



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 07:10 PM BST

PDB ID : 4U4R
Title : Crystal structure of Lactimidomycin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

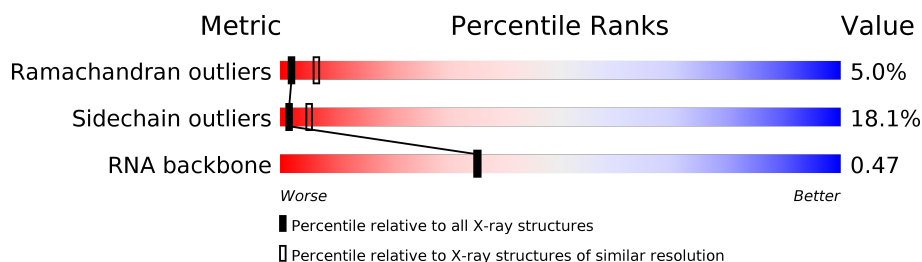
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	




















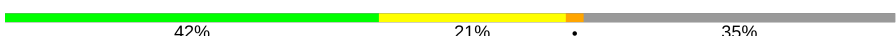





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	









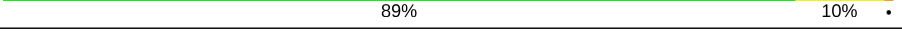
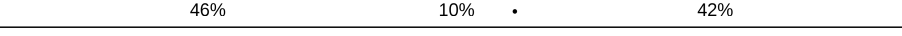

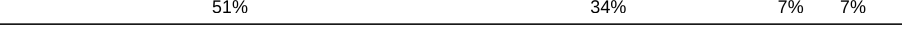

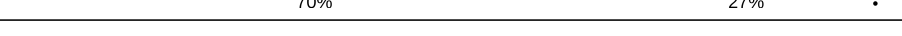


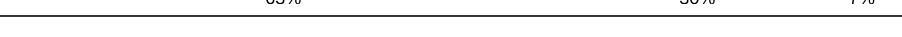

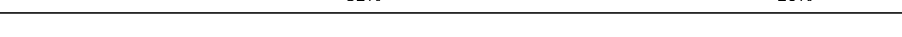
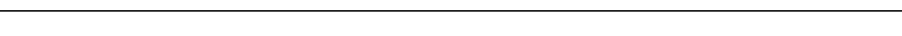

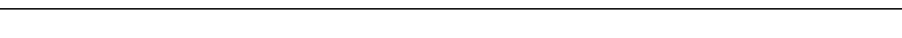
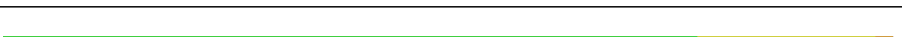


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	















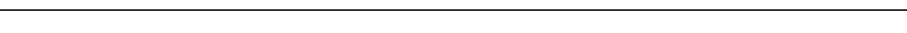




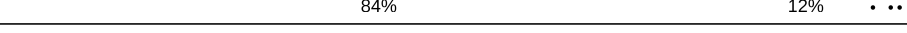





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	















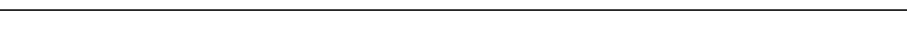




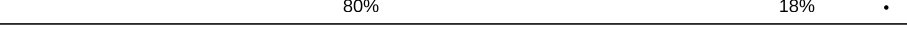





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	















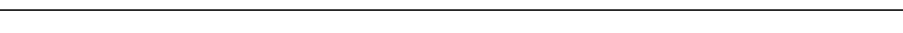




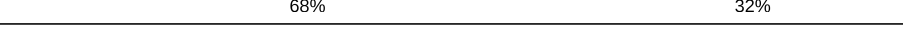





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	m9	188	 81% 19% .
56	N0	172	 82% 17% .
56	n0	172	 84% 15% .
57	N1	159	 80% 19% .
57	n1	159	 86% 12% .
58	N2	120	 72% 11% . 17%
58	n2	120	 69% 13% 18%
59	N3	136	 87% 13% .
59	n3	136	 90% 8% .
60	N4	155	 57% 5% . 37%
60	n4	155	 75% 10% . 13%
61	N5	141	 67% 18% . 14%
61	n5	141	 66% 18% . 15%
62	N6	126	 80% 17% .
62	n6	126	 76% 23% .
63	N7	135	 76% 23% .
63	n7	135	 78% 21% .
64	N8	148	 81% 16% .
64	n8	148	 80% 18% .
65	N9	58	 79% 21%
65	n9	58	 69% 28% .
66	O0	104	 78% 14% . 7%
66	o0	104	 79% 17% .
67	O1	112	 76% 20% . .
67	o1	112	 79% 17% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
68	O2	129	 85% 12% . .
68	o2	129	 82% 14% . .
69	O3	106	 85% 13% .
69	o3	106	 87% 12% .
70	O4	119	 77% 16% . 6%
70	o4	119	 81% 13% 6%
71	O5	119	 78% 20% .
71	o5	119	 76% 23% .
72	O6	99	 71% 28% .
72	o6	99	 69% 27% .
73	O7	87	 79% 21%
73	o7	87	 83% 17%
74	O8	77	 79% 21%
74	o8	77	 82% 17% .
75	O9	50	 80% 18% .
75	o9	50	 78% 22%
76	Q0	52	 83% 15% .
76	q0	52	 85% 13% .
77	Q1	25	 68% 32%
77	q1	25	 64% 32% .
78	Q2	105	 82% 17% .
78	q2	105	 79% 21%
79	Q3	91	 87% 13%
79	q3	91	 85% 15%
80	e0	62	 76% 23% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
81	m2	160	<div><div></div><div>94%</div><div>6%</div></div>
82	p0	311	<div><div></div><div>39%</div><div>7%</div><div>54%</div></div>
83	p1	47	<div><div></div><div>100%</div></div>
84	p2	46	<div><div></div><div>100%</div></div>

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411226 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1750	Total	C	N	O	P	0	0	0
			37283	16668	6591	12274	1750			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	S	0	0	0
			1481	951	265	265				
9	s7	186	Total	C	N	O	S	0	0	0
			1491	957	267	267				

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
c0	89	ALA	GLY	conflict	UNP Q08745

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47
c1	147	ALA	GLY	conflict	UNP P0CX47

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	C3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
21	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	D1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	D4	134	Total	C	N	O		0	0	0
			1073	676	208	189				
26	d4	134	Total	C	N	O		0	0	0
			1073	676	208	189				

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	D5	70	Total	C	N	O		0	0	0
			563	360	104	99				
27	d5	69	Total	C	N	O		0	0	0
			558	357	103	98				

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	D8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2441	1544	419	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				
35	sM	104	Total	C	N	O		0	0	0
			680	403	140	137				

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	13	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	14	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	15	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	16	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	18	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	19	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	M0	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	m0	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	m1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O		0	0	0
			1543	962	315	266				
49	m3	194	Total	C	N	O		0	0	0
			1548	965	316	267				

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O		0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O		0	0	0
			1227	764	238	225				

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	M8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	m8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O		0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O		0	0	0
			1521	935	326	260				

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	N1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	n1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	S	0	0	0
			796	516	131	149				
58	n2	98	Total	C	N	O	S	0	0	0
			778	505	127	146				

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	S	0	0	0
			993	625	192	176				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	N7	135	Total	C	N	O	0	0	0
			1092	710	202	180			
63	n7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	N8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	n8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	N9	58	Total	C	N	O	0	0	0
			462	289	100	73			
65	n9	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	o0	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	O1	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	o1	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	o5	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	O7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	S	0	0	0
			612	391	115	106				
74	o8	77	Total	C	N	O	S	0	0	0
			608	388	114	106				

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 81 is a protein called Unknown protein m2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
81	m2	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 83 is a protein called Unknown protein p1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
83	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 84 is a protein called Unknown protein p2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
84	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	n8	4	Total 4	Mg 4	0	0
85	o1	1	Total 1	Mg 1	0	0
85	N5	1	Total 1	Mg 1	0	0
85	6	147	Total 147	Mg 147	0	0
85	sM	2	Total 2	Mg 2	0	0
85	O4	1	Total 1	Mg 1	0	0
85	m5	1	Total 1	Mg 1	0	0
85	l3	1	Total 1	Mg 1	0	0
85	M1	1	Total 1	Mg 1	0	0
85	n0	2	Total 2	Mg 2	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	126	Total 126	Mg 126	0	0
85	O3	1	Total 1	Mg 1	0	0
85	L4	3	Total 3	Mg 3	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	504	Total 504	Mg 504	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	1	Total 1	Mg 1	0	0
85	s6	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	n9	2	Total 2	Mg 2	0	0
85	1	475	Total 475	Mg 475	0	0
85	d2	1	Total 1	Mg 1	0	0
85	n6	2	Total 2	Mg 2	0	0
85	S8	1	Total 1	Mg 1	0	0
85	m1	2	Total 2	Mg 2	0	0
85	d3	1	Total 1	Mg 1	0	0
85	q3	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0
85	M3	4	Total 4	Mg 4	0	0

Continued on next page...

Continued from previous page...

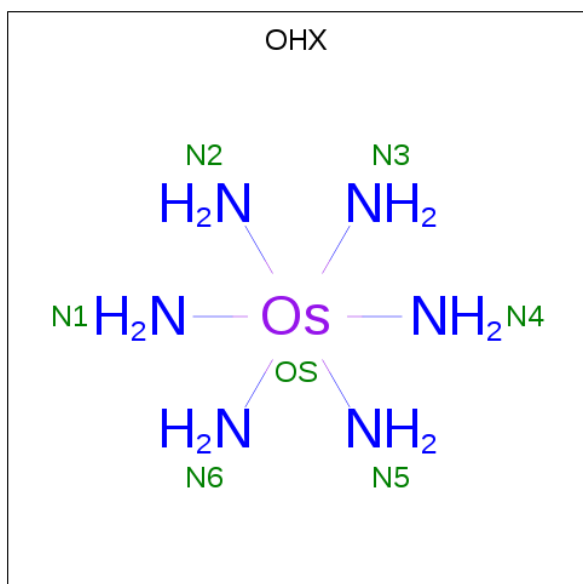
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N3	3	Total 3	Mg 3	0	0
85	N8	2	Total 2	Mg 2	0	0
85	4	21	Total 21	Mg 21	0	0
85	L2	1	Total 1	Mg 1	0	0
85	l5	3	Total 3	Mg 3	0	0
85	C3	1	Total 1	Mg 1	0	0
85	M7	6	Total 6	Mg 6	0	0
85	m4	1	Total 1	Mg 1	0	0
85	L6	1	Total 1	Mg 1	0	0
85	s1	1	Total 1	Mg 1	0	0
85	m6	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	15	Total 15	Mg 15	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	l2	2	Total 2	Mg 2	0	0
85	8	13	Total 13	Mg 13	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	3	14	Total	Mg	0	0
			14	14		

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total 7	N 6	Os 1	0	0
86	S8	1	Total 7	N 6	Os 1	0	0
86	C1	1	Total 7	N 6	Os 1	0	0
86	C3	1	Total 7	N 6	Os 1	0	0
86	C5	1	Total 7	N 6	Os 1	0	0
86	C8	1	Total 7	N 6	Os 1	0	0
86	D9	1	Total 7	N 6	Os 1	0	0
86	SR	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	3	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L4	1	Total	N	Os	0	0
			7	6	1		
86	L6	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		
86	M5	1	Total	N	Os	0	0
			7	6	1		
86	M5	1	Total	N	Os	0	0
			7	6	1		
86	M6	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	N9	1	Total	N	Os	0	0
			7	6	1		
86	O2	1	Total	N	Os	0	0
			7	6	1		
86	O3	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	O9	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	s1	1	Total	N	Os	0	0
			7	6	1		
86	s1	1	Total	N	Os	0	0
			7	6	1		
86	s4	1	Total	N	Os	0	0
			7	6	1		
86	s8	1	Total	N	Os	0	0
			7	6	1		
86	s9	1	Total	N	Os	0	0
			7	6	1		
86	c1	1	Total	N	Os	0	0
			7	6	1		
86	c3	1	Total	N	Os	0	0
			7	6	1		
86	c5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	8	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	13	1	Total 7	N 6	Os 1	0	0
86	14	1	Total 7	N 6	Os 1	0	0
86	14	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	15	1	Total 7	N 6	Os 1	0	0
86	19	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m1	1	Total 7	N 6	Os 1	0	0
86	m4	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o4	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

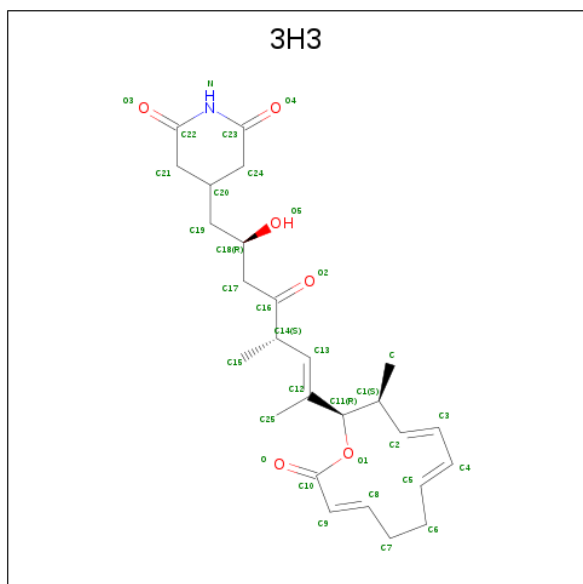
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q3	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		
87	D7	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		

- Molecule 88 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxooxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (three-letter code: 3H3) (formula: C₂₆H₃₅NO₆).



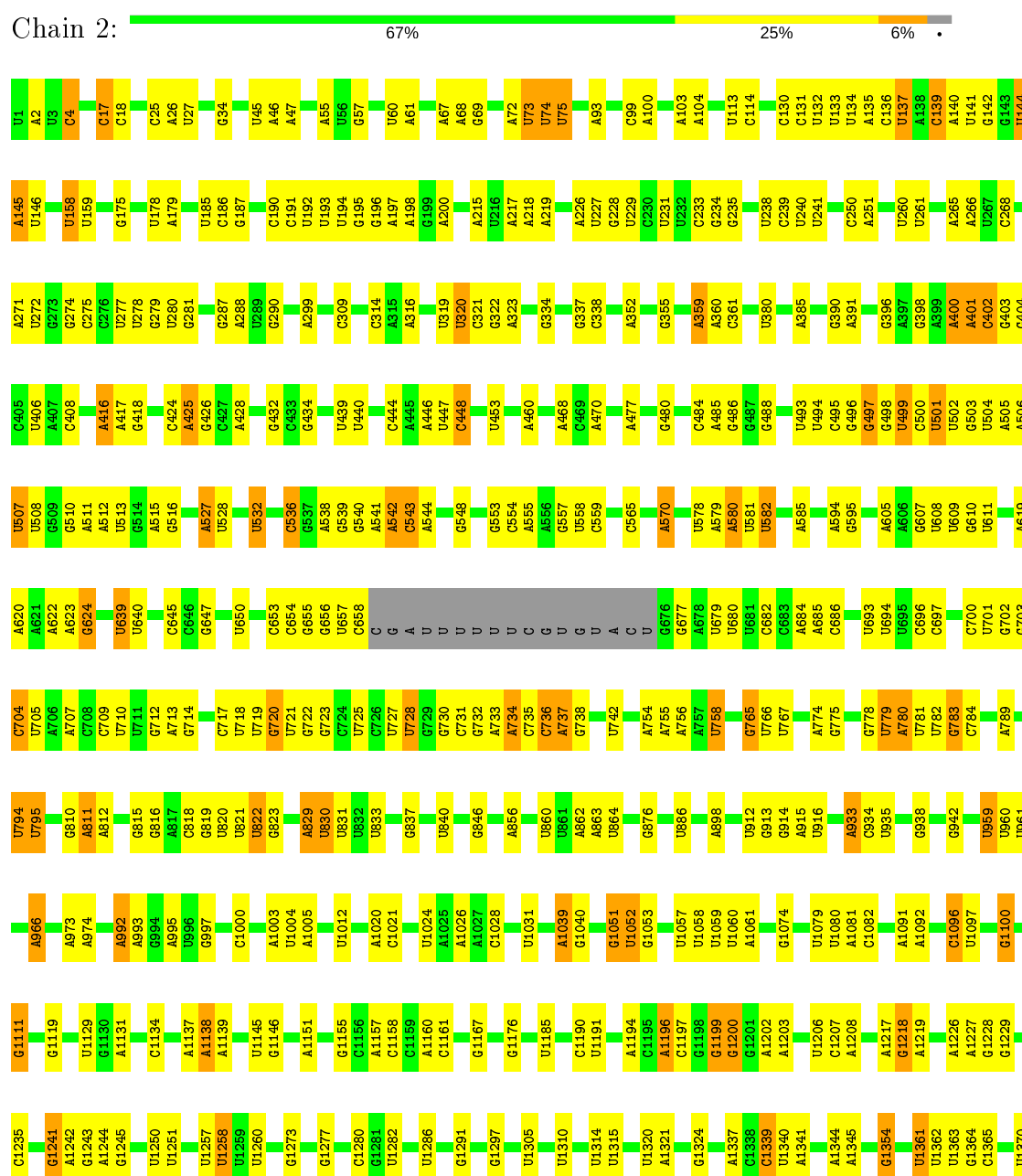
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			33	26	1	6		
88	5	1	Total	C	N	O	0	0
			33	26	1	6		

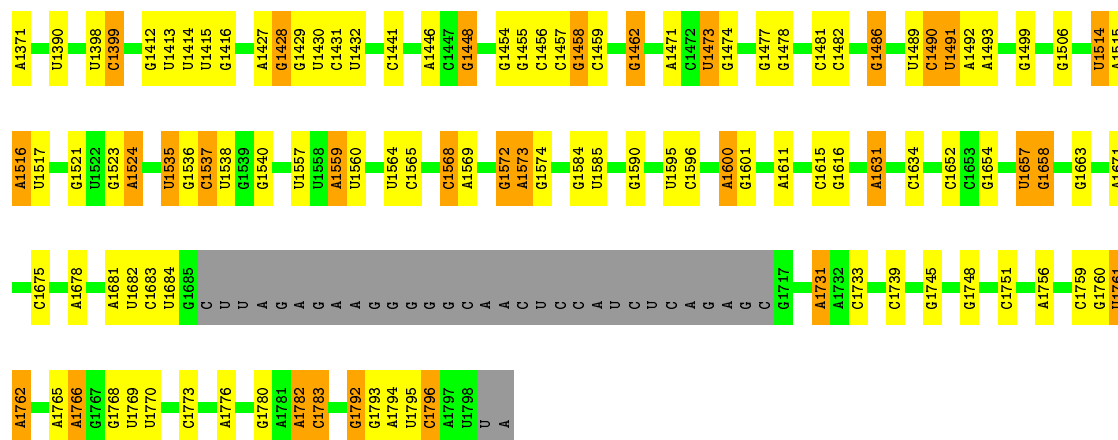
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

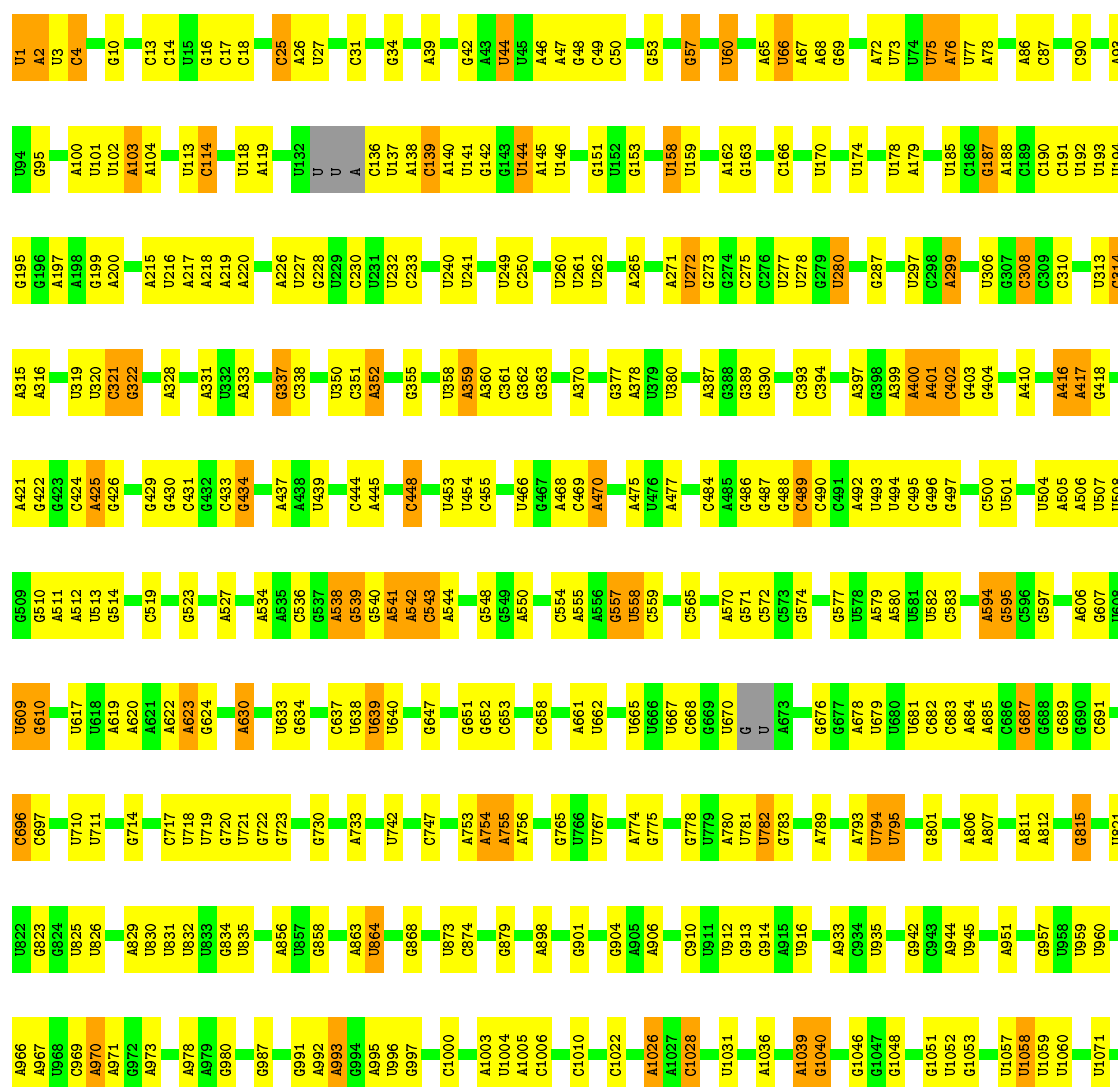
- Molecule 1: 18S ribosomal RNA

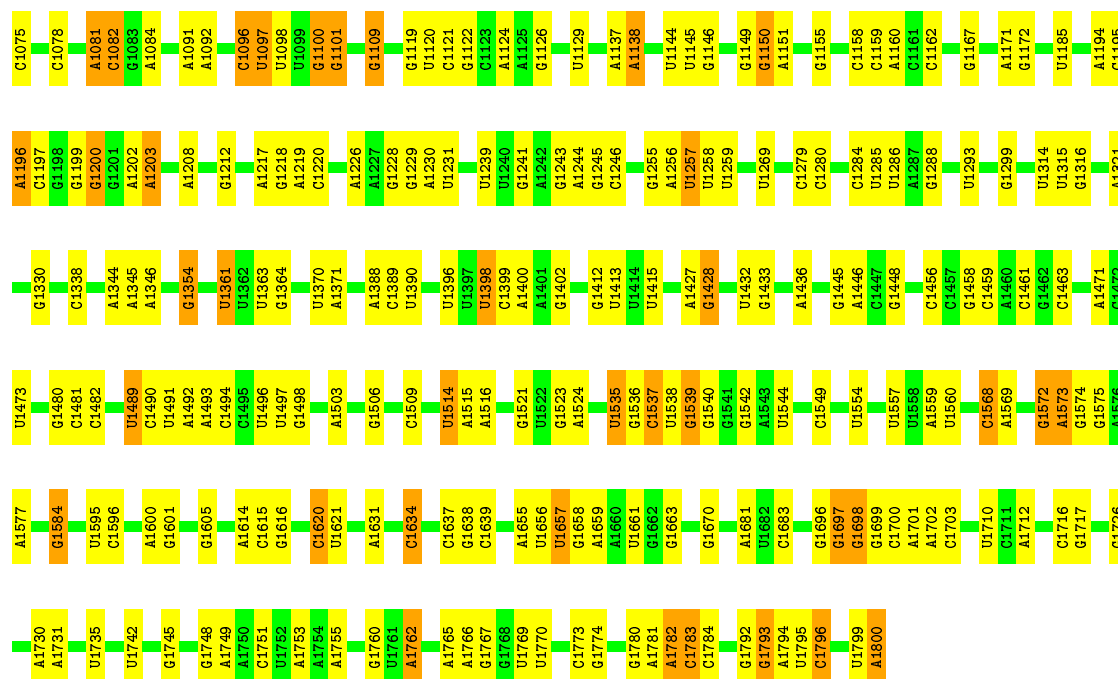




- Molecule 1: 18S ribosomal RNA

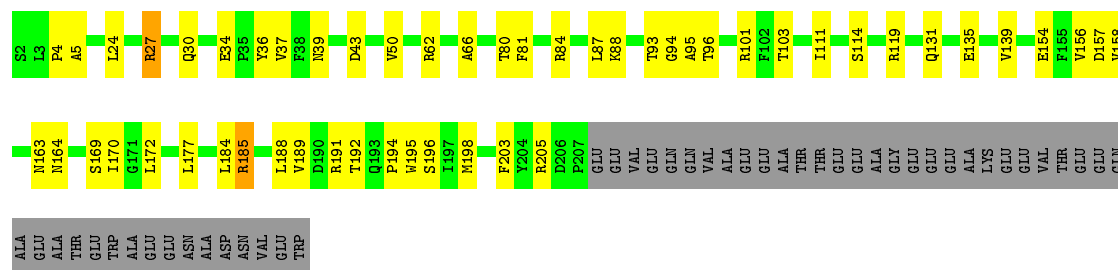
Chain 6: 65% 29% 6%





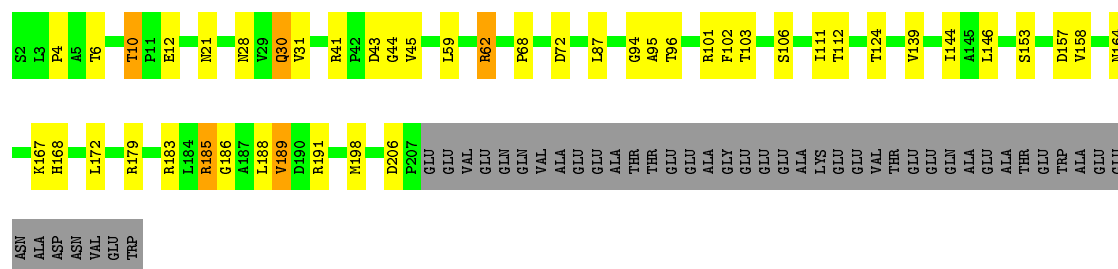
• Molecule 2: 40S ribosomal protein S0-A

