	129.05	126.00
80	B5	1509	A	N9-C4-C5	-5.09	103.77	105.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2396	G	C4-C5-N7	-5.09	108.77	110.80
80	B5	2633	U	C2-N3-C4	-5.09	123.95	127.00
80	B5	2716	U	N1-C2-N3	5.09	117.95	114.90
80	B5	3010	U	N1-C2-O2	5.09	126.36	122.80
80	B5	3127	A	C5-C6-N6	5.09	127.77	123.70
79	B2	324	U	N1-C2-N3	5.08	117.95	114.90
79	B2	760	A	N1-C6-N6	5.08	121.65	118.60
80	B5	1077	U	N1-C2-O2	-5.08	119.24	122.80
80	B5	1838	G	C5-N7-C8	5.08	106.84	104.30
79	B2	557	G	C5-C6-N1	-5.08	108.96	111.50
79	B2	597	G	C8-N9-C4	-5.08	104.37	106.40
80	B5	2207	A	C5-C6-N1	-5.08	115.16	117.70
80	B5	2606	G	N1-C2-N2	-5.08	111.63	116.20
80	B5	2913	C	N3-C2-O2	-5.08	118.34	121.90
80	B5	3132	C	C6-N1-C2	5.08	122.33	120.30
82	B8	26	U	C4-C5-C6	5.08	122.75	119.70
43	BI	69	ARG	NE-CZ-NH2	5.08	122.84	120.30
80	B5	2805	G	C5-C6-N1	5.08	114.04	111.50
80	B5	3313	U	N1-C2-N3	5.08	117.95	114.90
80	B5	2696	A	C5-C6-N6	5.08	127.76	123.70
80	B5	3259	U	N1-C2-N3	5.08	117.95	114.90
79	B2	1542	G	N9-C4-C5	5.08	107.43	105.40
80	B5	216	G	N9-C4-C5	-5.08	103.37	105.40
80	B5	1524	A	C4-C5-C6	5.08	119.54	117.00
80	B5	2364	G	C6-N1-C2	-5.08	122.05	125.10
80	B5	2407	C	N3-C2-O2	5.08	125.45	121.90
22	AN	114	ARG	NE-CZ-NH1	5.08	122.84	120.30
79	B2	270	C	C5-C6-N1	5.08	123.54	121.00
80	B5	1463	U	C5-C4-O4	-5.08	122.85	125.90
80	B5	2190	U	N3-C2-O2	-5.08	118.65	122.20
80	B5	2263	C	N3-C2-O2	-5.08	118.35	121.90
79	B2	1220	C	C6-N1-C2	5.08	122.33	120.30
80	B5	2945	G	C5-C6-O6	-5.08	125.56	128.60
80	B5	3049	A	N1-C6-N6	5.08	121.65	118.60
83	CV	490	VAL	N-CA-C	-5.08	97.30	111.00
79	B2	1605	G	N1-C2-N2	-5.07	111.63	116.20
80	B5	1144	U	N3-C2-O2	-5.07	118.65	122.20
80	B5	1660	C	C2-N3-C4	-5.07	117.36	119.90
80	B5	3199	G	C8-N9-C4	-5.07	104.37	106.40
85	CX	1	A	N9-C1'-C2'	-5.07	106.42	112.00
80	B5	2647	A	N1-C2-N3	5.07	131.84	129.30
81	B7	83	U	C5-C4-O4	5.07	128.94	125.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	356	C	C2-N3-C4	-5.07	117.36	119.90
80	B5	584	G	N1-C6-O6	-5.07	116.86	119.90
80	B5	958	C	C6-N1-C2	5.07	122.33	120.30
80	B5	2531	C	N3-C2-O2	-5.07	118.35	121.90
81	B7	1	G	N7-C8-N9	5.07	115.64	113.10
81	B7	57	G	C5-C6-O6	5.07	131.64	128.60
82	B8	23	U	N3-C2-O2	-5.07	118.65	122.20
84	CW	44	G	O4'-C1'-N9	5.07	112.26	108.20
79	B2	498	G	C4-N9-C1'	5.07	133.09	126.50
84	CW	75	C	C3'-C2'-C1'	5.07	105.56	101.50
79	B2	1037	C	C6-N1-C2	-5.07	118.27	120.30
80	B5	270	U	N1-C2-O2	5.07	126.35	122.80
80	B5	2283	G	C8-N9-C4	5.07	108.43	106.40
80	B5	2326	A	C5-C6-N1	5.07	120.23	117.70
81	B7	20	A	N1-C6-N6	5.07	121.64	118.60
79	B2	647	G	C8-N9-C1'	5.07	133.59	127.00
79	B2	1215	C	N3-C2-O2	-5.07	118.36	121.90
80	B5	874	U	C2-N1-C1'	-5.07	111.62	117.70
80	B5	1178	G	N3-C2-N2	-5.07	116.35	119.90
80	B5	1257	C	N1-C1'-C2'	-5.07	106.43	112.00
80	B5	1938	U	C2-N3-C4	-5.07	123.96	127.00
80	B5	2305	G	N3-C4-N9	5.07	129.04	126.00
80	B5	2386	A	N1-C6-N6	5.07	121.64	118.60
80	B5	2632	G	C6-N1-C2	5.07	128.14	125.10
80	B5	973	A	C6-N1-C2	-5.06	115.56	118.60
80	B5	3048	A	C5-C6-N6	-5.06	119.65	123.70
79	B2	6	G	N1-C2-N2	-5.06	111.64	116.20
79	B2	349	U	N1-C2-N3	5.06	117.94	114.90
79	B2	1734	U	C5-C4-O4	5.06	128.94	125.90
80	B5	1439	U	C5-C4-O4	-5.06	122.86	125.90
80	B5	1906	G	C5-C6-O6	-5.06	125.56	128.60
80	B5	2293	C	N3-C2-O2	-5.06	118.36	121.90
80	B5	3217	C	C2-N1-C1'	-5.06	113.23	118.80
81	B7	83	U	C6-N1-C1'	5.06	128.29	121.20
80	B5	916	G	C6-N1-C2	5.06	128.14	125.10
80	B5	1480	G	N3-C4-N9	5.06	129.04	126.00
80	B5	1938	U	N3-C4-C5	5.06	117.64	114.60
80	B5	2272	G	N7-C8-N9	-5.06	110.57	113.10
80	B5	2754	G	N3-C4-C5	-5.06	126.07	128.60
79	B2	132	U	C6-N1-C1'	5.06	128.28	121.20
80	B5	880	G	C8-N9-C4	5.06	108.42	106.40
80	B5	1049	C	C6-N1-C2	-5.06	118.28	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	1343	A	N1-C2-N3	5.06	131.83	129.30
80	B5	1481	A	C4-C5-C6	5.06	119.53	117.00
80	B5	1660	C	N1-C2-N3	5.06	122.74	119.20
79	B2	902	G	N1-C6-O6	5.06	122.94	119.90
79	B2	1780	G	N1-C6-O6	5.06	122.94	119.90
80	B5	2931	C	N1-C2-O2	-5.06	115.86	118.90
80	B5	3377	G	C6-C5-N7	-5.06	127.37	130.40
84	CW	61	C	C5-C4-N4	-5.06	116.66	120.20
44	BJ	92	ARG	NE-CZ-NH1	5.06	122.83	120.30
79	B2	335	U	N3-C2-O2	5.06	125.74	122.20
79	B2	1796	C	N3-C4-C5	-5.06	119.88	121.90
79	B2	1258	U	N1-C2-O2	5.05	126.34	122.80
79	B2	1268	G	N1-C6-O6	-5.05	116.87	119.90
80	B5	2364	G	C8-N9-C4	-5.05	104.38	106.40
80	B5	3066	U	N1-C2-O2	5.05	126.34	122.80
82	B8	4	C	C6-N1-C2	-5.05	118.28	120.30
79	B2	270	C	C2-N1-C1'	5.05	124.36	118.80
79	B2	1148	C	N1-C2-O2	5.05	121.93	118.90
80	B5	1004	U	C5-C4-O4	5.05	128.93	125.90
80	B5	2371	G	N7-C8-N9	-5.05	110.57	113.10
80	B5	3018	C	C6-N1-C2	-5.05	118.28	120.30
40	BF	177	GLY	N-CA-C	-5.05	100.47	113.10
80	B5	420	G	C6-C5-N7	-5.05	127.37	130.40
80	B5	622	A	C4-C5-N7	5.05	113.23	110.70
80	B5	635	G	N3-C4-N9	-5.05	122.97	126.00
80	B5	820	A	N1-C2-N3	5.05	131.82	129.30
80	B5	1301	A	C6-C5-N7	-5.05	128.76	132.30
80	B5	1901	A	N1-C6-N6	5.05	121.63	118.60
80	B5	2162	U	C5-C6-N1	-5.05	120.17	122.70
80	B5	3137	C	N3-C4-N4	-5.05	114.46	118.00
80	B5	3143	C	N3-C4-C5	-5.05	119.88	121.90
80	B5	3323	A	C2-N3-C4	-5.05	108.08	110.60
84	CW	76	A	C1'-O4'-C4'	-5.05	105.86	109.90
17	AI	172	ARG	NE-CZ-NH2	-5.05	117.78	120.30
51	BQ	38	ARG	NE-CZ-NH2	-5.05	117.78	120.30
53	BS	167	ARG	NE-CZ-NH1	5.05	122.82	120.30
79	B2	885	G	N1-C6-O6	5.05	122.93	119.90
80	B5	1432	C	N3-C2-O2	-5.05	118.37	121.90
80	B5	1887	A	C6-C5-N7	-5.05	128.76	132.30
80	B5	2303	A	N1-C2-N3	-5.05	126.78	129.30
80	B5	2525	G	N9-C4-C5	-5.05	103.38	105.40
80	B5	2774	C	N3-C4-N4	5.05	121.53	118.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	2919	A	C5-C6-N6	5.05	127.74	123.70
80	B5	524	U	C2-N3-C4	-5.05	123.97	127.00
70	Bj	5	THR	C-N-CD	5.05	139.00	128.40
79	B2	570	A	C2-N3-C4	5.05	113.12	110.60
80	B5	16	A	C5-C6-N1	5.05	120.22	117.70
80	B5	282	G	P-O3'-C3'	5.05	125.76	119.70
80	B5	432	G	N1-C2-N2	-5.05	111.66	116.20
80	B5	667	C	C5-C6-N1	-5.05	118.48	121.00
80	B5	1451	C	C6-N1-C2	5.05	122.32	120.30
84	CW	76	A	C5-C6-N1	-5.05	115.18	117.70
79	B2	158	U	N1-C2-O2	5.04	126.33	122.80
79	B2	1600	A	N1-C6-N6	5.04	121.63	118.60
80	B5	979	U	C5-C6-N1	5.04	125.22	122.70
80	B5	1338	C	N1-C2-O2	-5.04	115.87	118.90
80	B5	1462	A	C5-N7-C8	-5.04	101.38	103.90
80	B5	2748	A	C5-C6-N1	5.04	120.22	117.70
80	B5	3209	A	O4'-C1'-N9	5.04	112.24	108.20
82	B8	47	C	N3-C2-O2	-5.04	118.37	121.90
24	AP	42	ARG	NE-CZ-NH1	5.04	122.82	120.30
79	B2	73	U	C1'-O4'-C4'	-5.04	105.86	109.90
80	B5	356	C	C6-N1-C2	5.04	122.32	120.30
80	B5	2337	C	C5-C6-N1	-5.04	118.48	121.00
80	B5	2352	A	C4-C5-C6	5.04	119.52	117.00
81	B7	14	U	C2-N3-C4	-5.04	123.97	127.00
51	BQ	3	ILE	CB-CA-C	-5.04	101.52	111.60
79	B2	1600	A	C3'-C2'-C1'	-5.04	97.47	101.50
80	B5	1015	U	C2-N3-C4	5.04	130.03	127.00
80	B5	2639	G	N3-C4-N9	5.04	129.03	126.00
80	B5	3195	U	N1-C2-O2	5.04	126.33	122.80
80	B5	3200	G	N1-C6-O6	5.04	122.92	119.90
80	B5	141	C	C5-C6-N1	5.04	123.52	121.00
80	B5	2361	A	N1-C6-N6	-5.04	115.58	118.60
80	B5	2430	A	C4-C5-C6	5.04	119.52	117.00
80	B5	888	A	C2-N3-C4	-5.04	108.08	110.60
80	B5	1013	G	N3-C4-C5	-5.04	126.08	128.60
80	B5	1314	C	C4-C5-C6	5.04	119.92	117.40
80	B5	2215	A	N1-C6-N6	5.04	121.62	118.60
80	B5	2343	C	N1-C2-O2	-5.04	115.88	118.90
80	B5	2371	G	N1-C2-N2	-5.04	111.67	116.20
80	B5	3154	C	C6-N1-C2	-5.04	118.28	120.30
80	B5	3212	C	N1-C2-N3	5.04	122.73	119.20
80	B5	3266	G	N3-C4-N9	-5.04	122.98	126.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	B5	3273	A	C5-N7-C8	-5.04	101.38	103.90
80	B5	1240	A	C5-C6-N6	-5.04	119.67	123.70
79	B2	802	G	N3-C4-C5	-5.04	126.08	128.60
79	B2	1596	C	N1-C2-O2	5.04	121.92	118.90
80	B5	1804	A	N1-C6-N6	5.04	121.62	118.60
80	B5	2935	U	N1-C2-O2	5.04	126.33	122.80
80	B5	3039	C	C5-C6-N1	5.04	123.52	121.00
83	CV	191	TYR	CB-CG-CD1	5.04	124.02	121.00
79	B2	704	C	N3-C2-O2	-5.03	118.38	121.90
80	B5	840	C	C4-C5-C6	5.03	119.92	117.40
80	B5	1887	A	C4-C5-N7	5.03	113.22	110.70
80	B5	3183	A	N1-C6-N6	5.03	121.62	118.60
80	B5	3191	G	N7-C8-N9	-5.03	110.58	113.10
80	B5	3197	G	N3-C4-C5	5.03	131.12	128.60
79	B2	1629	G	N1-C2-N2	-5.03	111.67	116.20
80	B5	2572	C	C5-C6-N1	5.03	123.52	121.00
80	B5	2893	C	C5-C6-N1	-5.03	118.48	121.00
79	B2	270	C	C6-N1-C2	-5.03	118.29	120.30
80	B5	1100	U	C6-N1-C2	5.03	124.02	121.00
80	B5	2541	U	N1-C2-O2	5.03	126.32	122.80
80	B5	2857	C	C2-N3-C4	-5.03	117.39	119.90
80	B5	3249	C	C6-N1-C2	-5.03	118.29	120.30
82	B8	17	A	C6-C5-N7	-5.03	128.78	132.30
6	A5	106	TYR	N-CA-C	-5.03	97.42	111.00
13	AE	164	LEU	CA-CB-CG	5.03	126.87	115.30
80	B5	2361	A	C4-C5-N7	-5.03	108.19	110.70
80	B5	2733	A	N1-C2-N3	5.03	131.81	129.30
80	B5	2808	A	C8-N9-C1'	-5.03	118.65	127.70
80	B5	3087	A	C8-N9-C4	-5.03	103.79	105.80
80	B5	3211	C	C6-N1-C2	5.03	122.31	120.30
79	B2	819	G	P-O3'-C3'	5.03	125.73	119.70
79	B2	1441	C	C5-C6-N1	-5.03	118.49	121.00
79	B2	1568	C	P-O3'-C3'	5.03	125.73	119.70
80	B5	1529	A	C2-N3-C4	5.03	113.11	110.60
32	AX	111	GLY	N-CA-C	-5.03	100.54	113.10
79	B2	570	A	C4-C5-C6	5.03	119.51	117.00
79	B2	1311	U	C6-N1-C2	5.03	124.02	121.00
80	B5	587	U	C6-N1-C2	5.03	124.02	121.00
80	B5	982	C	C4-C5-C6	-5.03	114.89	117.40
80	B5	2603	G	N7-C8-N9	5.03	115.61	113.10
80	B5	2994	A	N1-C2-N3	5.03	131.81	129.30
84	CW	68	C	N3-C4-C5	-5.03	119.89	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	613	G	N3-C2-N2	5.02	123.42	119.90
80	B5	2847	A	C5-C6-N6	5.02	127.72	123.70
57	BW	23	ARG	NE-CZ-NH1	-5.02	117.79	120.30
80	B5	191	U	C2-N1-C1'	-5.02	111.67	117.70
80	B5	578	A	C2-N3-C4	5.02	113.11	110.60
80	B5	1414	G	C2-N3-C4	-5.02	109.39	111.90
80	B5	1461	A	C8-N9-C4	5.02	107.81	105.80
80	B5	1788	C	C6-N1-C2	-5.02	118.29	120.30
81	B7	116	C	C6-N1-C2	5.02	122.31	120.30
79	B2	553	G	C2-N3-C4	-5.02	109.39	111.90
80	B5	965	A	C5-C6-N1	5.02	120.21	117.70
80	B5	1237	G	P-O3'-C3'	-5.02	113.68	119.70
80	B5	1255	C	C5-C6-N1	5.02	123.51	121.00
80	B5	2813	A	C5-C6-N6	5.02	127.72	123.70
80	B5	3372	A	C8-N9-C4	-5.02	103.79	105.80
79	B2	432	G	C2-N3-C4	5.02	114.41	111.90
80	B5	1473	G	C8-N9-C4	5.02	108.41	106.40
80	B5	2271	A	C5-N7-C8	5.02	106.41	103.90
80	B5	2705	A	C6-N1-C2	-5.02	115.59	118.60
80	B5	2821	C	N1-C2-O2	-5.02	115.89	118.90
80	B5	2878	G	C5-C6-N1	5.02	114.01	111.50
24	AP	42	ARG	NE-CZ-NH2	-5.01	117.79	120.30
79	B2	1791	A	C5-C6-N1	5.01	120.21	117.70
80	B5	391	A	C8-N9-C4	5.01	107.81	105.80
80	B5	1303	A	C8-N9-C4	5.01	107.81	105.80
80	B5	2280	A	N3-C4-C5	5.01	130.31	126.80
80	B5	2306	C	C5-C6-N1	5.01	123.51	121.00
80	B5	2399	A	N1-C6-N6	5.01	121.61	118.60
80	B5	2618	G	N1-C6-O6	5.01	122.91	119.90
80	B5	2958	A	C4-N9-C1'	-5.01	117.28	126.30
79	B2	63	G	N1-C6-O6	-5.01	116.89	119.90
79	B2	345	U	N1-C2-N3	5.01	117.91	114.90
80	B5	1270	A	C5-C6-N1	-5.01	115.19	117.70
80	B5	2857	C	C5-C6-N1	-5.01	118.49	121.00
80	B5	3145	C	C5-C4-N4	-5.01	116.69	120.20
79	B2	914	G	C4-N9-C1'	5.01	133.01	126.50
79	B2	1649	G	N1-C2-N3	5.01	126.91	123.90
80	B5	2323	G	C5-C6-O6	5.01	131.61	128.60
80	B5	2974	U	C5-C6-N1	-5.01	120.19	122.70
84	CW	63	G	C5-C6-O6	-5.01	125.59	128.60
65	Be	111	ARG	NE-CZ-NH2	-5.01	117.80	120.30
79	B2	853	G	C4-C5-N7	5.01	112.80	110.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B2	992	A	C4-C5-C6	-5.01	114.50	117.00
79	B2	1679	G	N3-C2-N2	5.01	123.41	119.90
80	B5	701	G	C5-N7-C8	5.01	106.81	104.30
80	B5	1267	U	O4'-C1'-N1	5.01	112.21	108.20
80	B5	2122	G	N1-C6-O6	-5.01	116.89	119.90
81	B7	35	C	C2-N3-C4	-5.01	117.39	119.90
80	B5	2951	G	C8-N9-C4	5.01	108.40	106.40
82	B8	102	U	N1-C2-N3	5.01	117.91	114.90
79	B2	965	U	C4-C5-C6	-5.01	116.70	119.70
80	B5	582	G	N9-C4-C5	5.01	107.40	105.40
80	B5	654	C	N1-C2-O2	-5.01	115.90	118.90
84	CW	3	C	N3-C4-N4	5.01	121.50	118.00
79	B2	902	G	C6-C5-N7	-5.00	127.40	130.40
80	B5	2375	G	N3-C2-N2	5.00	123.40	119.90
80	B5	2434	U	N1-C2-N3	5.00	117.90	114.90
80	B5	3094	A	N7-C8-N9	-5.00	111.30	113.80
80	B5	822	G	N9-C4-C5	5.00	107.40	105.40
80	B5	1232	C	N3-C4-C5	-5.00	119.90	121.90
81	B7	88	G	N9-C4-C5	5.00	107.40	105.40
79	B2	334	G	N3-C4-N9	-5.00	123.00	126.00
79	B2	388	G	C2-N3-C4	5.00	114.40	111.90
79	B2	622	A	N9-C4-C5	5.00	107.80	105.80
79	B2	984	G	N3-C4-C5	5.00	131.10	128.60
79	B2	1051	G	C4-N9-C1'	5.00	133.00	126.50
80	B5	866	A	N1-C2-N3	-5.00	126.80	129.30
80	B5	2421	U	C2-N3-C4	-5.00	124.00	127.00
80	B5	2620	G	C4-C5-C6	-5.00	115.80	118.80
80	B5	3030	G	C5-C6-N1	-5.00	109.00	111.50
80	B5	3285	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (125) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A1	42	ASN	Peptide
6	A5	105	TYR	Peptide
6	A5	138	ARG	Peptide
8	A7	134	ASP	Sidechain
10	AB	131	ASP	Peptide
16	AH	131	PHE	Peptide
20	AL	127	GLN	Peptide
23	AO	124	ASP	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
26	AR	22	PRO	Peptide
26	AR	85	VAL	Peptide
34	AZ	54	VAL	Peptide
34	AZ	93	SER	Peptide
34	AZ	96	SER	Peptide
80	B5	1226	G	Sidechain
80	B5	1228	C	Sidechain
80	B5	1229	G	Sidechain
80	B5	1230	G	Sidechain
80	B5	1231	A	Sidechain
80	B5	1235	U	Sidechain
80	B5	1238	C	Sidechain
80	B5	1239	C	Sidechain
80	B5	1244	A	Sidechain
80	B5	1246	G	Sidechain
80	B5	1249	G	Sidechain
80	B5	1254	C	Sidechain
80	B5	1255	C	Sidechain
80	B5	1256	G	Sidechain
80	B5	1257	C	Sidechain
80	B5	1259	A	Sidechain
80	B5	1260	A	Sidechain
80	B5	1262	G	Sidechain
80	B5	1264	G	Sidechain
80	B5	1265	U	Sidechain
80	B5	1266	G	Sidechain
80	B5	1267	U	Sidechain
80	B5	1268	G	Sidechain
80	B5	1269	U	Sidechain
80	B5	1271	A	Sidechain
80	B5	1274	A	Sidechain
80	B5	1276	U	Sidechain
80	B5	1278	A	Sidechain
80	B5	1279	C	Sidechain
80	B5	1281	G	Sidechain
80	B5	1282	G	Sidechain
80	B5	1283	C	Sidechain
80	B5	1284	C	Sidechain
80	B5	1285	G	Sidechain
80	B5	2898	G	Sidechain
35	BA	143	GLU	Peptide
35	BA	211	HIS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
37	BC	91	GLY	Peptide
38	BD	271	LYS	Peptide
39	BE	129	GLU	Peptide
40	BF	192	GLY	Peptide
40	BF	226	GLY	Peptide
49	BO	110[A]	PRO	Peptide
49	BO	68[B]	ARG	Peptide
53	BS	133	ALA	Peptide
56	BV	41	GLY	Peptide
59	BY	111	LEU	Peptide
60	BZ	101	PHE	Peptide
61	Ba	26	ARG	Peptide
61	Ba	66	ALA	Peptide
61	Ba	75	LEU	Peptide
62	Bb	19	ASN	Peptide
76	Bq	16	ARG	Sidechain
76	Bq	185	LEU	Peptide
76	Bq	22	TYR	Sidechain
76	Bq	5	ARG	Sidechain
76	Bq	64	ARG	Sidechain
76	Bq	86	PHE	Sidechain
76	Bq	91	GLU	Peptide
77	Br	15	UNK	Peptide
83	CV	165	TYR	Sidechain
83	CV	2	ASP	Mainchain
83	CV	219	ARG	Sidechain
83	CV	227	LEU	Peptide
83	CV	320	ARG	Sidechain
83	CV	374	TYR	Sidechain
83	CV	375	VAL	Mainchain
83	CV	395	ILE	Mainchain
83	CV	4	ARG	Sidechain
83	CV	403	TYR	Sidechain
83	CV	465	SER	Mainchain
83	CV	47	PHE	Peptide
83	CV	523	ARG	Sidechain
83	CV	536	TYR	Sidechain
83	CV	547	TYR	Sidechain
83	CV	550	ILE	Peptide
83	CV	555	TYR	Sidechain
83	CV	62	TYR	Sidechain
84	CW	12	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
84	CW	14	A	Sidechain
84	CW	15	G	Sidechain
84	CW	16	U	Sidechain
84	CW	18	G	Sidechain
84	CW	19	G	Sidechain
84	CW	21	A	Sidechain
84	CW	26	A	Sidechain
84	CW	28	G	Sidechain
84	CW	30	G	Sidechain
84	CW	31	A	Sidechain
84	CW	33	U	Sidechain
84	CW	4	C	Sidechain
84	CW	40	C	Sidechain
84	CW	44	G	Sidechain
84	CW	45	U	Sidechain
84	CW	47	U	Sidechain
84	CW	48	C	Sidechain
84	CW	55	U	Sidechain
84	CW	6	G	Sidechain
84	CW	60	U	Sidechain
84	CW	63	G	Sidechain
84	CW	65	G	Sidechain
84	CW	66	U	Sidechain
84	CW	67	C	Sidechain
84	CW	68	C	Sidechain
84	CW	7	A	Sidechain
84	CW	70	G	Sidechain
84	CW	71	G	Sidechain
84	CW	74	C	Sidechain
84	CW	75	C	Sidechain
84	CW	8	U	Sidechain
85	CX	2	U	Sidechain
85	CX	3	G	Sidechain