Chain S0: 61% 20% 18%



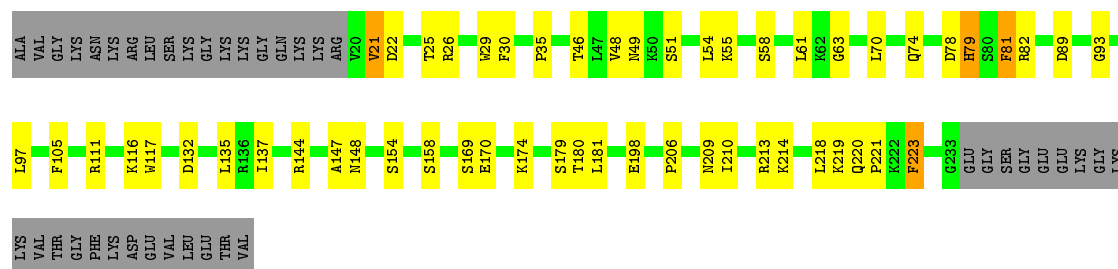
• Molecule 2: 40S ribosomal protein S0-A

Chain s0: 64% 16% 18%

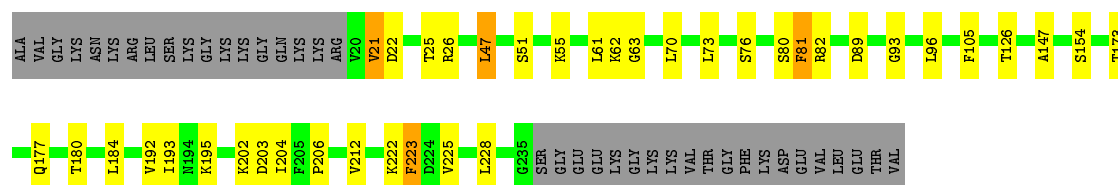


• Molecule 3: 40S ribosomal protein S1-A

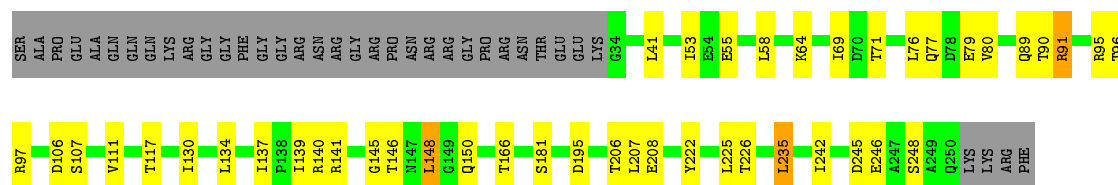
Chain S1: 63% 20% 16%



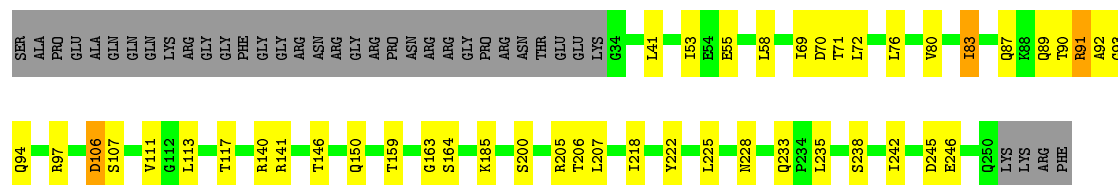
- Molecule 3: 40S ribosomal protein S1-A



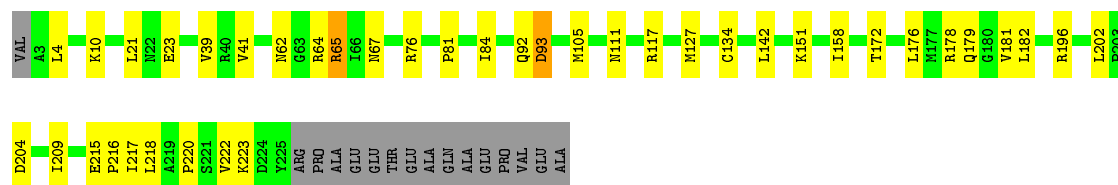
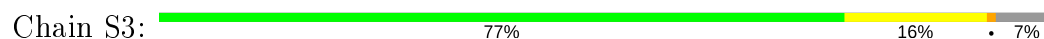
- Molecule 4: 40S ribosomal protein S2



- Molecule 4: 40S ribosomal protein S2

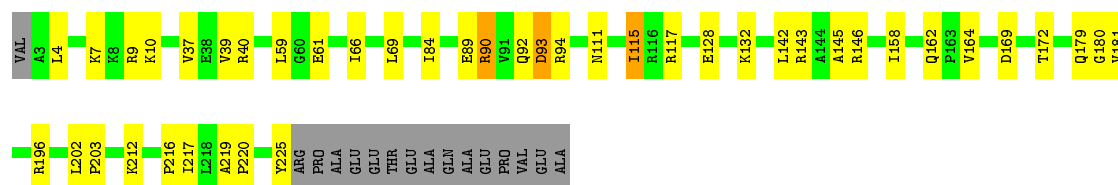


- Molecule 5: 40S ribosomal protein S3




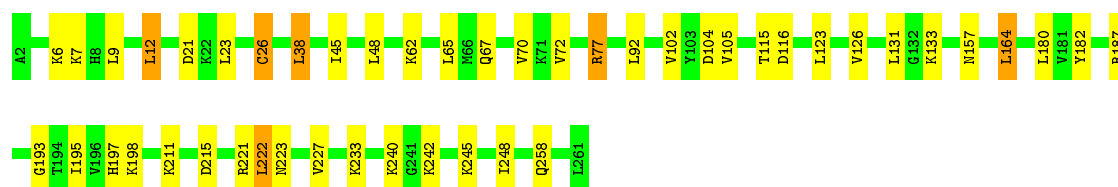
- Molecule 5: 40S ribosomal protein S3

Chain s3: 




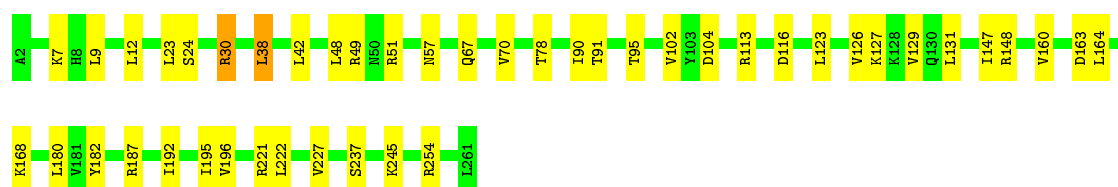
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 



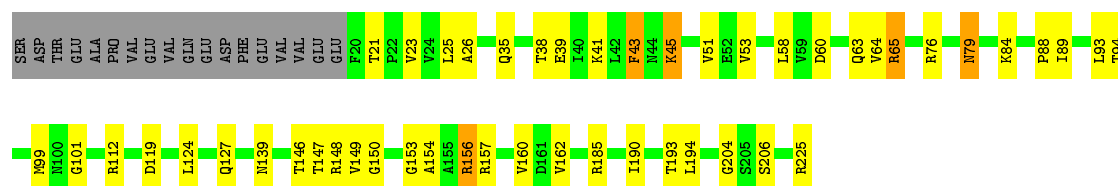
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 



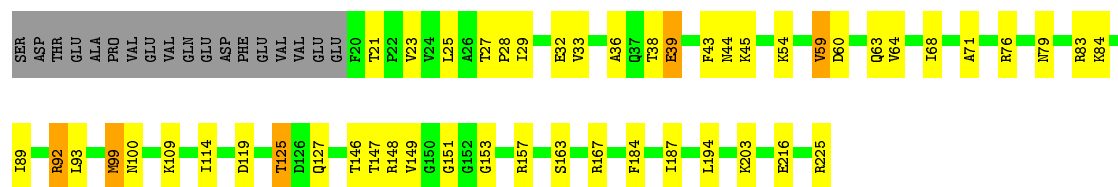
- Molecule 7: 40S ribosomal protein S5

Chain S5: 




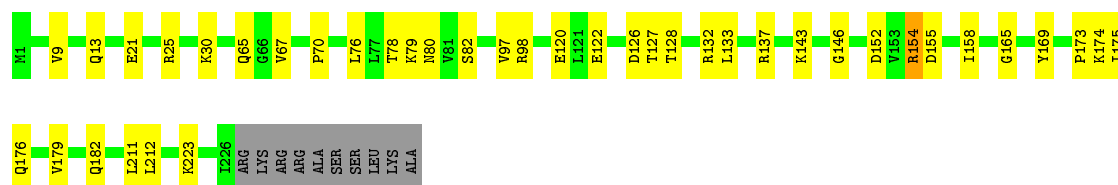
- Molecule 7: 40S ribosomal protein S5

Chain s5: 



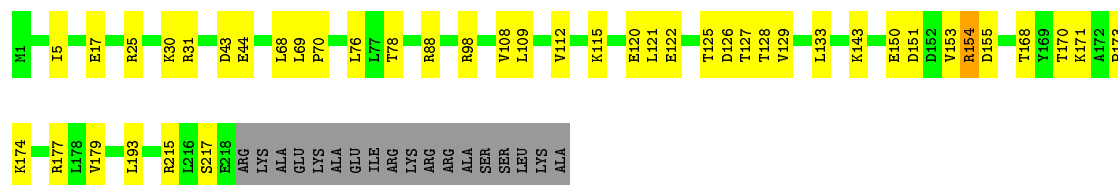
- Molecule 8: 40S ribosomal protein S6-A

Chain S6:  79% 17%




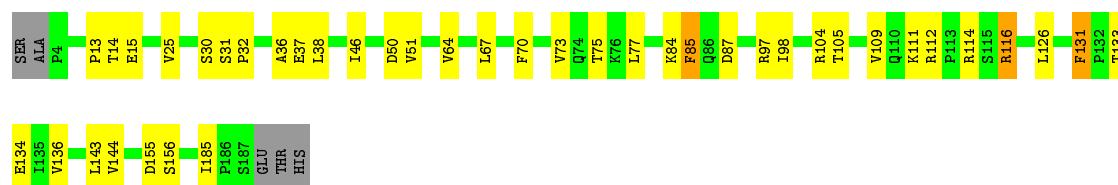
- Molecule 8: 40S ribosomal protein S6-A

Chain s6:  74% 18% 8%



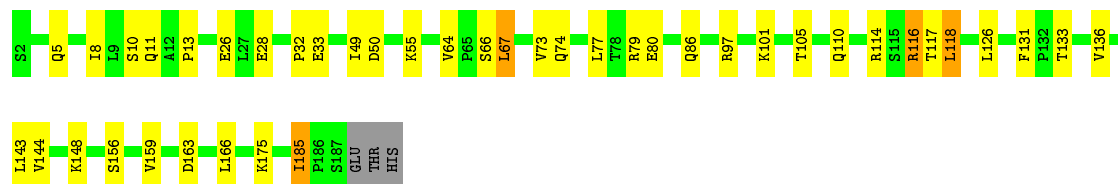
- Molecule 9: 40S ribosomal protein S7-A

Chain S7:  76% 20%




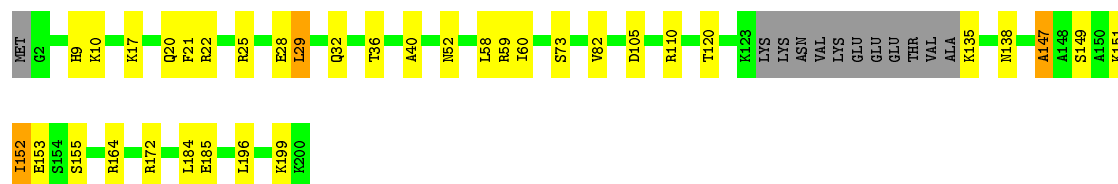
- Molecule 9: 40S ribosomal protein S7-A

Chain s7:  76% 20%




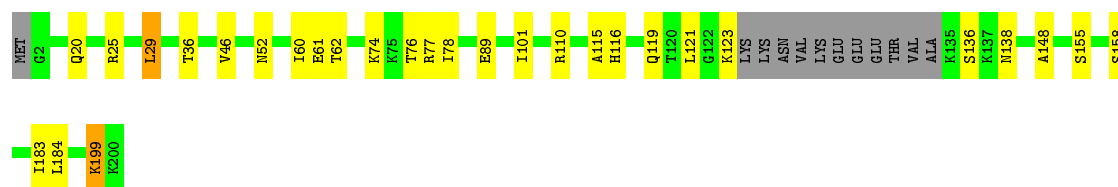
- Molecule 10: 40S ribosomal protein S8-A

Chain S8:  77% 16% 6%



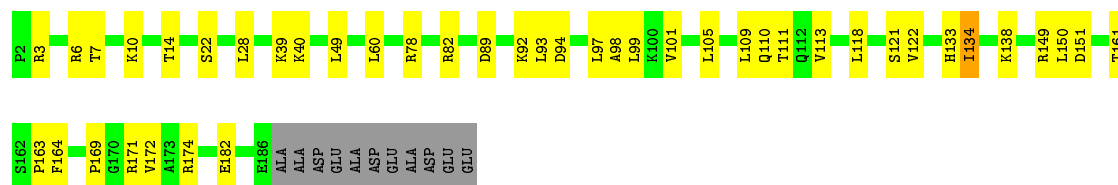
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 



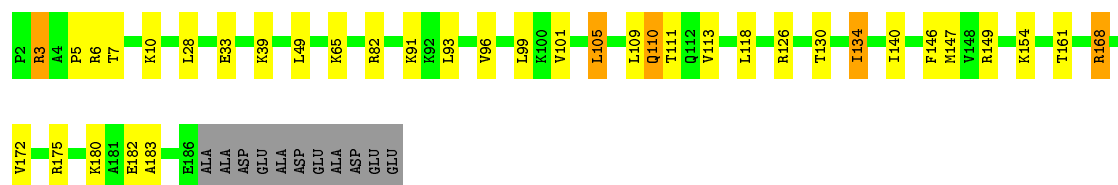
- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 



- Molecule 12: 40S ribosomal protein S10-A

Chain C0: 




- Molecule 12: 40S ribosomal protein S10-A

Chain c0: 

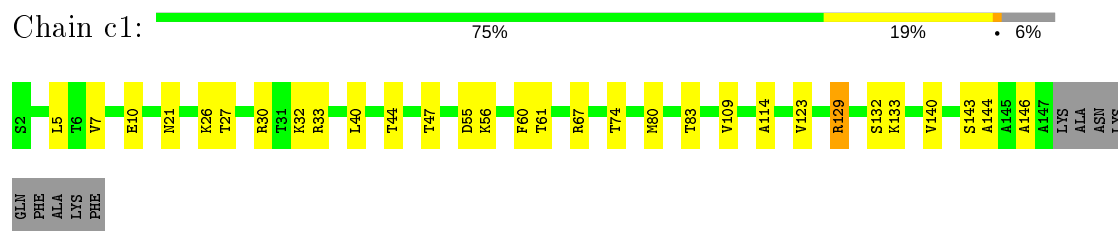


- Molecule 13: 40S ribosomal protein S11-A

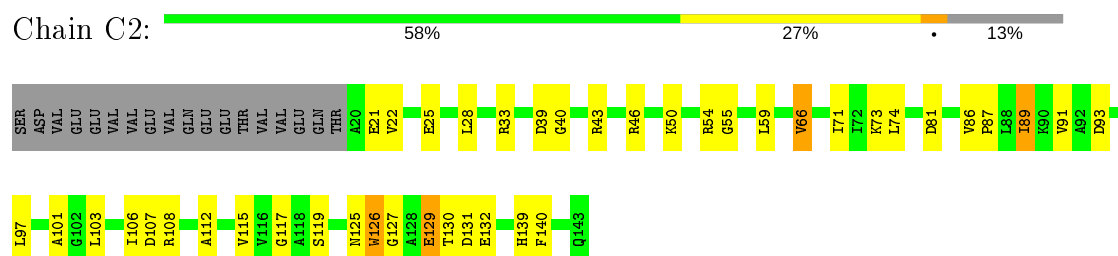
Chain C1: 



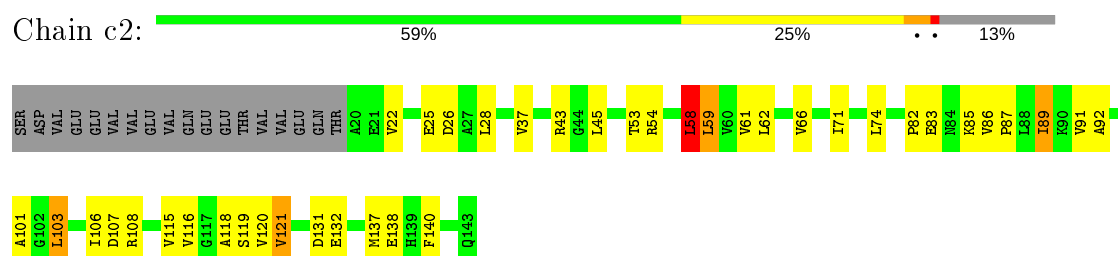
- Molecule 13: 40S ribosomal protein S11-A



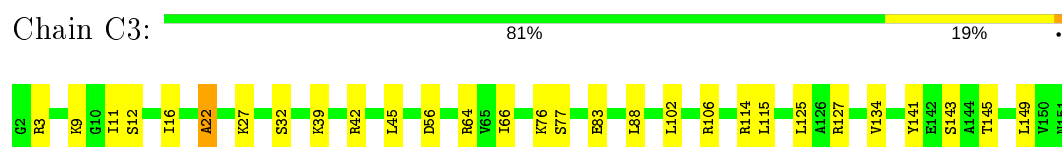
- Molecule 14: 40S ribosomal protein S12



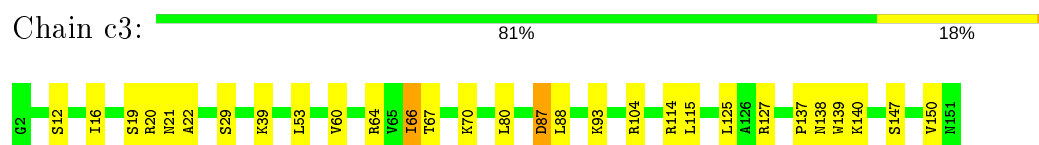
- Molecule 14: 40S ribosomal protein S12



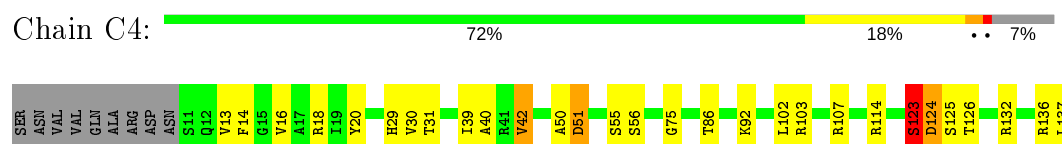
- Molecule 15: 40S ribosomal protein S13




- Molecule 15: 40S ribosomal protein S13



- Molecule 16: 40S ribosomal protein S14-A



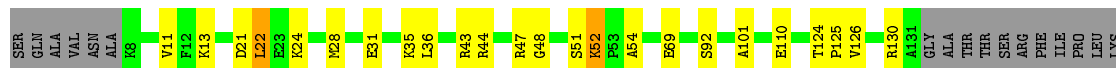
- Molecule 16: 40S ribosomal protein S14-A

Chain c4:  74% 15% 6%



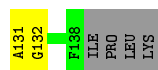
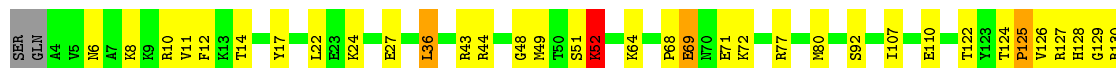
- Molecule 17: 40S ribosomal protein S15

Chain C5:  71% 16% 12%




- Molecule 17: 40S ribosomal protein S15

Chain c5:  70% 23% 7%




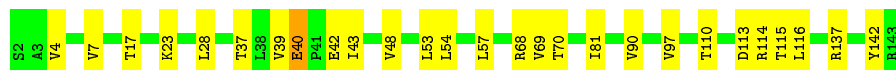
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:  80% 18% 2%



- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  81% 18% 1%

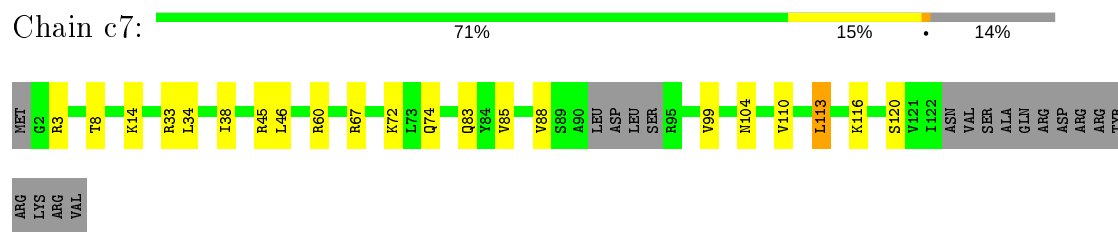


- Molecule 19: 40S ribosomal protein S17-A

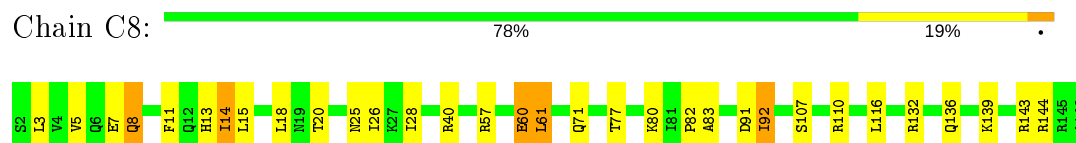
Chain C7:  66% 21% 12%



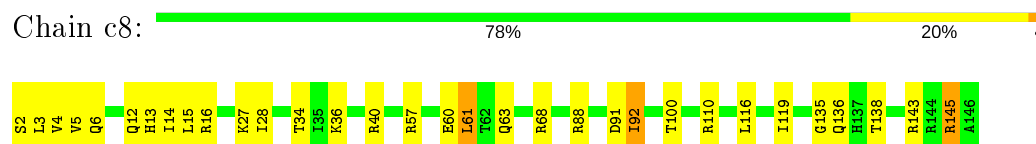
- Molecule 19: 40S ribosomal protein S17-A



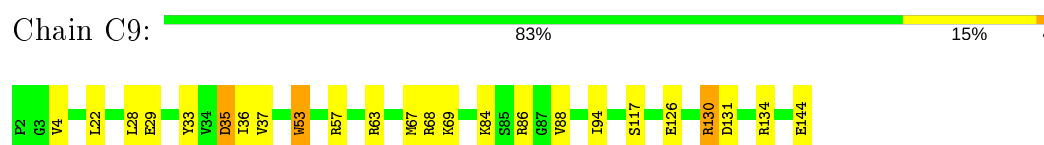
- Molecule 20: 40S ribosomal protein S18-A



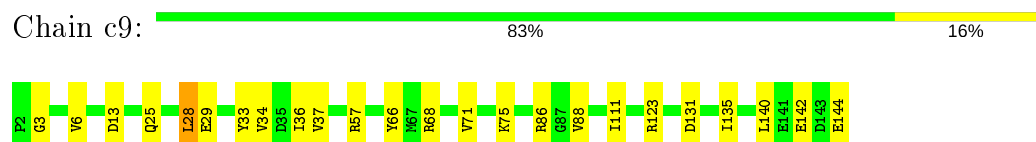
- Molecule 20: 40S ribosomal protein S18-A



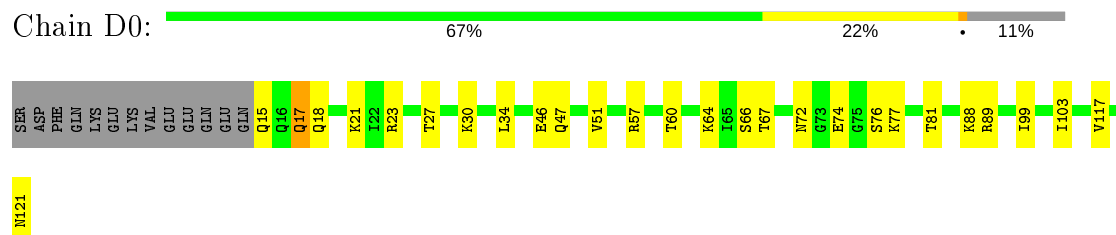
- Molecule 21: 40S ribosomal protein S19-A



- Molecule 21: 40S ribosomal protein S19-A

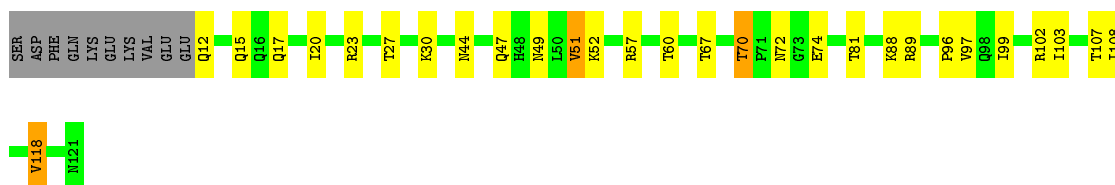


- Molecule 22: 40S ribosomal protein S20



- Molecule 22: 40S ribosomal protein S20





- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 77% 23%



- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 75% 25%



- Molecule 24: 40S ribosomal protein S22-A

Chain D2: 87% 12%



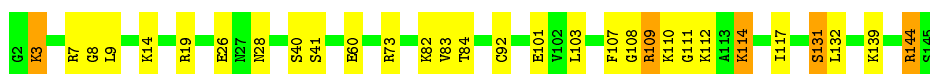
- Molecule 24: 40S ribosomal protein S22-A

Chain d2: 88% 12%



- Molecule 25: 40S ribosomal protein S23-A

Chain D3: 79% 17%




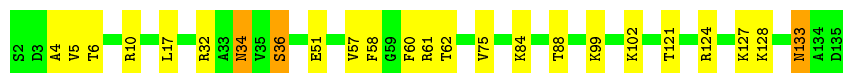
- Molecule 25: 40S ribosomal protein S23-A

Chain d3: 88% 10%




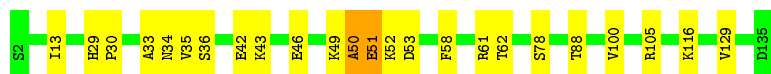
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:  82% 16%



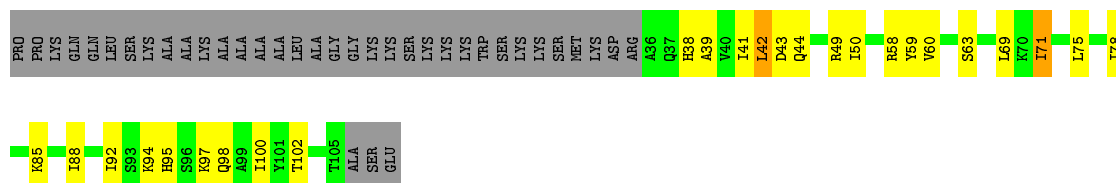
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:  82% 16%



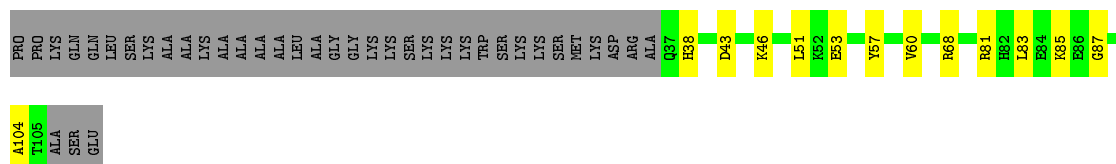
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:  42% 21% 35%



- Molecule 27: 40S ribosomal protein S25-A

Chain d5:  52% 12% 36%



- Molecule 28: 40S ribosomal protein S26-B

Chain D6:  74% 19% 5%




- Molecule 28: 40S ribosomal protein S26-B

Chain d6:  78% 21%

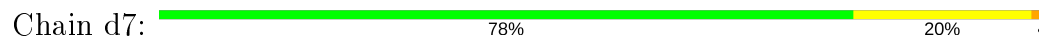


- Molecule 29: 40S ribosomal protein S27-A

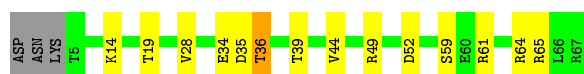
Chain D7:  80% 16%



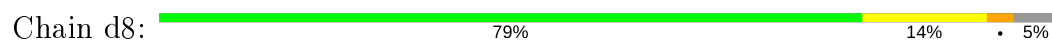
- Molecule 29: 40S ribosomal protein S27-A



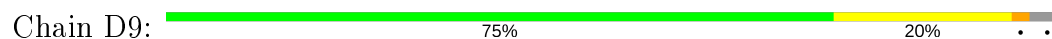
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



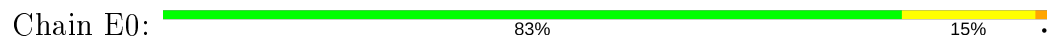
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A



- Molecule 33: Ubiquitin-40S ribosomal protein S31





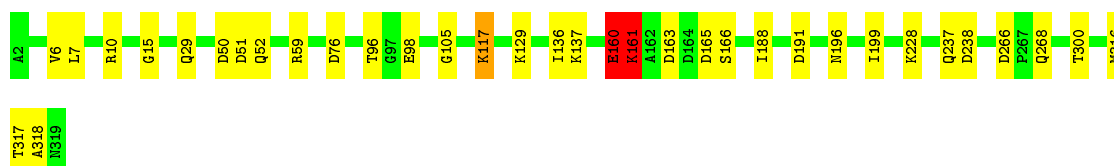
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 57% 37% 5% •



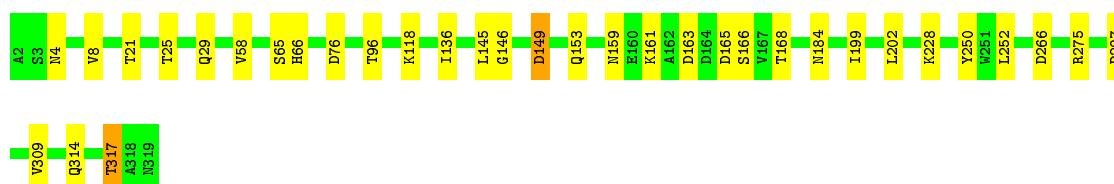
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR: 89% 10% •



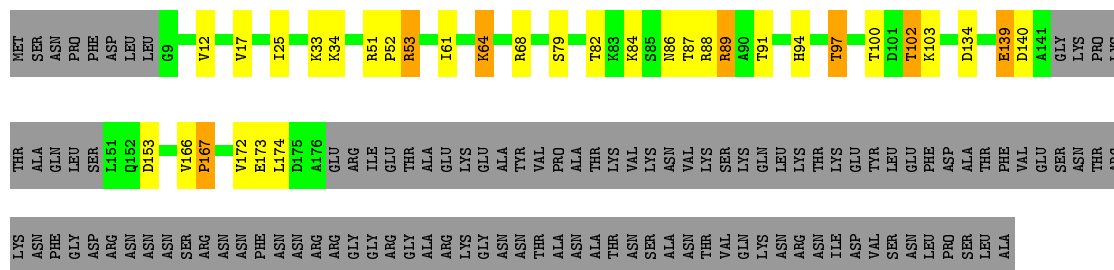
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 89% 10% •



- Molecule 35: Suppressor protein STM1

Chain SM: 46% 10% 42% •

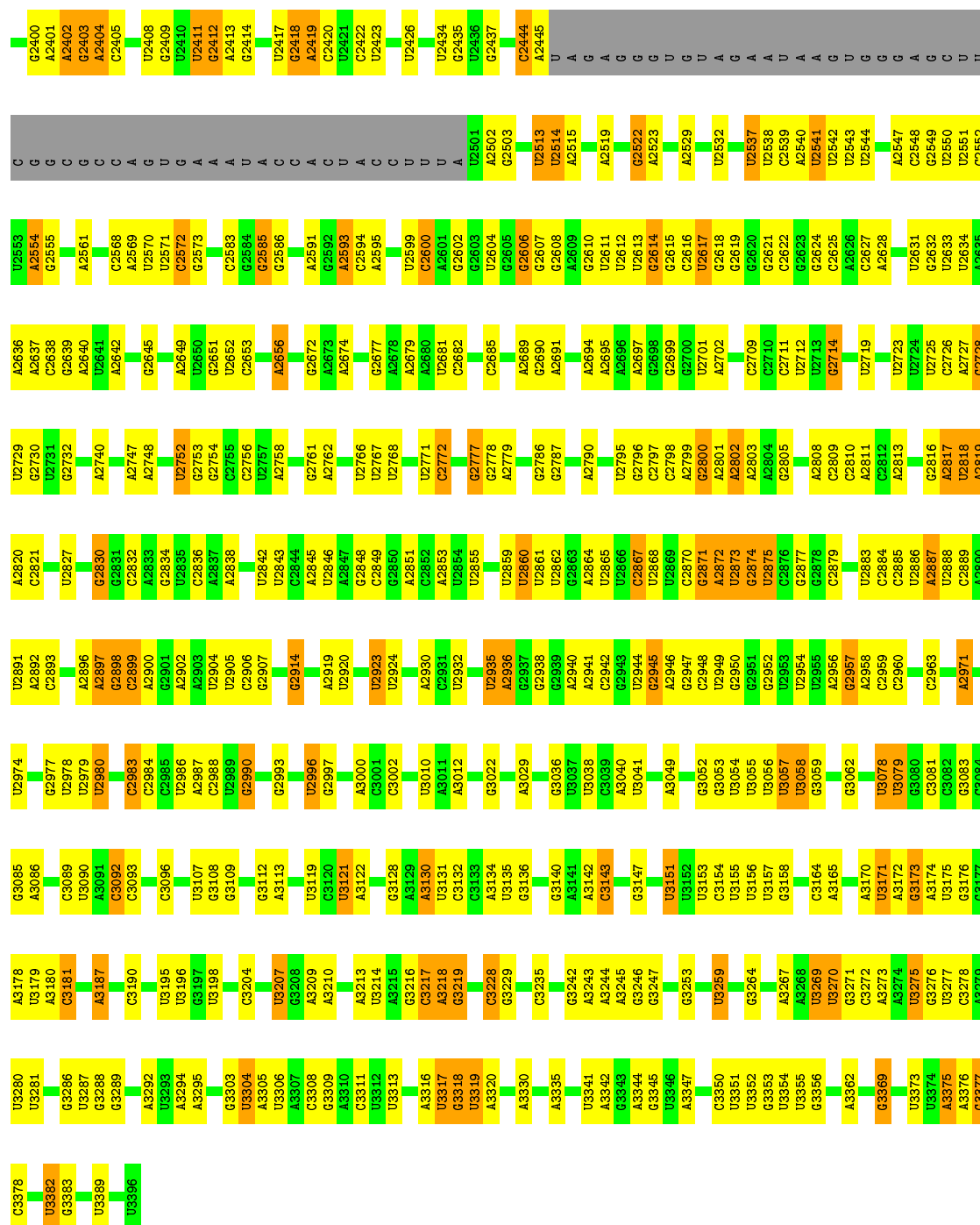


- Molecule 35: Suppressor protein STM1

Chain sM: 32% 5% 62% •

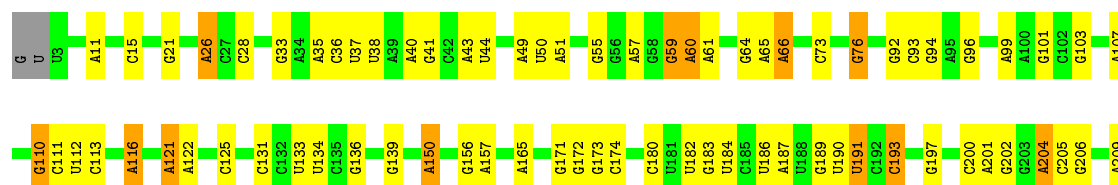






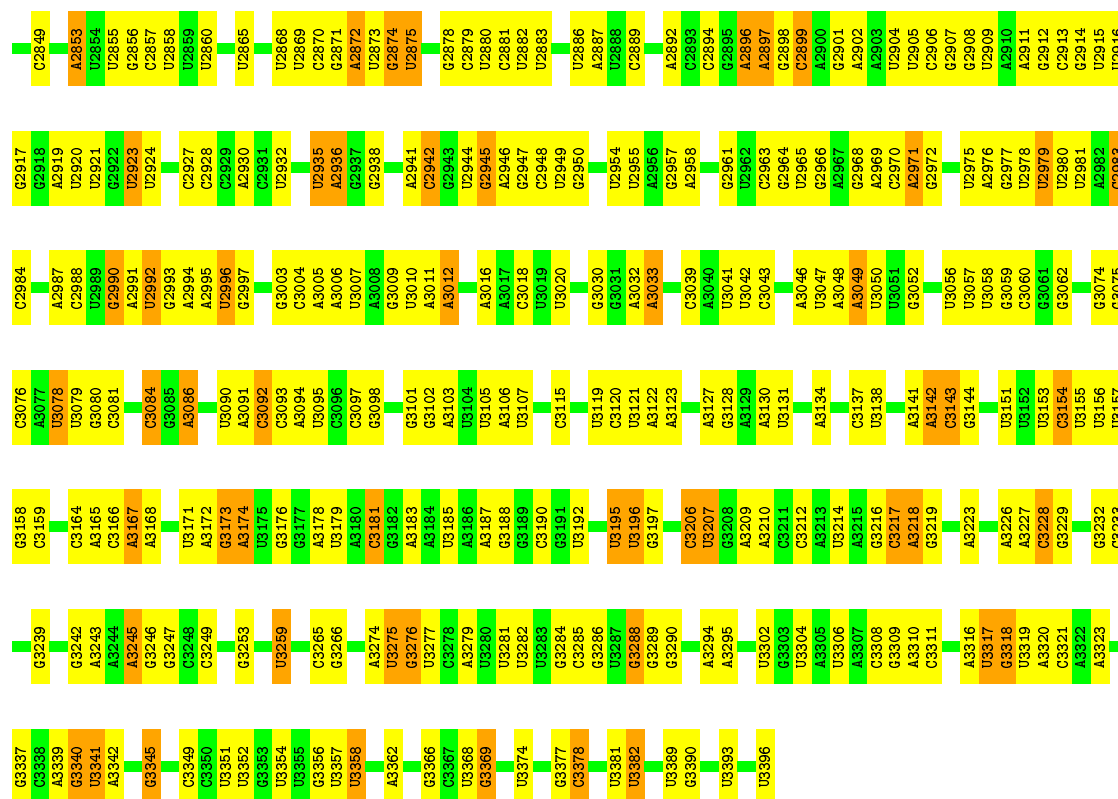
• Molecule 36: 25S ribosomal RNA

Chain 5: 51% 35% 7% 7%



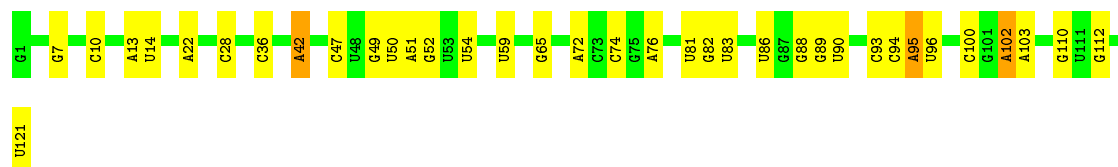
U1448	U1449	G1450	C1451	A1452	A1461	G1464	G1465	G1466	G1467	A1468	C1469	A1475	G1480	A1481	A1482	G1483	U1484	G1485	G1486	G1487	G1488	A1489	A1490	G1493	U1494	U1495	C1496	G1500	U1501	C1502	A1503	A1506	G1507	C1508	G1513	G1514	G1517	G1520	G1521	U1522	G1536	A1537	G1538	G1544	A1545	G1546	G1547																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
C1189	C1118	C1119	A1120	A1121	U1122	U1123	U1124	U1128	A1129	A1130	G1131	G1132	A1133	G1134	C1141	U1144	G1145	G1146	G1147	G1148	G1149	G1152	A1153	A1154	G1157	G1158	A1159	C1160	G1161	U1162	A1163	G1164	A1185	G1186	U1187	U1188	U1189	G1172	U1173	G1174	G1175	C1176	G1177	G1178	A1179	U1180	U1181	A1182	U1183	G1186	C1187	U1188																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
U1299	G1300	A1301	A1302	A1303	A1304	U1305	G1306	G1307	A1308	U1309	G1310	G1311	G1312	G1313	G1314	U1315	G1316	A1317	G1318	G1319	U1322	G1323	C1327	C1328	A1329	U1330	U1331	A1332	C1333	U1334	C1335	U1336	A1337	G1340	G1344	G1349	U1351	A1352	U1353	G1354	A1355	U1356	G1357	G1362	A1363	C1364	G1365	G1370	C1371	C1372																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G1373	G1374	C1375	C1376	G1379	G1380	A1381	G1382	C1385	A1386	G1387	U1388	G1389	A1390	C1391	G1395	C1396	G1397	U1398	A1399	G1400	A1401	C1402	G1403	G1404	A1405	A1406	U1407	G1408	G1409	U1410	C1411	G1412	A1418	A1419	C1420	G1421	C1426	U1427	A1428	G1429	U1430	G1431	C1432	A1433	G1434	A1435	U1436	C1437	U1438	U1439	U1445	A1446	G1447																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G1189	C1118	C1119	A1120	A1121	U1122	U1123	U1124	U1128	A1129	A1130	G1131	G1132	A1133	G1134	C1141	U1144	G1145	G1146	G1147	G1148	G1149	G1152	A1153	A1154	G1157	G1158	A1159	C1160	G1161	U1162	A1163	G1164	A1185	G1186	U1187	U1188	U1189	G1172	U1173	G1174	G1175	C1176	G1177	G1178	A1179	U1180	U1181	A1182	U1183	G1186	C1187	U1188																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C1298	U1299	G1300	A1301	A1302	A1303	A1304	U1305	G1306	G1307	A1308	U1309	G1310	G1311	G1312	G1313	G1314	U1315	G1316	A1317	G1318	G1319	U1322	G1323	C1327	C1328	A1329	U1330	U1331	A1332	C1333	U1334	C1335	U1336	A1337	G1340	G1344	G1349	U1351	A1352	U1353	G1354	A1355	U1356	G1357	G1362	A1363	C1364	G1365	G1370	C1371	C1372																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
A1373	G1374	C1375	C1376	G1379	G1380	A1381	G1382	C1385	A1386	G1387	U1388	G1389	A1390	C1391	G1395	C1396	G1397	U1398	A1399	G1400	A1401	C1402	G1403	G1404	A1405	A1406	U1407	G1408	G1409	U1410	C1411	G1412	A1418	A1419	C1420	G1421	C1426	U1427	A1428	G1429	U1430	G1431	C1432	A1433	G1434	A1435	U1436	C1437	U1438	U1439	U1445	A1446	G1447																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
U1448	A1449	G1450	C1451	A1452	A1461	G1464	G1465	G1466	G1467	A1468	C1469	A1475	G1480	A1481	A1482	G1483	U1484	G1485	G1486	G1487	G1488	A1489	A1490	G1493	U1494	U1495	C1496	G1500	U1501	C1502	A1503	A1506	G1507	C1508	G1513	G1514	G1517	G1520	G1521	U1522	G1536	A1537	G1538	G1544	A1545	G1546	G1547																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U210	A213	G216	U217	G218	A219	G220	A221	U230	G236	G237	A238	G239	U240	G244	C247	U249	U250	C251	U252	A253	A254	C259	G267	A268	G269	G277	U278	G282	G283	A284	A285	U286	G287	C288	U294	A295	A296	G297	U298	G299	G300	G301	G304	A307	U413																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C311	C312	A313	A318	A319	G320	G321	U322	A323	A324	A325	U326	U329	A336	G337	A338	C339	G340	G341	G345	A348	A349	C350	A351	A352	G353	C356	C359	U359	G360	A361	U362	G363	A366	U393	A397	A398	A399	G400	U401	A402	C403	G404	U405	A406	U411	G412	U413																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U414	G415	A416	A417	G420	G421	A422	A423	G424	A425	G426	C427	A428	A436	G437	A438	C439	A440	U441	G442	G443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	G460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	G1263	G1264	G1265	G1266	G1267	G1268	G1269	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330





• Molecule 37: 5S ribosomal RNA

Chain 3: 70% 27%



• Molecule 37: 5S ribosomal RNA

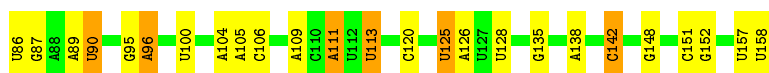
Chain 7: 63% 31% 6%



• Molecule 38: 5.8S ribosomal RNA

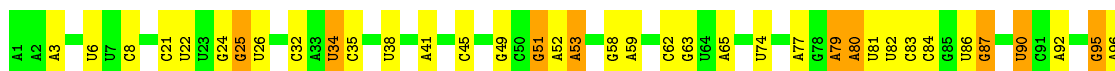
Chain 4: 58% 35% 7%





- Molecule 38: 5.8S ribosomal RNA

Chain 8: 63% 30% 7%



- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 84% 15%



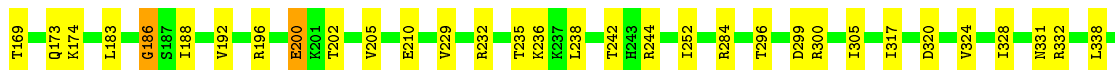
- Molecule 39: 60S ribosomal protein L2-A

Chain l2: 81% 16%



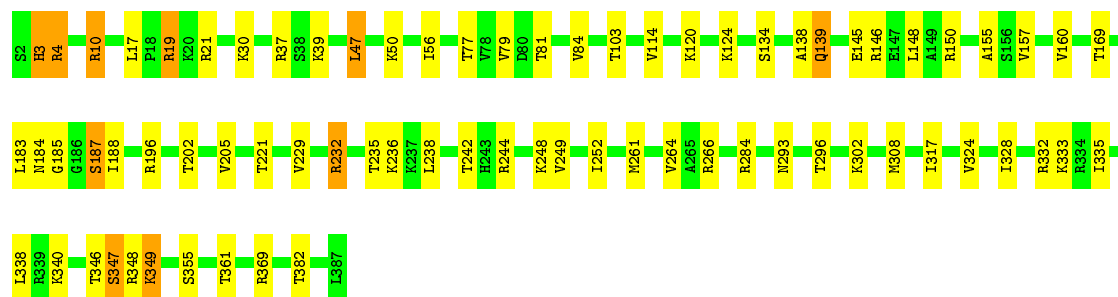
- Molecule 40: 60S ribosomal protein L3

Chain L3: 81% 18%



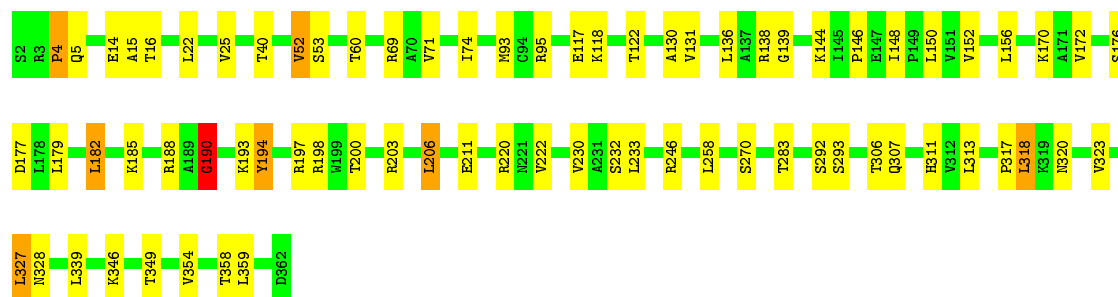
- Molecule 40: 60S ribosomal protein L3

Chain l3: 81% 17%



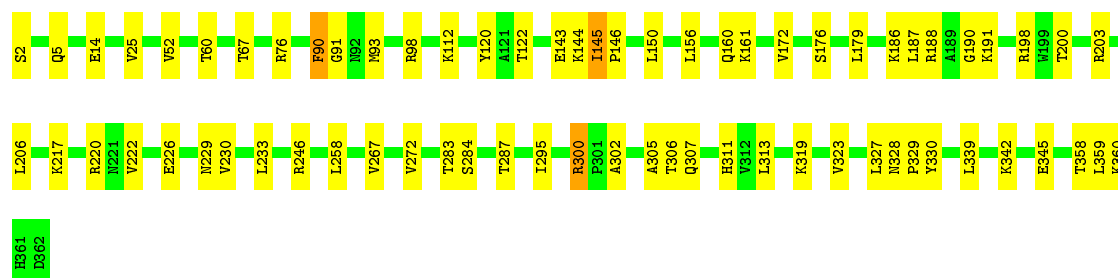
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 80% 18% .



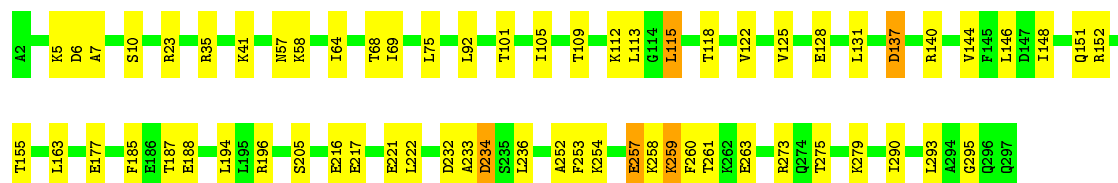
- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 81% 18% .



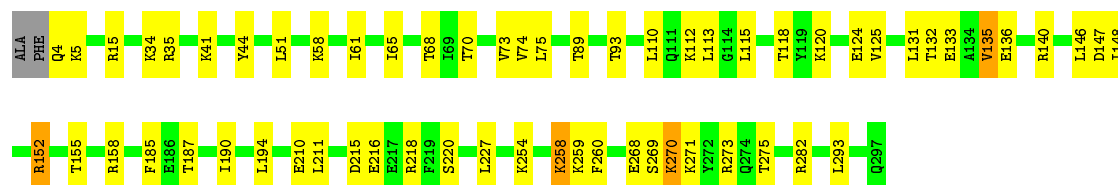
- Molecule 42: 60S ribosomal protein L5

Chain L5: 78% 20% .



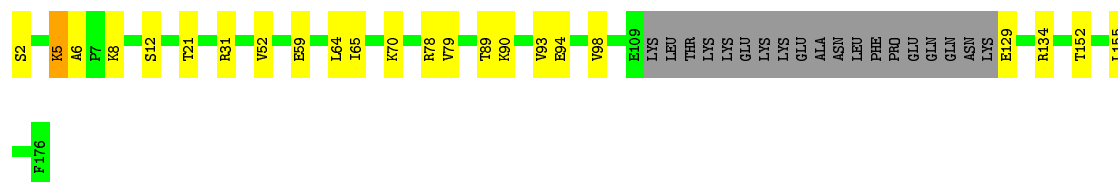
- Molecule 42: 60S ribosomal protein L5

Chain l5: 79% 19% ..