## 5.2 Too-close contacts

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



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	95/119 (80%)	57 (60%)	21 (22%)	17 (18%)	0	2
2	A1	79/82 (96%)	62 (78%)	13 (16%)	4 (5%)	2	19
3	A2	61/67 (91%)	47 (77%)	9 (15%)	5 (8%)	1	12
4	A3	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	3	23
5	A4	58/63 (92%)	49 (84%)	7 (12%)	2 (3%)	3	26
6	A5	50/152 (33%)	30 (60%)	9 (18%)	11 (22%)	0	1
7	A6	316/319 (99%)	273 (86%)	30 (10%)	13 (4%)	3	23
8	A7	120/273 (44%)	92 (77%)	17 (14%)	11 (9%)	1	10
9	AA	204/252 (81%)	143 (70%)	35 (17%)	26 (13%)	0	5
10	AB	212/255 (83%)	132 (62%)	42 (20%)	38 (18%)	0	2
11	AC	215/254 (85%)	187 (87%)	16 (7%)	12 (6%)	2	18
12	AD	221/240 (92%)	180 (81%)	27 (12%)	14 (6%)	1	16
13	AE	258/261 (99%)	201 (78%)	36 (14%)	21 (8%)	1	12
14	AF	204/225 (91%)	155 (76%)	30 (15%)	19 (9%)	0	10
15	AG	224/236 (95%)	190 (85%)	23 (10%)	11 (5%)	2	20
16	AH	182/190 (96%)	128 (70%)	27 (15%)	27 (15%)	0	3
17	AI	184/200 (92%)	155 (84%)	14 (8%)	15 (8%)	1	12
18	AJ	183/197 (93%)	153 (84%)	18 (10%)	12 (7%)	1	15
19	AK	94/105 (90%)	66 (70%)	18 (19%)	10 (11%)	0	8
20	AL	153/156 (98%)	125 (82%)	19 (12%)	9 (6%)	1	17
21	AM	122/143 (85%)	66 (54%)	23 (19%)	33 (27%)	0	0
22	AN	148/151 (98%)	125 (84%)	15 (10%)	8 (5%)	2	19
23	AO	125/137 (91%)	94 (75%)	16 (13%)	15 (12%)	0	6
24	AP	122/142 (86%)	92 (75%)	15 (12%)	15 (12%)	0	5
25	AQ	139/143 (97%)	114 (82%)	14 (10%)	11 (8%)	1	13

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	AR	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	0	8
27	AS	143/146 (98%)	110 (77%)	19 (13%)	14 (10%)	0	9
28	AT	141/144 (98%)	111 (79%)	18 (13%)	12 (8%)	1	11
29	AU	105/121 (87%)	87 (83%)	13 (12%)	5 (5%)	2	21
30	AV	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	6
31	AW	127/130 (98%)	114 (90%)	10 (8%)	3 (2%)	6	33
32	AX	142/145 (98%)	111 (78%)	13 (9%)	18 (13%)	0	5
33	AY	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	0	9
34	AZ	68/108 (63%)	46 (68%)	11 (16%)	11 (16%)	0	3
35	BA	250/253 (99%)	213 (85%)	30 (12%)	7 (3%)	5	30
36	BB	384/386 (100%)	341 (89%)	34 (9%)	9 (2%)	6	34
37	BC	359/361 (99%)	306 (85%)	32 (9%)	21 (6%)	1	18
38	BD	292/296 (99%)	267 (91%)	19 (6%)	6 (2%)	7	36
39	BE	153/175 (87%)	134 (88%)	15 (10%)	4 (3%)	5	31
40	BF	221/243 (91%)	201 (91%)	16 (7%)	4 (2%)	8	40
41	BG	229/255 (90%)	180 (79%)	28 (12%)	21 (9%)	1	10
42	BH	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	7	36
43	BI	209/220 (95%)	175 (84%)	22 (10%)	12 (6%)	1	18
44	BJ	167/173 (96%)	135 (81%)	19 (11%)	13 (8%)	1	13
46	BL	192/198 (97%)	161 (84%)	20 (10%)	11 (6%)	1	18
47	BM	135/137 (98%)	124 (92%)	10 (7%)	1 (1%)	22	63
48	BN	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	4	28
49	BO	352/218 (162%)	324 (92%)	18 (5%)	10 (3%)	5	30
50	BP	153/183 (84%)	142 (93%)	9 (6%)	2 (1%)	12	48
51	BQ	183/185 (99%)	168 (92%)	9 (5%)	6 (3%)	4	26
52	BR	186/188 (99%)	167 (90%)	16 (9%)	3 (2%)	9	44
53	BS	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	66
54	BT	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	12	48
55	BU	96/120 (80%)	80 (83%)	13 (14%)	3 (3%)	4	27
56	BV	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	10	46
57	BW	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	1	17

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	BX	118/141 (84%)	104 (88%)	6 (5%)	8 (7%)	1	15
59	BY	124/126 (98%)	107 (86%)	12 (10%)	5 (4%)	3	23
60	BZ	133/135 (98%)	107 (80%)	13 (10%)	13 (10%)	0	9
61	Ba	146/148 (99%)	123 (84%)	18 (12%)	5 (3%)	3	26
62	Bb	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1	11
63	Bc	98/104 (94%)	87 (89%)	8 (8%)	3 (3%)	4	27
64	Bd	107/112 (96%)	88 (82%)	13 (12%)	6 (6%)	2	18
65	Be	125/129 (97%)	110 (88%)	9 (7%)	6 (5%)	2	21
66	Bf	104/106 (98%)	96 (92%)	5 (5%)	3 (3%)	4	29
67	Bg	110/120 (92%)	93 (84%)	13 (12%)	4 (4%)	3	25
68	Bh	117/119 (98%)	99 (85%)	14 (12%)	4 (3%)	3	26
69	Bi	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	14
70	Bj	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	6	33
71	Bk	75/77 (97%)	61 (81%)	10 (13%)	4 (5%)	2	19
72	Bl	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	36
73	Bm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	7	38
74	Bn	23/25 (92%)	22 (96%)	0	1 (4%)	2	22
75	Bo	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	8	38
76	Bq	141/312 (45%)	105 (74%)	14 (10%)	22 (16%)	0	3
83	CV	555/586 (95%)	450 (81%)	61 (11%)	44 (8%)	1	13
All	All	11839/12944 (92%)	9833 (83%)	1245 (10%)	761 (6%)	2	16

All (761) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	19	LYS
1	A0	45	VAL
1	A0	46	GLU
1	A0	62	TYR
1	A0	65	PRO
1	A0	82	ARG
1	A0	84	VAL
1	A0	85	ARG
2	A1	38	PRO
2	A1	62	ILE

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
3	A2	36	THR
3	A2	51	ASN
4	A3	8	PHE
5	A4	47	VAL
6	A5	102	VAL
6	A5	103	LEU
6	A5	106	TYR
6	A5	111	GLU
6	A5	128	ALA
6	A5	148	TYR
7	A6	51	ASP
7	A6	160	GLU
7	A6	318	ALA
8	A7	47	ALA
8	A7	52	PRO
8	A7	85	SER
8	A7	87	THR
9	AA	4	PRO
9	AA	29	VAL
9	AA	30	GLN
9	AA	39	ASN
9	AA	66	ALA
9	AA	95	ALA
9	AA	111	ILE
9	AA	191	ARG
9	AA	203	PHE
9	AA	205	ARG
10	AB	21	VAL
10	AB	26	ARG
10	AB	49	ASN
10	AB	58	SER
10	AB	60	ALA
10	AB	63	GLY
10	AB	113	MET
10	AB	116	LYS
10	AB	176	VAL
10	AB	177	GLN
10	AB	179	SER
10	AB	182	ALA
10	AB	206	PRO
10	AB	221	PRO
11	AC	146	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	AC	148	LEU
12	AD	4	LEU
12	AD	62	ASN
12	AD	65	ARG
12	AD	93	ASP
12	AD	211	PRO
12	AD	212	LYS
12	AD	216	PRO
12	AD	220	PRO
13	AE	104	ASP
13	AE	142	HIS
13	AE	153	ASN
13	AE	164	LEU
13	AE	260	GLY
14	AF	26	ALA
14	AF	39	GLU
14	AF	43	PHE
14	AF	58	LEU
14	AF	63	GLN
14	AF	101	GLY
14	AF	153	GLY
14	AF	206	SER
15	AG	20	ASP
15	AG	25	ARG
15	AG	154	ARG
15	AG	173	PRO
15	AG	174	LYS
16	AH	31	SER
16	AH	36	ALA
16	AH	64	VAL
16	AH	67	LEU
16	AH	98	ILE
16	AH	105	THR
16	AH	111	LYS
16	AH	112	ARG
16	AH	131	PHE
16	AH	133	THR
16	AH	134	GLU
16	AH	155	ASP
17	AI	13	ALA
17	AI	22	ARG
17	AI	147	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
17	AI	149	SER
18	AJ	98	ALA
18	AJ	100	LYS
18	AJ	118	LEU
18	AJ	121	SER
18	AJ	164	PHE
19	AK	60	SER
19	AK	81	ASN
19	AK	87	VAL
19	AK	88	PRO
19	AK	93	GLN
20	AL	7	VAL
20	AL	29	LYS
20	AL	133	LYS
21	AM	21	GLU
21	AM	25	GLU
21	AM	45	LEU
21	AM	55	GLY
21	AM	83	GLU
21	AM	87	PRO
21	AM	89	ILE
21	AM	90	LYS
21	AM	93	ASP
21	AM	126	TRP
22	AN	19	SER
22	AN	22	ALA
23	AO	38	THR
23	AO	39	ILE
23	AO	124	ASP
23	AO	125	SER
23	AO	126	THR
24	AP	29	SER
24	AP	54	ALA
24	AP	125	PRO
24	AP	126	VAL
25	AQ	41	PRO
25	AQ	58	ASP
25	AQ	59	LYS
25	AQ	114	ARG
25	AQ	116	LEU
25	AQ	138	PHE
26	AR	6	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	AR	26	LEU
26	AR	85	VAL
26	AR	86	PRO
26	AR	88	VAL
26	AR	96	SER
26	AR	124	VAL
27	AS	14	ILE
27	AS	25	ASN
27	AS	28	ILE
27	AS	60	GLU
27	AS	91	ASP
27	AS	92	ILE
28	AT	31	PRO
28	AT	53	TRP
28	AT	69	LYS
29	AU	118	VAL
30	AV	4	ASP
30	AV	7	GLN
30	AV	11	LEU
32	AX	3	LYS
32	AX	41	SER
32	AX	96	VAL
32	AX	114	LYS
32	AX	128	SER
32	AX	131	SER
32	AX	137	LYS
32	AX	138	GLU
32	AX	144	ARG
33	AY	32	ARG
33	AY	36	SER
33	AY	78	SER
34	AZ	38	HIS
34	AZ	39	ALA
34	AZ	43	ASP
34	AZ	44	GLN
34	AZ	54	VAL
34	AZ	71	ILE
34	AZ	88	ILE
35	BA	96	LEU
36	BB	129	ALA
36	BB	140	ASP
36	BB	347	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
37	BC	14	GLU
37	BC	15	ALA
37	BC	90	PHE
37	BC	145	ILE
37	BC	302	ALA
37	BC	311	HIS
37	BC	329	PRO
37	BC	330	TYR
37	BC	361	HIS
38	BD	215	ASP
38	BD	260	PHE
39	BE	97	ASN
39	BE	98	VAL
40	BF	158	LYS
41	BG	25	PRO
41	BG	26	LEU
41	BG	34	PHE
41	BG	122	LYS
43	BI	25	ALA
43	BI	82	ARG
43	BI	170	LYS
43	BI	175	ASN
43	BI	187	ALA
44	BJ	8	PRO
44	BJ	10	ARG
44	BJ	12	LEU
44	BJ	94	ARG
44	BJ	95	ASN
44	BJ	108	GLU
44	BJ	115	LYS
44	BJ	167	TYR
46	BL	47	ALA
46	BL	129	ASN
46	BL	134	GLU
46	BL	150	PRO
47	BM	136	ALA
48	BN	49	ARG
48	BN	146	ALA
48	BN	147	ARG
49	BO	110[A]	PRO
49	BO	110[B]	PRO
49	BO	111[A]	PRO

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
49	BO	111[B]	PRO
49	BO	180[A]	SER
49	BO	180[B]	SER
49	BO	181[A]	ALA
49	BO	181[B]	ALA
51	BQ	41	ASP
51	BQ	99	THR
52	BR	35	ALA
53	BS	2	ALA
54	BT	136	ARG
56	BV	42	SER
57	BW	26	SER
57	BW	71	ARG
57	BW	76	VAL
58	BX	24	LEU
58	BX	25	LYS
58	BX	40	LEU
58	BX	44	PRO
58	BX	45	LYS
59	BY	77	LYS
59	BY	83	ASP
59	BY	84	LYS
59	BY	125	LYS
59	BY	126	LEU
60	BZ	5	LEU
60	BZ	125	GLY
60	BZ	129	TRP
61	Ba	76	ASP
62	Bb	21	ILE
62	Bb	23	LYS
62	Bb	25	LYS
62	Bb	39	PHE
63	Bc	100	ILE
63	Bc	104	LEU
64	Bd	7	VAL
64	Bd	45	GLY
64	Bd	84	ASP
65	Be	4	LEU
65	Be	5	PRO
65	Be	27	ARG
66	Bf	88	ASN
67	Bg	10	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
67	Bg	100	ILE
68	Bh	40	SER
68	Bh	82	ALA
69	Bi	33	ALA
69	Bi	63	ASN
69	Bi	64	SER
69	Bi	98	ARG
70	Bj	87	SER
71	Bk	17	ARG
71	Bk	18	ALA
72	Bl	3	ALA
75	Bo	78	LYS
76	Bq	36	GLN
76	Bq	37	GLN
76	Bq	91	GLU
76	Bq	105	VAL
76	Bq	107	ALA
76	Bq	186	THR
76	Bq	203	ASP
83	CV	60	ALA
83	CV	77	THR
83	CV	83	PHE
83	CV	187	ASN
83	CV	244	GLY
83	CV	352	GLY
83	CV	478	LYS
83	CV	493	GLN
83	CV	534	ALA
1	A0	36	ILE
1	A0	63	ALA
1	A0	75	VAL
1	A0	86	VAL
2	A1	63	LEU
3	A2	35	ASP
3	A2	61	ARG
4	A3	34	TYR
6	A5	118	ARG
6	A5	127	GLY
7	A6	3	SER
7	A6	28	GLY
7	A6	161	LYS
7	A6	217	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	A7	46	LYS
8	A7	82	THR
8	A7	89	ARG
8	A7	140	ASP
9	AA	5	ALA
9	AA	49	ASN
9	AA	81	PHE
9	AA	94	GLY
9	AA	190	ASP
9	AA	194	PRO
9	AA	196	SER
10	AB	23	PRO
10	AB	55	LYS
10	AB	72	ASP
10	AB	79	HIS
10	AB	82	ARG
10	AB	93	GLY
10	AB	108	ASP
10	AB	148	ASN
10	AB	181	LEU
10	AB	207	LEU
11	AC	35	TRP
11	AC	203	LYS
11	AC	248	SER
12	AD	44	THR
12	AD	218	LEU
13	AE	12	LEU
13	AE	152	PRO
13	AE	157	ASN
13	AE	195	ILE
13	AE	245	LYS
14	AF	35	GLN
14	AF	45	LYS
14	AF	127	GLN
14	AF	150	GLY
14	AF	223	SER
15	AG	24	ILE
15	AG	146	GLY
15	AG	152	ASP
15	AG	153	VAL
16	AH	32	PRO
16	AH	104	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	AH	156	SER
16	AH	186	PRO
17	AI	40	ALA
17	AI	105	ASP
17	AI	120	THR
17	AI	199	LYS
18	AJ	134	ILE
18	AJ	167	ALA
18	AJ	171	ARG
19	AK	30	ALA
19	AK	64	TYR
19	AK	82	LEU
21	AM	54	ARG
21	AM	63	VAL
21	AM	66	VAL
21	AM	84	ASN
21	AM	91	VAL
21	AM	113	ARG
21	AM	128	ALA
22	AN	13	SER
22	AN	28	LEU
22	AN	68	GLY
23	AO	40	ALA
23	AO	42	VAL
23	AO	46	MET
23	AO	50	ALA
23	AO	51	ASP
23	AO	114	ARG
24	AP	48	GLY
24	AP	51	SER
24	AP	101	ALA
25	AQ	40	GLU
25	AQ	113	ASP
26	AR	25	THR
27	AS	59	GLY
27	AS	61	LEU
27	AS	142	GLY
28	AT	11	ALA
28	AT	28	LEU
28	AT	50	ALA
29	AU	17	GLN
30	AV	12	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
31	AW	66	ASN
32	AX	8	GLY
32	AX	97	ASP
33	AY	5	VAL
33	AY	11	LYS
34	AZ	73	GLY
35	BA	24	GLN
35	BA	194	ASN
36	BB	235	THR
36	BB	293	ASN
37	BC	71	VAL
37	BC	190	GLY
37	BC	272	VAL
37	BC	345	GLU
37	BC	353	ALA
38	BD	125	VAL
38	BD	178	ASN
41	BG	81	THR
41	BG	121	SER
41	BG	188	THR
41	BG	203	VAL
41	BG	223	ALA
41	BG	240	ASN
42	BH	144	ILE
42	BH	189	GLU
43	BI	220	GLN
44	BJ	55	ARG
46	BL	135	ALA
46	BL	141	ALA
48	BN	184	LYS
50	BP	66	SER
50	BP	67	ILE
51	BQ	91	ALA
51	BQ	167	SER
55	BU	49	ASN
55	BU	91	ASP
56	BV	41	GLY
57	BW	63	ILE
57	BW	77	LYS
60	BZ	17	ARG
60	BZ	93	LYS
60	BZ	130	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
60	BZ	134	LEU
61	Ba	24	LYS
63	Bc	10	ILE
64	Bd	83	GLU
65	Be	6	HIS
65	Be	12	LYS
65	Be	124	GLY
66	Bf	91	ALA
68	Bh	119	LYS
74	Bn	23	ARG
76	Bq	33	VAL
76	Bq	92	PRO
76	Bq	104	ARG
76	Bq	204	ILE
76	Bq	205	THR
76	Bq	210	VAL
76	Bq	214	VAL
83	CV	56	THR
83	CV	73	LEU
83	CV	94	CYS
83	CV	138	TRP
83	CV	385	VAL
83	CV	433	VAL
83	CV	509	GLU
83	CV	526	LYS
1	A0	66	LYS
6	A5	138	ARG
7	A6	15	GLY
7	A6	96	THR
7	A6	98	GLU
9	AA	27	ARG
9	AA	103	THR
10	AB	35	PRO
10	AB	38	PHE
10	AB	62	LYS
10	AB	209	ASN
11	AC	106	ASP
11	AC	150	GLN
11	AC	235	LEU
12	AD	54	ARG
13	AE	200	ARG
14	AF	33	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	AF	156	ARG
16	AH	5	GLN
16	AH	29	ASN
16	AH	74	GLN
16	AH	75	THR
16	AH	110	GLN
17	AI	41	LYS
17	AI	136	SER
17	AI	153	GLU
18	AJ	163	PRO
20	AL	4	GLU
20	AL	55	ASP
20	AL	146	ALA
20	AL	153	PHE
20	AL	154	ALA
21	AM	22	VAL
21	AM	81	ASP
21	AM	82	PRO
21	AM	85	LYS
21	AM	112	ALA
21	AM	135	MET
22	AN	27	LYS
23	AO	18	ARG
23	AO	123	SER
24	AP	11	VAL
24	AP	22	LEU
24	AP	52	LYS
26	AR	83	GLN
26	AR	115	LEU
27	AS	10	SER
27	AS	80	LYS
27	AS	83	ALA
28	AT	25	GLN
29	AU	55	PRO
30	AV	2	GLU
30	AV	10	GLU
30	AV	15	ARG
32	AX	37	ALA
32	AX	40	SER
32	AX	89	ASN
33	AY	34	ASN
33	AY	51	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
33	AY	53	ASP
34	AZ	41	ILE
34	AZ	55	PRO
34	AZ	97	LYS
35	BA	56	ALA
35	BA	144	ASN
35	BA	249	SER
36	BB	138	ALA
36	BB	155	ALA
37	BC	146	PRO
38	BD	270	LYS
39	BE	10	TYR
39	BE	32	ALA
41	BG	39	ALA
41	BG	123	GLN
41	BG	133	LYS
41	BG	237	ILE
43	BI	83	ASP
43	BI	101	LYS
43	BI	174	THR
43	BI	176	LEU
46	BL	101	ARG
46	BL	140	SER
48	BN	181	ASN
49	BO	12[A]	LYS
49	BO	12[B]	LYS
55	BU	48	GLY
57	BW	74	LYS
57	BW	134	GLN
58	BX	38	LEU
58	BX	47	ALA
58	BX	55	ASN
60	BZ	16	GLY
61	Ba	47	LYS
64	Bd	5	LYS
64	Bd	86	LYS
67	Bg	79	SER
69	Bi	34	SER
76	Bq	81	LYS
76	Bq	187	VAL
76	Bq	200	SER
83	CV	16	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
83	CV	32	GLY
83	CV	41	GLN
83	CV	61	GLU
83	CV	79	GLY
83	CV	109	GLN
83	CV	280	THR
83	CV	283	PRO
83	CV	286	GLU
83	CV	290	LYS
83	CV	462	LYS
1	A0	64	LEU
3	A2	6	PRO
5	A4	50	VAL
6	A5	145	HIS
7	A6	136	ILE
7	A6	163	ASP
7	A6	237	GLN
9	AA	33	GLN
9	AA	158	VAL
9	AA	164	ASN
9	AA	185	ARG
9	AA	189	VAL
10	AB	54	LEU
10	AB	61	LEU
10	AB	81	PHE
10	AB	112	SER
10	AB	154	SER
10	AB	215	VAL
11	AC	39	THR
12	AD	217	ILE
13	AE	77	ARG
13	AE	80	THR
13	AE	163	ASP
13	AE	188	ASN
13	AE	193	GLY
14	AF	51	VAL
14	AF	79	ASN
15	AG	69	LEU
16	AH	13	PRO
16	AH	84	LYS
16	AH	132	PRO
17	AI	59	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
17	AI	152	ILE
19	AK	94	GLU
20	AL	145	ALA
21	AM	39	ASP
21	AM	68	GLU
21	AM	106	ILE
21	AM	107	ASP
21	AM	108	ARG
21	AM	129	GLU
21	AM	130	THR
22	AN	138	ASN
23	AO	69	ALA
25	AQ	142	TYR
26	AR	23	LYS
26	AR	72	LYS
28	AT	7	ARG
28	AT	23	GLN
28	AT	39	THR
30	AV	44	ARG
32	AX	92	CYS
32	AX	109	ARG
32	AX	112	LYS
33	AY	60	PHE
35	BA	143	GLU
36	BB	333	LYS
37	BC	233	LEU
37	BC	306	THR
37	BC	331	ALA
37	BC	342	LYS
38	BD	124	GLU
40	BF	191	VAL
41	BG	206	GLU
42	BH	167	VAL
43	BI	207	GLU
46	BL	60	ALA
46	BL	76	THR
48	BN	48	ALA
52	BR	147	ALA
57	BW	25	ASP
60	BZ	34	LYS
60	BZ	36	HIS
61	Ba	121	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
67	Bg	99	LYS
70	Bj	85	LYS
71	Bk	8	ILE
76	Bq	21	GLU
76	Bq	34	SER
83	CV	82	SER
83	CV	353	VAL
83	CV	399	GLU
83	CV	461	ILE
83	CV	503	GLU
83	CV	551	PRO
2	A1	51	GLN
8	A7	53	ARG
8	A7	102	THR
10	AB	64	ARG
11	AC	36	VAL
12	AD	59	LEU
13	AE	233	LYS
14	AF	21	THR
14	AF	64	VAL
16	AH	73	VAL
16	AH	185	ILE
18	AJ	162	SER
21	AM	101	ALA
24	AP	38	PRO
28	AT	29	GLU
29	AU	49	ASN
30	AV	46	ILE
30	AV	49	GLU
31	AW	67	GLY
31	AW	83	ILE
32	AX	70	LYS
33	AY	6	THR
33	AY	47	VAL
37	BC	5	GLN
40	BF	229	PHE
41	BG	69	LEU
41	BG	120	LYS
41	BG	124	ASP
42	BH	110	LYS
44	BJ	111	ASP
44	BJ	153	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
46	BL	121	SER
51	BQ	98	LYS
52	BR	183	ALA
54	BT	20	ARG
60	BZ	7	ALA
61	Ba	129	PHE
62	Bb	24	PRO
69	Bi	9	ILE
71	Bk	19	ASP
73	Bm	78	ILE
76	Bq	103	ASN
83	CV	154	SER
83	CV	267	MET
83	CV	400	ASP
83	CV	476	GLN
83	CV	505	VAL
1	A0	10	ARG
8	A7	88	ARG
9	AA	139	VAL
10	AB	78	ASP
10	AB	210	ILE
12	AD	89	GLU
13	AE	3	ARG
13	AE	53	LYS
16	AH	11	GLN
17	AI	10	LYS
17	AI	186	GLY
18	AJ	132	ARG
22	AN	60	VAL
24	AP	10	ARG
24	AP	23	GLU
24	AP	69	GLU
24	AP	130	ARG
27	AS	7	GLU
27	AS	34	THR
29	AU	117	VAL
33	AY	58	PHE
33	AY	77	ASN
36	BB	187	SER
37	BC	328	ASN
41	BG	202	GLU
43	BI	204	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
44	BJ	114	ILE
60	BZ	29	HIS
68	Bh	83	LYS
83	CV	136	TYR
13	AE	234	PRO
18	AJ	117	GLY
23	AO	48	VAL
25	AQ	97	VAL
40	BF	178	ILE
41	BG	190	VAL
76	Bq	196	VAL
83	CV	495	TYR
1	A0	50	VAL
1	A0	59	TYR
9	AA	117	GLU
21	AM	40	GLY
60	BZ	103	GLN
69	Bi	3	VAL
75	Bo	31	GLY
76	Bq	197	PHE
6	A5	147	VAL
10	AB	197	ILE
11	AC	145	GLY
25	AQ	29	ILE
28	AT	100	ILE
41	BG	73	PRO
44	BJ	118	PRO
51	BQ	42	ALA
83	CV	490	VAL
83	CV	508	VAL
11	AC	163	GLY
13	AE	45	ILE
15	AG	70	PRO
19	AK	89	GLY
21	AM	117	GLY
66	Bf	59	VAL
83	CV	506	GLY