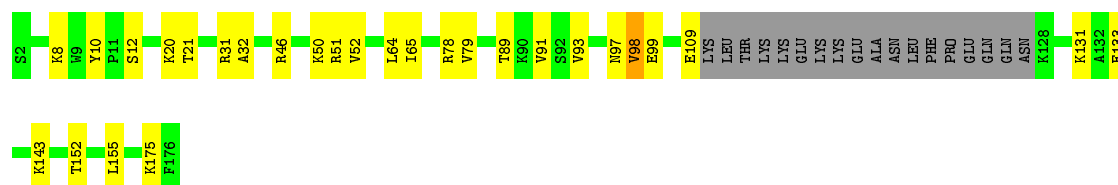
- Molecule 43: 60S ribosomal protein L6-A

Chain L6:  76% 13% • 11%




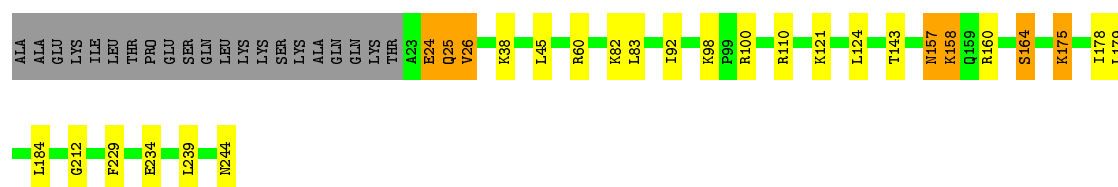
- Molecule 43: 60S ribosomal protein L6-A

Chain 16:  74% 15% 10%




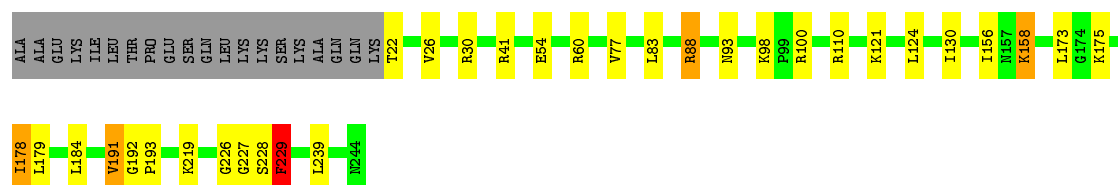
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:  80% 9% • 9%



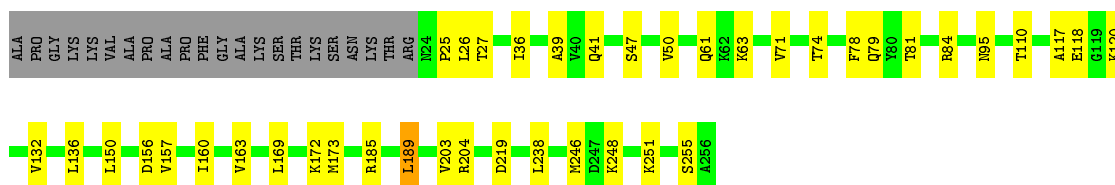
- Molecule 44: 60S ribosomal protein L7-A

Chain 17:  79% 11% • 8%



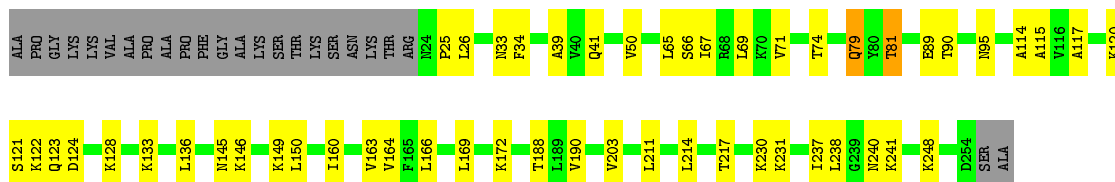
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:  75% 16% 9%



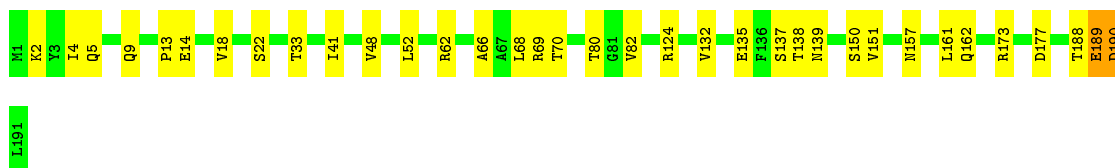
- Molecule 45: 60S ribosomal protein L8-A

Chain 18: 70% 20% 9%



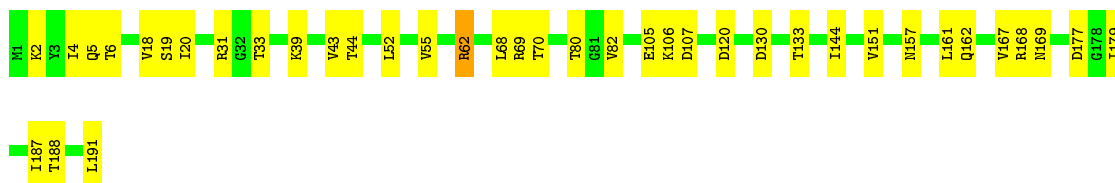
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 82% 17%



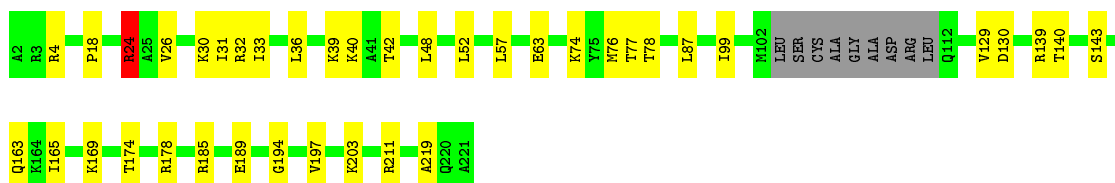
- Molecule 46: 60S ribosomal protein L9-A

Chain 19: 80% 20%



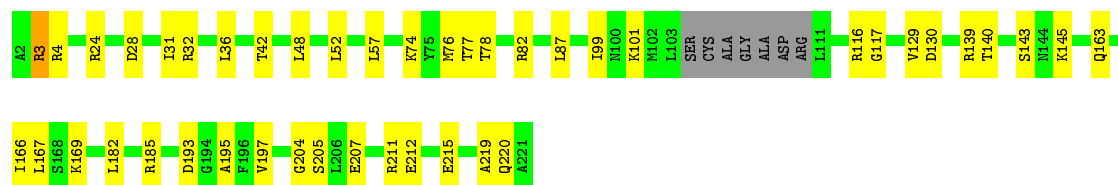
- Molecule 47: 60S ribosomal protein L10

Chain M0: 78% 17%



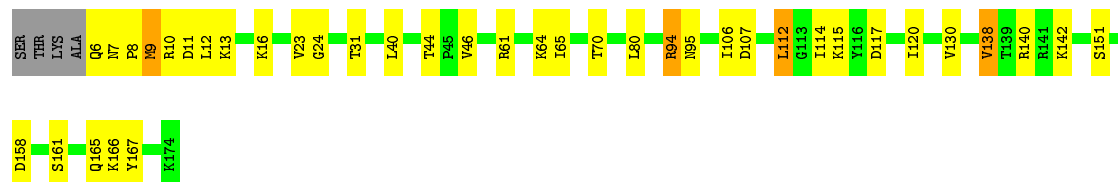
- Molecule 47: 60S ribosomal protein L10

Chain m0: 77% 20%



- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 75% 20% ..



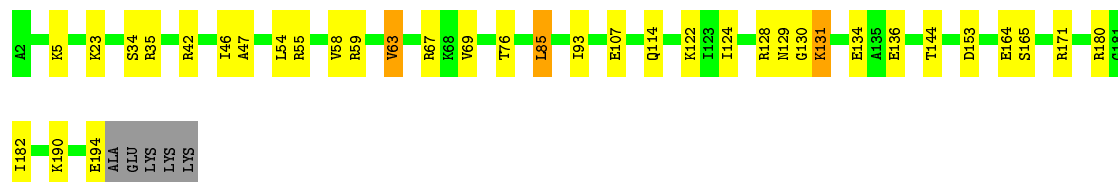
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 79% 17% ..



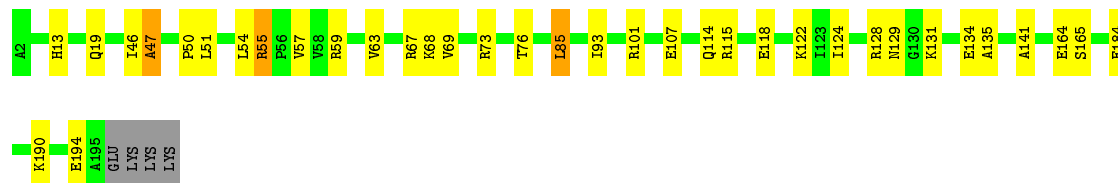
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 79% 17% ..



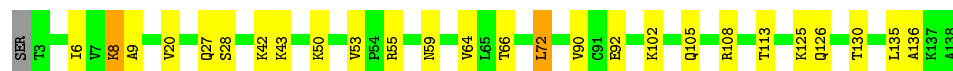
- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 80% 17% ..




- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 80% 18% ..




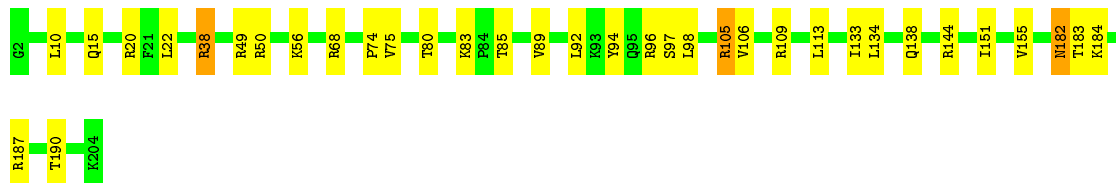
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:  87% 11%




- Molecule 51: 60S ribosomal protein L15-A

Chain M5:  83% 16%




- Molecule 51: 60S ribosomal protein L15-A

Chain m5:  85% 14%




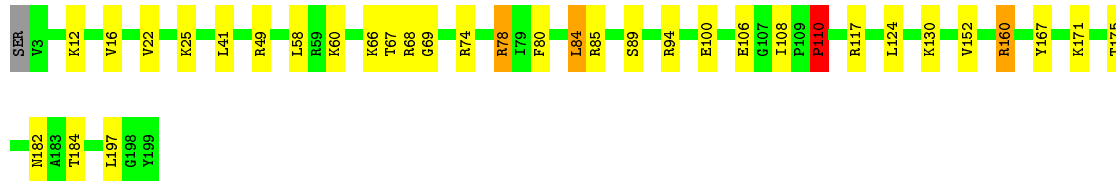
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:  84% 12%




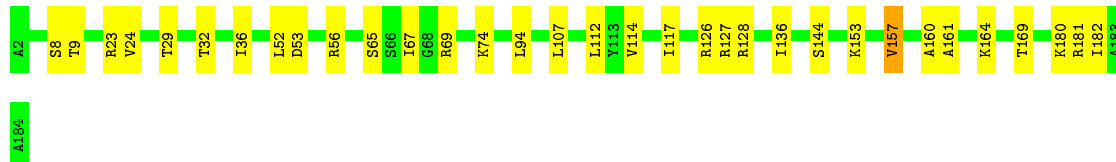
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:  82% 15%

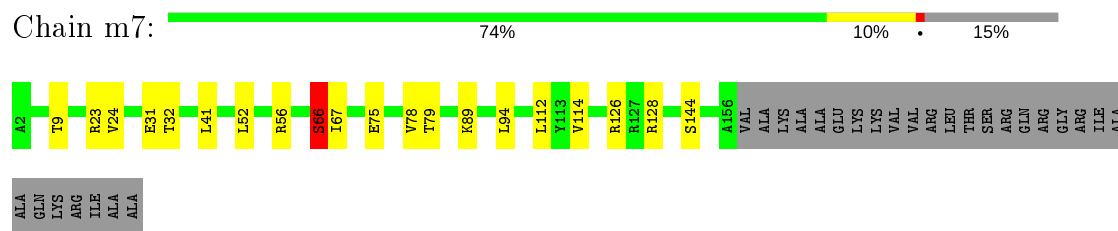


- Molecule 53: 60S ribosomal protein L17-A

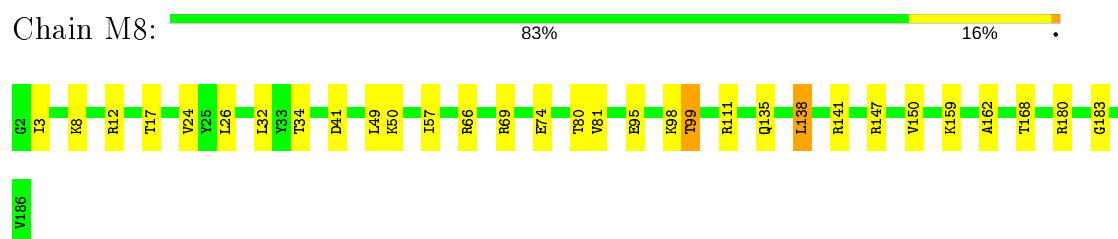
Chain M7:  82% 17%



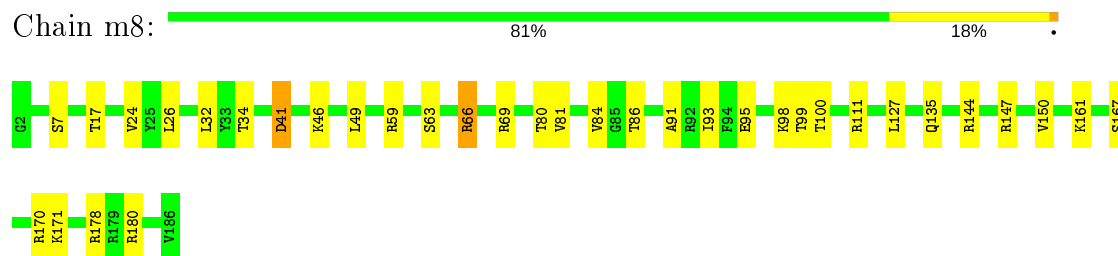
- Molecule 53: 60S ribosomal protein L17-A



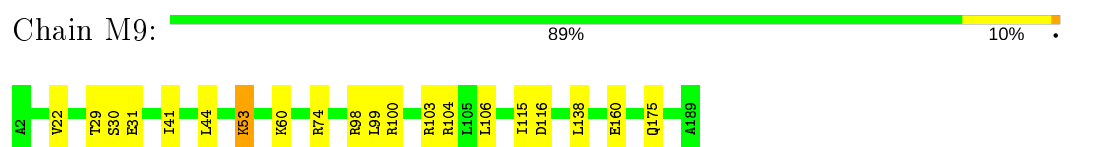
- Molecule 54: 60S ribosomal protein L18-A



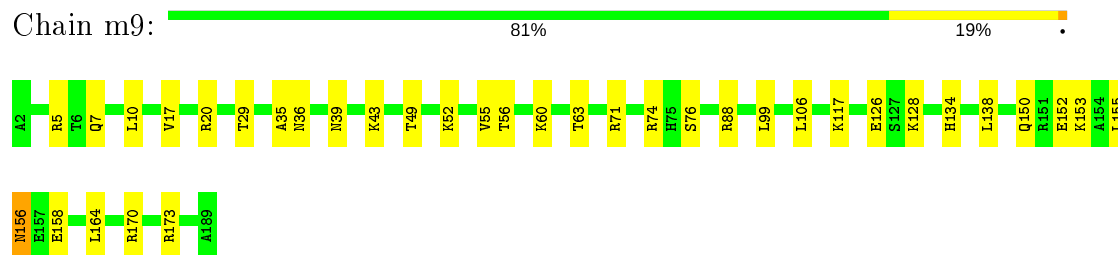
- Molecule 54: 60S ribosomal protein L18-A



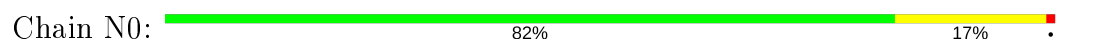
- Molecule 55: 60S ribosomal protein L19-A



- Molecule 55: 60S ribosomal protein L19-A

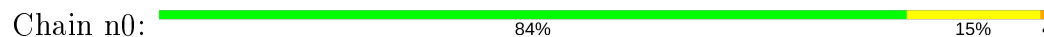


- Molecule 56: 60S ribosomal protein L20-A





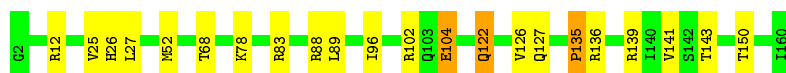
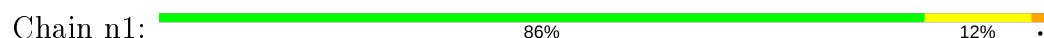
- Molecule 56: 60S ribosomal protein L20-A



- Molecule 57: 60S ribosomal protein L21-A



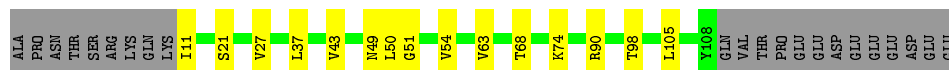
- Molecule 57: 60S ribosomal protein L21-A



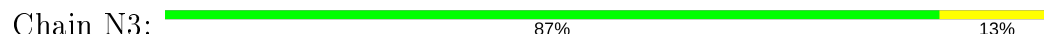
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L22-A



- Molecule 59: 60S ribosomal protein L23-A

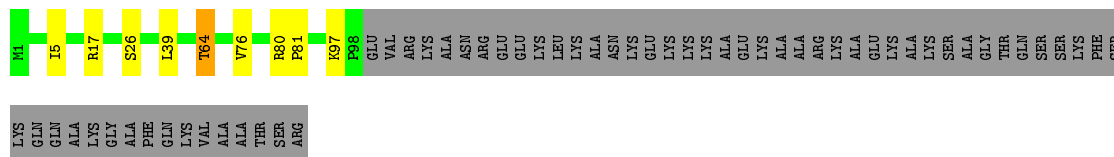


- Molecule 59: 60S ribosomal protein L23-A

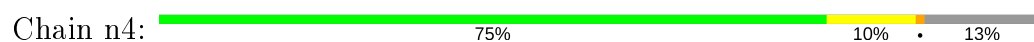




- Molecule 60: 60S ribosomal protein L24-A



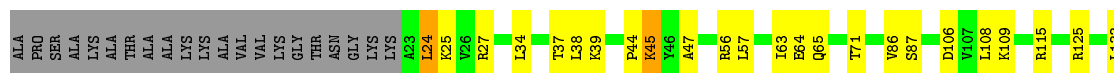
- Molecule 60: 60S ribosomal protein L24-A



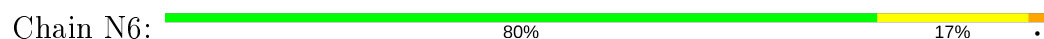
- Molecule 61: 60S ribosomal protein L25



- Molecule 61: 60S ribosomal protein L25



- Molecule 62: 60S ribosomal protein L26-A



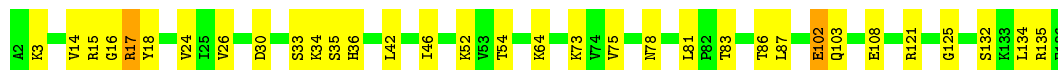
- Molecule 62: 60S ribosomal protein L26-A





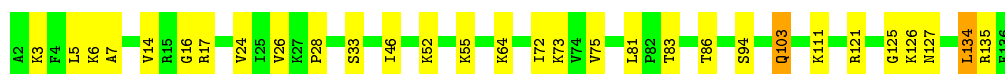
- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 76% 23% .



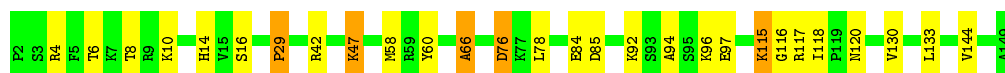
- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 78% 21% .



- Molecule 64: 60S ribosomal protein L28

Chain N8: 81% 16% .



- Molecule 64: 60S ribosomal protein L28

Chain n8: 80% 18% .



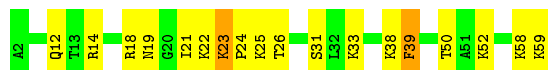
- Molecule 65: 60S ribosomal protein L29

Chain N9: 79% 21% .



- Molecule 65: 60S ribosomal protein L29

Chain n9: 69% 28% .

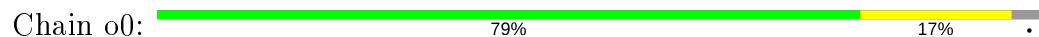


- Molecule 66: 60S ribosomal protein L30

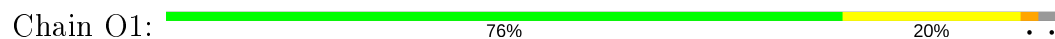
Chain O0: 78% 14% 7% .



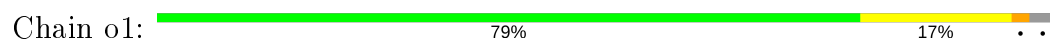
- Molecule 66: 60S ribosomal protein L30



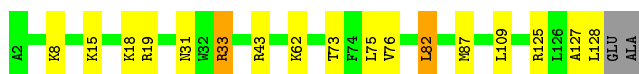
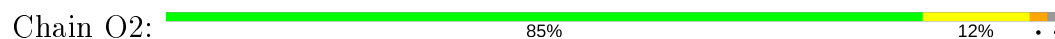
- Molecule 67: 60S ribosomal protein L31-A



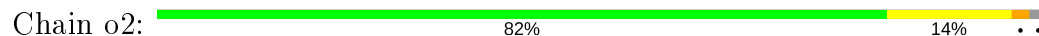
- Molecule 67: 60S ribosomal protein L31-A



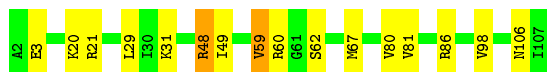
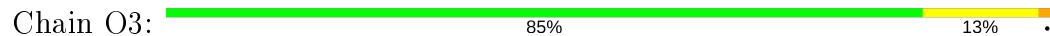
- Molecule 68: 60S ribosomal protein L32



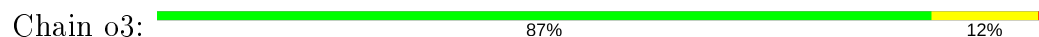
- Molecule 68: 60S ribosomal protein L32



- Molecule 69: 60S ribosomal protein L33-A

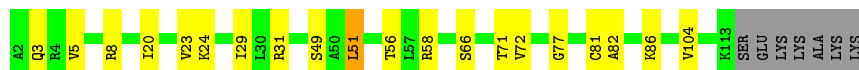
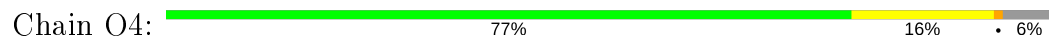


- Molecule 69: 60S ribosomal protein L33-A

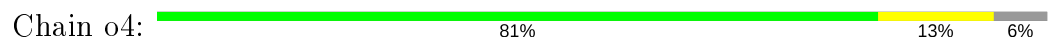




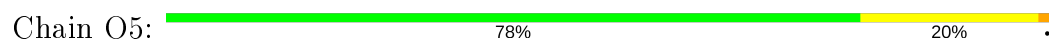
- Molecule 70: 60S ribosomal protein L34-A



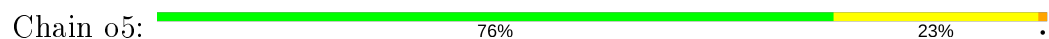
- Molecule 70: 60S ribosomal protein L34-A



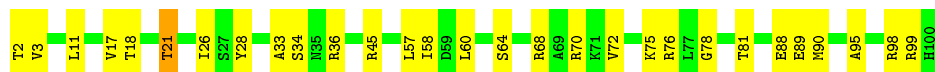
- Molecule 71: 60S ribosomal protein L35-A



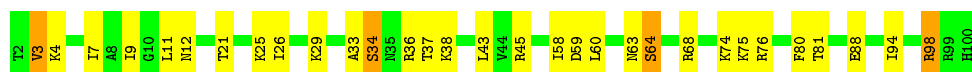
- Molecule 71: 60S ribosomal protein L35-A



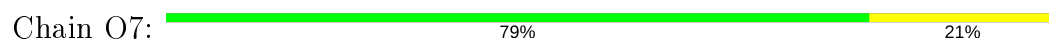
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A





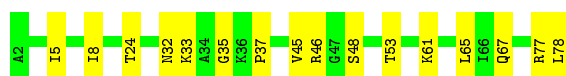
- Molecule 73: 60S ribosomal protein L37-A

Chain o7: 83% 17%



- Molecule 74: 60S ribosomal protein L38

Chain O8: 79% 21%



- Molecule 74: 60S ribosomal protein L38

Chain o8: 82% 17%



- Molecule 75: 60S ribosomal protein L39

Chain O9: 80% 18%



- Molecule 75: 60S ribosomal protein L39

Chain o9: 78% 22%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 83% 15%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 85% 13%



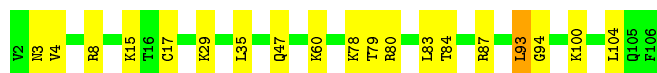
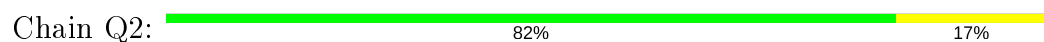
- Molecule 77: 60S ribosomal protein L41-A



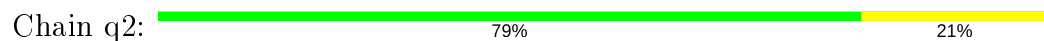
- Molecule 77: 60S ribosomal protein L41-A



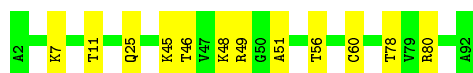
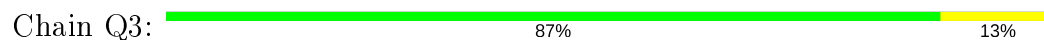
- Molecule 78: 60S ribosomal protein L42-A



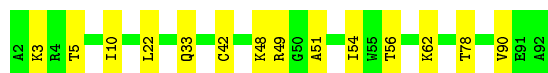
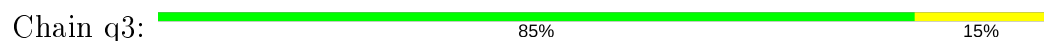
- Molecule 78: 60S ribosomal protein L42-A



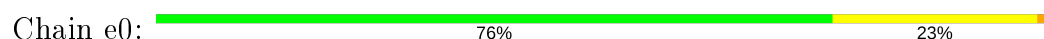
- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A



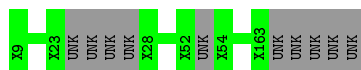
- Molecule 80: 40S ribosomal protein S30-A





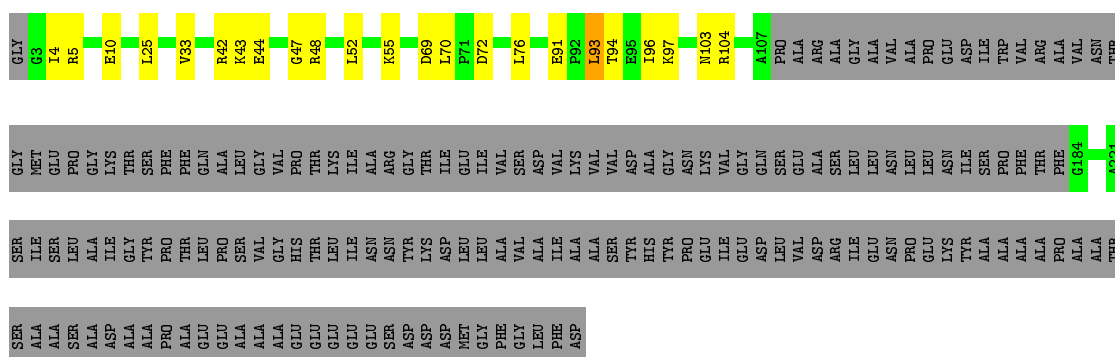
- Molecule 81: Unknown protein m2

Chain m2: 94% 6%



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 39% 7% 54%



- Molecule 83: Unknown protein p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein p2