### 5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	83/101 (82%)	65 (78%)	18 (22%)	1	6
2	A1	70/71 (99%)	62 (89%)	8 (11%)	5	21
3	A2	56/60 (93%)	38 (68%)	18 (32%)	0	2
4	A3	47/49 (96%)	38 (81%)	9 (19%)	1	8
5	A4	51/54 (94%)	43 (84%)	8 (16%)	2	14
6	A5	43/116 (37%)	32 (74%)	11 (26%)	0	3
7	A6	259/262 (99%)	221 (85%)	38 (15%)	3	15
8	A7	97/195 (50%)	74 (76%)	23 (24%)	1	4
9	AA	164/210 (78%)	122 (74%)	42 (26%)	0	3
10	AB	191/224 (85%)	137 (72%)	54 (28%)	0	2
11	AC	176/205 (86%)	130 (74%)	46 (26%)	0	3
12	AD	182/195 (93%)	138 (76%)	44 (24%)	0	4
13	AE	221/222 (100%)	166 (75%)	55 (25%)	0	3
14	AF	173/191 (91%)	137 (79%)	36 (21%)	1	7
15	AG	188/201 (94%)	149 (79%)	39 (21%)	1	7
16	AH	165/170 (97%)	124 (75%)	41 (25%)	0	3
17	AI	150/161 (93%)	118 (79%)	32 (21%)	1	6
18	AJ	158/166 (95%)	117 (74%)	41 (26%)	0	3
19	AK	77/98 (79%)	58 (75%)	19 (25%)	0	3
20	AL	129/137 (94%)	105 (81%)	24 (19%)	1	9
21	AM	88/119 (74%)	55 (62%)	33 (38%)	0	0
22	AN	127/128 (99%)	91 (72%)	36 (28%)	0	2
23	AO	81/105 (77%)	57 (70%)	24 (30%)	0	2
24	AP	101/118 (86%)	82 (81%)	19 (19%)	1	9
25	AQ	117/119 (98%)	83 (71%)	34 (29%)	0	2
26	AR	94/124 (76%)	70 (74%)	24 (26%)	0	3
27	AS	128/129 (99%)	87 (68%)	41 (32%)	0	2
28	AT	115/116 (99%)	84 (73%)	31 (27%)	0	3
29	AU	100/114 (88%)	71 (71%)	29 (29%)	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	AV	74/74 (100%)	56 (76%)	18 (24%)	0	4
31	AW	110/111 (99%)	84 (76%)	26 (24%)	1	4
32	AX	119/120 (99%)	97 (82%)	22 (18%)	1	10
33	AY	112/113 (99%)	84 (75%)	28 (25%)	0	3
34	AZ	61/89 (68%)	43 (70%)	18 (30%)	0	2
35	BA	192/195 (98%)	153 (80%)	39 (20%)	1	7
36	BB	320/322 (99%)	250 (78%)	70 (22%)	1	6
37	BC	288/288 (100%)	223 (77%)	65 (23%)	1	5
38	BD	243/244 (100%)	196 (81%)	47 (19%)	1	8
39	BE	135/152 (89%)	115 (85%)	20 (15%)	3	15
40	BF	187/204 (92%)	158 (84%)	29 (16%)	2	14
41	BG	177/207 (86%)	138 (78%)	39 (22%)	1	6
42	BH	171/171 (100%)	132 (77%)	39 (23%)	1	5
43	BI	179/186 (96%)	142 (79%)	37 (21%)	1	7
44	BJ	147/149 (99%)	114 (78%)	33 (22%)	1	6
46	BL	154/158 (98%)	124 (80%)	30 (20%)	1	8
47	BM	108/108 (100%)	84 (78%)	24 (22%)	1	6
48	BN	175/175 (100%)	143 (82%)	32 (18%)	1	10
49	BO	323/178 (182%)	267 (83%)	56 (17%)	2	11
50	BP	125/145 (86%)	103 (82%)	22 (18%)	2	11
51	BQ	150/150 (100%)	123 (82%)	27 (18%)	1	10
52	BR	153/153 (100%)	121 (79%)	32 (21%)	1	7
53	BS	156/156 (100%)	123 (79%)	33 (21%)	1	6
54	BT	136/136 (100%)	109 (80%)	27 (20%)	1	8
55	BU	85/106 (80%)	62 (73%)	23 (27%)	0	3
56	BV	104/104 (100%)	96 (92%)	8 (8%)	13	37
57	BW	100/129 (78%)	85 (85%)	15 (15%)	3	15
58	BX	104/117 (89%)	81 (78%)	23 (22%)	1	6
59	BY	109/109 (100%)	85 (78%)	24 (22%)	1	6
60	BZ	115/115 (100%)	89 (77%)	26 (23%)	1	5
61	Ba	118/118 (100%)	95 (80%)	23 (20%)	1	8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	Bb	46/46 (100%)	35 (76%)	11 (24%)	0	4
63	Bc	84/87 (97%)	68 (81%)	16 (19%)	1	9
64	Bd	94/96 (98%)	73 (78%)	21 (22%)	1	6
65	Be	109/110 (99%)	89 (82%)	20 (18%)	1	10
66	Bf	90/90 (100%)	79 (88%)	11 (12%)	5	20
67	Bg	95/102 (93%)	71 (75%)	24 (25%)	0	3
68	Bh	103/104 (99%)	77 (75%)	26 (25%)	0	3
69	Bi	80/81 (99%)	51 (64%)	29 (36%)	0	1
70	Bj	70/70 (100%)	53 (76%)	17 (24%)	0	4
71	Bk	67/68 (98%)	53 (79%)	14 (21%)	1	7
72	Bl	45/45 (100%)	34 (76%)	11 (24%)	0	4
73	Bm	47/116 (40%)	34 (72%)	13 (28%)	0	3
74	Bn	23/23 (100%)	16 (70%)	7 (30%)	0	2
75	Bo	90/90 (100%)	74 (82%)	16 (18%)	2	10
76	Bq	101/254 (40%)	91 (90%)	10 (10%)	8	26
83	CV	481/497 (97%)	450 (94%)	31 (6%)	17	42
All	All	9986/10821 (92%)	7877 (79%)	2109 (21%)	3	6

All (2109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	12	LYS
1	A0	36	ILE
1	A0	41	ILE
1	A0	44	ILE
1	A0	45	VAL
1	A0	53	LEU
1	A0	58	VAL
1	A0	61	GLU
1	A0	64	LEU
1	A0	66	LYS
1	A0	67	THR
1	A0	69	ASN
1	A0	70	LYS
1	A0	82	ARG
1	A0	83	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A0	85	ARG
1	A0	86	VAL
1	A0	90	GLU
2	A1	3	LEU
2	A1	4	VAL
2	A1	20	LYS
2	A1	29	ARG
2	A1	33	LEU
2	A1	34	ASP
2	A1	41	LEU
2	A1	67	THR
3	A2	5	THR
3	A2	13	ILE
3	A2	14	LYS
3	A2	15	VAL
3	A2	19	THR
3	A2	32	PHE
3	A2	33	LEU
3	A2	34	GLU
3	A2	38	ARG
3	A2	39	THR
3	A2	49	ARG
3	A2	52	ASP
3	A2	57	MET
3	A2	58	GLU
3	A2	59	SER
3	A2	62	GLU
3	A2	64	ARG
3	A2	65	ARG
4	A3	6	VAL
4	A3	8	PHE
4	A3	22	ARG
4	A3	25	SER
4	A3	30	LEU
4	A3	32	ARG
4	A3	36	LEU
4	A3	39	CYS
4	A3	48	ASN
5	A4	20	LYS
5	A4	25	GLU
5	A4	26	LYS
5	A4	28	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	A4	29	LYS
5	A4	42	ARG
5	A4	48	THR
5	A4	50	VAL
6	A5	102	VAL
6	A5	108	VAL
6	A5	120	GLU
6	A5	121	CYS
6	A5	125	THR
6	A5	130	VAL
6	A5	137	ASP
6	A5	140	TYR
6	A5	146	SER
6	A5	147	VAL
6	A5	151	ASN
7	A6	6	VAL
7	A6	7	LEU
7	A6	8	VAL
7	A6	46	LYS
7	A6	48	THR
7	A6	51	ASP
7	A6	52	GLN
7	A6	59	ARG
7	A6	71	CYS
7	A6	76	ASP
7	A6	87	LYS
7	A6	88	THR
7	A6	91	LEU
7	A6	94	VAL
7	A6	96	THR
7	A6	112	SER
7	A6	117	LYS
7	A6	118	LYS
7	A6	129	LYS
7	A6	134	TRP
7	A6	136	ILE
7	A6	137	LYS
7	A6	141	LEU
7	A6	149	ASP
7	A6	153	GLN
7	A6	165	ASP
7	A6	166	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A6	188	ILE
7	A6	199	ILE
7	A6	207	ASP
7	A6	221	MET
7	A6	238	ASP
7	A6	250	TYR
7	A6	266	ASP
7	A6	268	GLN
7	A6	292	LEU
7	A6	300	THR
7	A6	317	THR
8	A7	28	SER
8	A7	34	LYS
8	A7	46	LYS
8	A7	51	ARG
8	A7	61	ILE
8	A7	64	LYS
8	A7	65	THR
8	A7	68	ARG
8	A7	75	ASP
8	A7	78	ASP
8	A7	82	THR
8	A7	84	LYS
8	A7	88	ARG
8	A7	89	ARG
8	A7	94	HIS
8	A7	96	ARG
8	A7	97	THR
8	A7	100	THR
8	A7	102	THR
8	A7	105	LYS
8	A7	112	ASP
8	A7	130	GLU
8	A7	139	GLU
9	AA	7	PHE
9	AA	10	THR
9	AA	24	LEU
9	AA	27	ARG
9	AA	29	VAL
9	AA	33	GLN
9	AA	34	GLU
9	AA	37	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	AA	43	ASP
9	AA	45	VAL
9	AA	47	VAL
9	AA	50	VAL
9	AA	57	LEU
9	AA	59	LEU
9	AA	62	ARG
9	AA	76	ILE
9	AA	79	ARG
9	AA	84	ARG
9	AA	87	LEU
9	AA	88	LYS
9	AA	96	THR
9	AA	101	ARG
9	AA	103	THR
9	AA	110	TYR
9	AA	111	ILE
9	AA	114	SER
9	AA	117	GLU
9	AA	119	ARG
9	AA	123	VAL
9	AA	131	GLN
9	AA	135	GLU
9	AA	140	ASN
9	AA	154	GLU
9	AA	157	ASP
9	AA	162	CYS
9	AA	168	HIS
9	AA	172	LEU
9	AA	177	LEU
9	AA	184	LEU
9	AA	185	ARG
9	AA	196	SER
9	AA	197	ILE
10	AB	21	VAL
10	AB	22	ASP
10	AB	36	SER
10	AB	38	PHE
10	AB	47	LEU
10	AB	54	LEU
10	AB	55	LYS
10	AB	58	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	AB	61	LEU
10	AB	65	VAL
10	AB	68	VAL
10	AB	70	LEU
10	AB	73	LEU
10	AB	77	GLU
10	AB	78	ASP
10	AB	80	SER
10	AB	81	PHE
10	AB	83	LYS
10	AB	85	LYS
10	AB	89	ASP
10	AB	94	LYS
10	AB	96	LEU
10	AB	97	LEU
10	AB	105	PHE
10	AB	108	ASP
10	AB	109	LYS
10	AB	110	LEU
10	AB	115	ARG
10	AB	117	TRP
10	AB	124	ASN
10	AB	131	ASP
10	AB	135	LEU
10	AB	146	GLN
10	AB	148	ASN
10	AB	149	GLN
10	AB	154	SER
10	AB	166	LYS
10	AB	170	GLU
10	AB	177	GLN
10	AB	179	SER
10	AB	180	THR
10	AB	181	LEU
10	AB	183	GLN
10	AB	184	LEU
10	AB	193	ILE
10	AB	202	LYS
10	AB	214	LYS
10	AB	215	VAL
10	AB	218	LEU
10	AB	219	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	AB	220	GLN
10	AB	223	PHE
10	AB	225	VAL
10	AB	228	LEU
11	AC	41	LEU
11	AC	50	ILE
11	AC	53	ILE
11	AC	58	LEU
11	AC	64	LYS
11	AC	70	ASP
11	AC	71	THR
11	AC	72	LEU
11	AC	73	LEU
11	AC	76	LEU
11	AC	77	GLN
11	AC	80	VAL
11	AC	87	GLN
11	AC	89	GLN
11	AC	90	THR
11	AC	95	ARG
11	AC	96	THR
11	AC	97	ARG
11	AC	106	ASP
11	AC	111	VAL
11	AC	117	THR
11	AC	119	LYS
11	AC	130	ILE
11	AC	134	LEU
11	AC	137	ILE
11	AC	139	ILE
11	AC	140	ARG
11	AC	141	ARG
11	AC	146	THR
11	AC	148	LEU
11	AC	159	THR
11	AC	166	THR
11	AC	174	ARG
11	AC	185	LYS
11	AC	187	LEU
11	AC	201	ASN
11	AC	206	THR
11	AC	208	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	AC	221	THR
11	AC	222	TYR
11	AC	224	PHE
11	AC	226	THR
11	AC	237	VAL
11	AC	240	LEU
11	AC	245	ASP
11	AC	246	GLU
12	AD	4	LEU
12	AD	5	ILE
12	AD	7	LYS
12	AD	21	LEU
12	AD	23	GLU
12	AD	29	LEU
12	AD	37	VAL
12	AD	39	VAL
12	AD	53	THR
12	AD	57	ASP
12	AD	65	ARG
12	AD	66	ILE
12	AD	81	PRO
12	AD	84	ILE
12	AD	89	GLU
12	AD	90	ARG
12	AD	92	GLN
12	AD	93	ASP
12	AD	94	ARG
12	AD	96	LEU
12	AD	105	MET
12	AD	117	ARG
12	AD	127	MET
12	AD	129	SER
12	AD	134	CYS
12	AD	141	LYS
12	AD	142	LEU
12	AD	146	ARG
12	AD	151	LYS
12	AD	158	ILE
12	AD	170	THR
12	AD	172	THR
12	AD	176	LEU
12	AD	178	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	AD	181	VAL
12	AD	182	LEU
12	AD	187	LYS
12	AD	190	ARG
12	AD	204	ASP
12	AD	210	GLU
12	AD	215	GLU
12	AD	220	PRO
12	AD	221	SER
12	AD	222	VAL
13	AE	7	LYS
13	AE	9	LEU
13	AE	12	LEU
13	AE	23	LEU
13	AE	26	CYS
13	AE	38	LEU
13	AE	39	ARG
13	AE	45	ILE
13	AE	48	LEU
13	AE	56	LEU
13	AE	59	ARG
13	AE	62	LYS
13	AE	67	GLN
13	AE	68	ARG
13	AE	70	VAL
13	AE	72	VAL
13	AE	77	ARG
13	AE	92	LEU
13	AE	95	THR
13	AE	105	VAL
13	AE	116	ASP
13	AE	117	GLU
13	AE	123	LEU
13	AE	126	VAL
13	AE	129	VAL
13	AE	131	LEU
13	AE	133	LYS
13	AE	146	THR
13	AE	153	ASN
13	AE	155	LYS
13	AE	158	ASP
13	AE	164	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
13	AE	166	SER
13	AE	176	ASP
13	AE	180	LEU
13	AE	182	TYR
13	AE	187	ARG
13	AE	192	ILE
13	AE	197	HIS
13	AE	198	LYS
13	AE	206	ASP
13	AE	211	LYS
13	AE	215	ASP
13	AE	220	THR
13	AE	222	LEU
13	AE	226	PHE
13	AE	227	VAL
13	AE	237	SER
13	AE	240	LYS
13	AE	242	LYS
13	AE	246	LEU
13	AE	248	ILE
13	AE	258	GLN
13	AE	259	GLN
13	AE	261	LEU
14	AF	21	THR
14	AF	23	VAL
14	AF	24	VAL
14	AF	25	LEU
14	AF	27	THR
14	AF	32	GLU
14	AF	41	LYS
14	AF	42	LEU
14	AF	43	PHE
14	AF	45	LYS
14	AF	53	VAL
14	AF	63	GLN
14	AF	65	ARG
14	AF	68	ILE
14	AF	70	VAL
14	AF	76	ARG
14	AF	79	ASN
14	AF	84	LYS
14	AF	89	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	AF	93	LEU
14	AF	94	THR
14	AF	117	THR
14	AF	119	ASP
14	AF	130	ILE
14	AF	146	THR
14	AF	147	THR
14	AF	156	ARG
14	AF	157	ARG
14	AF	160	VAL
14	AF	162	VAL
14	AF	163	SER
14	AF	193	THR
14	AF	203	LYS
14	AF	206	SER
14	AF	216	GLU
14	AF	225	ARG
15	AG	21	GLU
15	AG	25	ARG
15	AG	45	PHE
15	AG	58	LYS
15	AG	59	GLN
15	AG	69	LEU
15	AG	70	PRO
15	AG	71	THR
15	AG	76	LEU
15	AG	78	THR
15	AG	79	LYS
15	AG	82	SER
15	AG	98	ARG
15	AG	105	ASP
15	AG	109	LEU
15	AG	115	LYS
15	AG	120	GLU
15	AG	124	LEU
15	AG	126	ASP
15	AG	127	THR
15	AG	129	VAL
15	AG	132	ARG
15	AG	133	LEU
15	AG	137	ARG
15	AG	143	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	AG	150	GLU
15	AG	151	ASP
15	AG	154	ARG
15	AG	155	ASP
15	AG	162	VAL
15	AG	170	THR
15	AG	175	ILE
15	AG	176	GLN
15	AG	177	ARG
15	AG	179	VAL
15	AG	211	LEU
15	AG	212	LEU
15	AG	217	SER
15	AG	223	LYS
16	AH	9	LEU
16	AH	25	VAL
16	AH	37	GLU
16	AH	38	LEU
16	AH	42	GLN
16	AH	46	ILE
16	AH	50	ASP
16	AH	51	VAL
16	AH	60	ILE
16	AH	66	SER
16	AH	67	LEU
16	AH	70	PHE
16	AH	71	HIS
16	AH	74	GLN
16	AH	75	THR
16	AH	77	LEU
16	AH	78	THR
16	AH	79	ARG
16	AH	80	GLU
16	AH	85	PHE
16	AH	87	ASP
16	AH	97	ARG
16	AH	103	SER
16	AH	105	THR
16	AH	109	VAL
16	AH	110	GLN
16	AH	114	ARG
16	AH	116	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	AH	117	THR
16	AH	126	LEU
16	AH	131	PHE
16	AH	143	LEU
16	AH	144	VAL
16	AH	148	LYS
16	AH	154	LEU
16	AH	162	ILE
16	AH	167	GLU
16	AH	181	ILE
16	AH	184	GLU
16	AH	185	ILE
16	AH	187	SER
17	AI	6	ASP
17	AI	7	SER
17	AI	8	ARG
17	AI	14	THR
17	AI	20	GLN
17	AI	21	PHE
17	AI	26	LYS
17	AI	28	GLU
17	AI	29	LEU
17	AI	36	THR
17	AI	46	VAL
17	AI	49	ARG
17	AI	58	LEU
17	AI	76	THR
17	AI	103	GLN
17	AI	107	THR
17	AI	120	THR
17	AI	121	LEU
17	AI	123	LYS
17	AI	135	LYS
17	AI	137	LYS
17	AI	138	ASN
17	AI	140	GLU
17	AI	142	LYS
17	AI	151	LYS
17	AI	152	ILE
17	AI	154	SER
17	AI	155	SER
17	AI	164	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
17	AI	184	LEU
17	AI	196	LEU
17	AI	199	LYS
18	AJ	3	ARG
18	AJ	6	ARG
18	AJ	7	THR
18	AJ	13	SER
18	AJ	14	THR
18	AJ	22	SER
18	AJ	28	LEU
18	AJ	39	LYS
18	AJ	46	SER
18	AJ	49	LEU
18	AJ	54	ARG
18	AJ	60	LEU
18	AJ	78	ARG
18	AJ	79	ARG
18	AJ	82	ARG
18	AJ	88	GLU
18	AJ	89	ASP
18	AJ	92	LYS
18	AJ	93	LEU
18	AJ	94	ASP
18	AJ	96	VAL
18	AJ	97	LEU
18	AJ	99	LEU
18	AJ	101	VAL
18	AJ	105	LEU
18	AJ	109	LEU
18	AJ	110	GLN
18	AJ	111	THR
18	AJ	120	LYS
18	AJ	130	THR
18	AJ	133	HIS
18	AJ	134	ILE
18	AJ	138	LYS
18	AJ	149	ARG
18	AJ	151	ASP
18	AJ	161	THR
18	AJ	171	ARG
18	AJ	172	VAL
18	AJ	174	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	AJ	175	ARG
18	AJ	182	GLU
19	AK	1	MET
19	AK	7	ASP
19	AK	8	ARG
19	AK	13	GLN
19	AK	20	VAL
19	AK	27	PHE
19	AK	29	GLN
19	AK	31	LYS
19	AK	32	HIS
19	AK	46	LEU
19	AK	49	LEU
19	AK	50	THR
19	AK	55	VAL
19	AK	56	LYS
19	AK	71	GLU
19	AK	76	LEU
19	AK	78	GLU
19	AK	80	LEU
19	AK	82	LEU
20	AL	3	THR
20	AL	7	VAL
20	AL	21	ASN
20	AL	27	THR
20	AL	29	LYS
20	AL	30	ARG
20	AL	40	LEU
20	AL	43	LYS
20	AL	44	THR
20	AL	54	ILE
20	AL	56	LYS
20	AL	67	ARG
20	AL	69	LYS
20	AL	74	THR
20	AL	79	LYS
20	AL	80	MET
20	AL	83	THR
20	AL	99	ARG
20	AL	109	VAL
20	AL	123	VAL
20	AL	131	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	AL	136	ARG
20	AL	140	VAL
20	AL	141	LYS
21	AM	25	GLU
21	AM	28	LEU
21	AM	33	ARG
21	AM	36	LEU
21	AM	43	ARG
21	AM	45	LEU
21	AM	50	LYS
21	AM	53	THR
21	AM	58	LEU
21	AM	59	LEU
21	AM	61	VAL
21	AM	62	LEU
21	AM	63	VAL
21	AM	71	ILE
21	AM	74	LEU
21	AM	75	VAL
21	AM	83	GLU
21	AM	85	LYS
21	AM	88	LEU
21	AM	89	ILE
21	AM	97	LEU
21	AM	103	LEU
21	AM	116	VAL
21	AM	119	SER
21	AM	121	VAL
21	AM	125	ASN
21	AM	126	TRP
21	AM	129	GLU
21	AM	132	GLU
21	AM	135	MET
21	AM	138	GLU
21	AM	139	HIS
21	AM	140	PHE
22	AN	3	ARG
22	AN	4	MET
22	AN	9	LYS
22	AN	12	SER
22	AN	16	ILE
22	AN	21	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	AN	27	LYS
22	AN	33	VAL
22	AN	36	GLN
22	AN	39	LYS
22	AN	42	ARG
22	AN	45	LEU
22	AN	50	ILE
22	AN	56	ASP
22	AN	58	HIS
22	AN	60	VAL
22	AN	64	ARG
22	AN	66	ILE
22	AN	67	THR
22	AN	76	LYS
22	AN	77	SER
22	AN	83	GLU
22	AN	84	ILE
22	AN	88	LEU
22	AN	94	LYS
22	AN	97	SER
22	AN	102	LEU
22	AN	105	ASN
22	AN	109	LYS
22	AN	114	ARG
22	AN	115	LEU
22	AN	125	LEU
22	AN	145	THR
22	AN	149	LEU
22	AN	150	VAL
22	AN	151	ASN
23	AO	13	VAL
23	AO	14	PHE
23	AO	16	VAL
23	AO	20	TYR
23	AO	24	ASN
23	AO	26	THR
23	AO	29	HIS
23	AO	31	THR
23	AO	39	ILE
23	AO	42	VAL
23	AO	43	THR
23	AO	51	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
23	AO	92	LYS
23	AO	99	GLN
23	AO	102	LEU
23	AO	103	ARG
23	AO	107	ARG
23	AO	108	SER
23	AO	118	VAL
23	AO	123	SER
23	AO	124	ASP
23	AO	125	SER
23	AO	133	ARG
23	AO	137	LEU
24	AP	14	THR
24	AP	22	LEU
24	AP	24	LYS
24	AP	26	LEU
24	AP	31	GLU
24	AP	35	LYS
24	AP	40	ARG
24	AP	44	ARG
24	AP	47	ARG
24	AP	50	THR
24	AP	52	LYS
24	AP	69	GLU
24	AP	86	VAL
24	AP	92	SER
24	AP	100	LYS
24	AP	110	GLU
24	AP	121	ILE
24	AP	125	PRO
24	AP	130	ARG
25	AQ	4	VAL
25	AQ	14	LYS
25	AQ	17	THR
25	AQ	23	LYS
25	AQ	26	LYS
25	AQ	28	LEU
25	AQ	36	ILE
25	AQ	44	LEU
25	AQ	45	ARG
25	AQ	52	LEU
25	AQ	53	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
25	AQ	54	LEU
25	AQ	57	LEU
25	AQ	58	ASP
25	AQ	59	LYS
25	AQ	63	ILE
25	AQ	66	ARG
25	AQ	68	ARG
25	AQ	69	VAL
25	AQ	76	SER
25	AQ	90	VAL
25	AQ	94	GLN
25	AQ	98	ASP
25	AQ	101	SER
25	AQ	106	LYS
25	AQ	115	THR
25	AQ	118	ILE
25	AQ	123	ARG
25	AQ	127	LYS
25	AQ	128	LYS
25	AQ	136	SER
25	AQ	137	ARG
25	AQ	138	PHE
25	AQ	141	SER
26	AR	5	ARG
26	AR	25	THR
26	AR	26	LEU
26	AR	29	GLN
26	AR	30	THR
26	AR	34	LEU
26	AR	36	ASP
26	AR	38	ILE
26	AR	44	LYS
26	AR	46	LEU
26	AR	49	LYS
26	AR	54	THR
26	AR	69	ILE
26	AR	72	LYS
26	AR	73	LEU
26	AR	78	ARG
26	AR	83	GLN
26	AR	84	TYR
26	AR	87	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	AR	105	GLN
26	AR	107	SER
26	AR	113	LEU
26	AR	115	LEU
26	AR	119	LEU
27	AS	3	LEU
27	AS	5	VAL
27	AS	8	GLN
27	AS	11	PHE
27	AS	12	GLN
27	AS	13	HIS
27	AS	14	ILE
27	AS	15	LEU
27	AS	17	LEU
27	AS	20	THR
27	AS	21	ASN
27	AS	26	ILE
27	AS	28	ILE
27	AS	34	THR
27	AS	38	VAL
27	AS	40	ARG
27	AS	46	VAL
27	AS	53	ASP
27	AS	54	LEU
27	AS	57	ARG
27	AS	60	GLU
27	AS	61	LEU
27	AS	71	GLN
27	AS	74	GLN
27	AS	77	THR
27	AS	80	LYS
27	AS	81	ILE
27	AS	86	LEU
27	AS	89	GLN
27	AS	92	ILE
27	AS	93	THR
27	AS	107	SER
27	AS	108	LYS
27	AS	110	ARG
27	AS	116	LEU
27	AS	119	ILE
27	AS	132	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
27	AS	136	GLN
27	AS	138	THR
27	AS	140	THR
27	AS	143	ARG
28	AT	4	VAL
28	AT	6	VAL
28	AT	13	ASP
28	AT	18	TYR
28	AT	22	LEU
28	AT	25	GLN
28	AT	28	LEU
28	AT	30	VAL
28	AT	33	TYR
28	AT	34	VAL
28	AT	35	ASP
28	AT	36	ILE
28	AT	37	VAL
28	AT	57	ARG
28	AT	63	ARG
28	AT	67	MET
28	AT	68	ARG
28	AT	84	LYS
28	AT	86	ARG
28	AT	88	VAL
28	AT	89	ARG
28	AT	92	LYS
28	AT	94	ILE
28	AT	103	LYS
28	AT	111	ILE
28	AT	126	GLU
28	AT	130	ARG
28	AT	131	ASP
28	AT	132	LEU
28	AT	134	ARG
28	AT	144	GLU
29	AU	15	GLN
29	AU	17	GLN
29	AU	18	GLN
29	AU	20	ILE
29	AU	22	ILE
29	AU	23	ARG
29	AU	27	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	AU	30	LYS
29	AU	31	VAL
29	AU	34	LEU
29	AU	35	GLU
29	AU	42	VAL
29	AU	47	GLN
29	AU	48	HIS
29	AU	51	VAL
29	AU	57	ARG
29	AU	58	LEU
29	AU	60	THR
29	AU	61	LYS
29	AU	66	SER
29	AU	74	GLU
29	AU	76	SER
29	AU	81	THR
29	AU	88	LYS
29	AU	89	ARG
29	AU	99	ILE
29	AU	103	ILE
29	AU	108	ILE
29	AU	121	ASN
30	AV	1	MET
30	AV	2	GLU
30	AV	3	ASN
30	AV	5	LYS
30	AV	7	GLN
30	AV	11	LEU
30	AV	25	LYS
30	AV	41	GLU
30	AV	49	GLU
30	AV	50	TYR
30	AV	52	THR
30	AV	60	ARG
30	AV	62	ARG
30	AV	68	SER
30	AV	69	LEU
30	AV	74	GLN
30	AV	76	ASP
30	AV	80	LYS
31	AW	3	ARG
31	AW	6	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
31	AW	7	LEU
31	AW	23	ARG
31	AW	24	GLN
31	AW	25	VAL
31	AW	27	ILE
31	AW	30	SER
31	AW	43	LYS
31	AW	53	ILE
31	AW	56	HIS
31	AW	65	LEU
31	AW	66	ASN
31	AW	69	LEU
31	AW	74	VAL
31	AW	76	SER
31	AW	83	ILE
31	AW	87	GLU
31	AW	93	LEU
31	AW	98	GLN
31	AW	103	ILE
31	AW	104	LEU
31	AW	105	THR
31	AW	114	GLU
31	AW	121	VAL
31	AW	129	VAL
32	AX	7	ARG
32	AX	9	LEU
32	AX	14	LYS
32	AX	18	HIS
32	AX	19	ARG
32	AX	28	ASN
32	AX	40	SER
32	AX	60	GLU
32	AX	82	LYS
32	AX	84	THR
32	AX	103	LEU
32	AX	107	PHE
32	AX	109	ARG
32	AX	110	LYS
32	AX	114	LYS
32	AX	117	ILE
32	AX	131	SER
32	AX	133	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	AX	137	LYS
32	AX	138	GLU
32	AX	140	LYS
32	AX	144	ARG
33	AY	17	LEU
33	AY	29	HIS
33	AY	32	ARG
33	AY	34	ASN
33	AY	44	LEU
33	AY	46	GLU
33	AY	47	VAL
33	AY	49	LYS
33	AY	51	GLU
33	AY	52	LYS
33	AY	57	VAL
33	AY	61	ARG
33	AY	62	THR
33	AY	75	VAL
33	AY	84	LYS
33	AY	88	THR
33	AY	93	ARG
33	AY	96	LEU
33	AY	99	LYS
33	AY	102	LYS
33	AY	105	ARG
33	AY	112	LYS
33	AY	123	LYS
33	AY	124	ARG
33	AY	127	LYS
33	AY	128	LYS
33	AY	129	VAL
33	AY	135	ASP
34	AZ	38	HIS
34	AZ	42	LEU
34	AZ	49	ARG
34	AZ	50	ILE
34	AZ	58	ARG
34	AZ	59	TYR
34	AZ	69	LEU
34	AZ	71	ILE
34	AZ	75	LEU
34	AZ	77	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
34	AZ	80	LEU
34	AZ	85	LYS
34	AZ	92	ILE
34	AZ	93	SER
34	AZ	95	HIS
34	AZ	96	SER
34	AZ	100	ILE
34	AZ	105	THR
35	BA	15	ILE
35	BA	23	ARG
35	BA	32	LEU
35	BA	41	ILE
35	BA	44	ILE
35	BA	45	VAL
35	BA	46	LYS
35	BA	48	ILE
35	BA	61	VAL
35	BA	62	VAL
35	BA	71	LEU
35	BA	96	LEU
35	BA	101	VAL
35	BA	104	LEU
35	BA	112	ILE
35	BA	113	VAL
35	BA	114	SER
35	BA	119	LYS
35	BA	134	VAL
35	BA	137	ILE
35	BA	142	ASP
35	BA	147	ARG
35	BA	155	LYS
35	BA	158	ILE
35	BA	169	ILE
35	BA	179	LEU
35	BA	180	LEU
35	BA	181	LYS
35	BA	193	ARG
35	BA	202	VAL
35	BA	207	VAL
35	BA	215	ASN
35	BA	224	THR
35	BA	226	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
35	BA	227	ARG
35	BA	230	VAL
35	BA	241	ARG
35	BA	243	THR
35	BA	246	LEU
36	BB	3	HIS
36	BB	4	ARG
36	BB	10	ARG
36	BB	17	LEU
36	BB	19	ARG
36	BB	20	LYS
36	BB	21	ARG
36	BB	24	SER
36	BB	30	LYS
36	BB	43	LEU
36	BB	47	LEU
36	BB	50	LYS
36	BB	56	ILE
36	BB	67	PHE
36	BB	70	ARG
36	BB	77	THR
36	BB	79	VAL
36	BB	81	THR
36	BB	84	VAL
36	BB	85	VAL
36	BB	89	VAL
36	BB	100	ARG
36	BB	103	THR
36	BB	114	VAL
36	BB	116	ARG
36	BB	139	GLN
36	BB	146	ARG
36	BB	148	LEU
36	BB	150	ARG
36	BB	153	LYS
36	BB	157	VAL
36	BB	169	THR
36	BB	175	LYS
36	BB	183	LEU
36	BB	187	SER
36	BB	188	ILE
36	BB	192	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
36	BB	196	ARG
36	BB	202	THR
36	BB	205	VAL
36	BB	213	GLU
36	BB	221	THR
36	BB	229	VAL
36	BB	232	ARG
36	BB	235	THR
36	BB	236	LYS
36	BB	238	LEU
36	BB	242	THR
36	BB	248	LYS
36	BB	252	ILE
36	BB	284	ARG
36	BB	291	GLU
36	BB	297	SER
36	BB	301	THR
36	BB	304	THR
36	BB	308	MET
36	BB	322	ILE
36	BB	324	VAL
36	BB	328	ILE
36	BB	332	ARG
36	BB	338	LEU
36	BB	340	LYS
36	BB	346	THR
36	BB	347	SER
36	BB	355	SER
36	BB	361	THR
36	BB	367	LYS
36	BB	369	ARG
36	BB	380	MET
36	BB	382	THR
37	BC	2	SER
37	BC	7	THR
37	BC	16	THR
37	BC	18	ASN
37	BC	25	VAL
37	BC	27	SER
37	BC	52	VAL
37	BC	53	SER
37	BC	55	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
37	BC	71	VAL
37	BC	85	SER
37	BC	93	MET
37	BC	99	MET
37	BC	112	LYS
37	BC	120	TYR
37	BC	122	THR
37	BC	136	LEU
37	BC	138	ARG
37	BC	144	LYS
37	BC	145	ILE
37	BC	150	LEU
37	BC	153	SER
37	BC	156	LEU
37	BC	158	SER
37	BC	161	LYS
37	BC	170	LYS
37	BC	176	SER
37	BC	177	ASP