Chain p2: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.64Å 287.69Å 304.39Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	300.66 – 2.80	Depositor
% Data completeness (in resolution range)	99.6 (300.66-2.80)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.208 , 0.246	Depositor
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.227	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411226	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3H3, OHX, 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	2	0.75	5/41698 (0.0%)	1.30	337/64972 (0.5%)
1	6	0.87	23/42765 (0.1%)	1.40	490/66634 (0.7%)
2	S0	0.47	0/1617	0.67	0/2215
2	s0	0.53	0/1623	0.76	2/2222 (0.1%)
3	S1	0.37	0/1735	0.62	0/2335
3	s1	0.52	0/1748	0.71	1/2352 (0.0%)
4	S2	0.51	0/1665	0.67	0/2263
4	s2	0.61	0/1665	0.79	0/2263
5	S3	0.50	0/1759	0.65	0/2368
5	s3	0.48	0/1759	0.62	0/2368
6	S4	0.51	0/2109	0.74	2/2839 (0.1%)
6	s4	0.57	0/2109	0.79	1/2839 (0.0%)
7	S5	0.43	0/1629	0.60	0/2202
7	s5	0.46	0/1629	0.66	1/2202 (0.0%)
8	S6	0.48	0/1823	0.65	0/2439
8	s6	0.58	0/1779	0.72	1/2379 (0.0%)
9	S7	0.46	0/1506	0.65	0/2028
9	s7	0.54	0/1516	0.70	1/2043 (0.0%)
10	S8	0.58	0/1514	0.79	3/2021 (0.1%)
10	s8	0.64	0/1514	0.77	1/2021 (0.0%)
11	S9	0.50	0/1519	0.69	0/2035
11	s9	0.59	0/1519	0.74	0/2035
12	C0	0.45	0/790	0.69	1/1069 (0.1%)
12	c0	0.40	0/777	0.63	3/1049 (0.3%)
13	C1	0.59	0/1240	0.71	0/1675
13	c1	0.66	0/1194	0.86	0/1610
14	C2	0.37	0/898	0.62	0/1220
14	c2	0.31	0/898	0.58	1/1220 (0.1%)
15	C3	0.50	0/1215	0.71	2/1638 (0.1%)
15	c3	0.61	0/1215	0.77	0/1638
16	C4	0.38	0/901	0.65	0/1217
16	c4	0.54	0/960	0.77	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.50	0/998	0.67	0/1341
17	c5	0.51	0/1060	0.68	1/1426 (0.1%)
18	C6	0.47	0/1125	0.74	3/1510 (0.2%)
18	c6	0.50	0/1131	0.69	0/1518
19	C7	0.46	0/935	0.65	0/1254
19	c7	0.50	0/914	0.70	0/1224
20	C8	0.49	0/1211	0.67	0/1628
20	c8	0.51	0/1211	0.73	1/1628 (0.1%)
21	C9	0.48	0/1130	0.68	0/1517
21	c9	0.51	0/1130	0.71	0/1517
22	D0	0.48	0/865	0.66	0/1169
22	d0	0.49	0/892	0.68	0/1205
23	D1	0.47	0/693	0.66	0/935
23	d1	0.57	0/693	0.80	0/935
24	D2	0.55	0/1038	0.75	1/1395 (0.1%)
24	d2	0.68	0/1038	0.75	0/1395
25	D3	0.63	0/1139	0.79	1/1518 (0.1%)
25	d3	0.73	0/1139	0.83	3/1518 (0.2%)
26	D4	0.48	0/1087	0.63	0/1449
26	d4	0.53	0/1087	0.72	0/1449
27	D5	0.42	0/571	0.71	0/768
27	d5	0.45	0/566	0.63	0/761
28	D6	0.47	0/782	0.67	0/1047
28	d6	0.59	0/782	0.75	0/1047
29	D7	0.46	0/620	0.68	1/838 (0.1%)
29	d7	0.52	0/620	0.73	0/838
30	D8	0.36	0/499	0.56	0/670
30	d8	0.44	0/499	0.67	0/670
31	D9	0.56	0/452	0.82	1/600 (0.2%)
31	d9	0.58	0/452	0.72	0/600
32	E0	0.49	0/483	0.65	0/643
33	E1	0.49	0/577	0.83	0/770
33	e1	0.43	0/619	0.75	1/822 (0.1%)
34	SR	1.06	2/2494 (0.1%)	1.50	6/3393 (0.2%)
34	sR	0.41	0/2495	0.58	0/3395
35	SM	0.55	0/1113	0.71	2/1502 (0.1%)
35	sM	0.51	0/683	0.68	1/923 (0.1%)
36	1	1.16	152/75394 (0.2%)	1.67	1955/117545 (1.7%)
36	5	1.20	176/75414 (0.2%)	1.69	1938/117575 (1.6%)
37	3	0.96	4/2883 (0.1%)	1.42	33/4491 (0.7%)
37	7	1.13	7/2883 (0.2%)	1.63	50/4491 (1.1%)
38	4	1.11	2/3746 (0.1%)	1.60	70/5832 (1.2%)
38	8	1.00	5/3746 (0.1%)	1.51	46/5832 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.75	0/1948	0.87	2/2617 (0.1%)
39	l2	0.82	1/1946 (0.1%)	0.95	5/2614 (0.2%)
40	L3	0.77	2/3146 (0.1%)	0.88	2/4228 (0.0%)
40	l3	0.85	1/3146 (0.0%)	0.96	11/4228 (0.3%)
41	L4	0.86	3/2800 (0.1%)	1.02	10/3790 (0.3%)
41	l4	0.79	0/2800	0.94	6/3790 (0.2%)
42	L5	0.59	0/2425	0.72	0/3271
42	l5	0.78	0/2408	0.83	3/3248 (0.1%)
43	L6	0.77	0/1260	0.85	3/1694 (0.2%)
43	l6	0.78	0/1269	0.85	0/1705
44	L7	0.85	1/1821 (0.1%)	0.90	0/2451
44	l7	0.86	1/1828 (0.1%)	0.91	5/2461 (0.2%)
45	L8	0.59	0/1836	0.69	1/2481 (0.0%)
45	l8	0.57	0/1795	0.69	0/2429
46	L9	0.70	0/1539	0.79	0/2073
46	l9	0.80	0/1539	0.85	0/2073
47	M0	0.76	0/1741	0.88	3/2335 (0.1%)
47	m0	0.82	0/1758	0.89	0/2358
48	M1	0.55	0/1374	0.74	1/1842 (0.1%)
48	m1	0.67	0/1374	0.83	2/1842 (0.1%)
49	M3	0.77	0/1568	0.91	3/2106 (0.1%)
49	m3	0.75	0/1573	0.89	4/2113 (0.2%)
50	M4	0.79	0/1068	0.87	2/1438 (0.1%)
50	m4	0.81	0/1074	0.84	1/1446 (0.1%)
51	M5	0.78	0/1757	0.97	3/2354 (0.1%)
51	m5	0.72	0/1757	0.83	0/2354
52	M6	0.93	3/1585 (0.2%)	1.00	7/2128 (0.3%)
52	m6	1.06	2/1585 (0.1%)	1.04	9/2128 (0.4%)
53	M7	0.84	0/1443	0.87	0/1944
53	m7	0.93	1/1250 (0.1%)	0.89	0/1683
54	M8	0.84	0/1465	0.95	4/1965 (0.2%)
54	m8	0.76	0/1465	0.94	2/1965 (0.1%)
55	M9	0.58	0/1538	0.68	0/2050
55	m9	0.65	0/1538	0.72	0/2050
56	N0	0.81	0/1481	0.87	3/1990 (0.2%)
56	n0	0.84	0/1481	0.92	1/1990 (0.1%)
57	N1	0.81	0/1300	0.86	0/1743
57	n1	0.86	1/1300 (0.1%)	0.86	0/1743
58	N2	0.46	0/812	0.61	0/1099
58	n2	0.53	0/794	0.66	0/1076
59	N3	0.78	0/1018	0.94	5/1369 (0.4%)
59	n3	0.85	0/1018	0.93	4/1369 (0.3%)
60	N4	0.61	0/712	0.69	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.68	0/1052	0.72	0/1398
61	N5	0.65	0/979	0.82	1/1321 (0.1%)
61	n5	0.68	0/974	0.84	0/1314
62	N6	0.76	0/1004	0.94	4/1341 (0.3%)
62	n6	0.68	0/1004	0.82	0/1341
63	N7	0.54	0/1118	0.72	0/1497
63	n7	0.52	0/1118	0.66	0/1497
64	N8	0.86	0/1204	0.97	4/1612 (0.2%)
64	n8	0.84	0/1204	0.97	4/1612 (0.2%)
65	N9	0.85	0/473	0.81	1/629 (0.2%)
65	n9	0.90	0/473	0.93	2/629 (0.3%)
66	O0	0.53	0/751	0.68	0/1008
66	o0	0.55	0/775	0.67	0/1040
67	O1	0.68	0/890	0.75	0/1196
67	o1	0.85	1/897 (0.1%)	0.86	0/1205
68	O2	0.87	0/1041	0.95	4/1394 (0.3%)
68	o2	0.89	0/1041	1.02	5/1394 (0.4%)
69	O3	0.92	0/868	0.90	3/1168 (0.3%)
69	o3	0.98	1/868 (0.1%)	0.92	2/1168 (0.2%)
70	O4	0.62	0/890	0.80	1/1189 (0.1%)
70	o4	0.67	0/890	0.74	0/1189
71	O5	0.71	1/978 (0.1%)	0.84	2/1301 (0.2%)
71	o5	0.62	0/974	0.71	0/1297
72	O6	0.68	0/778	0.84	0/1034
72	o6	0.60	0/777	0.74	0/1033
73	O7	0.89	1/696 (0.1%)	1.00	2/923 (0.2%)
73	o7	0.75	0/696	0.88	1/923 (0.1%)
74	O8	0.52	0/618	0.64	0/826
74	o8	0.49	0/614	0.67	0/822
75	O9	0.89	1/443 (0.2%)	0.96	1/588 (0.2%)
75	o9	0.81	0/443	0.95	0/588
76	Q0	0.73	0/423	0.90	1/562 (0.2%)
76	q0	0.89	0/423	0.92	1/562 (0.2%)
77	Q1	0.70	0/234	0.93	0/300
77	q1	0.94	0/234	1.05	1/300 (0.3%)
78	Q2	1.00	1/860 (0.1%)	0.99	2/1136 (0.2%)
78	q2	0.83	2/860 (0.2%)	0.87	0/1136
79	Q3	0.73	0/701	0.84	0/934
79	q3	0.78	0/701	0.88	0/934
80	e0	0.58	0/499	0.77	0/665
82	p0	0.46	0/1092	0.62	0/1474
All	All	0.92	400/430070 (0.1%)	1.33	5106/631356 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S0	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	2
17	c5	0	1
19	C7	0	1
22	d0	0	1
25	D3	0	1
25	d3	0	1
26	d4	0	2
27	D5	0	1
28	D6	0	3
31	d9	0	1
33	E1	0	1
34	SR	0	2
39	L2	0	1
39	l2	0	2
40	l3	0	2
41	L4	0	2
41	l4	0	1
42	L5	0	1
42	l5	0	2
43	l6	0	1
44	L7	0	1
44	l7	0	2
51	M5	0	1
52	M6	0	2
52	m6	0	1
53	M7	0	1
53	m7	0	1
57	N1	0	1
59	n3	0	1
62	n6	0	1
63	N7	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
67	O1	0	1
67	o1	0	1
72	O6	0	1
All	All	0	57

All (400) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SR	160	GLU	C-N	-38.52	0.45	1.34
34	SR	161	LYS	C-N	-29.42	0.66	1.34
78	Q2	17	CYS	CB-SG	16.03	2.09	1.82
36	5	1152	G	N9-C4	-13.26	1.27	1.38
39	l2	213	GLY	C-O	9.71	1.39	1.23
36	5	2899	C	N3-C4	-9.31	1.27	1.33
36	5	970	A	N9-C4	-9.17	1.32	1.37
36	5	1152	G	C2-N3	-8.92	1.25	1.32
52	m6	66	LYS	CE-NZ	8.54	1.70	1.49
36	5	2375	G	C6-N1	-8.24	1.33	1.39
36	5	2726	C	N3-C4	-8.16	1.28	1.33
1	6	1773	C	C4-N4	8.07	1.41	1.33
36	5	1152	G	N3-C4	-8.05	1.29	1.35
36	5	953	G	C5-C4	-7.92	1.32	1.38
1	6	538	A	N9-C4	7.89	1.42	1.37
36	5	2987	A	N7-C5	-7.85	1.34	1.39
1	6	163	G	N9-C4	-7.78	1.31	1.38
36	5	1152	G	N9-C8	7.74	1.43	1.37
36	1	2402	A	N9-C4	7.66	1.42	1.37
36	5	1115	G	N7-C5	-7.60	1.34	1.39
36	1	1103	A	C6-N1	7.54	1.40	1.35
1	6	337	G	C2-N2	7.54	1.42	1.34
36	5	2874	G	P-O5'	7.54	1.67	1.59
36	5	2412	G	N1-C2	-7.48	1.31	1.37
36	1	895	A	N9-C8	7.46	1.43	1.37
36	5	878	G	N7-C5	-7.32	1.34	1.39
36	1	980	A	N9-C4	7.26	1.42	1.37
36	1	2397	A	C6-N1	7.23	1.40	1.35
36	5	2635	A	N3-C4	-7.23	1.30	1.34
36	5	802	C	N1-C6	-7.21	1.32	1.37
36	5	2873	U	C2-N3	7.18	1.42	1.37
1	6	163	G	N3-C4	-7.16	1.30	1.35
69	o3	92	LYS	CE-NZ	7.09	1.66	1.49
36	5	691	A	N7-C5	-7.07	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1299	U	C4-O4	-6.98	1.18	1.23
36	5	1847	A	N9-C4	-6.97	1.33	1.37
36	1	1143	A	N9-C4	-6.95	1.33	1.37
53	m7	66	SER	C-O	6.94	1.36	1.23
36	1	895	A	N9-C4	-6.93	1.33	1.37
36	1	2726	C	N3-C4	-6.91	1.29	1.33
36	1	2403	G	N9-C4	6.89	1.43	1.38
36	1	2640	A	C6-N1	-6.87	1.30	1.35
36	1	1103	A	N9-C4	6.86	1.42	1.37
36	1	1114	U	C2-N3	-6.84	1.32	1.37
36	5	818	C	N3-C4	-6.84	1.29	1.33
36	5	1849	C	N1-C6	-6.79	1.33	1.37
36	5	1192	C	N1-C2	6.77	1.47	1.40
36	1	2977	G	C5-C4	-6.75	1.33	1.38
36	5	895	A	N9-C4	-6.74	1.33	1.37
36	5	437	G	N7-C5	6.74	1.43	1.39
36	1	96	G	N7-C5	-6.74	1.35	1.39
36	5	2371	G	C8-N7	-6.74	1.26	1.30
36	1	3181	C	N3-C4	-6.71	1.29	1.33
36	5	1332	A	N7-C5	-6.62	1.35	1.39
57	n1	104	GLU	CB-CG	6.62	1.64	1.52
36	1	2396	G	N7-C5	-6.60	1.35	1.39
78	q2	17	CYS	CB-SG	6.58	1.93	1.82
36	5	644	G	N7-C5	-6.55	1.35	1.39
36	5	795	G	N7-C5	-6.55	1.35	1.39
36	1	3209	A	C5-C4	6.53	1.43	1.38
36	5	2305	G	N7-C5	-6.50	1.35	1.39
36	5	3362	A	N9-C4	-6.49	1.33	1.37
36	5	1149	G	N9-C8	-6.45	1.33	1.37
36	5	2915	U	C2-O2	-6.43	1.16	1.22
36	1	910	G	N7-C5	-6.42	1.35	1.39
36	5	3209	A	C5-C4	6.42	1.43	1.38
36	1	2818	U	C2-O2	-6.42	1.16	1.22
36	5	2401	A	N9-C4	6.42	1.41	1.37
36	1	2617	U	N3-C4	-6.40	1.32	1.38
36	1	61	A	N7-C5	-6.40	1.35	1.39
36	1	2811	A	N3-C4	-6.39	1.31	1.34
36	5	2971	A	N9-C4	6.38	1.41	1.37
36	1	2134	G	C6-N1	-6.38	1.35	1.39
36	1	37	U	C2-O2	-6.37	1.16	1.22
36	1	921	A	N7-C5	-6.36	1.35	1.39
36	1	1112	A	N9-C4	-6.36	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2645	G	N3-C4	-6.35	1.31	1.35
36	5	1152	G	C5-C6	-6.35	1.36	1.42
36	1	2867	C	N3-C4	-6.34	1.29	1.33
36	5	2348	A	N3-C4	-6.33	1.31	1.34
36	1	637	C	C2-O2	-6.33	1.18	1.24
36	1	2867	C	C2-N3	-6.33	1.30	1.35
36	5	3245	A	N9-C4	-6.32	1.34	1.37
36	5	2385	G	N9-C4	-6.32	1.32	1.38
36	1	718	G	N9-C8	6.29	1.42	1.37
36	1	2899	C	N3-C4	-6.29	1.29	1.33
36	1	909	G	C5-C4	-6.24	1.33	1.38
40	L3	200	GLU	CG-CD	6.23	1.61	1.51
36	5	953	G	N9-C8	-6.23	1.33	1.37
36	1	2356	A	N9-C4	-6.23	1.34	1.37
36	5	872	U	C4-O4	-6.22	1.18	1.23
36	5	2954	U	C4-O4	6.22	1.28	1.23
36	5	1152	G	C8-N7	6.21	1.34	1.30
36	5	3005	A	N7-C5	-6.21	1.35	1.39
36	5	404	G	N7-C5	-6.19	1.35	1.39
36	5	2643	A	C6-N1	6.18	1.39	1.35
36	1	912	G	C5-C4	-6.16	1.34	1.38
36	5	1178	G	C2-N3	-6.16	1.27	1.32
36	5	909	G	C5-C4	-6.15	1.34	1.38
36	5	649	A	N7-C5	-6.15	1.35	1.39
36	1	2714	G	N9-C8	6.13	1.42	1.37
36	1	895	A	N3-C4	-6.12	1.31	1.34
36	5	661	G	N7-C5	-6.11	1.35	1.39
36	1	643	U	N1-C2	-6.09	1.33	1.38
36	5	2147	A	N7-C5	-6.09	1.35	1.39
38	8	80	A	N9-C4	6.08	1.41	1.37
36	1	803	C	C4-N4	-6.07	1.28	1.33
1	6	1765	A	N9-C4	-6.05	1.34	1.37
36	1	3209	A	C6-N1	6.04	1.39	1.35
36	1	938	C	C4-N4	-6.02	1.28	1.33
1	6	437	A	N3-C4	-6.02	1.31	1.34
36	1	1170	A	N9-C4	6.02	1.41	1.37
36	5	876	A	N3-C4	-6.01	1.31	1.34
36	5	1304	A	N3-C4	6.00	1.38	1.34
36	5	834	U	N1-C2	-5.99	1.33	1.38
36	5	2395	G	C5-C4	-5.97	1.34	1.38
36	5	2147	A	C5-C6	-5.96	1.35	1.41
38	8	41	A	C5-C6	-5.96	1.35	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	631	U	C2-N3	-5.95	1.33	1.37
38	8	25	G	N1-C2	-5.95	1.32	1.37
36	1	1858	A	N7-C5	-5.95	1.35	1.39
36	1	3216	G	N7-C5	-5.93	1.35	1.39
52	M6	34	VAL	CB-CG1	-5.93	1.40	1.52
36	1	1103	A	N3-C4	5.91	1.38	1.34
36	1	2800	G	C5-C4	-5.91	1.34	1.38
37	3	95	A	N7-C5	-5.91	1.35	1.39
36	1	2412	G	N7-C5	-5.91	1.35	1.39
36	5	2860	U	N3-C4	5.89	1.43	1.38
36	1	2147	A	N7-C5	-5.88	1.35	1.39
36	1	2404	A	C6-N1	5.88	1.39	1.35
36	5	1152	G	N1-C2	5.88	1.42	1.37
36	5	2975	U	C4-O4	-5.88	1.19	1.23
36	5	1311	G	C5-C4	-5.87	1.34	1.38
36	1	2836	C	N3-C4	-5.85	1.29	1.33
1	6	337	G	C2-N3	5.85	1.37	1.32
36	1	637	C	C3'-C2'	-5.83	1.46	1.52
36	5	960	U	N1-C2	5.83	1.43	1.38
36	5	2119	A	N7-C5	-5.83	1.35	1.39
36	1	2971	A	N9-C4	5.83	1.41	1.37
36	5	363	G	N3-C4	-5.82	1.31	1.35
1	6	65	A	N9-C4	-5.82	1.34	1.37
1	6	542	A	N7-C5	-5.82	1.35	1.39
36	1	368	G	N7-C5	-5.80	1.35	1.39
36	5	1103	A	N9-C4	5.80	1.41	1.37
36	1	2606	G	N7-C5	-5.79	1.35	1.39
36	1	426	G	N1-C2	-5.79	1.33	1.37
36	1	2805	G	C8-N7	-5.78	1.27	1.30
36	5	3107	U	C2-N3	-5.78	1.33	1.37
36	1	2396	G	N9-C8	-5.75	1.33	1.37
36	1	2761	G	N3-C4	-5.73	1.31	1.35
36	5	2872	A	C5-C6	5.71	1.46	1.41
36	5	426	G	C5-C4	-5.71	1.34	1.38
36	1	46	U	C2-O2	-5.70	1.17	1.22
36	1	818	C	N3-C4	-5.70	1.29	1.33
36	1	2986	U	C2-N3	-5.70	1.33	1.37
1	6	1655	A	N3-C4	-5.69	1.31	1.34
36	5	2899	C	C2-N3	-5.69	1.31	1.35
1	6	1681	A	N9-C4	-5.69	1.34	1.37
71	O5	64	GLU	CG-CD	5.68	1.60	1.51
36	5	420	G	C5-C4	-5.68	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2823	G	C5-C4	-5.67	1.34	1.38
36	5	2971	A	N7-C5	5.67	1.42	1.39
36	5	420	G	N9-C8	-5.67	1.33	1.37
36	5	94	G	C5-C4	-5.67	1.34	1.38
36	1	1164	G	N7-C5	-5.67	1.35	1.39
36	5	3052	G	N1-C2	-5.67	1.33	1.37
44	L7	234	GLU	CD-OE2	5.66	1.31	1.25
36	5	981	U	N1-C2	5.66	1.43	1.38
37	7	49	G	N9-C8	-5.65	1.33	1.37
36	5	1365	G	C6-N1	-5.63	1.35	1.39
36	1	2642	A	N7-C5	5.63	1.42	1.39
38	4	12	A	N9-C4	-5.62	1.34	1.37
36	1	960	U	C4-O4	5.62	1.28	1.23
36	1	2944	U	C4-O4	-5.62	1.19	1.23
36	5	2921	U	C4-O4	-5.62	1.19	1.23
52	m6	80	PHE	CB-CG	-5.61	1.41	1.51
36	5	2642	A	N9-C4	-5.61	1.34	1.37
36	1	2418	G	O3'-P	5.60	1.67	1.61
36	1	98	G	C6-N1	-5.59	1.35	1.39
36	5	2635	A	C6-N1	-5.59	1.31	1.35
36	5	2393	G	C8-N7	-5.58	1.27	1.30
36	1	279	U	C4-O4	-5.57	1.19	1.23
36	5	2873	U	C2-O2	5.57	1.27	1.22
36	5	1602	A	N7-C5	-5.57	1.35	1.39
36	5	2341	A	N9-C8	-5.56	1.33	1.37
36	1	1514	G	N1-C2	-5.56	1.33	1.37
36	1	2385	G	N9-C4	-5.56	1.33	1.38
36	1	2134	G	N1-C2	-5.55	1.33	1.37
36	1	2872	A	N7-C5	5.55	1.42	1.39
1	6	321	C	N1-C2	5.54	1.45	1.40
36	5	2700	G	C5-C4	-5.54	1.34	1.38
36	5	1113	G	N3-C4	-5.54	1.31	1.35
37	3	82	G	N9-C8	-5.52	1.33	1.37
36	5	877	C	C4-N4	-5.52	1.28	1.33
36	5	3106	A	N7-C5	-5.52	1.35	1.39
36	1	693	A	N7-C5	-5.52	1.35	1.39
36	5	1848	G	C5-C4	-5.52	1.34	1.38
36	1	2610	G	C8-N7	5.52	1.34	1.30
36	1	1330	A	N7-C5	-5.51	1.35	1.39
36	5	1899	G	N7-C5	-5.51	1.35	1.39
36	5	2314	U	C4-O4	5.51	1.28	1.23
41	L4	211	GLU	CG-CD	5.51	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1908	A	C6-N1	-5.50	1.31	1.35
36	1	1429	G	C2-N3	5.50	1.37	1.32
1	6	314	C	N3-C4	-5.50	1.30	1.33
36	5	2403	G	C2-N3	5.50	1.37	1.32
36	1	970	A	N9-C4	-5.49	1.34	1.37
36	1	1127	G	C5-C6	-5.49	1.36	1.42
36	5	2639	G	N7-C5	-5.49	1.35	1.39
36	5	1307	G	C3'-O3'	5.48	1.49	1.42
36	1	2397	A	N3-C4	5.48	1.38	1.34
36	1	661	G	N7-C5	-5.47	1.35	1.39
36	5	2897	A	N9-C8	-5.47	1.33	1.37
36	1	1395	G	C5-C4	-5.46	1.34	1.38
36	5	1482	A	N9-C4	-5.46	1.34	1.37
38	8	22	U	C4-O4	-5.46	1.19	1.23
36	1	2983	C	N3-C4	-5.46	1.30	1.33
36	5	2113	A	N9-C4	-5.45	1.34	1.37
36	5	1884	A	N7-C5	-5.45	1.35	1.39
36	1	2640	A	N3-C4	-5.44	1.31	1.34
36	5	2643	A	N9-C4	-5.44	1.34	1.37
36	5	2823	G	N7-C5	-5.44	1.35	1.39
36	1	968	G	C6-N1	-5.44	1.35	1.39
36	5	2899	C	N1-C6	-5.44	1.33	1.37
36	5	795	G	C5-C4	-5.43	1.34	1.38
36	5	2419	A	P-O5'	5.43	1.65	1.59
36	1	86	G	C6-N1	-5.43	1.35	1.39
36	1	278	U	C2-O2	-5.43	1.17	1.22
36	1	1103	A	N7-C5	5.43	1.42	1.39
1	2	1291	G	N3-C4	-5.42	1.31	1.35
36	1	2397	A	C5-C4	5.42	1.42	1.38
36	1	903	U	C4-O4	-5.42	1.19	1.23
36	5	2704	A	N9-C4	-5.42	1.34	1.37
36	1	2945	G	N7-C5	-5.42	1.35	1.39
36	1	94	G	N7-C5	-5.41	1.36	1.39
36	1	1305	U	C4-O4	-5.41	1.19	1.23
36	1	2371	G	C8-N7	-5.41	1.27	1.30
38	4	113	U	C2-N3	-5.39	1.33	1.37
36	5	1468	A	N9-C4	-5.39	1.34	1.37
1	2	992	A	N9-C4	-5.39	1.34	1.37
37	7	96	U	C4-O4	-5.38	1.19	1.23
36	1	1167	U	C4-O4	-5.38	1.19	1.23
36	1	637	C	C4-N4	-5.38	1.29	1.33
36	5	793	C	C4-C5	-5.38	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	3050	U	C2-N3	-5.37	1.33	1.37
36	5	2957	G	C8-N7	-5.37	1.27	1.30
36	5	3275	U	N1-C2	5.37	1.43	1.38
36	5	953	G	C5-C6	-5.36	1.36	1.42
36	5	1429	G	N9-C8	-5.36	1.34	1.37
36	5	3308	C	N3-C4	-5.36	1.30	1.33
36	1	3130	A	N7-C5	-5.33	1.36	1.39
36	5	2376	G	C6-N1	-5.33	1.35	1.39
73	O7	10	LYS	CE-NZ	5.33	1.62	1.49
1	6	607	G	C6-N1	-5.33	1.35	1.39
36	1	2761	G	N9-C4	-5.33	1.33	1.38
36	5	2164	A	N7-C5	-5.33	1.36	1.39
36	5	2272	G	C5-C4	-5.32	1.34	1.38
36	5	2971	A	C5-C4	5.32	1.42	1.38
36	1	1153	A	N3-C4	-5.31	1.31	1.34
40	L3	7	GLU	CB-CG	5.31	1.62	1.52
36	1	2988	C	C2-O2	-5.30	1.19	1.24
36	5	2813	A	N7-C5	-5.30	1.36	1.39
1	6	1537	C	N1-C6	5.30	1.40	1.37
36	1	2120	A	N7-C5	-5.29	1.36	1.39
36	5	2376	G	N9-C8	-5.28	1.34	1.37
36	5	652	G	N7-C5	-5.28	1.36	1.39
36	5	1373	A	C5-C4	-5.28	1.35	1.38
36	5	1331	U	C4-C5	-5.27	1.38	1.43
36	1	2145	A	N7-C5	-5.27	1.36	1.39
36	1	626	U	C2-N3	-5.27	1.34	1.37
36	5	2434	U	C2-N3	-5.27	1.34	1.37
36	1	1304	A	N9-C4	-5.26	1.34	1.37
36	1	1841	A	N9-C4	5.26	1.41	1.37
40	l3	349	LYS	CD-CE	5.26	1.64	1.51
38	8	79	A	N9-C4	5.26	1.41	1.37
1	6	967	A	N9-C4	5.25	1.41	1.37
1	6	1503	A	N9-C8	5.25	1.42	1.37
36	1	2945	G	C5-C4	-5.25	1.34	1.38
36	5	1902	G	C5-C4	-5.24	1.34	1.38
36	1	645	A	C2-N3	5.24	1.38	1.33
36	1	1507	G	N9-C8	-5.24	1.34	1.37
36	5	3274	A	N3-C4	-5.24	1.31	1.34
36	1	3362	A	N9-C4	-5.24	1.34	1.37
36	5	2138	A	N9-C8	-5.24	1.33	1.37
36	1	345	G	C5-C4	-5.24	1.34	1.38
36	5	937	G	C2-N3	5.23	1.36	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1173	U	C2-N3	-5.23	1.34	1.37
36	5	2403	G	N9-C4	5.23	1.42	1.38
36	1	2368	A	C5-C4	-5.23	1.35	1.38
67	o1	61	LYS	CD-CE	5.22	1.64	1.51
36	1	1592	G	N7-C5	-5.22	1.36	1.39
36	5	2412	G	C2-N3	-5.22	1.28	1.32
36	5	92	G	N1-C2	-5.22	1.33	1.37
36	1	3057	U	N3-C4	-5.22	1.33	1.38
36	5	2977	G	C6-N1	-5.21	1.35	1.39
36	1	1482	A	C5-C6	5.21	1.45	1.41
36	5	2958	A	N9-C4	-5.21	1.34	1.37
36	1	3136	G	C6-N1	-5.21	1.35	1.39
36	5	1103	A	N3-C4	5.21	1.38	1.34
36	1	2409	G	C6-N1	-5.20	1.35	1.39
36	1	2732	G	C6-N1	-5.20	1.35	1.39
36	1	2888	U	C4-O4	-5.20	1.19	1.23
36	1	3311	C	N3-C4	-5.20	1.30	1.33
1	2	1241	G	N9-C8	5.20	1.41	1.37
36	5	1103	A	C5-C4	5.20	1.42	1.38
36	5	2356	A	N3-C4	-5.20	1.31	1.34
36	1	2419	A	P-OP1	5.20	1.57	1.49
36	1	909	G	N9-C8	-5.19	1.34	1.37
36	5	818	C	N1-C2	-5.19	1.34	1.40
44	17	158	LYS	CB-CG	5.19	1.66	1.52
36	1	2198	A	C5-C4	-5.18	1.35	1.38
36	5	2874	G	C5'-C4'	5.18	1.57	1.51
36	5	1164	G	N7-C5	-5.17	1.36	1.39
36	1	2853	A	N7-C5	-5.17	1.36	1.39
36	1	3267	A	N7-C5	-5.16	1.36	1.39
37	7	76	A	N9-C4	-5.16	1.34	1.37
37	7	92	A	C5-C4	-5.16	1.35	1.38
36	1	1380	G	C6-N1	-5.16	1.35	1.39
36	5	1117	G	C5-C4	-5.16	1.34	1.38
36	5	2724	U	C2-O2	-5.16	1.17	1.22
36	1	2808	A	C6-N6	5.15	1.38	1.33
36	1	39	A	N9-C4	-5.15	1.34	1.37
36	1	2920	U	C2-N3	-5.15	1.34	1.37
36	1	2384	A	N7-C5	-5.14	1.36	1.39
36	5	2872	A	C6-N6	5.14	1.38	1.33
1	6	1109	G	C2-N3	-5.14	1.28	1.32
36	5	2341	A	N3-C4	5.14	1.38	1.34
36	5	3006	A	N3-C4	-5.14	1.31	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2403	G	C2-N3	5.14	1.36	1.32
36	5	794	U	N3-C4	-5.13	1.33	1.38
36	5	1902	G	N7-C5	-5.12	1.36	1.39
36	1	870	G	C5-C6	-5.12	1.37	1.42
36	5	966	U	C4-C5	-5.12	1.39	1.43
36	1	2870	C	O3'-P	5.12	1.67	1.61
36	1	2714	G	N9-C4	-5.12	1.33	1.38
36	5	2824	G	N7-C5	-5.12	1.36	1.39
36	1	2873	U	N1-C2	5.11	1.43	1.38
36	1	351	A	N9-C4	-5.11	1.34	1.37
36	1	407	A	C5-C6	-5.11	1.36	1.41
36	5	3218	A	C5-C6	-5.11	1.36	1.41
36	1	945	C	N1-C6	5.10	1.40	1.37
36	1	1379	G	C6-N1	-5.09	1.35	1.39
36	1	1402	C	C2-O2	-5.09	1.19	1.24
52	M6	4	GLU	CD-OE2	5.09	1.31	1.25
41	L4	117	GLU	CD-OE2	5.08	1.31	1.25
36	5	2930	A	N3-C4	5.08	1.37	1.34
36	5	1189	C	N1-C6	-5.08	1.34	1.37
52	M6	100	GLU	CD-OE2	5.08	1.31	1.25
36	5	2434	U	N3-C4	-5.08	1.33	1.38
36	1	291	C	N3-C4	-5.08	1.30	1.33
36	1	345	G	N9-C8	-5.08	1.34	1.37
36	1	970	A	N3-C4	-5.08	1.31	1.34
36	5	838	G	C6-N1	-5.08	1.35	1.39
36	5	3084	C	N1-C6	-5.08	1.34	1.37
36	1	2940	A	C8-N7	-5.07	1.27	1.31
36	1	1459	C	N3-C4	-5.07	1.30	1.33
36	5	611	A	N9-C8	-5.07	1.33	1.37
36	5	1582	C	N1-C6	5.07	1.40	1.37
36	1	1158	A	N7-C5	-5.06	1.36	1.39
36	5	2287	C	N1-C6	5.06	1.40	1.37
36	1	3277	U	N1-C2	5.06	1.43	1.38
1	6	630	A	C5-C6	-5.06	1.36	1.41
36	5	645	A	C2-N3	5.06	1.38	1.33
37	7	84	A	N7-C5	-5.06	1.36	1.39
36	5	1123	U	C2-N3	-5.05	1.34	1.37
36	1	585	A	N7-C5	-5.05	1.36	1.39
36	5	889	U	C4-O4	-5.05	1.19	1.23
37	3	82	G	N7-C5	-5.05	1.36	1.39
36	5	953	G	N7-C5	-5.05	1.36	1.39
36	5	3050	U	N3-C4	-5.05	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	2611	U	C4-O4	-5.04	1.19	1.23
41	L4	52	VAL	CB-CG2	-5.04	1.42	1.52
1	6	397	A	N9-C4	-5.04	1.34	1.37
36	1	2874	G	C5-C6	5.04	1.47	1.42
36	5	1404	G	N9-C8	-5.04	1.34	1.37
78	q2	60	LYS	CE-NZ	5.04	1.61	1.49
1	2	1100	G	N7-C5	-5.04	1.36	1.39
36	1	966	U	C4-O4	-5.03	1.19	1.23
36	5	2340	U	C4-O4	-5.03	1.19	1.23
36	5	2942	C	N1-C6	-5.02	1.34	1.37
36	5	2957	G	C5-C4	-5.02	1.34	1.38
36	1	106	A	N9-C4	-5.02	1.34	1.37
36	5	2977	G	N1-C2	-5.02	1.33	1.37
36	1	644	G	N7-C5	-5.02	1.36	1.39
36	5	2873	U	O3'-P	5.02	1.67	1.61
36	5	899	U	C4-O4	-5.02	1.19	1.23
36	5	2131	A	C5-C6	-5.02	1.36	1.41
36	5	2314	U	C2-N3	5.02	1.41	1.37
36	5	2872	A	N7-C5	5.02	1.42	1.39
36	5	283	G	C5-C6	-5.02	1.37	1.42
1	6	1800	A	N9-C4	5.01	1.40	1.37
36	1	1658	G	N7-C5	-5.01	1.36	1.39
37	3	83	U	C4-O4	-5.01	1.19	1.23
37	7	92	A	C5-C6	-5.01	1.36	1.41
36	5	2412	G	C6-N1	-5.01	1.36	1.39
1	2	1560	U	N3-C4	-5.01	1.33	1.38
75	O9	11	GLN	CG-CD	5.01	1.62	1.51
1	6	1600	A	N9-C4	-5.01	1.34	1.37
37	7	88	G	C6-N1	-5.01	1.36	1.39
36	5	2319	U	C2-N3	-5.00	1.34	1.37

All (5106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	SR	161	LYS	O-C-N	-48.73	44.74	122.70
34	SR	160	GLU	C-N-CA	-43.07	14.02	121.70
34	SR	160	GLU	CA-C-N	-38.98	31.43	117.20
36	5	1152	G	N3-C4-C5	26.73	141.96	128.60
36	5	1152	G	N3-C4-N9	-24.27	111.44	126.00
34	SR	160	GLU	O-C-N	-20.73	89.54	122.70
36	5	1152	G	C2-N3-C4	-20.72	101.54	111.90
36	1	1117	G	O5'-P-OP1	-18.27	88.78	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C2-N2	-17.50	107.65	119.90
36	5	1152	G	C5-N7-C8	-17.36	95.62	104.30
36	5	922	U	N1-C2-N3	16.97	125.08	114.90
1	6	1773	C	N3-C4-C5	-16.96	115.12	121.90
36	5	398	A	O5'-P-OP2	-16.88	90.44	110.70
1	2	553	G	N1-C6-O6	16.48	129.79	119.90
36	5	1152	G	N1-C6-O6	16.01	129.51	119.90
36	5	1152	G	C8-N9-C1'	15.19	146.75	127.00
1	6	163	G	N3-C4-N9	-15.18	116.89	126.00
36	5	922	U	C5-C6-N1	-14.62	115.39	122.70
36	1	1495	U	C5-C6-N1	-14.43	115.48	122.70
36	5	922	U	C2-N3-C4	-14.43	118.34	127.00
1	2	1200	G	N1-C6-O6	14.37	128.52	119.90
36	5	1152	G	C4-N9-C1'	-14.19	108.06	126.50
36	1	2373	A	O5'-P-OP1	-14.18	92.94	105.70
36	5	1419	A	O5'-P-OP2	-14.10	93.01	105.70
36	5	1117	G	O5'-P-OP1	-14.05	93.05	105.70
36	1	2617	U	C5-C4-O4	13.99	134.30	125.90
36	1	2714	G	N3-C4-C5	13.82	135.51	128.60
36	1	1495	U	C4-C5-C6	13.79	127.97	119.70
36	5	1879	A	O5'-P-OP1	13.78	127.24	110.70
36	1	895	A	C5-N7-C8	-13.70	97.05	103.90
36	1	1196	C	C6-N1-C2	13.63	125.75	120.30
36	5	2923	U	O5'-P-OP1	-13.58	93.47	105.70
36	5	3005	A	O5'-P-OP2	-13.50	93.55	105.70
36	5	776	U	C5-C6-N1	-13.47	115.97	122.70
36	1	2957	G	O5'-P-OP1	-13.45	93.59	105.70
36	1	2983	C	O5'-P-OP1	-13.36	93.67	105.70
36	1	2726	C	N3-C2-O2	-13.11	112.72	121.90
36	1	2938	G	O5'-P-OP1	-13.05	93.95	105.70
36	1	406	G	O4'-C1'-N9	13.04	118.64	108.20
36	5	2385	G	O5'-P-OP1	-13.01	93.99	105.70
36	1	1308	A	O5'-P-OP2	-12.98	94.02	105.70
36	5	1308	A	O5'-P-OP2	-12.95	94.05	105.70
34	SR	161	LYS	CA-C-N	12.79	145.33	117.20
36	5	1152	G	C4-C5-N7	12.79	115.91	110.80
36	5	2121	G	O5'-P-OP2	-12.76	94.22	105.70
1	6	609	U	C5-C6-N1	-12.75	116.33	122.70
36	5	3018	C	O5'-P-OP2	-12.73	94.24	105.70
36	5	2945	G	O5'-P-OP2	-12.72	94.25	105.70
36	1	218	G	O5'-P-OP2	-12.70	94.27	105.70
36	1	2978	U	O5'-P-OP2	-12.67	94.30	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2617	U	N3-C4-O4	-12.58	110.59	119.40
52	M6	78	ARG	NE-CZ-NH1	12.58	126.59	120.30
36	1	817	A	O5'-P-OP1	-12.50	94.45	105.70
36	1	2848	G	O5'-P-OP2	-12.39	94.55	105.70
40	l3	19	ARG	NE-CZ-NH2	-12.31	114.15	120.30
36	1	1400	G	O5'-P-OP2	-12.21	94.71	105.70
36	1	802	C	O5'-P-OP1	-12.17	94.75	105.70
1	6	1657	U	O5'-P-OP2	-12.14	94.78	105.70
36	5	2373	A	O5'-P-OP1	-12.06	94.85	105.70
36	1	1495	U	N1-C2-N3	12.05	122.13	114.90
36	5	3245	A	C2-N3-C4	-12.03	104.59	110.60
1	6	1773	C	N3-C4-N4	11.94	126.36	118.00
36	5	2882	U	O5'-P-OP2	-11.93	94.97	105.70
36	5	2393	G	O5'-P-OP2	-11.84	95.05	105.70
1	6	163	G	N3-C4-C5	11.83	134.51	128.60
36	5	2278	C	C6-N1-C2	-11.81	115.58	120.30
36	5	776	U	C4-C5-C6	11.78	126.77	119.70
36	1	2846	U	N3-C2-O2	-11.72	113.99	122.20
36	1	1320	C	O5'-P-OP2	-11.71	95.16	105.70
36	5	1513	G	C8-N9-C4	-11.62	101.75	106.40
36	5	2704	A	O5'-P-OP1	-11.59	95.27	105.70
36	1	2983	C	N3-C2-O2	-11.52	113.84	121.90
36	1	3362	A	C2-N3-C4	-11.50	104.85	110.60
36	5	2315	G	O5'-P-OP1	-11.47	95.37	105.70
36	1	2618	G	N1-C6-O6	-11.47	113.02	119.90
36	5	2726	C	C5-C4-N4	11.44	128.21	120.20
36	5	1551	C	O5'-P-OP1	-11.44	95.40	105.70
36	1	776	U	C4-C5-C6	11.37	126.52	119.70
36	1	2617	U	C5-C6-N1	-11.36	117.02	122.70
36	1	2714	G	N3-C4-N9	-11.27	119.24	126.00
1	6	163	G	C2-N3-C4	-11.27	106.26	111.90
36	5	3245	A	C5-N7-C8	-11.27	98.27	103.90
36	1	2631	U	N3-C4-O4	-11.25	111.53	119.40
36	1	944	C	C5-C6-N1	11.23	126.61	121.00
36	5	960	U	C2-N3-C4	-11.15	120.31	127.00
36	5	645	A	C6-N1-C2	-11.13	111.92	118.60
36	5	1152	G	C5-C6-O6	-11.13	121.92	128.60
36	1	2726	C	N3-C4-N4	-11.05	110.27	118.00
36	1	895	A	N7-C8-N9	11.04	119.32	113.80
36	1	2281	A	O5'-P-OP2	-11.04	95.76	105.70
36	5	2983	C	O5'-P-OP1	-11.03	95.77	105.70
36	5	2634	U	C2-N3-C4	-11.01	120.39	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	144	U	N3-C2-O2	-10.91	114.56	122.20
36	1	2403	G	N3-C4-C5	-10.89	123.15	128.60
1	2	553	G	C5-C6-O6	-10.85	122.09	128.60
36	5	806	A	O5'-P-OP1	-10.82	95.96	105.70
36	5	2340	U	N3-C4-O4	-10.72	111.89	119.40
36	1	954	U	O5'-P-OP2	-10.72	96.05	105.70
36	5	2289	U	N1-C2-O2	10.72	130.30	122.80
36	1	611	A	O5'-P-OP1	10.70	123.54	110.70
1	6	1773	C	C4-C5-C6	10.67	122.74	117.40
36	1	637	C	O4'-C1'-N1	10.65	116.72	108.20
1	6	1537	C	C6-N1-C2	-10.65	116.04	120.30
36	5	406	G	O4'-C1'-N9	10.64	116.71	108.20
36	5	590	G	O5'-P-OP1	-10.62	96.15	105.70
36	1	979	U	C6-N1-C2	-10.57	114.66	121.00
36	1	2412	G	C8-N9-C4	-10.56	102.17	106.40
36	1	3278	C	N3-C2-O2	-10.54	114.52	121.90
36	1	718	G	N3-C4-C5	10.53	133.87	128.60
36	5	776	U	N1-C2-N3	10.53	121.22	114.90
1	2	1291	G	N3-C4-N9	-10.52	119.69	126.00
36	5	2412	G	C8-N9-C4	-10.50	102.20	106.40
36	5	922	U	C4-C5-C6	10.50	126.00	119.70
1	6	337	G	C6-C5-N7	-10.49	124.11	130.40
36	1	2726	C	C6-N1-C2	-10.45	116.12	120.30
36	5	2800	G	N3-C2-N2	-10.44	112.59	119.90
36	5	2726	C	C6-N1-C2	-10.43	116.13	120.30
36	5	877	C	N3-C4-C5	10.39	126.06	121.90
36	5	1313	G	O5'-P-OP2	-10.38	96.36	105.70
36	1	637	C	C6-N1-C1'	10.38	133.25	120.80
36	1	2726	C	C5-C4-N4	10.37	127.46	120.20
1	2	639	U	N3-C2-O2	-10.36	114.94	122.20
38	4	113	U	C5-C4-O4	10.36	132.11	125.90
36	5	1115	G	C8-N9-C4	-10.35	102.26	106.40
36	1	3362	A	C5-N7-C8	-10.30	98.75	103.90
36	1	1381	A	O5'-P-OP2	10.30	123.06	110.70
1	2	1200	G	C5-C6-O6	-10.28	122.43	128.60
38	4	113	U	C5-C6-N1	-10.24	117.58	122.70
36	5	2632	G	C5-C6-O6	10.24	134.74	128.60
36	1	2977	G	N7-C8-N9	-10.23	107.98	113.10
37	3	10	C	O5'-P-OP2	-10.21	96.52	105.70
36	1	2860	U	N3-C2-O2	10.16	129.31	122.20
36	1	1414	G	O5'-P-OP2	-10.15	96.57	105.70
1	6	352	A	O5'-P-OP1	-10.13	96.58	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2977	G	C8-N9-C4	10.12	110.45	106.40
37	7	120	C	C6-N1-C2	10.07	124.33	120.30
36	1	3214	U	N3-C2-O2	-10.06	115.16	122.20
36	1	1555	U	C2-N1-C1'	-10.05	105.64	117.70
36	5	2899	C	N3-C2-O2	-10.04	114.87	121.90
37	3	86	U	C5-C4-O4	-10.03	119.88	125.90
36	1	2836	C	C5-C4-N4	10.00	127.20	120.20
36	1	2617	U	N1-C2-N3	10.00	120.90	114.90
36	1	979	U	N1-C2-N3	9.98	120.89	114.90
36	1	2550	U	N3-C2-O2	-9.97	115.22	122.20
36	1	608	A	N1-C6-N6	9.94	124.56	118.60
36	5	2398	A	C8-N9-C4	-9.92	101.83	105.80
1	6	1773	C	N1-C2-O2	-9.91	112.95	118.90
36	1	645	A	C6-N1-C2	-9.88	112.67	118.60
36	5	835	G	O4'-C1'-N9	9.86	116.09	108.20
36	1	2419	A	O5'-P-OP2	-9.86	96.83	105.70
36	5	2619	G	C5-C6-O6	-9.85	122.69	128.60
36	5	2865	U	N1-C2-O2	9.84	129.69	122.80
36	5	3107	U	N3-C2-O2	-9.80	115.34	122.20
36	1	2772	C	C2-N1-C1'	9.80	129.58	118.80
1	2	1200	G	N3-C2-N2	-9.79	113.05	119.90
1	6	542	A	N7-C8-N9	9.79	118.69	113.80
36	5	2836	C	C5-C4-N4	9.79	127.05	120.20
36	5	1371	G	N1-C6-O6	-9.75	114.05	119.90
36	5	3052	G	C5-C6-O6	9.75	134.45	128.60
38	8	80	A	C8-N9-C4	-9.73	101.91	105.80
36	5	2818	U	O5'-P-OP1	-9.71	96.96	105.70
36	5	922	U	N3-C2-O2	-9.63	115.46	122.20
36	1	776	U	C5-C6-N1	-9.62	117.89	122.70
36	5	3214	U	N3-C2-O2	-9.61	115.47	122.20
70	O4	51	LEU	CA-CB-CG	9.59	137.35	115.30
36	1	2867	C	N3-C4-N4	-9.57	111.30	118.00
36	1	3306	U	N1-C2-N3	9.57	120.64	114.90
36	5	2385	G	N3-C4-C5	9.55	133.38	128.60
36	1	2862	U	N3-C2-O2	-9.54	115.52	122.20
1	2	1596	C	N3-C2-O2	-9.53	115.23	121.90
36	1	909	G	N7-C8-N9	-9.52	108.34	113.10
36	1	949	C	C6-N1-C2	-9.52	116.49	120.30
36	1	2618	G	C5-C6-N1	9.51	116.26	111.50
62	N6	13	ARG	NE-CZ-NH2	-9.51	115.54	120.30
1	6	453	U	N3-C2-O2	-9.51	115.55	122.20
36	5	1152	G	N1-C2-N2	9.50	124.75	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3362	A	C2-N3-C4	-9.50	105.85	110.60
36	5	1845	G	O5'-P-OP1	-9.49	97.16	105.70
36	5	2632	G	N1-C6-O6	-9.48	114.21	119.90
36	1	3214	U	C5-C4-O4	9.47	131.58	125.90
1	2	553	G	N3-C2-N2	-9.46	113.28	119.90
36	1	280	U	C5-C4-O4	-9.45	120.23	125.90
36	5	648	C	O5'-P-OP1	-9.44	97.20	105.70
36	1	2434	U	C5-C4-O4	9.43	131.56	125.90
1	6	687	G	N3-C2-N2	-9.42	113.31	119.90
36	1	1164	G	C5-C6-O6	9.42	134.25	128.60
36	1	718	G	N3-C4-N9	-9.41	120.35	126.00
36	1	3344	A	N7-C8-N9	9.41	118.50	113.80
36	1	3306	U	N3-C4-O4	-9.40	112.82	119.40
1	6	337	G	C4-N9-C1'	9.39	138.71	126.50
36	1	2846	U	C5-C4-O4	9.39	131.53	125.90
36	1	1450	G	O5'-P-OP1	-9.39	97.25	105.70
1	6	1537	C	N3-C4-C5	-9.38	118.15	121.90
36	1	895	A	C4-C5-N7	9.37	115.38	110.70
36	1	895	A	C8-N9-C4	-9.36	102.06	105.80
1	2	1631	A	O5'-P-OP1	-9.34	97.30	105.70
38	4	74	U	O5'-P-OP1	-9.34	97.29	105.70
36	1	968	G	C8-N9-C4	-9.34	102.67	106.40
36	5	3245	A	N7-C8-N9	9.33	118.47	113.80
36	1	439	C	N1-C2-O2	9.33	124.50	118.90
1	6	1596	C	N3-C2-O2	-9.32	115.38	121.90
36	1	3362	A	N7-C8-N9	9.31	118.46	113.80
36	1	729	C	O5'-P-OP2	-9.31	97.32	105.70
1	6	1634	C	N1-C2-O2	9.29	124.48	118.90
36	1	1450	G	C8-N9-C4	9.29	110.12	106.40
36	1	909	G	C8-N9-C4	9.29	110.11	106.40
36	1	2808	A	N1-C6-N6	9.28	124.17	118.60
36	1	3214	U	N1-C2-N3	9.26	120.46	114.90
36	1	2572	C	N1-C2-O2	9.24	124.44	118.90
36	1	2550	U	C5-C4-O4	9.23	131.44	125.90
36	1	1328	C	O5'-P-OP1	-9.22	97.40	105.70
36	1	1419	A	O5'-P-OP2	-9.22	97.40	105.70
36	5	2968	G	N1-C6-O6	-9.22	114.37	119.90
36	1	2617	U	N3-C2-O2	-9.20	115.76	122.20
36	1	2944	U	N3-C4-C5	9.19	120.12	114.60
36	5	887	G	N3-C2-N2	9.19	126.33	119.90
36	1	3181	C	N3-C2-O2	-9.18	115.47	121.90
36	5	909	G	N1-C6-O6	-9.18	114.39	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D9	36	LEU	CA-CB-CG	9.17	136.39	115.30
36	1	2867	C	N3-C2-O2	-9.15	115.50	121.90
36	5	1120	A	N1-C6-N6	-9.15	113.11	118.60
36	1	2797	C	C6-N1-C2	9.14	123.96	120.30
36	5	2860	U	C5-C4-O4	-9.14	120.41	125.90
36	5	2694	A	C8-N9-C4	-9.14	102.14	105.80
36	5	1439	U	C5-C4-O4	-9.14	120.42	125.90
1	6	542	A	N1-C6-N6	9.12	124.07	118.60
1	6	337	G	C8-N9-C1'	-9.12	115.14	127.00
36	5	1314	C	N3-C4-C5	9.11	125.55	121.90
36	5	2375	G	N1-C6-O6	-9.11	114.43	119.90
1	2	1783	C	O5'-P-OP2	-9.10	97.52	105.70
36	1	2176	U	N3-C2-O2	-9.09	115.83	122.20
36	1	1189	C	N1-C2-O2	-9.08	113.45	118.90
36	1	2634	U	C2-N3-C4	-9.08	121.55	127.00
36	1	2978	U	O5'-P-OP1	9.08	121.59	110.70
40	l3	266	ARG	NE-CZ-NH2	-9.07	115.77	120.30
36	1	439	C	C2-N1-C1'	9.06	128.77	118.80
49	M3	85	LEU	CA-CB-CG	9.04	136.10	115.30
1	6	65	A	C2-N3-C4	-9.04	106.08	110.60
36	5	1501	U	C5-C6-N1	9.03	127.22	122.70
36	5	3259	U	O5'-P-OP2	-9.00	97.60	105.70
36	1	2130	G	N1-C6-O6	-9.00	114.50	119.90
36	5	1419	A	O5'-P-OP1	8.99	121.49	110.70
36	1	2945	G	O5'-P-OP2	-8.99	97.61	105.70
36	1	347	G	C5-C6-O6	-8.99	123.21	128.60
36	1	637	C	C2-N1-C1'	-8.98	108.92	118.80
1	6	1145	U	O5'-P-OP2	-8.98	97.62	105.70
36	1	960	U	C2-N3-C4	-8.97	121.62	127.00
1	6	163	G	N3-C2-N2	-8.96	113.63	119.90
38	4	113	U	N1-C2-N3	8.95	120.27	114.90
1	6	57	G	O5'-P-OP2	-8.95	97.64	105.70
36	5	1178	G	N3-C2-N2	-8.95	113.63	119.90
36	1	200	C	N1-C2-O2	8.93	124.26	118.90
36	1	967	A	N1-C6-N6	-8.93	113.24	118.60
36	5	1189	C	N3-C2-O2	8.93	128.15	121.90
1	6	542	A	C6-C5-N7	-8.93	126.05	132.30
36	1	2572	C	C2-N1-C1'	8.92	128.62	118.80
1	6	1096	C	N1-C2-O2	8.92	124.25	118.90
36	5	116	A	O4'-C1'-N9	8.91	115.33	108.20
36	5	216	G	N1-C6-O6	8.90	125.24	119.90
36	5	634	C	N3-C4-C5	8.89	125.46	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3050	U	N3-C2-O2	-8.88	115.99	122.20
36	5	637	C	C2-N1-C1'	-8.87	109.05	118.80
36	5	2415	C	O5'-P-OP2	-8.86	97.72	105.70
36	5	2836	C	N3-C4-N4	-8.86	111.80	118.00
36	1	200	C	N3-C2-O2	-8.85	115.70	121.90
1	2	553	G	C6-C5-N7	-8.85	125.09	130.40
36	5	957	C	N3-C4-C5	8.85	125.44	121.90
36	5	2119	A	N1-C6-N6	8.85	123.91	118.60
36	5	2385	G	C8-N9-C4	8.84	109.94	106.40
1	6	434	G	O5'-P-OP2	-8.83	97.75	105.70
36	1	2385	G	O5'-P-OP1	-8.83	97.75	105.70
36	1	2818	U	O5'-P-OP1	-8.83	97.76	105.70
36	5	3012	A	C8-N9-C4	8.83	109.33	105.80
36	5	2327	U	C5-C6-N1	-8.82	118.29	122.70
36	1	3306	U	N3-C2-O2	-8.82	116.03	122.20
36	5	2382	G	N1-C6-O6	-8.82	114.61	119.90
36	1	2409	G	N1-C6-O6	-8.81	114.62	119.90
36	1	2884	C	N3-C4-C5	8.80	125.42	121.90
36	5	1879	A	N1-C6-N6	8.80	123.88	118.60
36	5	960	U	N3-C4-C5	8.79	119.88	114.60
36	5	2142	A	C5-C6-N1	8.79	122.09	117.70
36	5	2978	U	O5'-P-OP2	-8.78	97.80	105.70
36	1	633	C	C6-N1-C2	8.77	123.81	120.30
36	1	3092	C	C2-N1-C1'	-8.77	109.15	118.80
1	6	1	U	O4'-C1'-N1	8.77	115.22	108.20
36	1	870	G	C5-C6-O6	-8.75	123.35	128.60
1	2	1199	G	O5'-P-OP2	-8.75	97.83	105.70
36	5	2403	G	N1-C6-O6	-8.75	114.65	119.90
36	5	3092	C	O4'-C1'-N1	8.75	115.20	108.20
36	1	59	G	O5'-P-OP2	-8.73	97.84	105.70
36	1	2860	U	N1-C2-O2	-8.73	116.69	122.80
1	6	1560	U	N3-C2-O2	-8.72	116.10	122.20
36	5	1879	A	C4-C5-N7	8.71	115.06	110.70
1	6	18	C	C6-N1-C2	-8.71	116.82	120.30
36	1	636	C	O5'-P-OP1	-8.70	97.87	105.70
36	5	2978	U	N3-C2-O2	-8.69	116.11	122.20
36	1	776	U	N1-C2-N3	8.69	120.12	114.90
36	1	967	A	N9-C4-C5	8.69	109.28	105.80
1	6	17	C	O5'-P-OP2	-8.69	97.88	105.70
1	6	1596	C	C6-N1-C2	-8.69	116.83	120.30
36	5	1181	U	C5-C6-N1	-8.69	118.36	122.70
36	1	960	U	C5-C4-O4	-8.67	120.70	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3154	C	N1-C2-O2	8.66	124.10	118.90
36	1	1411	C	N3-C2-O2	-8.66	115.84	121.90
36	5	2726	C	N3-C2-O2	-8.66	115.84	121.90
36	1	346	C	C5-C6-N1	-8.65	116.67	121.00
36	1	3207	U	C6-N1-C1'	8.65	133.32	121.20
36	5	1879	A	C5-N7-C8	-8.65	99.58	103.90
36	5	1536	G	O5'-P-OP2	-8.65	97.92	105.70
36	1	3207	U	C2-N1-C1'	-8.64	107.34	117.70
1	6	308	C	C5-C6-N1	-8.63	116.69	121.00
36	5	1406	A	O5'-P-OP1	-8.63	97.94	105.70
36	5	2340	U	N3-C4-C5	8.63	119.78	114.60
36	5	2366	C	C5-C6-N1	8.62	125.31	121.00