37	BC	179	LEU
37	BC	182	LEU
37	BC	186	LYS
37	BC	187	LEU
37	BC	198	ARG
37	BC	203	ARG
37	BC	206	LEU
37	BC	220	ARG
37	BC	222	VAL
37	BC	230	VAL
37	BC	246	ARG
37	BC	258	LEU
37	BC	259	ASP
37	BC	265	GLU
37	BC	267	VAL
37	BC	283	THR
37	BC	287	THR
37	BC	289	ILE
37	BC	290	ILE
37	BC	300	ARG
37	BC	307	GLN
37	BC	313	LEU
37	BC	319	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
37	BC	323	VAL
37	BC	327	LEU
37	BC	333	VAL
37	BC	339	LEU
37	BC	342	LYS
37	BC	345	GLU
37	BC	349	THR
37	BC	354	VAL
37	BC	356	THR
37	BC	357	GLU
37	BC	358	THR
37	BC	359	LEU
37	BC	360	LYS
37	BC	362	ASP
38	BD	4	GLN
38	BD	5	LYS
38	BD	13	SER
38	BD	34	LYS
38	BD	35	ARG
38	BD	41	LYS
38	BD	51	LEU
38	BD	65	ILE
38	BD	68	THR
38	BD	70	THR
38	BD	74	VAL
38	BD	81	HIS
38	BD	89	THR
38	BD	93	THR
38	BD	110	LEU
38	BD	112	LYS
38	BD	113	LEU
38	BD	118	THR
38	BD	124	GLU
38	BD	131	LEU
38	BD	133	GLU
38	BD	136	GLU
38	BD	146	LEU
38	BD	148	ILE
38	BD	152	ARG
38	BD	155	THR
38	BD	164	LYS
38	BD	185	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	BD	186	GLU
38	BD	189	GLU
38	BD	190	ILE
38	BD	191	ASP
38	BD	194	LEU
38	BD	205	SER
38	BD	211	LEU
38	BD	218	ARG
38	BD	227	LEU
38	BD	232	ASP
38	BD	251	PRO
38	BD	254	LYS
38	BD	258	LYS
38	BD	259	LYS
38	BD	262	LYS
38	BD	268	GLU
38	BD	273	ARG
38	BD	275	THR
38	BD	282	ARG
39	BE	5	LYS
39	BE	8	LYS
39	BE	20	LYS
39	BE	21	THR
39	BE	46	ARG
39	BE	50	LYS
39	BE	64	LEU
39	BE	65	ILE
39	BE	76	LEU
39	BE	78	ARG
39	BE	79	VAL
39	BE	89	THR
39	BE	93	VAL
39	BE	98	VAL
39	BE	99	GLU
39	BE	109	GLU
39	BE	143	LYS
39	BE	152	THR
39	BE	155	LEU
39	BE	162	SER
40	BF	22	THR
40	BF	24	GLU
40	BF	26	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
40	BF	39	GLU
40	BF	41	ARG
40	BF	45	LEU
40	BF	53	LYS
40	BF	54	GLU
40	BF	56	GLU
40	BF	60	ARG
40	BF	83	LEU
40	BF	88	ARG
40	BF	98	LYS
40	BF	101	LYS
40	BF	121	LYS
40	BF	124	LEU
40	BF	130	ILE
40	BF	156	ILE
40	BF	158	LYS
40	BF	159	GLN
40	BF	173	LEU
40	BF	175	LYS
40	BF	179	LEU
40	BF	184	LEU
40	BF	196	LYS
40	BF	206	LYS
40	BF	219	LYS
40	BF	229	PHE
40	BF	239	LEU
41	BG	26	LEU
41	BG	41	GLN
41	BG	50	VAL
41	BG	68	ARG
41	BG	70	LYS
41	BG	74	THR
41	BG	79	GLN
41	BG	81	THR
41	BG	85	ASN
41	BG	89	GLU
41	BG	92	LYS
41	BG	95	ASN
41	BG	110	THR
41	BG	126	SER
41	BG	128	LYS
41	BG	136	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
41	BG	145	ASN
41	BG	146	LYS
41	BG	149	LYS
41	BG	150	LEU
41	BG	153	ILE
41	BG	160	ILE
41	BG	169	LEU
41	BG	172	LYS
41	BG	173	MET
41	BG	183	LYS
41	BG	185	ARG
41	BG	189	LEU
41	BG	208	GLU
41	BG	213	LYS
41	BG	214	LEU
41	BG	216	SER
41	BG	217	THR
41	BG	219	ASP
41	BG	222	PHE
41	BG	230	LYS
41	BG	241	LYS
41	BG	245	LYS
41	BG	248	LYS
42	BH	4	ILE
42	BH	5	GLN
42	BH	6	THR
42	BH	18	VAL
42	BH	19	SER
42	BH	20	ILE
42	BH	31	ARG
42	BH	33	THR
42	BH	43	VAL
42	BH	44	THR
42	BH	52	LEU
42	BH	55	VAL
42	BH	62	ARG
42	BH	63	LYS
42	BH	68	LEU
42	BH	69	ARG
42	BH	70	THR
42	BH	80	THR
42	BH	82	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
42	BH	92	TYR
42	BH	106	LYS
42	BH	121	LYS
42	BH	123	ILE
42	BH	129	ARG
42	BH	130	ASP
42	BH	132	VAL
42	BH	133	THR
42	BH	134	ILE
42	BH	138	THR
42	BH	144	ILE
42	BH	151	VAL
42	BH	157	ASN
42	BH	161	LEU
42	BH	162	GLN
42	BH	164	ILE
42	BH	169	ASN
42	BH	177	ASP
42	BH	179	ILE
42	BH	191	LEU
43	BI	4	ARG
43	BI	24	ARG
43	BI	26	VAL
43	BI	36	LEU
43	BI	42	THR
43	BI	52	LEU
43	BI	57	LEU
43	BI	58	GLU
43	BI	63	GLU
43	BI	71	CYS
43	BI	74	LYS
43	BI	76	MET
43	BI	78	THR
43	BI	83	ASP
43	BI	87	LEU
43	BI	91	VAL
43	BI	99	ILE
43	BI	129	VAL
43	BI	139	ARG
43	BI	140	THR
43	BI	143	SER
43	BI	144	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
43	BI	145	LYS
43	BI	153	ARG
43	BI	163	GLN
43	BI	167	LEU
43	BI	169	LYS
43	BI	174	THR
43	BI	177	ASP
43	BI	178	ARG
43	BI	185	ARG
43	BI	200	LEU
43	BI	206	LEU
43	BI	211	ARG
43	BI	212	GLU
43	BI	215	GLU
43	BI	217	PHE
44	BJ	10	ARG
44	BJ	12	LEU
44	BJ	13	LYS
44	BJ	16	LYS
44	BJ	22	SER
44	BJ	29	ARG
44	BJ	30	LEU
44	BJ	31	THR
44	BJ	34	SER
44	BJ	35	LYS
44	BJ	44	THR
44	BJ	46	VAL
44	BJ	80	LEU
44	BJ	87	LYS
44	BJ	92	ARG
44	BJ	94	ARG
44	BJ	106	ILE
44	BJ	107	ASP
44	BJ	112	LEU
44	BJ	114	ILE
44	BJ	129	VAL
44	BJ	130	VAL
44	BJ	132	ASN
44	BJ	137	ARG
44	BJ	138	VAL
44	BJ	140	ARG
44	BJ	142	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
44	BJ	147	THR
44	BJ	158	ASP
44	BJ	159	THR
44	BJ	160	VAL
44	BJ	161	SER
44	BJ	165	GLN
46	BL	45	LYS
46	BL	46	ILE
46	BL	54	LEU
46	BL	55	ARG
46	BL	59	ARG
46	BL	63	VAL
46	BL	67	ARG
46	BL	68	LYS
46	BL	69	VAL
46	BL	73	ARG
46	BL	85	LEU
46	BL	100	ARG
46	BL	107	GLU
46	BL	114	GLN
46	BL	115	ARG
46	BL	118	GLU
46	BL	121	SER
46	BL	123	ILE
46	BL	124	ILE
46	BL	128	ARG
46	BL	131	LYS
46	BL	152	THR
46	BL	154	VAL
46	BL	157	ARG
46	BL	164	GLU
46	BL	171	ARG
46	BL	175	SER
46	BL	184	GLU
46	BL	189	GLU
46	BL	194	GLU
47	BM	3	THR
47	BM	10	SER
47	BM	13	ARG
47	BM	20	VAL
47	BM	24	LYS
47	BM	42	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
47	BM	53	VAL
47	BM	62	GLN
47	BM	63	VAL
47	BM	64	VAL
47	BM	72	LEU
47	BM	74	ARG
47	BM	80	THR
47	BM	82	SER
47	BM	92	GLU
47	BM	106	ARG
47	BM	107	GLU
47	BM	124	ARG
47	BM	126	GLN
47	BM	128	ARG
47	BM	130	THR
47	BM	132	LYS
47	BM	133	LYS
47	BM	135	LEU
48	BN	5	LYS
48	BN	7	LEU
48	BN	8	GLU
48	BN	10	LEU
48	BN	12	ARG
48	BN	15	GLN
48	BN	18	VAL
48	BN	22	LEU
48	BN	24	ARG
48	BN	41	ARG
48	BN	49	ARG
48	BN	54	LYS
48	BN	68	ARG
48	BN	80	THR
48	BN	85	THR
48	BN	92	LEU
48	BN	93	LYS
48	BN	96	ARG
48	BN	97	SER
48	BN	104	GLU
48	BN	105	ARG
48	BN	109	ARG
48	BN	117	ASN
48	BN	134	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
48	BN	138	GLN
48	BN	155	VAL
48	BN	159	ARG
48	BN	170	LYS
48	BN	184	LYS
48	BN	190	THR
48	BN	196	THR
48	BN	204	LYS
49	BO	3[A]	VAL
49	BO	3[B]	SER
49	BO	12[A]	LYS
49	BO	12[B]	LYS
49	BO	16[B]	LEU
49	BO	22[B]	THR
49	BO	27[B]	VAL
49	BO	34[A]	VAL
49	BO	34[B]	VAL
49	BO	41[A]	LEU
49	BO	41[B]	LEU
49	BO	58[A]	LEU
49	BO	58[B]	LEU
49	BO	59[A]	ARG
49	BO	59[B]	ARG
49	BO	67[A]	THR
49	BO	67[B]	THR
49	BO	74[A]	ARG
49	BO	74[B]	ARG
49	BO	78[A]	ARG
49	BO	78[B]	ARG
49	BO	80[B]	LEU
49	BO	85[A]	ARG
49	BO	85[B]	ARG
49	BO	100[A]	GLU
49	BO	100[B]	GLU
49	BO	106[A]	GLU
49	BO	106[B]	GLU
49	BO	108[A]	ILE
49	BO	108[B]	ILE
49	BO	117[A]	ARG
49	BO	117[B]	ARG
49	BO	124[A]	LEU
49	BO	124[B]	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
49	BO	126[A]	VAL
49	BO	126[B]	VAL
49	BO	128[A]	ARG
49	BO	128[B]	ARG
49	BO	129[A]	LEU
49	BO	129[B]	LEU
49	BO	130[A]	LYS
49	BO	130[B]	LYS
49	BO	144[A]	SER
49	BO	144[B]	SER
49	BO	160[A]	ARG
49	BO	160[B]	ARG
49	BO	163[B]	ARG
49	BO	166[A]	GLU
49	BO	166[B]	GLU
49	BO	171[A]	LYS
49	BO	171[B]	LYS
49	BO	175[A]	THR
49	BO	175[B]	THR
49	BO	182[A]	ASN
49	BO	184[A]	THR
49	BO	197[A]	LEU
50	BP	9	THR
50	BP	24	VAL
50	BP	29	THR
50	BP	31	GLU
50	BP	32	THR
50	BP	41	LEU
50	BP	52	LEU
50	BP	56	ARG
50	BP	69	ARG
50	BP	74	LYS
50	BP	78	VAL
50	BP	79	THR
50	BP	80	LYS
50	BP	89	LYS
50	BP	94	LEU
50	BP	103	GLU
50	BP	112	LEU
50	BP	114	VAL
50	BP	119	VAL
50	BP	126	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
50	BP	128	ARG
50	BP	138	LYS
51	BQ	3	ILE
51	BQ	7	SER
51	BQ	17	THR
51	BQ	24	VAL
51	BQ	26	LEU
51	BQ	31	LYS
51	BQ	32	LEU
51	BQ	34	THR
51	BQ	49	LEU
51	BQ	57	ILE
51	BQ	64	VAL
51	BQ	80	THR
51	BQ	81	VAL
51	BQ	86	THR
51	BQ	93	ILE
51	BQ	98	LYS
51	BQ	100	THR
51	BQ	105	ARG
51	BQ	113	LYS
51	BQ	135	GLN
51	BQ	138	LEU
51	BQ	147	ARG
51	BQ	150	VAL
51	BQ	161	LYS
51	BQ	165	ILE
51	BQ	166	LEU
51	BQ	170	ARG
52	BR	5	ARG
52	BR	7	GLN
52	BR	10	LEU
52	BR	17	VAL
52	BR	20	ARG
52	BR	27	ASN
52	BR	29	THR
52	BR	36	ASN
52	BR	39	ASN
52	BR	43	LYS
52	BR	49	THR
52	BR	55	VAL
52	BR	56	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
52	BR	63	THR
52	BR	70	LYS
52	BR	71	ARG
52	BR	74	ARG
52	BR	98	ARG
52	BR	99	LEU
52	BR	105	LEU
52	BR	106	LEU
52	BR	114	LYS
52	BR	126	GLU
52	BR	138	LEU
52	BR	152	GLU
52	BR	153	LYS
52	BR	158	GLU
52	BR	162	ARG
52	BR	164	LEU
52	BR	167	ARG
52	BR	173	ARG
52	BR	180	LYS
53	BS	1	MET
53	BS	13	ARG
53	BS	15	PRO
53	BS	17	GLU
53	BS	21	GLU
53	BS	23	LYS
53	BS	40	ARG
53	BS	50	LYS
53	BS	51	VAL
53	BS	52	LYS
53	BS	61	ILE
53	BS	71	LYS
53	BS	74	ASN
53	BS	80	ARG
53	BS	87	THR
53	BS	96	ASP
53	BS	97	VAL
53	BS	100	VAL
53	BS	104	GLU
53	BS	105	THR
53	BS	115	ARG
53	BS	117	ARG
53	BS	130	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
53	BS	136	LYS
53	BS	146	LYS
53	BS	148	LEU
53	BS	149	LYS
53	BS	155	ARG
53	BS	161	LYS
53	BS	162	THR
53	BS	166	LYS
53	BS	169	SER
53	BS	172	TYR
54	BT	17	ARG
54	BT	25	VAL
54	BT	26	HIS
54	BT	27	LEU
54	BT	35	LYS
54	BT	36	VAL
54	BT	47	SER
54	BT	55	LYS
54	BT	68	THR
54	BT	71	SER
54	BT	78	LYS
54	BT	80	VAL
54	BT	83	ARG
54	BT	88	ARG
54	BT	89	LEU
54	BT	96	ILE
54	BT	102	ARG
54	BT	104	GLU
54	BT	118	GLU
54	BT	126	VAL
54	BT	131	GLN
54	BT	135	PRO
54	BT	139	ARG
54	BT	143	THR
54	BT	149	GLN
54	BT	150	THR
54	BT	160	ILE
55	BU	13	LYS
55	BU	14	THR
55	BU	16	THR
55	BU	21	SER
55	BU	23	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
55	BU	27	VAL
55	BU	28	PHE
55	BU	37	LEU
55	BU	39	ASP
55	BU	43	VAL
55	BU	50	LEU
55	BU	52	ASN
55	BU	54	VAL
55	BU	55	THR
55	BU	58	GLU
55	BU	61	THR
55	BU	62	VAL
55	BU	63	VAL
55	BU	68	THR
55	BU	90	ARG
55	BU	98	THR
55	BU	100	THR
55	BU	105	LEU
56	BV	13	ILE
56	BV	14	SER
56	BV	48	ARG
56	BV	70	ARG
56	BV	88	ARG
56	BV	91	VAL
56	BV	110	LYS
56	BV	115	THR
57	BW	1	MET
57	BW	5	ILE
57	BW	25	ASP
57	BW	47	ARG
57	BW	56	ARG
57	BW	57	LYS
57	BW	63	ILE
57	BW	95	SER
57	BW	97	LYS
57	BW	100	VAL
57	BW	105	ARG
57	BW	107	GLU
57	BW	126	GLU
57	BW	127	LYS
57	BW	135	SER
58	BX	24	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
58	BX	27	ARG
58	BX	34	LEU
58	BX	37	THR
58	BX	38	LEU
58	BX	40	LEU
58	BX	56	ARG
58	BX	57	LEU
58	BX	63	ILE
58	BX	70	GLU
58	BX	71	THR
58	BX	73	MET
58	BX	74	LYS
58	BX	86	VAL
58	BX	101	GLU
58	BX	108	LEU
58	BX	109	LYS
58	BX	115	ARG
58	BX	121	LYS
58	BX	125	ARG
58	BX	133	LEU
58	BX	135	ILE
58	BX	142	ILE
59	BY	12	ARG
59	BY	13	ARG
59	BY	14	LYS
59	BY	17	LYS
59	BY	37	LYS
59	BY	40	ARG
59	BY	43	TYR
59	BY	45	ILE
59	BY	50	ILE
59	BY	52	ARG
59	BY	57	LEU
59	BY	59	VAL
59	BY	66	GLN
59	BY	71	SER
59	BY	74	TYR
59	BY	76	LEU
59	BY	80	VAL
59	BY	83	ASP
59	BY	87	LYS
59	BY	94	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
59	BY	95	VAL
59	BY	97	ILE
59	BY	103	LYS
59	BY	120	GLN
60	BZ	3	LYS
60	BZ	14	VAL
60	BZ	17	ARG
60	BZ	24	VAL
60	BZ	30	ASP
60	BZ	31	GLU
60	BZ	34	LYS
60	BZ	55	LYS
60	BZ	65	ARG
60	BZ	72	ILE
60	BZ	81	LEU
60	BZ	83	THR
60	BZ	86	THR
60	BZ	89	VAL
60	BZ	93	LYS
60	BZ	95	VAL
60	BZ	99	GLU
60	BZ	100	THR
60	BZ	102	GLU
60	BZ	103	GLN
60	BZ	105	SER
60	BZ	121	ARG
60	BZ	126	LYS
60	BZ	127	ASN
60	BZ	134	LEU
60	BZ	135	ARG
61	Ba	6	THR
61	Ba	8	THR
61	Ba	10	LYS
61	Ba	12	ARG
61	Ba	16	SER
61	Ba	24	LYS
61	Ba	34	MET
61	Ba	42	ARG
61	Ba	44	ASN
61	Ba	47	LYS
61	Ba	60	TYR
61	Ba	78	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
61	Ba	80	THR
61	Ba	82	ILE
61	Ba	85	ASP
61	Ba	91	LEU
61	Ba	97	GLU
61	Ba	98	THR
61	Ba	115	LYS
61	Ba	128	ARG
61	Ba	130	VAL
61	Ba	132	LYS
61	Ba	133	LEU
62	Bb	14	ARG
62	Bb	15	LYS
62	Bb	21	ILE
62	Bb	22	LYS
62	Bb	26	THR
62	Bb	33	LYS
62	Bb	38	LYS
62	Bb	50	THR
62	Bb	52	LYS
62	Bb	58	LYS
62	Bb	59	LYS
63	Bc	8	GLU
63	Bc	9	SER
63	Bc	18	ILE
63	Bc	19	LYS
63	Bc	30	THR
63	Bc	33	SER
63	Bc	34	LEU
63	Bc	40	LYS
63	Bc	41	LEU
63	Bc	48	THR
63	Bc	61	MET
63	Bc	68	TYR
63	Bc	86	ARG
63	Bc	87	VAL
63	Bc	99	ASP
63	Bc	100	ILE
64	Bd	6	ASP
64	Bd	8	VAL
64	Bd	13	THR
64	Bd	16	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
64	Bd	26	LYS
64	Bd	31	ARG
64	Bd	34	LYS
64	Bd	44	MET
64	Bd	55	LEU
64	Bd	61	LYS
64	Bd	76	SER
64	Bd	82	GLU
64	Bd	89	LEU
64	Bd	90	PHE
64	Bd	96	VAL
64	Bd	100	SER
64	Bd	102	LYS
64	Bd	104	LEU
64	Bd	105	GLN
64	Bd	106	THR
64	Bd	110	GLU
65	Be	4	LEU
65	Be	14	THR
65	Be	16	LYS
65	Be	18	LYS
65	Be	19	ARG
65	Be	27	ARG
65	Be	31	ASN
65	Be	33	ARG
65	Be	35	GLN
65	Be	51	SER
65	Be	61	LYS
65	Be	73	THR
65	Be	75	LEU
65	Be	82	LEU
65	Be	87	MET
65	Be	91	THR
65	Be	106	VAL
65	Be	109	LEU
65	Be	125	ARG
65	Be	126	LEU
66	Bf	4	SER
66	Bf	10	LYS
66	Bf	20	LYS
66	Bf	28	SER
66	Bf	31	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
66	Bf	49	ILE
66	Bf	70	LYS
66	Bf	81	VAL
66	Bf	84	THR
66	Bf	98	VAL
66	Bf	107	ILE
67	Bg	5	VAL
67	Bg	9	ARG
67	Bg	16	ARG
67	Bg	19	LYS
67	Bg	20	ILE
67	Bg	23	VAL
67	Bg	24	LYS
67	Bg	29	ILE
67	Bg	30	LEU
67	Bg	31	ARG
67	Bg	35	VAL
67	Bg	36	LYS
67	Bg	44	CYS
67	Bg	54	ILE
67	Bg	58	ARG
67	Bg	65	VAL
67	Bg	70	LYS
67	Bg	79	SER
67	Bg	85	VAL
67	Bg	86	LYS
67	Bg	88	ARG
67	Bg	90	ILE
67	Bg	98	GLN
67	Bg	104	VAL
68	Bh	15	GLU
68	Bh	20	GLN
68	Bh	21	LEU
68	Bh	27	GLU
68	Bh	28	LEU
68	Bh	38	ARG
68	Bh	40	SER
68	Bh	45	LYS
68	Bh	47	VAL
68	Bh	48	ARG
68	Bh	57	VAL
68	Bh	62	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
68	Bh	66	VAL
68	Bh	69	LEU
68	Bh	79	ASP
68	Bh	81	ARG
68	Bh	84	LYS
68	Bh	85	THR
68	Bh	86	ARG
68	Bh	89	ARG
68	Bh	90	ARG
68	Bh	98	SER
68	Bh	100	VAL
68	Bh	101	THR
68	Bh	107	LYS
68	Bh	119	LYS
69	Bi	3	VAL
69	Bi	7	ILE
69	Bi	9	ILE
69	Bi	11	LEU
69	Bi	17	VAL
69	Bi	18	THR
69	Bi	21	THR
69	Bi	26	ILE
69	Bi	29	LYS
69	Bi	34	SER
69	Bi	36	ARG
69	Bi	37	THR
69	Bi	38	LYS
69	Bi	43	LEU
69	Bi	45	ARG
69	Bi	57	LEU
69	Bi	58	ILE
69	Bi	60	LEU
69	Bi	61	ILE
69	Bi	66	GLU
69	Bi	68	ARG
69	Bi	74	LYS
69	Bi	75	LYS
69	Bi	76	ARG
69	Bi	81	THR
69	Bi	88	GLU
69	Bi	90	MET
69	Bi	94	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
69	Bi	98	ARG
70	Bj	3	LYS
70	Bj	11	ARG
70	Bj	17	THR
70	Bj	25	ARG
70	Bj	33	THR
70	Bj	36	SER
70	Bj	44	THR
70	Bj	55	ARG
70	Bj	58	THR
70	Bj	59	THR
70	Bj	64	MET
70	Bj	65	ARG
70	Bj	67	LEU
70	Bj	68	LYS
70	Bj	75	LYS
70	Bj	80	THR
70	Bj	84	SER
71	Bk	5	ILE
71	Bk	12	LEU
71	Bk	24	THR
71	Bk	31	LEU
71	Bk	39	ARG
71	Bk	41	THR
71	Bk	46	ARG
71	Bk	50	SER
71	Bk	53	THR
71	Bk	61	LYS
71	Bk	64	LYS
71	Bk	65	LEU
71	Bk	67	GLN
71	Bk	68	SER
72	Bl	11	GLN
72	Bl	15	LYS
72	Bl	17	LYS
72	Bl	21	ARG
72	Bl	23	LEU
72	Bl	27	ILE
72	Bl	29	LEU
72	Bl	41	ARG
72	Bl	45	ARG
72	Bl	47	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
72	B <sub>l</sub>	51	ILE
73	B <sub>m</sub>	78	ILE
73	B <sub>m</sub>	79	GLU
73	B <sub>m</sub>	83	LYS
73	B <sub>m</sub>	85	LEU
73	B <sub>m</sub>	88	LYS
73	B <sub>m</sub>	91	CYS
73	B <sub>m</sub>	93	LYS
73	B <sub>m</sub>	106	ARG
73	B <sub>m</sub>	112	LYS
73	B <sub>m</sub>	113	ARG
73	B <sub>m</sub>	114	LYS
73	B <sub>m</sub>	126	LYS
73	B <sub>m</sub>	127	LEU
74	B <sub>n</sub>	6	ARG
74	B <sub>n</sub>	9	ARG
74	B <sub>n</sub>	13	LEU
74	B <sub>n</sub>	16	LYS
74	B <sub>n</sub>	21	ARG
74	B <sub>n</sub>	23	ARG
74	B <sub>n</sub>	24	SER
75	B <sub>o</sub>	7	THR
75	B <sub>o</sub>	8	ARG
75	B <sub>o</sub>	18	ARG
75	B <sub>o</sub>	46	LYS
75	B <sub>o</sub>	47	GLN
75	B <sub>o</sub>	61	LYS
75	B <sub>o</sub>	63	LYS
75	B <sub>o</sub>	71	ARG
75	B <sub>o</sub>	78	LYS
75	B <sub>o</sub>	79	THR
75	B <sub>o</sub>	83	LEU
75	B <sub>o</sub>	84	THR
75	B <sub>o</sub>	89	LYS
75	B <sub>o</sub>	93	LEU
75	B <sub>o</sub>	104	LEU
75	B <sub>o</sub>	105	GLN
76	B <sub>q</sub>	6	GLU
76	B <sub>q</sub>	14	LYS
76	B <sub>q</sub>	17	GLU
76	B <sub>q</sub>	26	PHE
76	B <sub>q</sub>	39	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
76	Bq	53	MET
76	Bq	60	ARG
76	Bq	64	ARG
76	Bq	89	THR
76	Bq	186	THR
83	CV	16	THR
83	CV	23	ASP
83	CV	69	VAL
83	CV	110	GLN
83	CV	126	VAL
83	CV	133	ASP
83	CV	235	LEU
83	CV	243	PHE
83	CV	251	LEU
83	CV	255	TYR
83	CV	267	MET
83	CV	294	VAL
83	CV	310	ASN
83	CV	322	LEU
83	CV	336	ASP
83	CV	387	ARG
83	CV	401	ARG
83	CV	415	PRO
83	CV	420	GLU
83	CV	422	LYS
83	CV	435	TYR
83	CV	451	GLU
83	CV	485	GLU
83	CV	495	TYR
83	CV	509	GLU
83	CV	525	GLN
83	CV	538	LYS
83	CV	553	ASN
83	CV	575	ASP
83	CV	580	ILE
83	CV	582	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
4	A3	48	ASN
4	A3	53	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A6	17	ASN
8	A7	108	GLN
9	AA	168	HIS
10	AB	101	HIS
10	AB	146	GLN
10	AB	149	GLN
10	AB	177	GLN
11	AC	89	GLN
11	AC	94	GLN
12	AD	179	GLN
13	AE	16	HIS
13	AE	98	ASN
14	AF	103	ASN
14	AF	104	ASN
14	AF	128	ASN
14	AF	170	GLN
15	AG	13	GLN
15	AG	22	HIS
15	AG	189	HIS
17	AI	44	HIS
17	AI	64	ASN
17	AI	103	GLN
18	AJ	110	GLN
18	AJ	131	GLN
18	AJ	133	HIS
20	AL	110	HIS
21	AM	125	ASN
25	AQ	74	HIS
27	AS	89	GLN
27	AS	136	GLN
29	AU	18	GLN
29	AU	72	ASN
30	AV	74	GLN
31	AW	16	ASN
31	AW	24	GLN
31	AW	80	ASN
32	AX	48	HIS
34	AZ	95	HIS
35	BA	50	HIS
35	BA	194	ASN
35	BA	209	HIS
35	BA	215	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
36	BB	243	HIS
37	BC	48	GLN
37	BC	114	ASN
37	BC	221	ASN
38	BD	40	HIS
38	BD	63	GLN
38	BD	81	HIS
39	BE	167	ASN
41	BG	59	GLN
42	BH	58	HIS
44	BJ	101	ASN
44	BJ	109	HIS
44	BJ	132	ASN
48	BN	90	ASN
50	BP	55	GLN
51	BQ	158	HIS
52	BR	166	ASN
54	BT	26	HIS
54	BT	49	GLN
55	BU	40	HIS
56	BV	33	ASN
60	BZ	57	HIS
61	Ba	44	ASN
61	Ba	62	HIS
61	Ba	64	GLN
64	Bd	43	HIS
66	Bf	77	ASN
67	Bg	33	GLN
68	Bh	20	GLN
70	Bj	79	GLN
72	Bl	4	GLN
72	Bl	19	GLN
76	Bq	39	HIS
76	Bq	56	ASN
76	Bq	103	ASN
83	CV	65	GLN
83	CV	95	ASN
83	CV	109	GLN
83	CV	153	GLN
83	CV	184	GLN
83	CV	310	ASN
83	CV	432	ASN