36	5	2289	U	N3-C2-O2	-8.61	116.17	122.20
36	1	2327	U	O5'-P-OP1	-8.61	97.95	105.70
36	5	1064	A	N1-C6-N6	8.61	123.77	118.60
36	1	2614	G	N1-C6-O6	-8.61	114.73	119.90
36	1	421	G	N3-C4-N9	8.61	131.16	126.00
36	1	1484	U	P-O3'-C3'	8.60	130.02	119.70
36	1	2340	U	N3-C4-O4	-8.60	113.38	119.40
36	1	1196	C	C5-C6-N1	-8.60	116.70	121.00
36	5	960	U	C5-C6-N1	-8.59	118.41	122.70
36	1	3278	C	N1-C2-O2	8.58	124.05	118.90
36	5	1212	A	O5'-P-OP2	-8.58	97.98	105.70
36	1	2836	C	C4-C5-C6	8.58	121.69	117.40
36	1	3055	U	C5-C4-O4	-8.58	120.75	125.90
36	5	637	C	C6-N1-C1'	8.58	131.09	120.80
36	5	2719	U	O5'-P-OP2	-8.56	97.99	105.70
1	6	1600	A	C2-N3-C4	-8.56	106.32	110.60
36	5	945	C	C6-N1-C2	8.56	123.72	120.30
36	5	776	U	C5-C4-O4	8.56	131.04	125.90
36	1	765	C	N1-C2-O2	8.55	124.03	118.90
36	1	633	C	C5-C6-N1	-8.55	116.72	121.00
36	5	110	G	O5'-P-OP2	-8.55	98.01	105.70
36	5	909	G	C4-C5-N7	-8.55	107.38	110.80
36	5	2860	U	N3-C2-O2	8.55	128.18	122.20
36	5	2638	C	N1-C2-O2	-8.54	113.77	118.90
36	1	1841	A	C2-N3-C4	8.54	114.87	110.60
36	1	2772	C	O4'-C1'-N1	8.53	115.03	108.20
36	1	2244	A	O5'-P-OP1	8.53	120.94	110.70
36	5	2865	U	C5-C6-N1	8.53	126.96	122.70
36	1	2827	U	C2-N1-C1'	-8.53	107.47	117.70
36	1	2875	U	O5'-P-OP2	-8.53	98.03	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2302	G	C5-C6-O6	8.52	133.71	128.60
36	1	3344	A	C5-N7-C8	-8.52	99.64	103.90
36	5	971	G	N7-C8-N9	-8.52	108.84	113.10
36	1	2818	U	C5-C6-N1	8.51	126.95	122.70
36	1	2679	A	C2-N3-C4	-8.50	106.35	110.60
36	5	2278	C	C5-C6-N1	8.50	125.25	121.00
36	5	2618	G	C5-C6-O6	-8.50	123.50	128.60
18	C6	40	GLU	C-N-CD	-8.49	101.91	120.60
36	5	2426	U	N3-C4-O4	-8.49	113.45	119.40
1	2	1773	C	N3-C4-C5	-8.49	118.50	121.90
36	5	2984	C	C2-N3-C4	-8.49	115.66	119.90
36	1	1082	U	C6-N1-C2	-8.47	115.92	121.00
36	5	3048	A	O5'-P-OP2	-8.46	98.09	105.70
37	3	88	G	N1-C6-O6	-8.45	114.83	119.90
36	5	662	U	O5'-P-OP1	-8.45	98.10	105.70
36	5	3245	A	C4-C5-N7	8.45	114.92	110.70
36	5	961	C	N1-C2-O2	8.45	123.97	118.90
1	6	543	C	C5-C6-N1	8.44	125.22	121.00
1	6	1039	A	O4'-C1'-N9	8.43	114.95	108.20
36	5	2978	U	N3-C4-O4	-8.43	113.50	119.40
1	6	1473	U	N3-C2-O2	-8.43	116.30	122.20
36	1	937	G	C8-N9-C4	8.41	109.77	106.40
36	1	2400	G	N1-C6-O6	8.41	124.95	119.90
36	1	2618	G	N3-C4-C5	-8.41	124.39	128.60
36	1	3209	A	N1-C6-N6	8.40	123.64	118.60
36	5	838	G	N1-C6-O6	-8.39	114.86	119.90
36	5	2572	C	N1-C2-O2	8.39	123.94	118.90
36	1	944	C	C6-N1-C2	-8.38	116.95	120.30
36	1	709	A	C8-N9-C4	8.37	109.15	105.80
38	8	80	A	N7-C8-N9	8.37	117.99	113.80
36	5	1452	A	C8-N9-C4	8.37	109.15	105.80
36	1	2298	U	C5-C6-N1	-8.37	118.52	122.70
36	1	2384	A	N1-C6-N6	8.36	123.62	118.60
68	o2	27	ARG	NE-CZ-NH2	-8.36	116.12	120.30
36	1	2249	G	N1-C6-O6	-8.36	114.88	119.90
36	1	2184	U	C5-C4-O4	-8.36	120.89	125.90
36	5	649	A	C8-N9-C4	-8.35	102.46	105.80
36	5	200	C	C2-N1-C1'	8.35	127.99	118.80
38	8	99	C	C6-N1-C2	8.35	123.64	120.30
1	2	1096	C	C2-N1-C1'	8.35	127.98	118.80
36	5	2932	U	N3-C2-O2	-8.35	116.36	122.20
36	1	342	A	O5'-P-OP2	-8.34	98.19	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	641	C	C6-N1-C2	-8.34	116.96	120.30
36	5	2634	U	N1-C2-O2	-8.34	116.97	122.80
36	5	2932	U	N1-C2-O2	8.33	128.63	122.80
38	8	98	U	C5-C4-O4	-8.33	120.90	125.90
36	5	2726	C	N3-C4-C5	-8.32	118.57	121.90
36	5	2964	G	O5'-P-OP2	-8.31	98.22	105.70
36	1	2550	U	N1-C2-N3	8.31	119.89	114.90
36	1	1331	U	C5-C4-O4	-8.31	120.92	125.90
36	1	1329	U	N1-C1'-C2'	-8.30	102.87	112.00
36	5	2412	G	N9-C4-C5	8.30	108.72	105.40
36	5	2272	G	O4'-C1'-N9	8.29	114.83	108.20
36	1	2165	G	O5'-P-OP2	-8.29	98.24	105.70
36	5	2392	C	C2-N3-C4	-8.28	115.76	119.90
36	1	2899	C	N3-C2-O2	-8.27	116.11	121.90
1	6	795	U	N3-C2-O2	-8.27	116.41	122.20
36	5	2376	G	C8-N9-C4	8.26	109.70	106.40
36	1	2883	U	C5-C6-N1	8.25	126.83	122.70
1	2	934	C	C2-N1-C1'	8.24	127.87	118.80
36	5	2913	C	O5'-P-OP1	-8.24	98.28	105.70
37	7	88	G	N1-C6-O6	-8.24	114.95	119.90
36	5	2393	G	C5-C6-O6	-8.24	123.66	128.60
1	2	1773	C	C6-N1-C2	-8.23	117.01	120.30
36	5	1902	G	C5-C6-O6	-8.23	123.66	128.60
36	5	890	C	O5'-P-OP2	-8.22	98.30	105.70
36	1	2142	A	C6-N1-C2	-8.22	113.67	118.60
36	1	2987	A	O5'-P-OP1	-8.22	98.30	105.70
36	1	14	U	O5'-P-OP2	-8.21	98.31	105.70
36	5	663	C	C2-N3-C4	-8.21	115.80	119.90
1	6	389	G	N1-C6-O6	-8.21	114.98	119.90
36	5	1327	C	N3-C4-N4	-8.21	112.26	118.00
36	1	2214	A	N1-C6-N6	8.20	123.52	118.60
36	5	2248	C	C6-N1-C2	8.20	123.58	120.30
36	1	611	A	O5'-P-OP2	-8.20	98.32	105.70
64	n8	21	ARG	NE-CZ-NH1	8.20	124.40	120.30
36	1	1555	U	C5-C6-N1	-8.20	118.60	122.70
36	1	1156	C	N3-C4-N4	-8.19	112.27	118.00
36	1	3214	U	C6-N1-C2	-8.19	116.09	121.00
36	5	909	G	C6-C5-N7	8.19	135.31	130.40
38	4	73	U	N3-C4-C5	8.18	119.51	114.60
36	1	1136	A	C5-C6-N1	8.18	121.79	117.70
36	5	637	C	N1-C2-O2	-8.18	113.99	118.90
36	5	2860	U	N1-C2-O2	-8.16	117.09	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2978	U	C5-C4-O4	8.16	130.79	125.90
36	5	2889	C	N3-C2-O2	-8.15	116.19	121.90
36	1	1589	A	O4'-C1'-N9	-8.15	101.68	108.20
36	5	2915	U	N1-C2-N3	8.14	119.79	114.90
36	1	2409	G	C5-C6-O6	8.14	133.48	128.60
36	5	2896	A	N1-C6-N6	-8.14	113.72	118.60
36	5	2730	G	N1-C6-O6	8.13	124.78	119.90
36	5	2601	A	O5'-P-OP2	-8.13	98.39	105.70
1	6	542	A	C5-N7-C8	-8.12	99.84	103.90
36	5	2800	G	N9-C4-C5	8.12	108.65	105.40
36	5	1513	G	N1-C6-O6	-8.12	115.03	119.90
36	5	3143	C	O5'-P-OP2	-8.12	98.40	105.70
36	1	980	A	C8-N9-C4	-8.11	102.56	105.80
1	6	1026	A	O5'-P-OP1	-8.11	98.40	105.70
36	5	1124	U	N3-C4-C5	8.11	119.46	114.60
36	5	2730	G	C5-C6-O6	-8.11	123.74	128.60
36	1	3362	A	N1-C6-N6	8.10	123.46	118.60
36	5	92	G	N1-C6-O6	-8.10	115.04	119.90
36	1	2395	G	N1-C6-O6	-8.10	115.04	119.90
38	4	113	U	N3-C2-O2	-8.10	116.53	122.20
38	4	79	A	C8-N9-C4	-8.09	102.56	105.80
36	1	33	G	C8-N9-C4	-8.09	103.17	106.40
36	1	960	U	N1-C2-O2	-8.08	117.14	122.80
36	1	2714	G	C2-N3-C4	-8.08	107.86	111.90
1	6	139	C	C6-N1-C2	-8.08	117.07	120.30
36	5	96	G	O5'-P-OP2	-8.08	98.43	105.70
1	2	1305	U	C5-C4-O4	8.08	130.75	125.90
1	2	1560	U	N3-C2-O2	-8.08	116.55	122.20
36	5	2813	A	C8-N9-C4	-8.08	102.57	105.80
36	1	3306	U	C5-C4-O4	8.07	130.74	125.90
36	1	360	G	N9-C4-C5	-8.07	102.17	105.40
36	5	716	A	O5'-P-OP1	-8.07	98.44	105.70
36	5	1848	G	C5-C6-O6	-8.07	123.76	128.60
36	1	2226	U	O5'-P-OP1	-8.06	98.44	105.70
36	1	1202	A	O5'-P-OP2	-8.06	98.44	105.70
36	1	3362	A	C6-C5-N7	-8.06	126.66	132.30
36	5	3107	U	N1-C2-O2	8.05	128.43	122.80
36	1	949	C	N3-C4-C5	-8.04	118.68	121.90
1	2	1560	U	C5-C4-O4	8.04	130.72	125.90
36	1	1168	U	N3-C2-O2	-8.04	116.57	122.20
36	1	3092	C	O4'-C1'-N1	8.04	114.63	108.20
36	1	2616	C	O5'-P-OP1	-8.03	98.47	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1902	G	C4-C5-N7	8.03	114.01	110.80
36	1	1405	U	N3-C4-C5	8.02	119.41	114.60
36	1	2121	G	O5'-P-OP2	-8.02	98.48	105.70
36	1	3218	A	C8-N9-C4	-8.02	102.59	105.80
36	5	437	G	N3-C4-N9	-8.02	121.19	126.00
36	5	971	G	C5-N7-C8	8.02	108.31	104.30
36	1	2758	A	C2-N3-C4	8.02	114.61	110.60
1	2	1339	C	P-O3'-C3'	8.02	129.32	119.70
36	1	371	G	O5'-P-OP2	-8.01	98.49	105.70
36	1	2867	C	N1-C2-O2	8.01	123.71	118.90
36	5	1189	C	N1-C2-O2	-8.00	114.10	118.90
37	7	110	G	O5'-P-OP2	-8.00	98.50	105.70
36	5	2360	C	C4-C5-C6	7.99	121.40	117.40
1	6	1634	C	C2-N1-C1'	7.99	127.59	118.80
36	1	3362	A	C4-C5-N7	7.99	114.69	110.70
1	6	308	C	C2-N3-C4	-7.99	115.91	119.90
36	1	2836	C	N3-C4-C5	-7.98	118.71	121.90
36	1	689	U	N1-C2-O2	7.98	128.39	122.80
36	5	1496	C	O5'-P-OP1	7.98	120.28	110.70
36	5	1152	G	N7-C8-N9	7.98	117.09	113.10
36	5	2389	C	C2-N3-C4	-7.97	115.91	119.90
36	5	2857	C	N3-C4-C5	7.97	125.09	121.90
36	5	3142	A	C8-N9-C4	7.97	108.99	105.80
36	5	2980	U	OP1-P-OP2	-7.96	107.66	119.60
1	6	687	G	N3-C4-N9	-7.96	121.23	126.00
36	5	2726	C	N1-C2-N3	7.95	124.77	119.20
36	5	671	U	C5-C4-O4	-7.94	121.13	125.90
36	1	369	A	C8-N9-C4	-7.94	102.62	105.80
38	8	25	G	N1-C6-O6	-7.94	115.14	119.90
36	5	2283	G	O5'-P-OP2	-7.94	98.56	105.70
1	6	163	G	N9-C4-C5	7.93	108.57	105.40
36	1	2215	A	C8-N9-C4	7.92	108.97	105.80
1	6	337	G	C4-C5-N7	7.92	113.97	110.80
36	1	114	A	N1-C6-N6	7.92	123.35	118.60
38	8	45	C	C6-N1-C2	-7.92	117.13	120.30
36	1	2391	G	N1-C6-O6	-7.92	115.15	119.90
1	6	1537	C	N1-C2-O2	-7.92	114.15	118.90
36	5	1308	A	C8-N9-C4	-7.91	102.64	105.80
36	5	1856	C	C6-N1-C2	-7.91	117.14	120.30
52	m6	160	ARG	NE-CZ-NH2	-7.91	116.34	120.30
36	1	3264	G	C8-N9-C4	7.91	109.56	106.40
36	5	3052	G	N1-C6-O6	-7.91	115.16	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	54	C	N3-C4-N4	-7.90	112.47	118.00
36	5	878	G	OP1-P-O3'	7.90	122.58	105.20
36	5	712	G	O5'-P-OP2	-7.89	98.59	105.70
36	5	816	A	C8-N9-C4	-7.89	102.64	105.80
36	1	1314	C	C6-N1-C2	-7.89	117.14	120.30
36	5	2979	U	N3-C2-O2	7.89	127.72	122.20
36	1	2936	A	O5'-P-OP2	7.89	120.17	110.70
1	2	448	C	O5'-P-OP2	-7.88	98.61	105.70
36	5	1480	G	O4'-C1'-N9	7.88	114.51	108.20
38	4	113	U	C4-C5-C6	7.88	124.43	119.70
36	1	1134	G	O5'-P-OP2	-7.88	98.61	105.70
36	1	2827	U	N1-C2-N3	7.87	119.62	114.90
1	6	543	C	C6-N1-C2	-7.86	117.15	120.30
36	5	2531	C	C2-N1-C1'	7.86	127.45	118.80
1	2	1773	C	N3-C4-N4	7.86	123.50	118.00
1	2	75	U	N1-C2-O2	7.86	128.30	122.80
36	1	116	A	O4'-C1'-N9	7.86	114.49	108.20
36	1	1201	C	O5'-P-OP1	-7.86	98.63	105.70
36	5	1004	U	N1-C2-O2	7.85	128.30	122.80
36	1	3277	U	N3-C2-O2	-7.85	116.71	122.20
36	1	2241	U	O5'-P-OP1	-7.84	98.64	105.70
36	1	770	G	O4'-C1'-N9	7.84	114.47	108.20
1	6	337	G	C5-C6-O6	-7.84	123.89	128.60
1	2	1654	G	C5-C6-O6	-7.84	123.90	128.60
36	1	1480	G	O4'-C1'-N9	7.83	114.47	108.20
36	5	1513	G	N3-C4-C5	-7.83	124.68	128.60
36	5	2142	A	C6-N1-C2	-7.82	113.91	118.60
36	5	3245	A	C6-C5-N7	-7.82	126.82	132.30
36	1	2758	A	N1-C2-N3	-7.82	125.39	129.30
36	5	2919	A	N1-C6-N6	-7.82	113.91	118.60
36	1	609	G	C5-C6-O6	-7.81	123.91	128.60
36	1	1111	U	O5'-P-OP1	-7.81	98.67	105.70
36	1	3181	C	N1-C2-N3	7.81	124.67	119.20
36	1	612	U	C2-N3-C4	-7.81	122.31	127.00
36	1	3362	A	N1-C2-N3	7.81	133.20	129.30
1	2	145	A	C8-N9-C4	-7.80	102.68	105.80
36	1	1607	U	P-O3'-C3'	7.80	129.06	119.70
36	1	2802	A	C2-N3-C4	7.80	114.50	110.60
36	5	2278	C	C4-C5-C6	-7.80	113.50	117.40
36	1	806	A	C8-N9-C4	7.80	108.92	105.80
36	1	2593	A	O5'-P-OP2	-7.80	98.68	105.70
36	1	609	G	O5'-P-OP2	-7.79	98.69	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2772	C	C6-N1-C1'	-7.79	111.45	120.80
1	6	448	C	O5'-P-OP2	-7.79	98.69	105.70
36	1	1166	G	N3-C2-N2	7.79	125.35	119.90
36	1	2886	U	C5-C4-O4	-7.79	121.23	125.90
36	5	1116	G	N1-C6-O6	-7.79	115.23	119.90
36	1	1419	A	O5'-P-OP1	7.78	120.04	110.70
36	5	2719	U	C2-N1-C1'	-7.78	108.36	117.70
36	1	905	U	N1-C2-O2	-7.78	117.36	122.80
1	2	1291	G	N3-C4-C5	7.78	132.49	128.60
64	n8	21	ARG	NE-CZ-NH2	-7.78	116.41	120.30
36	1	1389	G	C4-C5-N7	7.78	113.91	110.80
36	5	189	G	N1-C6-O6	-7.78	115.23	119.90
36	5	1064	A	N9-C4-C5	-7.77	102.69	105.80
36	1	420	G	C8-N9-C4	7.77	109.51	106.40
1	6	1514	U	C5-C4-O4	7.77	130.56	125.90
36	5	2870	C	C2-N1-C1'	-7.77	110.25	118.80
1	2	453	U	C2-N1-C1'	7.77	127.02	117.70
36	5	1513	G	C5-C6-O6	7.77	133.26	128.60
36	1	2768	U	O5'-P-OP2	-7.76	98.71	105.70
36	5	1304	A	O5'-P-OP1	-7.76	98.72	105.70
36	5	1390	A	N9-C4-C5	7.76	108.91	105.80
36	5	1434	G	O5'-P-OP2	-7.76	98.72	105.70
36	1	407	A	N1-C2-N3	-7.75	125.42	129.30
36	1	2134	G	N1-C6-O6	-7.75	115.25	119.90
36	5	1133	A	N1-C6-N6	-7.75	113.95	118.60
36	1	2726	C	N1-C2-N3	7.75	124.62	119.20
36	1	2357	A	O5'-P-OP2	-7.75	98.73	105.70
36	5	1402	C	N3-C2-O2	-7.74	116.48	121.90
36	1	1114	U	C6-N1-C2	7.74	125.64	121.00
36	1	2403	G	N3-C4-N9	7.74	130.64	126.00
36	5	1838	G	OP1-P-O3'	7.74	122.23	105.20
36	5	2341	A	C8-N9-C4	7.73	108.89	105.80
36	1	895	A	C2-N3-C4	-7.73	106.74	110.60
36	1	521	A	N1-C6-N6	7.72	123.23	118.60
36	1	217	U	OP1-P-O3'	7.71	122.17	105.20
36	1	859	G	N3-C2-N2	7.71	125.30	119.90
36	1	3143	C	C6-N1-C2	7.71	123.38	120.30
36	5	2964	G	C5-C6-N1	7.71	115.35	111.50
36	5	3185	U	O5'-P-OP2	-7.71	98.76	105.70
1	6	609	U	C5-C4-O4	7.71	130.52	125.90
36	5	1001	G	O5'-P-OP1	-7.70	98.77	105.70
36	5	1445	U	C5-C4-O4	-7.70	121.28	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3107	U	O5'-P-OP2	-7.70	98.77	105.70
36	5	2385	G	C4-N9-C1'	-7.70	116.49	126.50
36	5	2572	C	C2-N1-C1'	7.70	127.27	118.80
36	1	1082	U	C5-C6-N1	7.69	126.55	122.70
36	5	3192	U	O5'-P-OP1	-7.69	98.78	105.70
36	5	2883	U	N3-C2-O2	-7.69	116.81	122.20
38	8	38	U	C5-C6-N1	-7.69	118.85	122.70
36	5	2113	A	C8-N9-C4	7.69	108.88	105.80
36	1	504	A	N7-C8-N9	-7.68	109.96	113.80
36	5	2719	U	N1-C2-O2	-7.68	117.43	122.80
36	5	2993	G	N9-C4-C5	-7.68	102.33	105.40
36	1	2816	G	O4'-C1'-N9	7.68	114.34	108.20
36	5	3101	G	N1-C6-O6	-7.68	115.29	119.90
1	2	1282	U	N3-C2-O2	-7.67	116.83	122.20
36	1	835	G	O4'-C1'-N9	7.67	114.34	108.20
36	1	776	U	C5-C4-O4	7.67	130.50	125.90
36	5	1876	U	C5-C6-N1	7.67	126.54	122.70
36	1	2861	U	O5'-P-OP1	-7.67	98.80	105.70
36	5	1374	G	C8-N9-C4	7.67	109.47	106.40
1	6	387	A	N1-C6-N6	-7.67	114.00	118.60
36	1	797	U	C2-N3-C4	-7.67	122.40	127.00
36	5	437	G	N9-C4-C5	7.67	108.47	105.40
36	5	3197	G	N3-C4-N9	-7.67	121.40	126.00
36	1	907	G	O4'-C1'-N9	7.66	114.33	108.20
36	5	2694	A	O5'-P-OP2	-7.66	98.80	105.70
36	1	3306	U	C2-N3-C4	-7.66	122.40	127.00
36	1	716	A	O5'-P-OP1	-7.66	98.81	105.70
36	1	2873	U	N3-C2-O2	-7.66	116.84	122.20
36	1	2602	G	O5'-P-OP2	-7.65	98.81	105.70
1	2	1745	G	O5'-P-OP2	-7.65	98.81	105.70
36	1	1495	U	C2-N3-C4	-7.65	122.41	127.00
36	1	2378	C	N3-C4-C5	-7.65	118.84	121.90
36	1	1496	C	C5-C6-N1	7.65	124.82	121.00
36	1	3209	A	N9-C4-C5	-7.64	102.74	105.80
36	5	1859	A	O5'-P-OP2	-7.64	98.82	105.70
36	1	339	C	N3-C2-O2	-7.64	116.55	121.90
36	1	1170	A	C5-N7-C8	7.64	107.72	103.90
36	1	637	C	N1-C2-N3	7.64	124.55	119.20