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
79	B2	1764/1800 (98%)	545 (30%)	86 (4%)
80	B5	3140/3396 (92%)	741 (23%)	131 (4%)
81	B7	120/121 (99%)	18 (15%)	0
82	B8	157/158 (99%)	32 (20%)	3 (1%)
84	CW	74/76 (97%)	23 (31%)	5 (6%)
85	CX	2/3 (66%)	0	0
All	All	5257/5554 (94%)	1359 (25%)	225 (4%)

All (1359) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
79	B2	2	A
79	B2	4	C
79	B2	8	U
79	B2	16	G
79	B2	20	G
79	B2	25	C
79	B2	26	A
79	B2	27	U
79	B2	34	G
79	B2	39	A
79	B2	41	A
79	B2	42	G
79	B2	45	U
79	B2	46	A
79	B2	47	A
79	B2	50	C
79	B2	57	G
79	B2	60	U
79	B2	67	A
79	B2	68	A
79	B2	69	G
79	B2	72	A
79	B2	73	U
79	B2	74	U
79	B2	75	U
79	B2	76	A
79	B2	77	U
79	B2	78	A
79	B2	97	C
79	B2	100	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	101	U
79	B2	104	A
79	B2	114	C
79	B2	126	A
79	B2	127	G
79	B2	131	C
79	B2	132	U
79	B2	133	U
79	B2	134	U
79	B2	135	A
79	B2	136	C
79	B2	137	U
79	B2	138	A
79	B2	139	C
79	B2	140	A
79	B2	141	U
79	B2	144	U
79	B2	145	A
79	B2	146	U
79	B2	153	G
79	B2	158	U
79	B2	159	U
79	B2	175	G
79	B2	178	U
79	B2	179	A
79	B2	185	U
79	B2	186	C
79	B2	187	G
79	B2	188	A
79	B2	189	C
79	B2	190	C
79	B2	191	C
79	B2	192	U
79	B2	193	U
79	B2	194	U
79	B2	195	G
79	B2	196	G
79	B2	197	A
79	B2	198	A
79	B2	199	G
79	B2	200	A
79	B2	215	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	218	A
79	B2	219	A
79	B2	223	U
79	B2	225	A
79	B2	226	A
79	B2	227	U
79	B2	228	G
79	B2	229	U
79	B2	233	C
79	B2	234	G
79	B2	235	G
79	B2	236	A
79	B2	238	U
79	B2	239	C
79	B2	240	U
79	B2	241	U
79	B2	242	U
79	B2	249	U
79	B2	250	C
79	B2	261	U
79	B2	262	U
79	B2	265	A
79	B2	266	A
79	B2	271	A
79	B2	272	U
79	B2	274	G
79	B2	275	C
79	B2	276	C
79	B2	277	U
79	B2	278	U
79	B2	279	G
79	B2	280	U
79	B2	281	G
79	B2	288	A
79	B2	290	G
79	B2	299	A
79	B2	301	A
79	B2	306	U
79	B2	308	C
79	B2	309	C
79	B2	314	C
79	B2	316	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	319	U
79	B2	320	U
79	B2	321	C
79	B2	322	G
79	B2	337	G
79	B2	338	C
79	B2	341	A
79	B2	348	U
79	B2	352	A
79	B2	359	A
79	B2	360	A
79	B2	361	C
79	B2	399	A
79	B2	400	A
79	B2	401	A
79	B2	402	C
79	B2	403	G
79	B2	404	G
79	B2	411	C
79	B2	416	A
79	B2	418	G
79	B2	423	G
79	B2	424	C
79	B2	425	A
79	B2	426	G
79	B2	428	A
79	B2	434	G
79	B2	439	U
79	B2	444	C
79	B2	445	A
79	B2	446	A
79	B2	448	C
79	B2	467	G
79	B2	468	A
79	B2	470	A
79	B2	475	A
79	B2	477	A
79	B2	484	C
79	B2	485	A
79	B2	486	G
79	B2	487	G
79	B2	488	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	493	U
79	B2	494	U
79	B2	495	C
79	B2	496	G
79	B2	497	G
79	B2	498	G
79	B2	499	U
79	B2	500	C
79	B2	502	U
79	B2	503	G
79	B2	504	U
79	B2	505	A
79	B2	506	A
79	B2	507	U
79	B2	508	U
79	B2	510	G
79	B2	511	A
79	B2	512	A
79	B2	513	U
79	B2	515	A
79	B2	516	G
79	B2	519	C
79	B2	525	A
79	B2	527	A
79	B2	532	U
79	B2	538	A
79	B2	539	G
79	B2	540	G
79	B2	541	A
79	B2	542	A
79	B2	543	C
79	B2	544	A
79	B2	545	A
79	B2	548	G
79	B2	555	A
79	B2	556	A
79	B2	557	G
79	B2	558	U
79	B2	559	C
79	B2	565	C
79	B2	570	A
79	B2	575	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	579	A
79	B2	580	A
79	B2	582	U
79	B2	583	C
79	B2	585	A
79	B2	594	A
79	B2	595	G
79	B2	597	G
79	B2	605	A
79	B2	607	G
79	B2	611	U
79	B2	619	A
79	B2	620	A
79	B2	622	A
79	B2	623	A
79	B2	624	G
79	B2	630	A
79	B2	639	U
79	B2	640	U
79	B2	650	U
79	B2	653	C
79	B2	655	G
79	B2	656	G
79	B2	657	U
79	B2	658	C
79	B2	677	G
79	B2	679	U
79	B2	680	U
79	B2	684	A
79	B2	685	A
79	B2	686	C
79	B2	692	C
79	B2	694	U
79	B2	696	C
79	B2	697	C
79	B2	699	U
79	B2	700	C
79	B2	701	U
79	B2	702	G
79	B2	703	G
79	B2	704	C
79	B2	705	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	706	A
79	B2	707	A
79	B2	709	C
79	B2	710	U
79	B2	712	G
79	B2	713	A
79	B2	714	G
79	B2	717	C
79	B2	718	U
79	B2	719	U
79	B2	720	G
79	B2	721	U
79	B2	722	G
79	B2	723	G
79	B2	725	U
79	B2	727	U
79	B2	728	U
79	B2	729	G
79	B2	730	G
79	B2	731	C
79	B2	732	G
79	B2	733	A
79	B2	734	A
79	B2	735	C
79	B2	736	C
79	B2	737	A
79	B2	738	G
79	B2	742	U
79	B2	743	U
79	B2	745	U
79	B2	754	A
79	B2	755	A
79	B2	756	A
79	B2	758	U
79	B2	765	G
79	B2	766	U
79	B2	771	A
79	B2	774	A
79	B2	775	G
79	B2	778	G
79	B2	779	U
79	B2	780	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	781	U
79	B2	782	U
79	B2	783	G
79	B2	784	C
79	B2	785	U
79	B2	787	G
79	B2	789	A
79	B2	793	A
79	B2	794	U
79	B2	795	U
79	B2	806	A
79	B2	811	A
79	B2	812	A
79	B2	813	U
79	B2	815	G
79	B2	816	G
79	B2	818	C
79	B2	819	G
79	B2	820	U
79	B2	821	U
79	B2	823	G
79	B2	824	G
79	B2	829	A
79	B2	830	U
79	B2	831	U
79	B2	832	U
79	B2	833	U
79	B2	837	G
79	B2	838	G
79	B2	840	U
79	B2	846	G
79	B2	848	C
79	B2	849	C
79	B2	854	U
79	B2	862	A
79	B2	863	A
79	B2	864	U
79	B2	873	U
79	B2	876	G
79	B2	892	A
79	B2	896	U
79	B2	898	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	912	U
79	B2	913	G
79	B2	914	G
79	B2	921	U
79	B2	928	U
79	B2	933	A
79	B2	935	U
79	B2	942	G
79	B2	944	A
79	B2	951	A
79	B2	959	U
79	B2	960	U
79	B2	961	U
79	B2	966	A
79	B2	968	U
79	B2	982	U
79	B2	988	A
79	B2	992	A
79	B2	993	A
79	B2	995	A
79	B2	997	G
79	B2	1003	A
79	B2	1004	U
79	B2	1005	A
79	B2	1020	A
79	B2	1021	C
79	B2	1026	A
79	B2	1028	C
79	B2	1031	U
79	B2	1039	A
79	B2	1040	G
79	B2	1052	U
79	B2	1053	G
79	B2	1058	U
79	B2	1059	U
79	B2	1060	U
79	B2	1061	A
79	B2	1064	G
79	B2	1073	G
79	B2	1074	G
79	B2	1079	U
79	B2	1080	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	1082	C
79	B2	1083	G
79	B2	1084	A
79	B2	1086	A
79	B2	1087	A
79	B2	1091	A
79	B2	1092	A
79	B2	1093	A
79	B2	1096	C
79	B2	1097	U
79	B2	1100	G
79	B2	1104	U
79	B2	1111	G
79	B2	1138	A
79	B2	1139	A
79	B2	1146	G
79	B2	1149	G
79	B2	1151	A
79	B2	1152	A
79	B2	1155	G
79	B2	1157	A
79	B2	1158	C
79	B2	1160	A
79	B2	1162	C
79	B2	1167	G
79	B2	1185	U
79	B2	1188	G
79	B2	1191	U
79	B2	1194	A
79	B2	1196	A
79	B2	1197	C
79	B2	1199	G
79	B2	1200	G
79	B2	1202	A
79	B2	1207	C
79	B2	1208	A
79	B2	1217	A
79	B2	1218	G
79	B2	1219	A
79	B2	1221	A
79	B2	1226	A
79	B2	1227	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	1228	G
79	B2	1229	G
79	B2	1235	C
79	B2	1243	G
79	B2	1244	A
79	B2	1245	G
79	B2	1250	U
79	B2	1251	U
79	B2	1257	U
79	B2	1258	U
79	B2	1260	U
79	B2	1269	U
79	B2	1286	U
79	B2	1301	U
79	B2	1314	U
79	B2	1315	U
79	B2	1321	A
79	B2	1329	A
79	B2	1337	A
79	B2	1339	C
79	B2	1340	U
79	B2	1341	A
79	B2	1344	A
79	B2	1345	A
79	B2	1349	G
79	B2	1354	G
79	B2	1361	U
79	B2	1363	U
79	B2	1364	G
79	B2	1370	U
79	B2	1371	A
79	B2	1372	U
79	B2	1379	C
79	B2	1382	A
79	B2	1383	G
79	B2	1388	A
79	B2	1390	U
79	B2	1398	U
79	B2	1399	C
79	B2	1400	A
79	B2	1412	G
79	B2	1413	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	1414	U
79	B2	1415	U
79	B2	1420	C
79	B2	1421	A
79	B2	1427	A
79	B2	1428	G
79	B2	1429	G
79	B2	1431	C
79	B2	1445	G
79	B2	1446	A
79	B2	1448	G
79	B2	1454	G
79	B2	1457	C
79	B2	1459	C
79	B2	1461	C
79	B2	1462	G
79	B2	1471	A
79	B2	1473	U
79	B2	1474	G
79	B2	1475	A
79	B2	1478	G
79	B2	1482	C
79	B2	1486	G
79	B2	1488	G
79	B2	1489	U
79	B2	1490	C
79	B2	1491	U
79	B2	1492	A
79	B2	1493	A
79	B2	1499	G
79	B2	1500	C
79	B2	1506	G
79	B2	1514	U
79	B2	1516	A
79	B2	1518	C
79	B2	1521	G
79	B2	1523	G
79	B2	1524	A
79	B2	1535	U
79	B2	1536	G
79	B2	1537	C
79	B2	1538	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	1539	G
79	B2	1540	G
79	B2	1557	U
79	B2	1559	A
79	B2	1569	A
79	B2	1573	A
79	B2	1574	G
79	B2	1575	G
79	B2	1584	G
79	B2	1590	G
79	B2	1601	G
79	B2	1616	G
79	B2	1619	C
79	B2	1624	C
79	B2	1625	C
79	B2	1631	A
79	B2	1635	A
79	B2	1649	G
79	B2	1657	U
79	B2	1658	G
79	B2	1663	G
79	B2	1680	G
79	B2	1682	U
79	B2	1683	C
79	B2	1684	U
79	B2	1685	G
79	B2	1686	C
79	B2	1687	U
79	B2	1693	A
79	B2	1712	A
79	B2	1713	G
79	B2	1716	C
79	B2	1717	G
79	B2	1727	G
79	B2	1729	C
79	B2	1731	A
79	B2	1759	C
79	B2	1760	G
79	B2	1761	U
79	B2	1762	A
79	B2	1766	A
79	B2	1768	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	1769	U
79	B2	1770	U
79	B2	1780	G
79	B2	1782	A
79	B2	1783	C
79	B2	1789	G
79	B2	1792	G
79	B2	1793	G
79	B2	1794	A
79	B2	1795	U
79	B2	1796	C
80	B5	14	U
80	B5	15	C
80	B5	16	A
80	B5	26	A
80	B5	38	U
80	B5	40	A
80	B5	43	A
80	B5	49	A
80	B5	60	A
80	B5	65	A
80	B5	66	A
80	B5	74	G
80	B5	76	G
80	B5	77	A
80	B5	92	G
80	B5	93	C
80	B5	96	G
80	B5	99	A
80	B5	109	A
80	B5	110	G
80	B5	111	C
80	B5	116	A
80	B5	121	A
80	B5	122	A
80	B5	133	U
80	B5	134	U
80	B5	135	C
80	B5	136	G
80	B5	146	U
80	B5	150	A
80	B5	152	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	156	G
80	B5	157	A
80	B5	160	G
80	B5	166	C
80	B5	170	G
80	B5	171	G
80	B5	174	C
80	B5	178	U
80	B5	180	C
80	B5	182	U
80	B5	183	G
80	B5	184	U
80	B5	187	A
80	B5	190	U
80	B5	191	U
80	B5	200	C
80	B5	201	A
80	B5	210	U
80	B5	218	G
80	B5	219	A
80	B5	221	A
80	B5	235	A
80	B5	236	G
80	B5	238	A
80	B5	239	G
80	B5	240	U
80	B5	242	C
80	B5	244	G
80	B5	248	U
80	B5	249	U
80	B5	250	U
80	B5	251	G
80	B5	252	U
80	B5	253	A
80	B5	254	A
80	B5	258	G
80	B5	259	C
80	B5	269	G
80	B5	283	G
80	B5	284	A
80	B5	286	U
80	B5	294	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	295	A
80	B5	305	U
80	B5	322	U
80	B5	323	A
80	B5	329	U
80	B5	334	A
80	B5	339	C
80	B5	349	A
80	B5	350	C
80	B5	351	A
80	B5	352	A
80	B5	370	U
80	B5	376	G
80	B5	390	G
80	B5	395	A
80	B5	398	A
80	B5	399	A
80	B5	401	U
80	B5	402	A
80	B5	403	C
80	B5	421	G
80	B5	422	A
80	B5	436	A
80	B5	437	G
80	B5	438	A
80	B5	439	C
80	B5	440	A
80	B5	441	U
80	B5	442	G
80	B5	443	G
80	B5	492	U
80	B5	493	G
80	B5	495	G
80	B5	520	U
80	B5	521	A
80	B5	531	G
80	B5	535	G
80	B5	538	G
80	B5	546	C
80	B5	547	G
80	B5	548	G
80	B5	551	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	553	U
80	B5	555	U
80	B5	557	A
80	B5	559	A
80	B5	578	A
80	B5	579	G
80	B5	592	A
80	B5	594	U
80	B5	595	G
80	B5	600	G
80	B5	604	G
80	B5	609	G
80	B5	610	G
80	B5	611	A
80	B5	612	U
80	B5	619	A
80	B5	620	U
80	B5	621	A
80	B5	630	A
80	B5	636	C
80	B5	649	A
80	B5	653	A
80	B5	656	A
80	B5	660	A
80	B5	675	C
80	B5	677	A
80	B5	681	U
80	B5	705	A
80	B5	708	G
80	B5	712	G
80	B5	715	A
80	B5	716	A
80	B5	719	U
80	B5	720	A
80	B5	725	G
80	B5	726	G
80	B5	735	A
80	B5	736	A
80	B5	750	G
80	B5	758	C
80	B5	766	U
80	B5	767	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	768	C
80	B5	776	U
80	B5	777	U
80	B5	780	A
80	B5	781	G
80	B5	785	G
80	B5	786	A
80	B5	806	A
80	B5	809	G
80	B5	817	A
80	B5	830	A
80	B5	846	A
80	B5	851	C
80	B5	861	C
80	B5	862	U
80	B5	871	U
80	B5	874	U
80	B5	879	U
80	B5	891	G
80	B5	893	C
80	B5	896	A
80	B5	897	U
80	B5	907	G
80	B5	908	G
80	B5	914	A
80	B5	916	G
80	B5	917	A
80	B5	921	A
80	B5	923	C
80	B5	924	G
80	B5	937	G
80	B5	944	C
80	B5	946	U
80	B5	947	G
80	B5	958	C
80	B5	959	C
80	B5	960	U
80	B5	974	G
80	B5	979	U
80	B5	980	A
80	B5	981	U
80	B5	983	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	994	G
80	B5	1000	C
80	B5	1001	G
80	B5	1002	A
80	B5	1003	A
80	B5	1010	G
80	B5	1014	U
80	B5	1015	U
80	B5	1016	C
80	B5	1017	C
80	B5	1018	G
80	B5	1020	G
80	B5	1021	G
80	B5	1023	C
80	B5	1024	G
80	B5	1025	A
80	B5	1026	A
80	B5	1027	A
80	B5	1028	U
80	B5	1029	G
80	B5	1032	C
80	B5	1034	U
80	B5	1035	G
80	B5	1047	A
80	B5	1049	C
80	B5	1057	A
80	B5	1064	A
80	B5	1065	A
80	B5	1071	U
80	B5	1072	G
80	B5	1081	U
80	B5	1082	U
80	B5	1085	A
80	B5	1093	A
80	B5	1094	U
80	B5	1095	U
80	B5	1096	U
80	B5	1097	G
80	B5	1098	A
80	B5	1103	A
80	B5	1104	G
80	B5	1117	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	1131	G
80	B5	1153	A
80	B5	1159	A
80	B5	1160	C
80	B5	1174	G
80	B5	1178	G
80	B5	1179	A
80	B5	1180	A
80	B5	1181	U
80	B5	1182	A
80	B5	1191	U
80	B5	1192	C
80	B5	1193	A
80	B5	1201	C
80	B5	1209	G
80	B5	1213	G
80	B5	1229	G
80	B5	1230	G
80	B5	1231	A
80	B5	1232	C
80	B5	1233	G
80	B5	1236	G
80	B5	1237	G
80	B5	1239	C
80	B5	1240	A
80	B5	1241	U
80	B5	1242	G
80	B5	1244	A
80	B5	1245	A
80	B5	1246	G
80	B5	1247	U
80	B5	1248	C
80	B5	1258	U
80	B5	1259	A
80	B5	1261	G
80	B5	1262	G
80	B5	1263	A
80	B5	1264	G
80	B5	1265	U
80	B5	1266	G
80	B5	1271	A
80	B5	1272	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	1278	A
80	B5	1279	C
80	B5	1280	C
80	B5	1282	G
80	B5	1283	C
80	B5	1284	C
80	B5	1285	G
80	B5	1294	A
80	B5	1307	G
80	B5	1308	A
80	B5	1309	U
80	B5	1312	C
80	B5	1330	A
80	B5	1332	A
80	B5	1348	U
80	B5	1349	G
80	B5	1350	A
80	B5	1351	U
80	B5	1352	A
80	B5	1353	U
80	B5	1354	G
80	B5	1355	A
80	B5	1356	U
80	B5	1357	G
80	B5	1366	A
80	B5	1385	C
80	B5	1386	A
80	B5	1387	G
80	B5	1399	A
80	B5	1400	G
80	B5	1403	C
80	B5	1419	A
80	B5	1422	G
80	B5	1428	A
80	B5	1434	G
80	B5	1437	C
80	B5	1440	G
80	B5	1446	A
80	B5	1450	G
80	B5	1460	A
80	B5	1481	A
80	B5	1482	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	1490	A
80	B5	1495	U
80	B5	1502	C
80	B5	1503	A
80	B5	1508	C
80	B5	1527	C
80	B5	1541	G
80	B5	1542	G
80	B5	1549	U
80	B5	1554	U
80	B5	1555	U
80	B5	1556	C
80	B5	1557	A
80	B5	1560	G
80	B5	1561	G
80	B5	1562	C
80	B5	1563	C
80	B5	1565	G
80	B5	1566	A
80	B5	1567	U
80	B5	1568	U
80	B5	1569	U
80	B5	1570	U
80	B5	1571	A
80	B5	1572	U
80	B5	1574	C
80	B5	1575	A
80	B5	1576	G
80	B5	1577	G
80	B5	1578	C
80	B5	1580	A
80	B5	1581	C
80	B5	1582	C
80	B5	1583	A
80	B5	1587	A
80	B5	1589	A
80	B5	1593	A
80	B5	1605	A
80	B5	1607	U
80	B5	1608	C
80	B5	1620	U
80	B5	1629	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	1633	C
80	B5	1635	G
80	B5	1639	C
80	B5	1641	U
80	B5	1643	A
80	B5	1644	C
80	B5	1645	U
80	B5	1655	G
80	B5	1657	C
80	B5	1680	G
80	B5	1683	A
80	B5	1716	U
80	B5	1717	U
80	B5	1718	G
80	B5	1724	U
80	B5	1725	C
80	B5	1736	G
80	B5	1750	A
80	B5	1751	G
80	B5	1754	G
80	B5	1758	G
80	B5	1760	A
80	B5	1762	C
80	B5	1764	U
80	B5	1765	U
80	B5	1766	G
80	B5	1767	C
80	B5	1770	G
80	B5	1778	G
80	B5	1780	G
80	B5	1783	U
80	B5	1797	A
80	B5	1810	A
80	B5	1812	G
80	B5	1814	A
80	B5	1815	U
80	B5	1816	A
80	B5	1817	G
80	B5	1818	U
80	B5	1820	U
80	B5	1821	U
80	B5	1835	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	1841	A
80	B5	1842	A
80	B5	1846	C
80	B5	1849	C
80	B5	1850	A
80	B5	1855	U
80	B5	1871	U
80	B5	1876	U
80	B5	1878	G
80	B5	1879	A
80	B5	1880	U
80	B5	1905	G
80	B5	1906	G
80	B5	1909	A
80	B5	1918	C
80	B5	1927	G
80	B5	1940	G
80	B5	1953	G
80	B5	2100	A
80	B5	2101	C
80	B5	2102	U
80	B5	2112	U
80	B5	2113	A
80	B5	2114	C
80	B5	2121	G
80	B5	2122	G
80	B5	2128	C
80	B5	2131	A
80	B5	2134	G
80	B5	2139	A
80	B5	2144	A
80	B5	2158	A
80	B5	2169	G
80	B5	2170	U
80	B5	2171	G
80	B5	2192	C
80	B5	2201	G
80	B5	2205	U
80	B5	2210	G
80	B5	2213	A
80	B5	2222	A
80	B5	2223	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	2228	A
80	B5	2229	A
80	B5	2244	A
80	B5	2250	G
80	B5	2253	G
80	B5	2255	A
80	B5	2256	A
80	B5	2257	C
80	B5	2258	U
80	B5	2264	U
80	B5	2270	A
80	B5	2273	G
80	B5	2276	G
80	B5	2278	C
80	B5	2279	A
80	B5	2288	G
80	B5	2290	C
80	B5	2294	U
80	B5	2298	U
80	B5	2307	G
80	B5	2310	U
80	B5	2313	A
80	B5	2315	G
80	B5	2324	A
80	B5	2329	C
80	B5	2334	U
80	B5	2335	G
80	B5	2336	U
80	B5	2373	A
80	B5	2374	C
80	B5	2375	G
80	B5	2377	G
80	B5	2385	G
80	B5	2388	U
80	B5	2393	G
80	B5	2394	G
80	B5	2396	G
80	B5	2397	A
80	B5	2398	A
80	B5	2400	G
80	B5	2401	A
80	B5	2402	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	2403	G
80	B5	2404	A
80	B5	2405	C
80	B5	2406	C
80	B5	2411	U
80	B5	2418	G
80	B5	2435	G
80	B5	2436	U
80	B5	2437	G
80	B5	2438	A
80	B5	2439	A
80	B5	2440	G
80	B5	2441	A
80	B5	2443	A
80	B5	2504	U
80	B5	2505	U
80	B5	2506	U
80	B5	2507	C
80	B5	2508	U
80	B5	2510	U
80	B5	2511	A
80	B5	2512	C
80	B5	2513	U
80	B5	2514	U
80	B5	2515	A
80	B5	2518	C
80	B5	2523	A
80	B5	2524	A
80	B5	2526	C
80	B5	2530	G
80	B5	2531	C
80	B5	2532	U
80	B5	2534	G
80	B5	2538	U
80	B5	2539	C
80	B5	2540	A
80	B5	2543	U
80	B5	2544	U
80	B5	2549	G
80	B5	2552	C
80	B5	2555	G
80	B5	2562	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	2567	C
80	B5	2568	C
80	B5	2569	A
80	B5	2570	U
80	B5	2571	U
80	B5	2572	C
80	B5	2573	G
80	B5	2574	G
80	B5	2584	G
80	B5	2585	G
80	B5	2589	G
80	B5	2590	A
80	B5	2591	A
80	B5	2593	A
80	B5	2594	C
80	B5	2598	G
80	B5	2599	U
80	B5	2606	G
80	B5	2607	G
80	B5	2610	G
80	B5	2614	G
80	B5	2615	G
80	B5	2622	C
80	B5	2637	A
80	B5	2639	G
80	B5	2652	U
80	B5	2656	A
80	B5	2662	G
80	B5	2663	G
80	B5	2667	A
80	B5	2674	A
80	B5	2677	G
80	B5	2678	A
80	B5	2681	U
80	B5	2683	U
80	B5	2689	A
80	B5	2691	A
80	B5	2694	A
80	B5	2696	A
80	B5	2714	G
80	B5	2723	U
80	B5	2728	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	2729	U
80	B5	2752	U
80	B5	2753	G
80	B5	2762	A
80	B5	2771	U
80	B5	2772	C
80	B5	2773	C
80	B5	2776	C
80	B5	2777	G
80	B5	2778	G
80	B5	2779	A
80	B5	2796	G
80	B5	2799	A
80	B5	2800	G
80	B5	2801	A
80	B5	2810	C
80	B5	2817	A
80	B5	2818	U
80	B5	2819	A
80	B5	2822	U
80	B5	2829	U
80	B5	2839	G
80	B5	2844	C
80	B5	2845	A
80	B5	2853	A
80	B5	2871	G
80	B5	2872	A
80	B5	2873	U
80	B5	2875	U
80	B5	2887	A
80	B5	2889	C
80	B5	2896	A
80	B5	2897	A
80	B5	2898	G
80	B5	2899	C
80	B5	2904	U
80	B5	2910	A
80	B5	2923	U
80	B5	2928	C
80	B5	2935	U
80	B5	2936	A
80	B5	2941	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	2942	C
80	B5	2945	G
80	B5	2947	G
80	B5	2954	U
80	B5	2957	G
80	B5	2970	C
80	B5	2971	A
80	B5	2972	G
80	B5	2979	U
80	B5	2983	C
80	B5	2987	A
80	B5	2990	G
80	B5	2996	U
80	B5	2997	G
80	B5	3012	A
80	B5	3028	G
80	B5	3050	U
80	B5	3056	U
80	B5	3057	U
80	B5	3059	G
80	B5	3078	U
80	B5	3079	U
80	B5	3080	G
80	B5	3086	A
80	B5	3087	A
80	B5	3092	C
80	B5	3130	A
80	B5	3131	U
80	B5	3139	A
80	B5	3142	A
80	B5	3143	C
80	B5	3148	U
80	B5	3153	U
80	B5	3154	C
80	B5	3155	U
80	B5	3156	U
80	B5	3157	U
80	B5	3158	G
80	B5	3159	C
80	B5	3164	C
80	B5	3165	A
80	B5	3166	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	3168	A
80	B5	3171	U
80	B5	3172	A
80	B5	3173	G
80	B5	3174	A
80	B5	3175	U
80	B5	3176	G
80	B5	3177	G
80	B5	3179	U
80	B5	3180	A
80	B5	3181	C
80	B5	3187	A
80	B5	3195	U
80	B5	3196	U
80	B5	3207	U
80	B5	3217	C
80	B5	3218	A
80	B5	3219	G
80	B5	3222	U
80	B5	3223	A
80	B5	3224	G
80	B5	3227	A
80	B5	3229	G
80	B5	3238	G
80	B5	3245	A
80	B5	3246	G
80	B5	3247	G
80	B5	3251	U
80	B5	3253	G
80	B5	3259	U
80	B5	3260	G
80	B5	3269	U
80	B5	3270	U
80	B5	3273	A
80	B5	3275	U
80	B5	3276	G
80	B5	3277	U
80	B5	3279	A
80	B5	3280	U
80	B5	3282	U
80	B5	3284	G
80	B5	3285	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	3286	G
80	B5	3288	G
80	B5	3289	G
80	B5	3290	G
80	B5	3292	A
80	B5	3294	A
80	B5	3304	U
80	B5	3307	A
80	B5	3313	U
80	B5	3316	A
80	B5	3317	U
80	B5	3318	G
80	B5	3319	U
80	B5	3320	A
80	B5	3330	A
80	B5	3333	G
80	B5	3335	A
80	B5	3336	A
80	B5	3341	U
80	B5	3342	A
80	B5	3343	G
80	B5	3345	G
80	B5	3349	C
80	B5	3351	U
80	B5	3352	U
80	B5	3354	U
80	B5	3355	U
80	B5	3356	G
80	B5	3357	U
80	B5	3358	U
80	B5	3369	G
80	B5	3378	C
80	B5	3382	U
80	B5	3383	G
80	B5	3389	U
80	B5	3390	G
80	B5	3393	U
80	B5	3396	U
81	B7	7	G
81	B7	22	A
81	B7	27	A
81	B7	33	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
81	B7	38	U
81	B7	42	A
81	B7	54	U
81	B7	61	G
81	B7	65	G
81	B7	66	A
81	B7	73	C
81	B7	74	C
81	B7	93	C
81	B7	101	G
81	B7	102	A
81	B7	103	A
81	B7	104	A
81	B7	112	G
82	B8	21	C
82	B8	34	U
82	B8	35	C
82	B8	48	A
82	B8	52	A
82	B8	53	A
82	B8	59	A
82	B8	62	C
82	B8	63	G
82	B8	79	A
82	B8	80	A
82	B8	81	U
82	B8	83	C
82	B8	84	C
82	B8	86	U
82	B8	87	G
82	B8	90	U
82	B8	95	G
82	B8	104	A
82	B8	105	A
82	B8	106	C
82	B8	111	A
82	B8	113	U
82	B8	122	U
82	B8	125	U
82	B8	126	A
82	B8	127	U
82	B8	138	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
82	B8	152	G
82	B8	156	U
82	B8	157	U
82	B8	158	U
84	CW	2	C
84	CW	3	C
84	CW	8	U
84	CW	17	C
84	CW	18	G
84	CW	19	G
84	CW	20	U
84	CW	21	A
84	CW	22	G
84	CW	37	A
84	CW	42	C
84	CW	46	G
84	CW	48	C
84	CW	52	G
84	CW	57	G
84	CW	60	U
84	CW	61	C
84	CW	68	C
84	CW	72	C
84	CW	73	A
84	CW	74	C
84	CW	75	C
84	CW	76	A

All (225) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
79	B2	2	A
79	B2	25	C
79	B2	45	U
79	B2	68	A
79	B2	73	U
79	B2	74	U
79	B2	76	A
79	B2	103	A
79	B2	114	C
79	B2	126	A
79	B2	130	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	131	C
79	B2	132	U
79	B2	133	U
79	B2	136	C
79	B2	139	C
79	B2	144	U
79	B2	158	U
79	B2	187	G
79	B2	217	A
79	B2	218	A
79	B2	232	U
79	B2	239	C
79	B2	240	U
79	B2	278	U
79	B2	280	U
79	B2	320	U
79	B2	400	A
79	B2	417	A
79	B2	484	C
79	B2	495	C
79	B2	497	G
79	B2	498	G
79	B2	499	U
79	B2	501	U
79	B2	503	G
79	B2	507	U
79	B2	512	A
79	B2	542	A
79	B2	543	C
79	B2	555	A
79	B2	558	U
79	B2	582	U
79	B2	685	A
79	B2	704	C
79	B2	720	G
79	B2	721	U
79	B2	734	A
79	B2	755	A
79	B2	781	U
79	B2	782	U
79	B2	794	U
79	B2	811	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
79	B2	815	G
79	B2	819	G
79	B2	823	G
79	B2	829	A
79	B2	913	G
79	B2	1051	G
79	B2	1058	U
79	B2	1081	A
79	B2	1137	A
79	B2	1157	A
79	B2	1187	U
79	B2	1195	C
79	B2	1196	A
79	B2	1207	C
79	B2	1226	A
79	B2	1234	A
79	B2	1244	A
79	B2	1250	U
79	B2	1339	C
79	B2	1344	A
79	B2	1370	U
79	B2	1428	G
79	B2	1481	C
79	B2	1489	U
79	B2	1490	C
79	B2	1521	G
79	B2	1568	C
79	B2	1572	G
79	B2	1573	A
79	B2	1615	C
79	B2	1657	U
79	B2	1711	C
79	B2	1761	U
80	B5	43	A
80	B5	65	A
80	B5	93	C
80	B5	151	A
80	B5	169	U
80	B5	183	G
80	B5	217	U
80	B5	238	A
80	B5	282	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	397	A
80	B5	436	A
80	B5	438	A
80	B5	439	C
80	B5	545	U
80	B5	546	C
80	B5	588	G
80	B5	611	A
80	B5	619	A
80	B5	647	A
80	B5	705	A
80	B5	715	A
80	B5	719	U
80	B5	726	G
80	B5	735	A
80	B5	765	C
80	B5	786	A
80	B5	816	A
80	B5	873	C
80	B5	896	A
80	B5	908	G
80	B5	916	G
80	B5	937	G
80	B5	979	U
80	B5	993	G
80	B5	1027	A
80	B5	1033	U
80	B5	1064	A
80	B5	1081	U
80	B5	1085	A
80	B5	1094	U
80	B5	1152	G
80	B5	1181	U
80	B5	1192	C
80	B5	1230	G
80	B5	1231	A
80	B5	1236	G
80	B5	1238	C
80	B5	1241	U
80	B5	1256	G
80	B5	1258	U
80	B5	1284	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	1307	G
80	B5	1317	A
80	B5	1329	U
80	B5	1331	U
80	B5	1352	A
80	B5	1355	A
80	B5	1434	G
80	B5	1481	A
80	B5	1507	G
80	B5	1514	G
80	B5	1554	U
80	B5	1560	G
80	B5	1568	U
80	B5	1574	C
80	B5	1580	A
80	B5	1589	A
80	B5	1607	U
80	B5	1716	U
80	B5	1724	U
80	B5	1815	U
80	B5	1816	A
80	B5	1817	G
80	B5	1819	U
80	B5	1841	A
80	B5	1842	A
80	B5	1849	C
80	B5	1878	G
80	B5	1879	A
80	B5	2101	C
80	B5	2112	U
80	B5	2116	G
80	B5	2204	C
80	B5	2209	U
80	B5	2249	G
80	B5	2255	A
80	B5	2257	C
80	B5	2372	A
80	B5	2374	C
80	B5	2440	G
80	B5	2507	C
80	B5	2513	U
80	B5	2531	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
80	B5	2537	U
80	B5	2539	C
80	B5	2583	C
80	B5	2585	G
80	B5	2593	A
80	B5	2662	G
80	B5	2682	C
80	B5	2689	A
80	B5	2714	G
80	B5	2728	G
80	B5	2752	U
80	B5	2772	C
80	B5	2777	G
80	B5	2801	A
80	B5	2817	A
80	B5	2818	U
80	B5	2887	A
80	B5	2896	A
80	B5	2970	C
80	B5	2971	A
80	B5	2996	U
80	B5	3056	U
80	B5	3078	U
80	B5	3154	C
80	B5	3155	U
80	B5	3167	A
80	B5	3195	U
80	B5	3218	A
80	B5	3228	C
80	B5	3259	U
80	B5	3269	U
80	B5	3275	U
80	B5	3289	G
80	B5	3317	U
80	B5	3330	A
80	B5	3340	G
80	B5	3341	U
80	B5	3357	U
82	B8	111	A
82	B8	126	A
82	B8	156	U
84	CW	17	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
84	CW	20	U
84	CW	68	C
84	CW	69	G
84	CW	73	A

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

9 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
83	HSO	CV	296	83	6,10,10	2.30	2 (33%)	4,12,12	2.25	2 (50%)
83	HSO	CV	556	83	6,10,10	2.35	2 (33%)	4,12,12	2.02	2 (50%)
83	HSO	CV	541	83	6,10,10	2.66	2 (33%)	4,12,12	1.64	2 (50%)
83	HSO	CV	295	83	6,10,10	2.10	1 (16%)	4,12,12	1.46	1 (25%)
83	HSO	CV	105	83	6,10,10	2.30	2 (33%)	4,12,12	1.84	2 (50%)
83	HSO	CV	80	83	6,10,10	2.37	2 (33%)	4,12,12	1.35	0
83	HSO	CV	554	83	6,10,10	2.44	2 (33%)	4,12,12	1.50	1 (25%)
83	HSO	CV	229	83	6,10,10	2.01	1 (16%)	4,12,12	1.69	1 (25%)
83	HSO	CV	13	83	6,10,10	2.17	1 (16%)	4,12,12	1.46	1 (25%)

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
83	HSO	CV	296	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	556	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	541	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	295	83	-	2/6/6/6	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	HSO	CV	105	83	-	3/6/6/6	0/1/1/1
83	HSO	CV	80	83	-	4/6/6/6	0/1/1/1
83	HSO	CV	554	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	229	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	13	83	-	5/6/6/6	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	CV	296	HSO	O-C	-4.65	1.22	1.42
83	CV	556	HSO	O-C	-4.65	1.22	1.42
83	CV	541	HSO	O-C	-4.64	1.22	1.42
83	CV	295	HSO	O-C	-4.63	1.22	1.42
83	CV	13	HSO	O-C	-4.60	1.23	1.42
83	CV	80	HSO	O-C	-4.59	1.23	1.42
83	CV	105	HSO	O-C	-4.59	1.23	1.42
83	CV	554	HSO	O-C	-4.58	1.23	1.42
83	CV	229	HSO	O-C	-4.55	1.23	1.42
83	CV	541	HSO	C-CA	-4.05	1.46	1.52
83	CV	554	HSO	C-CA	-3.22	1.47	1.52
83	CV	105	HSO	C-CA	-2.96	1.47	1.52
83	CV	556	HSO	C-CA	-2.92	1.47	1.52
83	CV	296	HSO	C-CA	-2.80	1.48	1.52
83	CV	80	HSO	C-CA	-2.51	1.48	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	CV	296	HSO	CB-CA-C	-3.71	105.49	112.21
83	CV	556	HSO	CB-CA-C	-2.84	107.07	112.21
83	CV	556	HSO	O-C-CA	2.64	121.97	111.52
83	CV	105	HSO	CB-CA-C	-2.64	107.44	112.21
83	CV	229	HSO	O-C-CA	2.63	121.91	111.52
83	CV	13	HSO	O-C-CA	2.43	121.14	111.52
83	CV	296	HSO	O-C-CA	2.39	120.95	111.52
83	CV	541	HSO	CB-CA-C	-2.28	108.09	112.21
83	CV	105	HSO	O-C-CA	2.24	120.36	111.52
83	CV	541	HSO	O-C-CA	2.12	119.89	111.52
83	CV	295	HSO	O-C-CA	2.03	119.56	111.52
83	CV	554	HSO	O-C-CA	2.03	119.54	111.52

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	CV	13	HSO	N-CA-CB-CG
83	CV	13	HSO	O-C-CA-CB
83	CV	13	HSO	CA-CB-CG-ND1
83	CV	13	HSO	CA-CB-CG-CD2
83	CV	80	HSO	N-CA-CB-CG
83	CV	80	HSO	C-CA-CB-CG
83	CV	105	HSO	O-C-CA-N
83	CV	105	HSO	O-C-CA-CB
83	CV	105	HSO	CA-CB-CG-ND1
83	CV	229	HSO	O-C-CA-N
83	CV	229	HSO	O-C-CA-CB
83	CV	295	HSO	O-C-CA-CB
83	CV	296	HSO	O-C-CA-N
83	CV	541	HSO	O-C-CA-CB
83	CV	554	HSO	O-C-CA-N
83	CV	554	HSO	CA-CB-CG-ND1
83	CV	556	HSO	O-C-CA-N
83	CV	556	HSO	O-C-CA-CB
83	CV	80	HSO	O-C-CA-CB
83	CV	296	HSO	O-C-CA-CB
83	CV	13	HSO	O-C-CA-N
83	CV	80	HSO	O-C-CA-N
83	CV	295	HSO	O-C-CA-N
83	CV	541	HSO	O-C-CA-N

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 443 ligands modelled in this entry, 232 are monoatomic - leaving 211 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	$\# Z  > 2$
88	OHX	B2	2071	-	0,6,6	-	-	-		
88	OHX	B2	2056	-	0,6,6	-	-	-		
88	OHX	B2	1954	-	0,6,6	-	-	-		
88	OHX	B2	1987	-	0,6,6	-	-	-		
88	OHX	B2	2015	-	0,6,6	-	-	-		
88	OHX	AI	301	-	0,6,6	-	-	-		
88	OHX	B7	219	87	0,6,6	-	-	-		
88	OHX	B2	2001	-	0,6,6	-	-	-		
88	OHX	B2	2080	-	0,6,6	-	-	-		
88	OHX	B7	220	-	0,6,6	-	-	-		
88	OHX	B2	1936	-	0,6,6	-	-	-		
88	OHX	B2	1924	-	0,6,6	-	-	-		
88	OHX	B2	1950	-	0,6,6	-	-	-		
88	OHX	B2	2058	-	0,6,6	-	-	-		
88	OHX	B2	1996	-	0,6,6	-	-	-		
89	GCP	CV	602	-	27,34,34	2.12	6 (22%)	34,54,54	2.52	9 (26%)
88	OHX	B2	1923	-	0,6,6	-	-	-		
88	OHX	B2	2039	-	0,6,6	-	-	-		
88	OHX	B2	1971	-	0,6,6	-	-	-		
88	OHX	B2	1914	-	0,6,6	-	-	-		
88	OHX	B2	1990	-	0,6,6	-	-	-		
88	OHX	B2	2025	-	0,6,6	-	-	-		
88	OHX	B2	1926	-	0,6,6	-	-	-		
88	OHX	B2	1945	-	0,6,6	-	-	-		
88	OHX	B2	2053	-	0,6,6	-	-	-		
88	OHX	B2	2074	-	0,6,6	-	-	-		
88	OHX	B2	1974	-	0,6,6	-	-	-		
88	OHX	B2	1927	-	0,6,6	-	-	-		
88	OHX	B2	1938	-	0,6,6	-	-	-		
88	OHX	B2	1977	-	0,6,6	-	-	-		
88	OHX	B2	1952	-	0,6,6	-	-	-		
88	OHX	B2	1913	-	0,6,6	-	-	-		
88	OHX	B2	1928	-	0,6,6	-	-	-		
88	OHX	B2	1998	-	0,6,6	-	-	-		
88	OHX	B2	1917	-	0,6,6	-	-	-		
88	OHX	B2	1972	-	0,6,6	-	-	-		
88	OHX	B7	214	-	0,6,6	-	-	-		
88	OHX	B2	2052	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	B2	2000	-	0,6,6	-	-	-		
88	OHX	Bn	101	-	0,6,6	-	-	-		
88	OHX	B2	1941	-	0,6,6	-	-	-		
88	OHX	B2	1982	-	0,6,6	-	-	-		
88	OHX	B2	2006	-	0,6,6	-	-	-		
88	OHX	B2	2020	-	0,6,6	-	-	-		
88	OHX	B2	1964	-	0,6,6	-	-	-		
88	OHX	B2	1975	-	0,6,6	-	-	-		
88	OHX	B7	210	-	0,6,6	-	-	-		
88	OHX	B2	2066	-	0,6,6	-	-	-		
88	OHX	B2	1995	-	0,6,6	-	-	-		
88	OHX	B2	2065	-	0,6,6	-	-	-		
88	OHX	B2	2003	-	0,6,6	-	-	-		
88	OHX	B2	1957	-	0,6,6	-	-	-		
88	OHX	B2	2024	-	0,6,6	-	-	-		
88	OHX	B2	2076	-	0,6,6	-	-	-		
88	OHX	B2	1966	-	0,6,6	-	-	-		
88	OHX	B2	2007	-	0,6,6	-	-	-		
88	OHX	B2	1956	-	0,6,6	-	-	-		
88	OHX	B2	2059	-	0,6,6	-	-	-		
88	OHX	B2	2069	79	0,6,6	-	-	-		
88	OHX	B2	2032	-	0,6,6	-	-	-		
88	OHX	B2	1953	-	0,6,6	-	-	-		
88	OHX	B2	1919	-	0,6,6	-	-	-		
88	OHX	B2	2057	-	0,6,6	-	-	-		
88	OHX	A3	102	-	0,6,6	-	-	-		
88	OHX	B2	1969	-	0,6,6	-	-	-		
88	OHX	B2	2008	-	0,6,6	-	-	-		
88	OHX	A6	401	-	0,6,6	-	-	-		
88	OHX	B2	2049	-	0,6,6	-	-	-		
88	OHX	B5	3402	-	0,6,6	-	-	-		
88	OHX	B2	1962	-	0,6,6	-	-	-		
88	OHX	B2	1903	-	0,6,6	-	-	-		
88	OHX	B2	1901	-	0,6,6	-	-	-		
88	OHX	B2	1939	-	0,6,6	-	-	-		
88	OHX	B2	2068	-	0,6,6	-	-	-		
88	OHX	B2	1931	-	0,6,6	-	-	-		
88	OHX	B2	1965	-	0,6,6	-	-	-		
88	OHX	B2	2082	-	0,6,6	-	-	-		
88	OHX	B2	1915	-	0,6,6	-	-	-		
88	OHX	B2	1947	-	0,6,6	-	-	-		
88	OHX	B2	2009	-	0,6,6	-	-	-		
88	OHX	B2	2050	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	B7	206	-	0,6,6	-	-	-		
88	OHX	B2	2060	-	0,6,6	-	-	-		
88	OHX	B2	1993	-	0,6,6	-	-	-		
88	OHX	B2	1904	-	0,6,6	-	-	-		
88	OHX	B2	2062	87,88	0,6,6	-	-	-		
88	OHX	B2	2026	-	0,6,6	-	-	-		
88	OHX	B2	2012	-	0,6,6	-	-	-		
88	OHX	B2	2038	-	0,6,6	-	-	-		
88	OHX	B2	2044	-	0,6,6	-	-	-		
88	OHX	CX	101	-	0,6,6	-	-	-		
88	OHX	B2	1918	88	0,6,6	-	-	-		
88	OHX	B2	1909	88	0,6,6	-	-	-		
88	OHX	B2	2077	-	0,6,6	-	-	-		
88	OHX	AN	201	-	0,6,6	-	-	-		
88	OHX	B2	2043	-	0,6,6	-	-	-		
88	OHX	B2	1906	87	0,6,6	-	-	-		
88	OHX	B2	1970	-	0,6,6	-	-	-		
88	OHX	B2	2078	-	0,6,6	-	-	-		
88	OHX	B2	2023	-	0,6,6	-	-	-		
88	OHX	B7	204	-	0,6,6	-	-	-		
88	OHX	B2	2018	-	0,6,6	-	-	-		
88	OHX	B2	1920	-	0,6,6	-	-	-		
88	OHX	B2	1944	-	0,6,6	-	-	-		
88	OHX	B5	3401	-	0,6,6	-	-	-		
88	OHX	B2	1930	-	0,6,6	-	-	-		
88	OHX	B2	1997	-	0,6,6	-	-	-		
88	OHX	B2	1907	-	0,6,6	-	-	-		
88	OHX	B7	212	-	0,6,6	-	-	-		
88	OHX	B2	1916	-	0,6,6	-	-	-		
88	OHX	B2	2048	87	0,6,6	-	-	-		
88	OHX	B2	1992	-	0,6,6	-	-	-		
88	OHX	B7	201	-	0,6,6	-	-	-		
88	OHX	B2	2005	-	0,6,6	-	-	-		
88	OHX	B2	2028	-	0,6,6	-	-	-		
88	OHX	B2	1943	-	0,6,6	-	-	-		
88	OHX	AC	301	-	0,6,6	-	-	-		
88	OHX	B2	1960	-	0,6,6	-	-	-		
88	OHX	B7	205	-	0,6,6	-	-	-		
88	OHX	B2	1999	-	0,6,6	-	-	-		
88	OHX	B7	203	-	0,6,6	-	-	-		
88	OHX	B2	1988	-	0,6,6	-	-	-		
88	OHX	B2	2036	-	0,6,6	-	-	-		
88	OHX	B2	2064	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	B7	215	-	0,6,6	-	-	-		
88	OHX	B2	1908	-	0,6,6	-	-	-		
88	OHX	B2	1955	-	0,6,6	-	-	-		
88	OHX	B2	1981	-	0,6,6	-	-	-		
88	OHX	B2	1991	-	0,6,6	-	-	-		
88	OHX	B5	3403	-	0,6,6	-	-	-		
88	OHX	B2	1935	-	0,6,6	-	-	-		
88	OHX	B2	2040	-	0,6,6	-	-	-		
88	OHX	B2	1994	-	0,6,6	-	-	-		
88	OHX	B2	1933	-	0,6,6	-	-	-		
88	OHX	B2	1984	-	0,6,6	-	-	-		
88	OHX	B2	2054	-	0,6,6	-	-	-		
88	OHX	B2	2070	-	0,6,6	-	-	-		
88	OHX	B2	2079	-	0,6,6	-	-	-		
88	OHX	B2	2081	-	0,6,6	-	-	-		
88	OHX	B2	1973	-	0,6,6	-	-	-		
88	OHX	B2	2061	-	0,6,6	-	-	-		
88	OHX	B2	1980	-	0,6,6	-	-	-		
88	OHX	B2	1967	-	0,6,6	-	-	-		
88	OHX	B2	1986	-	0,6,6	-	-	-		
88	OHX	B2	1946	-	0,6,6	-	-	-		
88	OHX	B2	2035	-	0,6,6	-	-	-		
88	OHX	B2	1949	-	0,6,6	-	-	-		
88	OHX	B2	2072	-	0,6,6	-	-	-		
88	OHX	B2	2047	-	0,6,6	-	-	-		
88	OHX	B2	2073	-	0,6,6	-	-	-		
88	OHX	B2	2030	-	0,6,6	-	-	-		
88	OHX	B2	1932	-	0,6,6	-	-	-		
88	OHX	AP	201	-	0,6,6	-	-	-		
88	OHX	B2	1905	-	0,6,6	-	-	-		
88	OHX	B2	2004	-	0,6,6	-	-	-		
88	OHX	B2	1961	-	0,6,6	-	-	-		
88	OHX	B2	2021	-	0,6,6	-	-	-		
88	OHX	B2	2031	-	0,6,6	-	-	-		
88	OHX	B2	2042	-	0,6,6	-	-	-		
88	OHX	B7	202	-	0,6,6	-	-	-		
88	OHX	B2	1951	-	0,6,6	-	-	-		
88	OHX	B2	2027	-	0,6,6	-	-	-		
88	OHX	B2	1959	-	0,6,6	-	-	-		
88	OHX	B2	2067	-	0,6,6	-	-	-		
88	OHX	B2	1979	-	0,6,6	-	-	-		
88	OHX	CV	601	-	0,6,6	-	-	-		
88	OHX	B2	2063	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	AL	201	-	0,6,6	-	-	-		
88	OHX	B2	1922	-	0,6,6	-	-	-		
88	OHX	B2	2013	-	0,6,6	-	-	-		
88	OHX	B2	2033	-	0,6,6	-	-	-		
88	OHX	B2	2022	-	0,6,6	-	-	-		
88	OHX	B2	1921	-	0,6,6	-	-	-		
88	OHX	B2	2037	-	0,6,6	-	-	-		
88	OHX	B2	1963	-	0,6,6	-	-	-		
88	OHX	B2	2041	-	0,6,6	-	-	-		
88	OHX	B2	2075	-	0,6,6	-	-	-		
88	OHX	B2	2017	-	0,6,6	-	-	-		
88	OHX	B7	221	-	0,6,6	-	-	-		
88	OHX	B2	1912	-	0,6,6	-	-	-		
88	OHX	B2	2011	-	0,6,6	-	-	-		
88	OHX	B2	2051	-	0,6,6	-	-	-		
88	OHX	B2	1958	-	0,6,6	-	-	-		
88	OHX	B2	2034	-	0,6,6	-	-	-		
88	OHX	B2	2019	-	0,6,6	-	-	-		
88	OHX	B2	2014	-	0,6,6	-	-	-		
88	OHX	B2	2046	-	0,6,6	-	-	-		
88	OHX	B2	2055	-	0,6,6	-	-	-		
88	OHX	B2	1985	-	0,6,6	-	-	-		
88	OHX	B2	1910	-	0,6,6	-	-	-		
88	OHX	B2	2045	-	0,6,6	-	-	-		
88	OHX	B2	1989	-	0,6,6	-	-	-		
88	OHX	B2	1968	-	0,6,6	-	-	-		
88	OHX	B2	1978	-	0,6,6	-	-	-		
88	OHX	B2	1902	-	0,6,6	-	-	-		
88	OHX	B2	1983	-	0,6,6	-	-	-		
88	OHX	BR	201	-	0,6,6	-	-	-		
88	OHX	B2	1925	-	0,6,6	-	-	-		
88	OHX	B2	2002	-	0,6,6	-	-	-		
88	OHX	B2	1934	-	0,6,6	-	-	-		
88	OHX	B2	1940	-	0,6,6	-	-	-		
88	OHX	B2	2029	88	0,6,6	-	-	-		
88	OHX	B2	1911	-	0,6,6	-	-	-		
88	OHX	B2	2016	-	0,6,6	-	-	-		
88	OHX	B2	1942	-	0,6,6	-	-	-		
88	OHX	B2	1976	-	0,6,6	-	-	-		
88	OHX	B2	2010	-	0,6,6	-	-	-		
88	OHX	B2	1929	-	0,6,6	-	-	-		
88	OHX	AI	302	-	0,6,6	-	-	-		
88	OHX	B2	1937	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	B2	1948	-	0,6,6	-	-	-	-	-

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
89	GCP	CV	602	-	-	1/15/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	CV	602	GCP	C2'-C1'	-6.48	1.43	1.53
89	CV	602	GCP	C6-N1	5.32	1.42	1.33
89	CV	602	GCP	C4-N3	2.81	1.40	1.35
89	CV	602	GCP	C8-N7	-2.35	1.30	1.34
89	CV	602	GCP	PB-O3A	-2.31	1.55	1.58
89	CV	602	GCP	C2-N1	2.31	1.39	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	CV	602	GCP	O3G-PG-C3B	-7.36	88.55	106.40
89	CV	602	GCP	C5-C6-N1	-7.05	113.79	123.43
89	CV	602	GCP	C2-N1-C6	5.19	124.18	115.93
89	CV	602	GCP	N3-C2-N1	-3.57	122.46	127.22
89	CV	602	GCP	C4-C5-C6	-2.97	117.96	120.80
89	CV	602	GCP	O1B-PB-C3B	2.89	116.72	109.07
89	CV	602	GCP	C1'-N9-C4	-2.75	121.81	126.64
89	CV	602	GCP	O2G-PG-O1G	2.71	119.54	112.39
89	CV	602	GCP	O4'-C1'-C2'	-2.01	103.98	106.93

There are no chirality outliers.

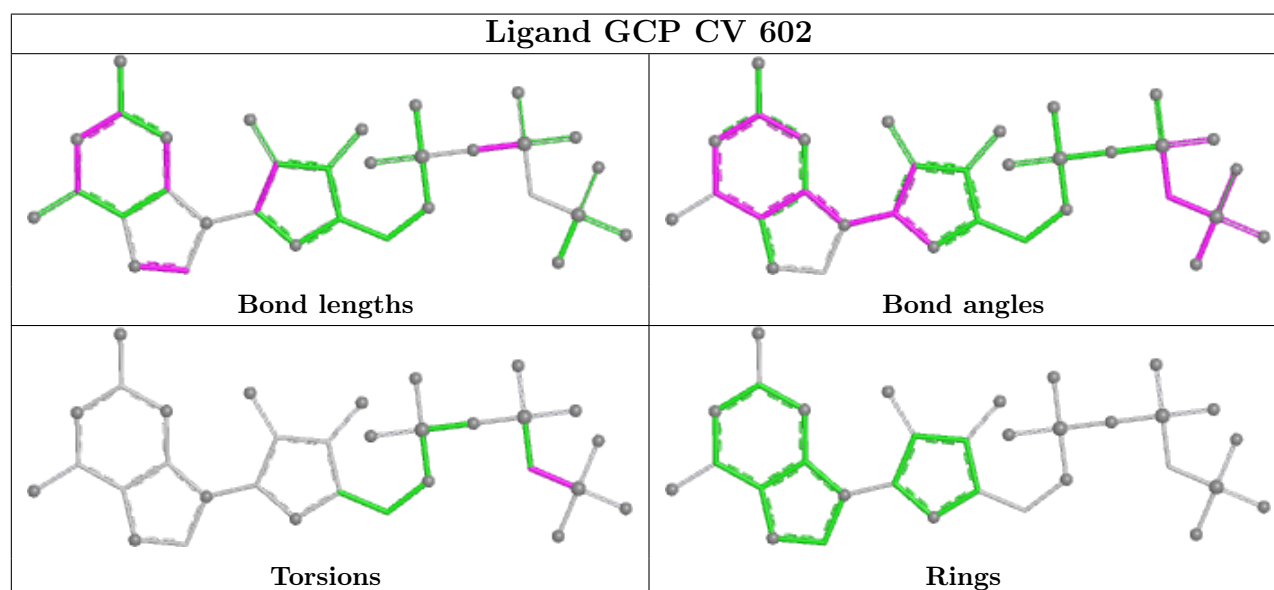
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	CV	602	GCP	PB-C3B-PG-O1G

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
80	B5	1
84	CW	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B5	1285:G	O3'	1286:A	P	6.77

*Continued on next page...*

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CW	33:U	O3'	34:C	P	4.25

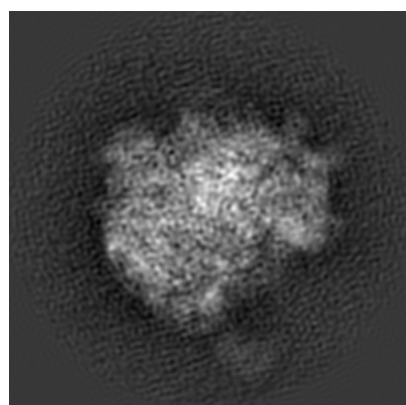
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2422. These allow visual inspection of the internal detail of the map and identification of artifacts.

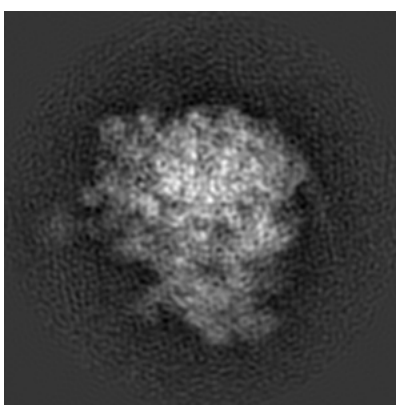
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

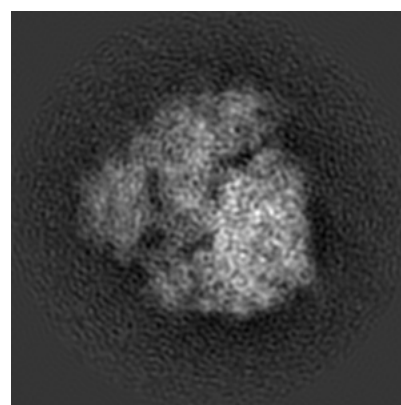
#### 6.1.1 Primary map



X



Y

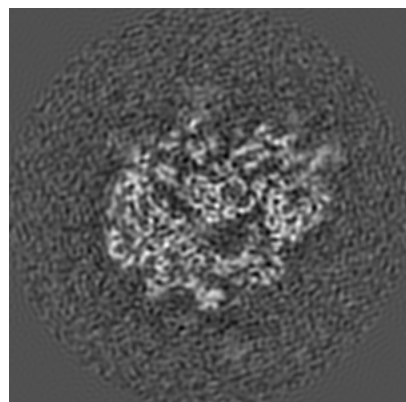


Z

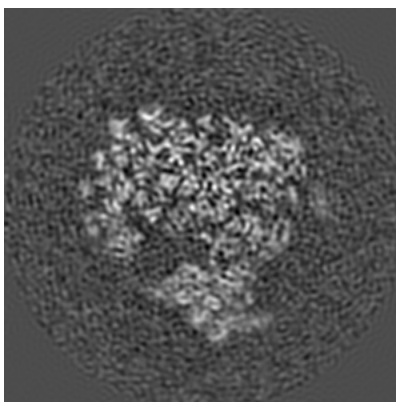
The images above show the map projected in three orthogonal directions.

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

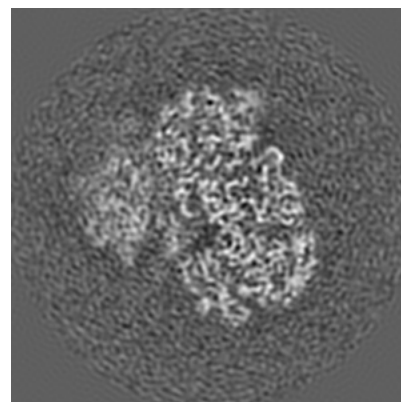
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

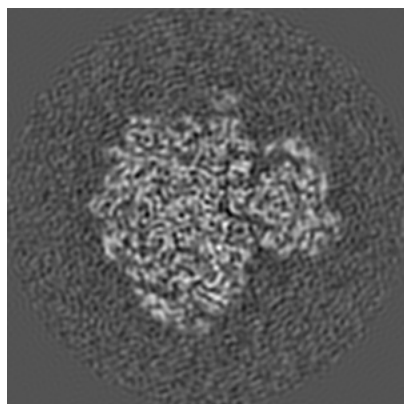


Z Index: 120

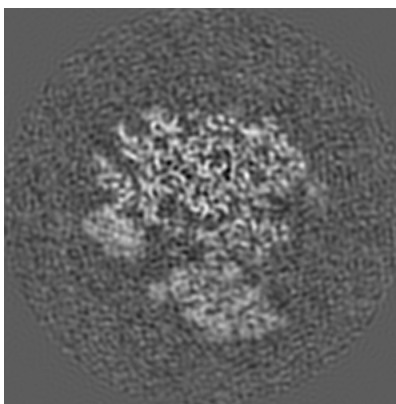
The images above show central slices of the map in three orthogonal directions.

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

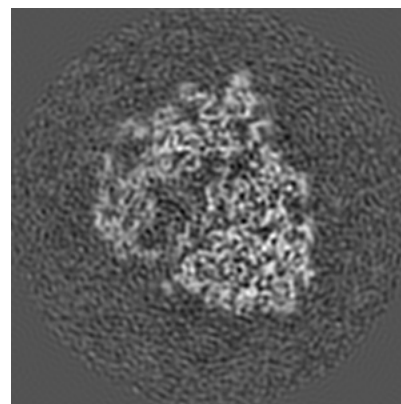
### 6.3.1 Primary map



X Index: 133



Y Index: 124

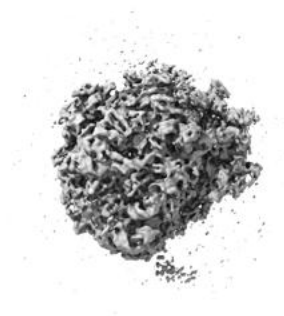


Z Index: 113

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

## 6.4 Orthogonal surface views [i](#)

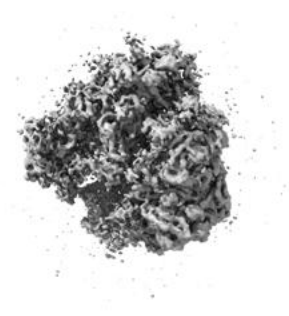
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

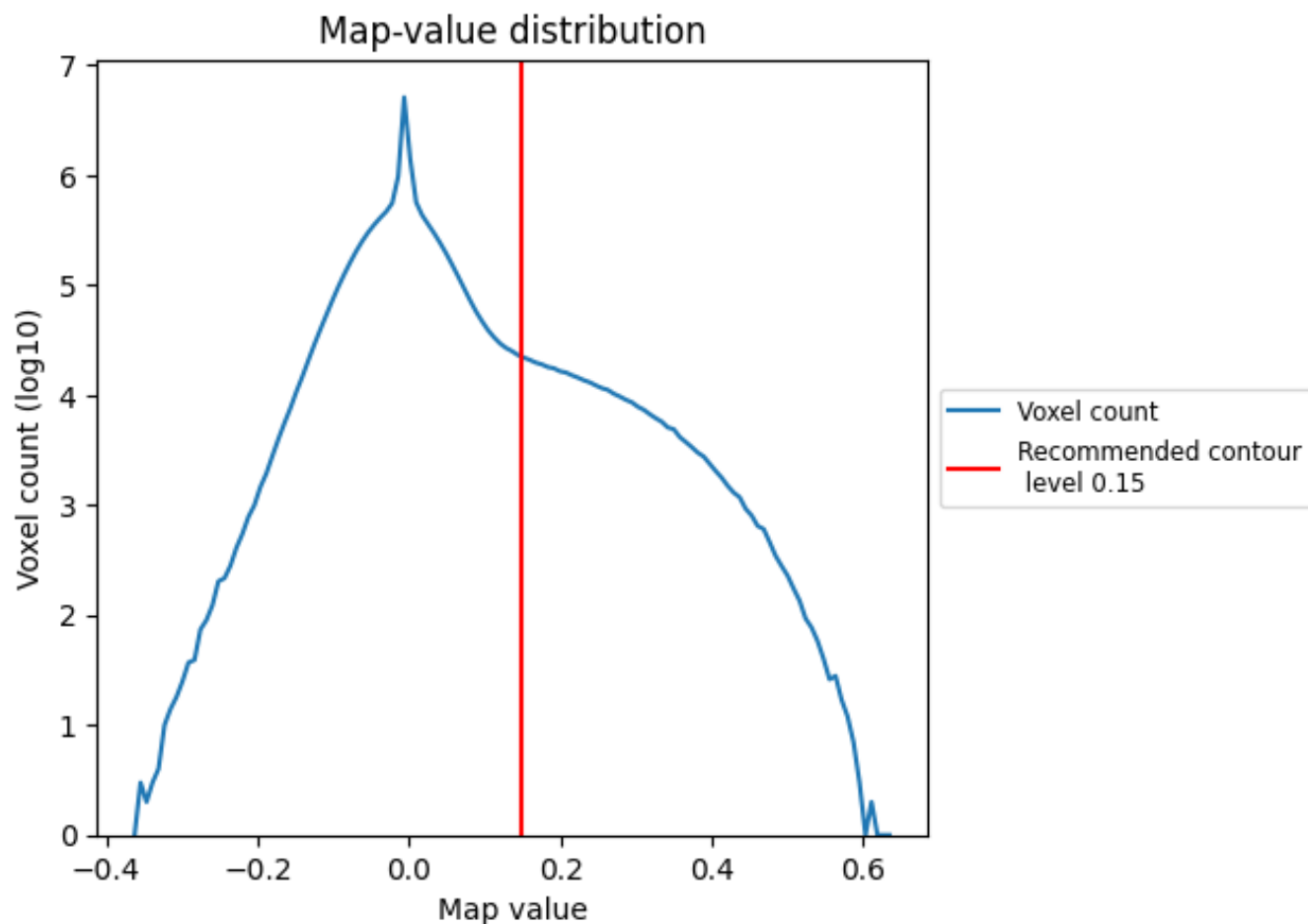
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

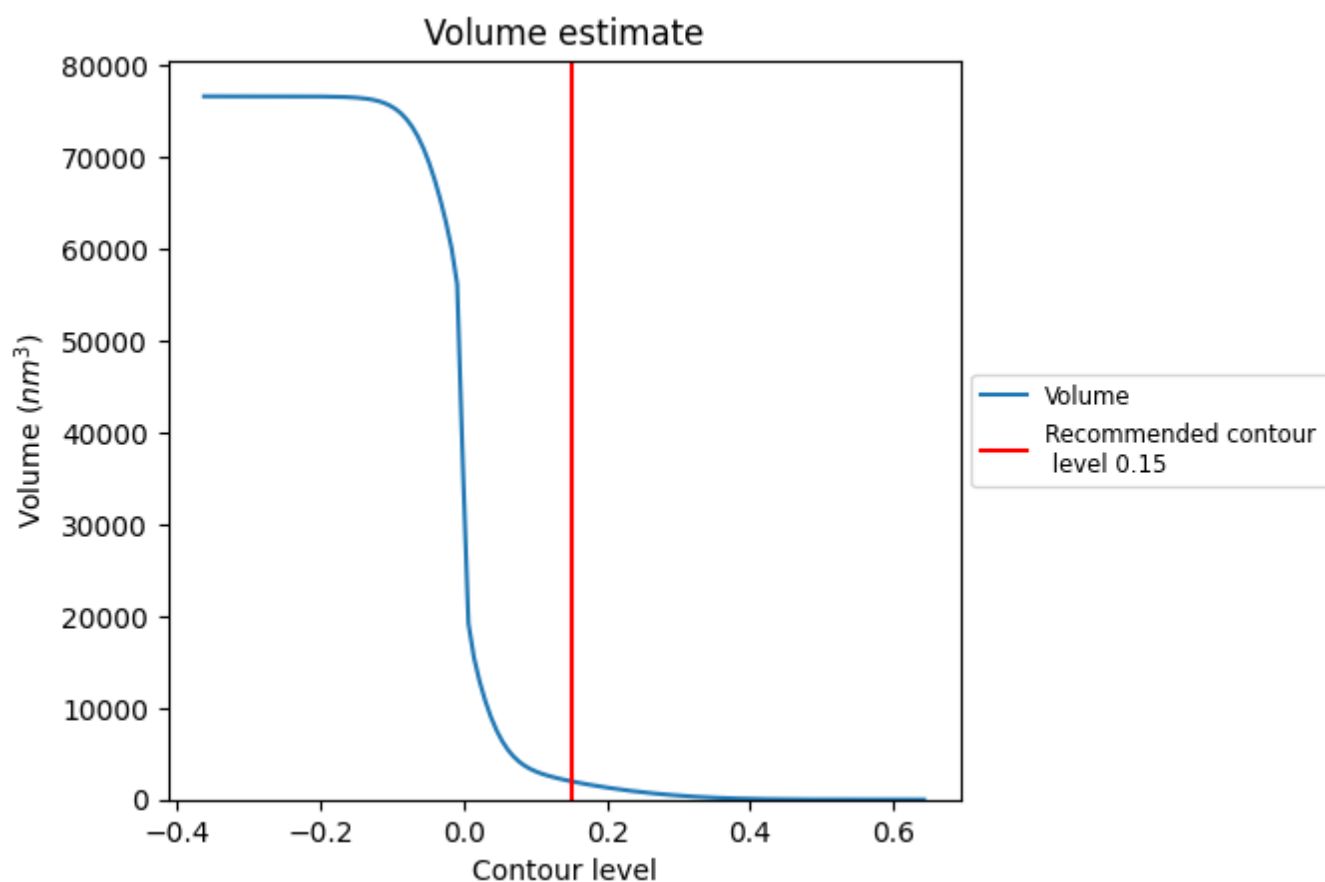
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

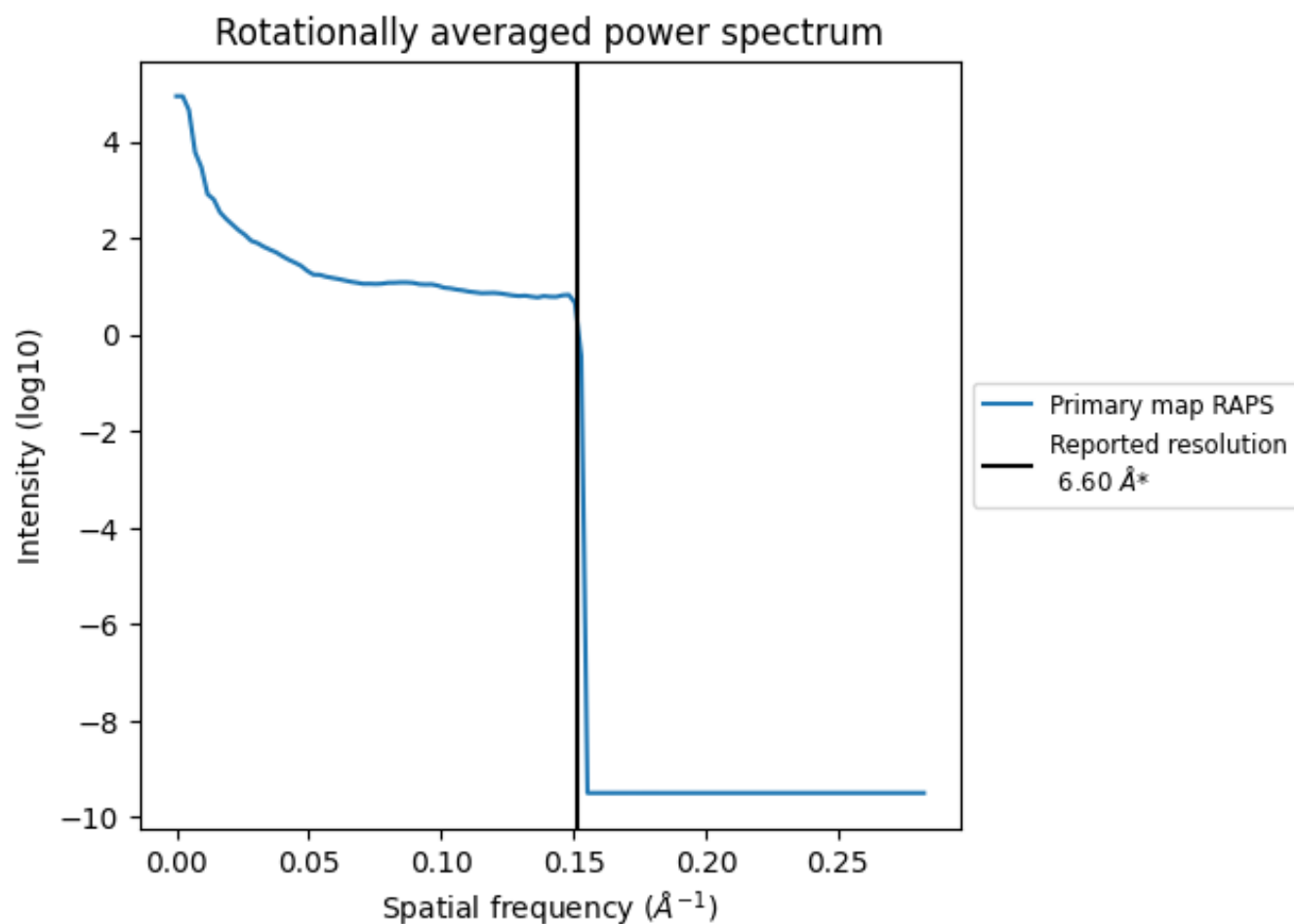
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1997 nm<sup>3</sup>; this corresponds to an approximate mass of 1804 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.152  $\text{\AA}^{-1}$

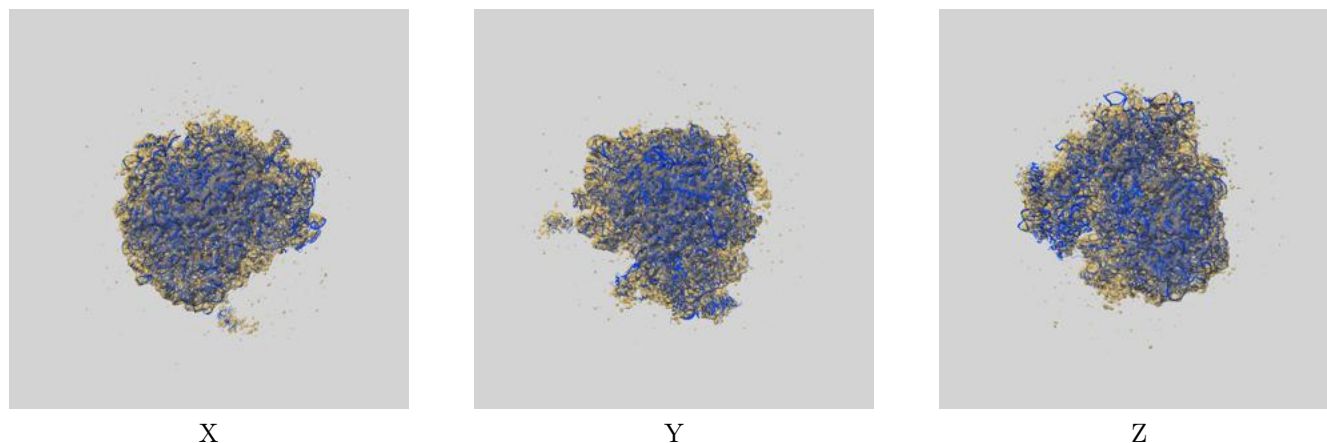
## 8 Fourier-Shell correlation

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

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

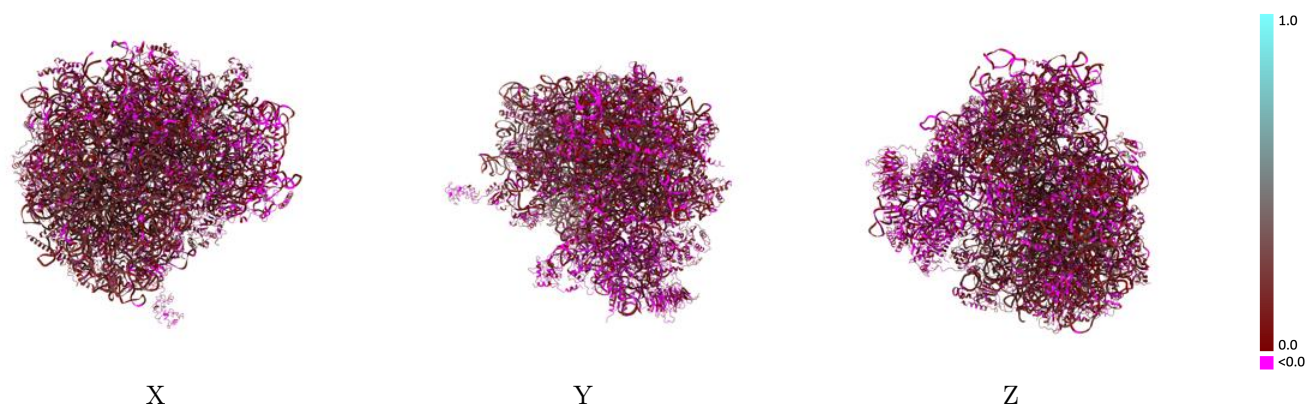
This section contains information regarding the fit between EMDB map EMD-2422 and PDB model 4V8Z. Per-residue inclusion information can be found in section [3](#) on page [35](#).

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



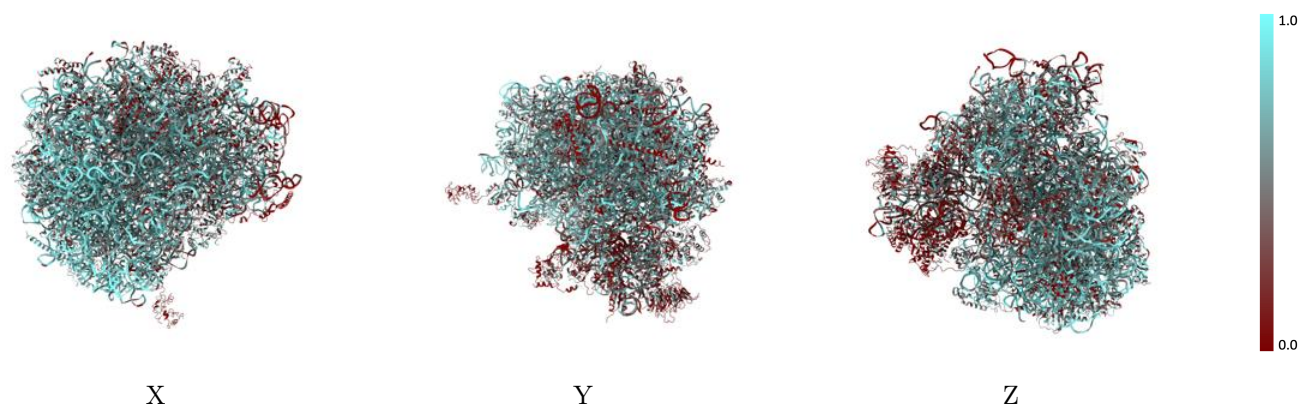
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



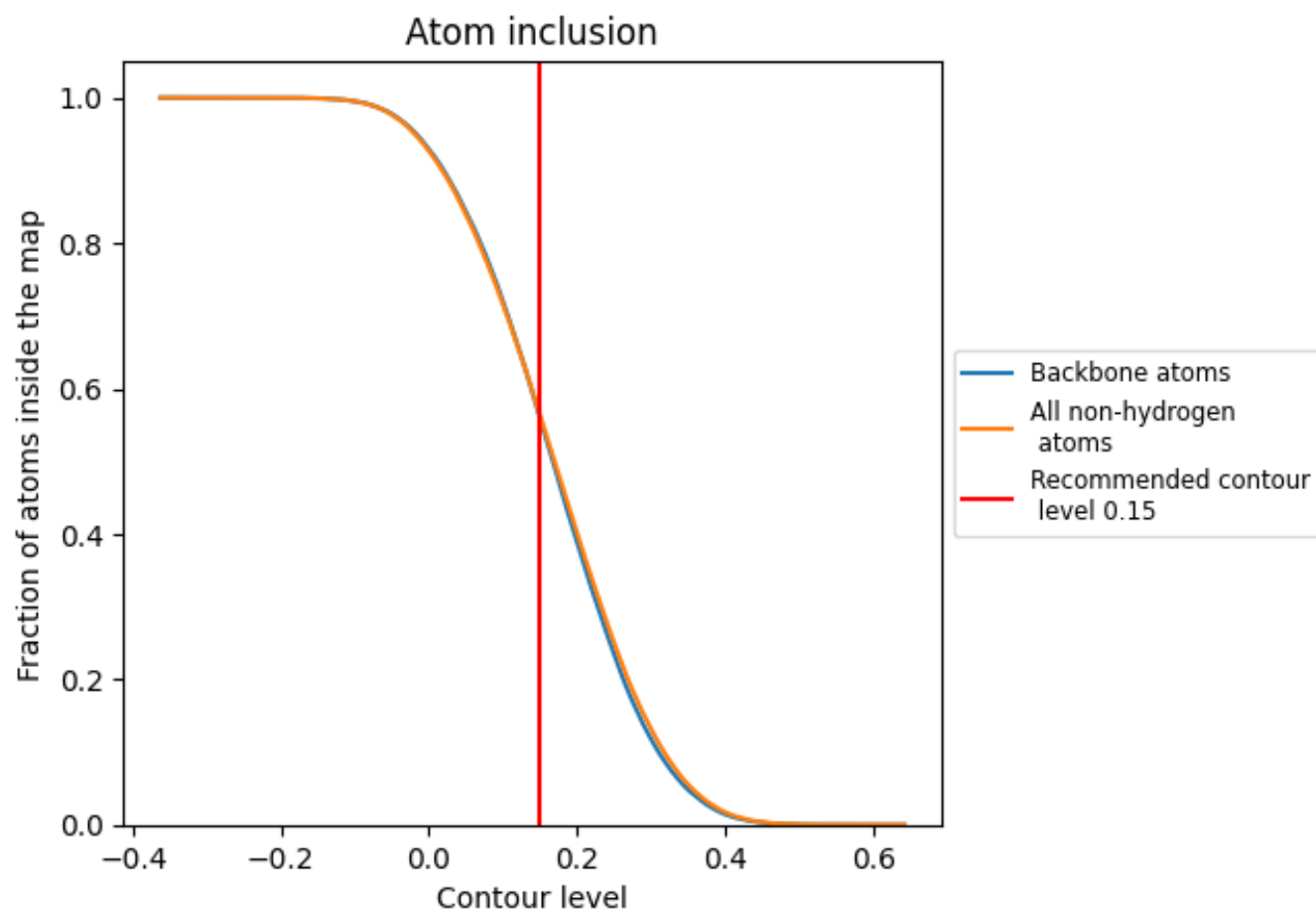
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.5647	 0.1080
A0	 0.3315	 -0.0020
A1	 0.4120	 0.0760
A2	 0.1153	 -0.0000
A3	 0.3687	 0.0080
A4	 0.3791	 0.0510
A5	 0.0512	 -0.0100
A6	 0.2510	 0.0200
A7	 0.1377	 0.0190
AA	 0.4135	 0.0530
AB	 0.2238	 0.0100
AC	 0.3921	 0.0420
AD	 0.2866	 -0.0120
AE	 0.4218	 0.0540
AF	 0.1330	 -0.0030
AG	 0.3766	 0.0160
AH	 0.5544	 0.1420
AI	 0.4252	 0.0370
AJ	 0.4317	 0.0580
AK	 0.2863	 -0.0190
AL	 0.4349	 0.0800
AM	 0.2034	 0.0190
AN	 0.4652	 0.1190
AO	 0.3701	 -0.0040
AP	 0.2320	 0.0100
AQ	 0.3114	 0.0080
AR	 0.3944	 0.0960
AS	 0.2199	 0.0110
AT	 0.3006	 0.0260
AU	 0.2414	 0.0090
AV	 0.4277	 0.0470
AW	 0.4880	 0.1130
AX	 0.4388	 0.1160
AY	 0.4467	 0.0390
AZ	 0.0530	 0.0150



*Continued on next page...*





















*Continued from previous page...*

Chain	Atom inclusion	Q-score
B2	 0.5483	 0.0840
B5	 0.7489	 0.1610
B7	 0.8476	 0.1770
B8	 0.7513	 0.1470
BA	 0.3855	 0.0620
BB	 0.4890	 0.1010
BC	 0.5558	 0.1160
BD	 0.5696	 0.1270
BE	 0.5990	 0.1360
BF	 0.5954	 0.1490
BG	 0.4714	 0.0510
BH	 0.5436	 0.1110
BI	 0.5398	 0.1340
BJ	 0.5392	 0.1260
BK	 0.4409	 0.0840
BL	 0.4926	 0.0910
BM	 0.6357	 0.1480
BN	 0.4465	 0.0670
BO	 0.5482	 0.1400
BP	 0.5214	 0.0980
BQ	 0.5333	 0.1170
BR	 0.3288	 0.0290
BS	 0.5673	 0.1260
BT	 0.5298	 0.1380
BU	 0.4254	 0.0610
BV	 0.4433	 0.1270
BW	 0.2184	 0.0370
BX	 0.3938	 0.0650
BY	 0.5559	 0.0940
BZ	 0.4556	 0.0410
Ba	 0.4825	 0.1010
Bb	 0.4934	 0.1510
Bc	 0.4106	 0.0580
Bd	 0.4877	 0.0570
Be	 0.5372	 0.1380
Bf	 0.5505	 0.1240
Bg	 0.4007	 0.0400
Bh	 0.4973	 0.1060
Bi	 0.4664	 0.0640
Bj	 0.4787	 0.0670
Bk	 0.4286	 0.0610
Bl	 0.4169	 0.0610

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
Bm	 0.4851	 0.1270
Bn	 0.1781	 0.0130
Bo	 0.4662	 0.1040
Bq	 0.4815	 0.1050
Br	 0.1356	 0.0410
Bs	 0.1169	 0.0360
CV	 0.4618	 0.1390
CW	 0.5950	 0.2240
CX	 0.5797	 0.1470