36	1	1130	A	C2-N3-C4	7.63	114.42	110.60
36	1	2645	G	N3-C2-N2	-7.63	114.56	119.90
36	1	3022	G	O4'-C1'-N9	7.63	114.31	108.20
36	5	931	C	C2-N3-C4	-7.63	116.08	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2393	G	N1-C6-O6	7.63	124.48	119.90
36	5	2635	A	N9-C4-C5	7.63	108.85	105.80
36	1	2403	G	C8-N9-C4	-7.62	103.35	106.40
36	1	304	G	N1-C2-N2	7.62	123.05	116.20
1	2	1486	G	N7-C8-N9	7.61	116.91	113.10
36	5	2968	G	C5-N7-C8	7.61	108.11	104.30
1	6	194	U	C2-N1-C1'	7.61	126.83	117.70
36	5	3259	U	C5-C6-N1	7.61	126.50	122.70
36	1	1049	C	O5'-P-OP2	-7.60	98.86	105.70
36	1	2914	G	O5'-P-OP2	-7.60	98.86	105.70
36	1	3181	C	C5-C4-N4	7.60	125.52	120.20
36	1	2983	C	N3-C4-N4	-7.60	112.68	118.00
36	1	2790	A	O5'-P-OP2	-7.60	98.86	105.70
36	5	580	C	C6-N1-C2	-7.60	117.26	120.30
36	5	1513	G	N7-C8-N9	7.60	116.90	113.10
36	5	2993	G	C4-C5-N7	7.60	113.84	110.80
36	1	646	A	O5'-P-OP2	-7.59	98.86	105.70
36	1	967	A	C4-C5-N7	-7.59	106.90	110.70
36	1	2954	U	C6-N1-C2	7.59	125.56	121.00
1	2	639	U	N1-C2-O2	7.59	128.12	122.80
36	5	3362	A	O4'-C1'-N9	7.59	114.28	108.20
36	5	2211	U	N1-C2-N3	7.59	119.45	114.90
36	5	2875	U	O5'-P-OP2	-7.59	98.87	105.70
36	1	2884	C	C6-N1-C2	7.58	123.33	120.30
36	5	2524	A	O4'-C1'-N9	7.58	114.27	108.20
1	2	1600	A	C2-N3-C4	-7.58	106.81	110.60
1	2	1486	G	C5-N7-C8	-7.58	100.51	104.30
36	5	2870	C	C6-N1-C1'	7.58	129.89	120.80
36	5	1665	C	N3-C4-N4	-7.57	112.70	118.00
36	5	1493	G	O4'-C1'-N9	7.57	114.25	108.20
36	1	3362	A	O4'-C1'-N9	7.56	114.25	108.20
36	5	2975	U	N3-C4-C5	7.56	119.14	114.60
36	1	2978	U	O4'-C1'-N1	7.56	114.25	108.20
1	6	163	G	C5-N7-C8	-7.56	100.52	104.30
36	1	1308	A	N7-C8-N9	7.56	117.58	113.80
36	1	360	G	C5-C6-O6	-7.55	124.07	128.60
1	2	99	C	O5'-P-OP2	-7.55	98.91	105.70
36	1	353	G	C8-N9-C4	-7.55	103.38	106.40
36	5	2290	C	N3-C4-C5	7.55	124.92	121.90
36	5	2728	G	O4'-C1'-N9	7.55	114.24	108.20
36	1	2281	A	C2-N3-C4	-7.55	106.83	110.60
36	1	967	A	C5-C6-N6	7.54	129.73	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2827	U	C6-N1-C1'	7.54	131.76	121.20
1	6	1280	C	N3-C4-C5	-7.54	118.88	121.90
36	5	1202	A	O5'-P-OP1	-7.54	98.92	105.70
36	5	1305	U	C5-C4-O4	-7.54	121.38	125.90
1	2	453	U	N3-C2-O2	-7.53	116.93	122.20
36	1	1327	C	N3-C4-C5	7.53	124.91	121.90
36	1	2732	G	N3-C2-N2	7.53	125.17	119.90
36	1	3055	U	O5'-P-OP2	-7.53	98.92	105.70
36	5	1064	A	C5-C6-N6	-7.53	117.67	123.70
36	1	2983	C	C5-C4-N4	7.53	125.47	120.20
38	4	53	A	C2-N3-C4	7.53	114.36	110.60
36	5	2813	A	N9-C4-C5	7.53	108.81	105.80
36	5	971	G	C4-C5-N7	-7.52	107.79	110.80
1	2	543	C	N3-C2-O2	-7.52	116.64	121.90
36	5	2287	C	C6-N1-C2	-7.51	117.29	120.30
1	2	1761	U	C6-N1-C2	-7.51	116.49	121.00
36	5	2395	G	N7-C8-N9	-7.51	109.34	113.10
36	5	2915	U	C2-N3-C4	-7.51	122.49	127.00
68	o2	43	ARG	NE-CZ-NH1	7.51	124.06	120.30
36	5	201	A	OP1-P-OP2	-7.51	108.34	119.60
1	2	581	U	C2-N1-C1'	7.51	126.71	117.70
1	6	1120	U	N3-C4-O4	-7.51	114.15	119.40
1	6	163	G	C8-N9-C1'	7.50	136.75	127.00
36	5	417	A	N1-C6-N6	-7.50	114.10	118.60
36	1	3079	U	O5'-P-OP1	-7.50	98.95	105.70
36	1	2176	U	N1-C2-O2	7.50	128.05	122.80
1	2	1096	C	N1-C2-O2	7.50	123.40	118.90
36	1	2631	U	N3-C4-C5	7.50	119.10	114.60
36	1	2714	G	C5-N7-C8	-7.50	100.55	104.30
36	5	2372	A	C8-N9-C4	-7.50	102.80	105.80
36	5	3245	A	N1-C6-N6	7.50	123.10	118.60
1	6	358	U	O5'-P-OP1	-7.49	98.96	105.70
36	5	931	C	N3-C4-C5	7.49	124.90	121.90
36	1	971	G	N7-C8-N9	-7.49	109.36	113.10
36	1	2130	G	C5-C6-O6	7.49	133.09	128.60
36	1	938	C	N3-C4-C5	7.49	124.89	121.90
36	1	664	U	C2-N3-C4	-7.48	122.52	127.00
52	M6	78	ARG	NE-CZ-NH2	-7.47	116.56	120.30
36	1	46	U	N3-C2-O2	-7.47	116.97	122.20
36	1	645	A	C5-C6-N1	7.47	121.44	117.70
36	1	1103	A	C2-N3-C4	7.47	114.33	110.60
36	1	928	C	C6-N1-C2	-7.47	117.31	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1114	U	N3-C4-C5	7.47	119.08	114.60
36	1	99	A	O5'-P-OP2	-7.46	98.98	105.70
1	2	554	C	N3-C4-C5	-7.46	118.92	121.90
36	5	2426	U	N1-C2-O2	7.46	128.02	122.80
40	l3	4	ARG	NE-CZ-NH1	7.46	124.03	120.30
36	1	2138	A	N1-C2-N3	7.46	133.03	129.30
36	1	2178	A	N1-C6-N6	-7.45	114.13	118.60
36	5	2639	G	C5-C6-O6	-7.45	124.13	128.60
36	1	2651	G	N3-C4-C5	7.45	132.32	128.60
36	5	73	C	C6-N1-C2	7.45	123.28	120.30
36	5	1395	G	N1-C6-O6	7.45	124.37	119.90
36	5	817	A	O5'-P-OP1	-7.45	99.00	105.70
36	5	908	G	C6-C5-N7	-7.44	125.93	130.40
36	1	999	G	OP2-P-O3'	7.44	121.57	105.20
36	5	1426	C	N3-C4-C5	7.44	124.88	121.90
1	2	830	U	N3-C2-O2	-7.44	116.99	122.20
52	m6	69	GLY	N-CA-C	-7.43	94.51	113.10
36	1	935	U	C5-C6-N1	-7.43	118.98	122.70
36	5	3052	G	C4-C5-N7	-7.43	107.83	110.80
36	5	612	U	O5'-P-OP1	-7.43	99.01	105.70
36	5	2621	G	N1-C6-O6	7.43	124.36	119.90
36	1	1342	C	N3-C4-C5	7.42	124.87	121.90
36	5	641	C	N1-C2-O2	-7.42	114.44	118.90
36	1	1156	C	N3-C2-O2	-7.42	116.70	121.90
1	6	308	C	N3-C4-N4	-7.41	112.81	118.00
36	5	2799	A	O5'-P-OP2	-7.41	99.03	105.70
36	1	2632	G	N1-C6-O6	-7.41	115.45	119.90
36	5	929	A	C8-N9-C4	7.41	108.76	105.80
36	5	2718	U	O5'-P-OP2	-7.41	99.03	105.70
1	6	65	A	N1-C6-N6	7.41	123.04	118.60
36	1	2617	U	C2-N3-C4	-7.40	122.56	127.00
40	l3	19	ARG	NE-CZ-NH1	7.40	124.00	120.30
36	1	417	A	O5'-P-OP2	-7.40	99.04	105.70
36	5	1128	U	O5'-P-OP2	-7.40	99.04	105.70
36	1	2940	A	C5-N7-C8	7.40	107.60	103.90
36	1	103	G	C5-C6-O6	7.40	133.04	128.60
1	6	1036	A	N1-C6-N6	-7.40	114.16	118.60
1	2	1200	G	C6-C5-N7	-7.40	125.96	130.40
36	5	797	U	C5-C4-O4	-7.39	121.46	125.90
36	5	2404	A	N9-C1'-C2'	-7.39	103.87	112.00
36	1	2149	A	O5'-P-OP2	7.38	119.56	110.70
36	5	348	A	C8-N9-C4	7.38	108.75	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	121	U	N3-C2-O2	-7.38	117.03	122.20
36	1	94	G	O5'-P-OP1	-7.38	99.06	105.70
36	1	2988	C	C5-C4-N4	7.38	125.36	120.20
42	15	35	ARG	NE-CZ-NH1	-7.38	116.61	120.30
36	5	1149	G	O5'-P-OP2	-7.38	99.06	105.70
36	1	3181	C	N3-C4-N4	-7.38	112.84	118.00
36	5	1410	U	O5'-P-OP2	-7.37	99.06	105.70
36	5	2948	C	N3-C4-N4	-7.37	112.84	118.00
36	5	2255	A	O5'-P-OP1	-7.37	99.07	105.70
36	5	2765	C	C5-C6-N1	7.37	124.68	121.00
36	1	2633	U	N3-C2-O2	-7.36	117.05	122.20
36	1	968	G	N1-C6-O6	-7.36	115.48	119.90
1	6	337	G	N3-C4-N9	7.36	130.42	126.00
36	1	33	G	O5'-P-OP2	-7.36	99.08	105.70
38	4	125	U	N1-C2-O2	7.36	127.95	122.80
36	1	359	U	C2-N3-C4	-7.36	122.59	127.00
36	1	859	G	O5'-P-OP1	-7.36	99.08	105.70
36	5	671	U	N1-C2-O2	-7.36	117.65	122.80
1	6	557	G	N1-C6-O6	-7.35	115.49	119.90
36	1	960	U	N3-C4-C5	7.35	119.01	114.60
36	1	2642	A	C8-N9-C4	7.35	108.74	105.80
36	5	2405	C	O5'-P-OP1	-7.35	99.09	105.70
36	1	25	U	C5-C4-O4	-7.35	121.49	125.90
36	5	922	U	N3-C4-O4	-7.35	114.26	119.40
36	1	2870	C	C2-N1-C1'	-7.34	110.72	118.80
36	1	1846	C	N1-C2-O2	-7.34	114.50	118.90
36	1	2411	U	N3-C4-O4	-7.34	114.26	119.40
1	6	1549	C	C6-N1-C2	-7.34	117.36	120.30
36	1	765	C	N3-C2-O2	-7.34	116.77	121.90
36	1	2617	U	C4-C5-C6	7.34	124.10	119.70
36	5	2294	U	N1-C2-N3	7.34	119.30	114.90
36	5	3106	A	N1-C2-N3	-7.34	125.63	129.30
36	1	1890	U	C5-C6-N1	-7.33	119.03	122.70
36	1	2836	C	C6-N1-C2	-7.33	117.37	120.30
36	5	1284	C	C6-N1-C2	-7.33	117.37	120.30
1	2	1454	G	N1-C6-O6	-7.32	115.51	119.90
36	5	817	A	C8-N9-C4	-7.32	102.87	105.80
36	1	1495	U	N3-C2-O2	-7.32	117.08	122.20
36	1	2278	C	C4-C5-C6	-7.32	113.74	117.40
36	5	2290	C	C2-N3-C4	-7.32	116.24	119.90
36	5	3046	A	N1-C2-N3	-7.32	125.64	129.30
40	13	232	ARG	NE-CZ-NH2	-7.32	116.64	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	93	C	N1-C2-O2	-7.31	114.51	118.90
36	1	2651	G	C8-N9-C4	7.31	109.32	106.40
36	5	908	G	C4-N9-C1'	7.31	136.00	126.50
36	1	806	A	N9-C4-C5	-7.31	102.88	105.80
36	1	1060	U	C5-C6-N1	-7.30	119.05	122.70
36	1	1381	A	O5'-P-OP1	-7.30	99.13	105.70
36	1	2618	G	C6-N1-C2	-7.30	120.72	125.10
36	5	3142	A	N9-C4-C5	-7.30	102.88	105.80
36	5	931	C	C5-C6-N1	-7.30	117.35	121.00
36	5	2231	C	C2-N1-C1'	7.30	126.83	118.80
36	1	2938	G	OP1-P-OP2	7.30	130.54	119.60
36	5	1175	C	C6-N1-C2	-7.29	117.38	120.30
36	1	2418	G	OP1-P-O3'	7.29	121.25	105.20
36	5	341	G	C5-C6-O6	-7.29	124.22	128.60
36	1	664	U	C5-C6-N1	-7.29	119.05	122.70
36	5	1879	A	OP1-P-OP2	-7.29	108.66	119.60
36	5	3123	A	C8-N9-C4	7.29	108.72	105.80
1	2	1039	A	O4'-C1'-N9	7.29	114.03	108.20
36	5	702	C	C6-N1-C2	-7.29	117.39	120.30
36	5	856	G	C5-C6-O6	-7.29	124.23	128.60
36	1	2779	A	O5'-P-OP2	-7.28	99.14	105.70
36	1	2865	U	N3-C4-C5	7.28	118.97	114.60
38	8	25	G	N3-C2-N2	7.28	125.00	119.90
1	2	554	C	C2-N3-C4	7.28	123.54	119.90
36	1	2194	G	O5'-P-OP2	-7.28	99.15	105.70
36	1	2302	G	N1-C6-O6	-7.28	115.53	119.90
36	5	3127	A	N1-C6-N6	-7.28	114.23	118.60
36	1	1196	C	N3-C2-O2	7.28	127.00	121.90
36	1	1308	A	C8-N9-C4	-7.28	102.89	105.80
36	5	1331	U	N3-C2-O2	7.28	127.30	122.20
36	5	341	G	C4-C5-N7	7.28	113.71	110.80
36	5	909	G	C2-N3-C4	7.28	115.54	111.90
36	5	968	G	N3-C2-N2	7.27	124.99	119.90
36	1	766	U	O5'-P-OP1	-7.27	99.16	105.70
36	1	3029	A	C8-N9-C4	-7.27	102.89	105.80
1	6	973	A	O5'-P-OP2	-7.27	99.16	105.70
36	5	914	A	C2-N3-C4	-7.27	106.96	110.60
36	5	3218	A	C2-N3-C4	-7.27	106.96	110.60
36	1	797	U	C5-C6-N1	-7.27	119.06	122.70
36	1	2414	G	N3-C2-N2	-7.27	114.81	119.90
36	1	1160	C	O5'-P-OP1	-7.27	99.16	105.70
36	5	1496	C	OP1-P-OP2	-7.27	108.70	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	402	C	O5'-P-OP1	-7.27	99.16	105.70
36	1	53	G	O5'-P-OP2	-7.27	99.16	105.70
36	5	3197	G	N3-C4-C5	7.27	132.23	128.60
36	1	2811	A	C6-N1-C2	-7.26	114.24	118.60
36	1	2572	C	N3-C2-O2	-7.26	116.82	121.90
36	5	304	G	C2-N3-C4	7.25	115.53	111.90
36	5	922	U	C5-C4-O4	7.25	130.25	125.90
36	1	2950	G	C4-C5-N7	7.25	113.70	110.80
38	4	51	G	C5-C6-O6	-7.25	124.25	128.60
36	5	1314	C	C2-N3-C4	-7.25	116.28	119.90
1	2	1012	U	C2-N3-C4	7.24	131.35	127.00
36	5	3362	A	C5-N7-C8	-7.24	100.28	103.90
36	1	718	G	C5-N7-C8	-7.24	100.68	104.30
1	2	1535	U	C2-N1-C1'	7.24	126.39	117.70
36	5	2300	G	N1-C6-O6	-7.24	115.56	119.90
36	5	277	G	N1-C6-O6	-7.24	115.56	119.90
52	m6	94	ARG	NE-CZ-NH1	-7.23	116.68	120.30
36	1	2411	U	O5'-P-OP1	-7.23	99.19	105.70
36	1	3207	U	N1-C2-O2	-7.23	117.74	122.80
36	5	1421	G	O5'-P-OP2	-7.23	99.19	105.70
36	1	2411	U	N3-C4-C5	7.23	118.94	114.60
47	M0	57	LEU	CA-CB-CG	7.23	131.92	115.30
1	6	1537	C	C6-N1-C1'	7.23	129.47	120.80
36	5	3197	G	N3-C2-N2	-7.22	114.84	119.90
36	1	1556	C	C2-N1-C1'	7.22	126.74	118.80
1	6	1473	U	C6-N1-C2	-7.22	116.67	121.00
1	6	453	U	C2-N1-C1'	7.22	126.36	117.70
36	1	959	C	C5-C4-N4	-7.21	115.15	120.20
36	5	2899	C	N1-C2-N3	7.21	124.25	119.20
36	5	3020	U	C5-C4-O4	-7.21	121.57	125.90
36	5	2572	C	N3-C2-O2	-7.21	116.85	121.90
36	1	196	G	O5'-P-OP2	-7.21	99.21	105.70
1	2	1339	C	C6-N1-C2	-7.21	117.42	120.30
36	5	1931	U	C2-N1-C1'	-7.21	109.05	117.70
36	5	426	G	N7-C8-N9	-7.20	109.50	113.10
36	1	2719	U	N1-C2-O2	-7.20	117.76	122.80
36	1	1120	A	N1-C6-N6	-7.20	114.28	118.60
36	1	2388	U	N1-C2-O2	-7.20	117.76	122.80
34	SR	161	LYS	C-N-CA	7.20	139.69	121.70
36	1	1168	U	N1-C2-O2	7.20	127.84	122.80
36	5	2382	G	C5-C6-O6	7.20	132.92	128.60
36	1	345	G	C5-C6-N1	7.19	115.10	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1396	C	C6-N1-C2	7.19	123.18	120.30
36	5	1489	A	N1-C6-N6	7.19	122.91	118.60
36	5	2988	C	N3-C2-O2	-7.19	116.87	121.90
36	5	3047	U	N3-C4-O4	-7.19	114.37	119.40
36	1	608	A	C5-C6-N6	-7.18	117.95	123.70
36	1	401	U	C5-C4-O4	-7.18	121.59	125.90
36	1	1313	G	O5'-P-OP2	-7.18	99.24	105.70
36	5	2968	G	N7-C8-N9	-7.18	109.51	113.10
1	6	542	A	O5'-P-OP1	-7.17	99.24	105.70
1	2	287	G	O4'-C1'-N9	7.17	113.94	108.20
36	5	339	C	C6-N1-C1'	7.17	129.41	120.80
36	1	2363	A	N1-C6-N6	-7.17	114.30	118.60
36	5	2142	A	OP1-P-OP2	-7.17	108.85	119.60
36	5	2223	A	O5'-P-OP1	-7.17	99.25	105.70
36	5	1858	A	C8-N9-C4	-7.17	102.93	105.80
36	5	3006	A	C8-N9-C4	-7.17	102.93	105.80
36	1	817	A	O5'-P-OP2	7.16	119.30	110.70
36	1	2864	A	C8-N9-C4	-7.16	102.94	105.80
59	N3	87	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	6	755	A	O4'-C1'-N9	7.16	113.93	108.20
36	5	838	G	C5-C6-O6	7.16	132.90	128.60
36	1	1715	A	O4'-C1'-N9	-7.16	102.47	108.20
36	5	869	G	O5'-P-OP2	-7.16	99.26	105.70
10	s8	29	LEU	CA-CB-CG	7.15	131.75	115.30
36	5	3214	U	N3-C4-O4	-7.15	114.39	119.40
36	1	847	A	N1-C6-N6	7.15	122.89	118.60
36	5	1380	G	O5'-P-OP2	-7.15	99.26	105.70
36	5	671	U	N3-C2-O2	7.15	127.20	122.20
36	5	2356	A	C2-N3-C4	-7.15	107.03	110.60
36	5	3047	U	N3-C4-C5	7.15	118.89	114.60
36	1	3119	U	N3-C4-O4	-7.14	114.40	119.40
36	5	3052	G	C5-N7-C8	7.14	107.87	104.30
36	5	3308	C	C6-N1-C2	-7.14	117.44	120.30
36	1	439	C	C6-N1-C1'	-7.14	112.23	120.80
36	1	215	G	C8-N9-C4	-7.14	103.55	106.40
38	4	30	C	N3-C4-N4	-7.14	113.00	118.00
36	5	1307	G	P-O3'-C3'	7.14	128.26	119.70
36	1	2376	G	N3-C4-N9	7.13	130.28	126.00
36	5	2928	C	C4-C5-C6	7.13	120.97	117.40
36	5	3050	U	N1-C2-O2	7.13	127.79	122.80
36	5	2808	A	N9-C4-C5	-7.13	102.95	105.80
36	1	2827	U	C5-C4-O4	7.13	130.18	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1509	C	N1-C2-O2	7.13	123.18	118.90
36	5	92	G	C5-C6-N1	7.13	115.06	111.50
36	1	2697	A	N1-C6-N6	-7.13	114.32	118.60
36	1	3121	U	OP1-P-O3'	7.13	120.88	105.20
36	1	2408	U	O5'-P-OP1	-7.12	99.29	105.70
36	5	2278	C	N3-C4-N4	-7.12	113.02	118.00
36	5	307	A	N1-C6-N6	-7.12	114.33	118.60
36	5	2333	C	N1-C2-O2	-7.12	114.63	118.90
36	1	859	G	N3-C4-N9	7.12	130.27	126.00
36	1	721	G	C5-C6-O6	-7.12	124.33	128.60
36	5	1799	A	N1-C2-N3	-7.12	125.74	129.30
38	4	32	C	N1-C2-O2	-7.11	114.63	118.90
62	N6	13	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	2	137	U	N3-C2-O2	-7.11	117.22	122.20
36	1	2983	C	C4-C5-C6	7.11	120.95	117.40
36	5	2796	G	C5-N7-C8	-7.11	100.75	104.30
36	1	2149	A	C5-C6-N1	-7.11	114.15	117.70
36	5	1168	U	N3-C4-C5	7.11	118.86	114.60
36	1	937	G	N7-C8-N9	-7.10	109.55	113.10
36	1	1297	C	O5'-P-OP1	-7.10	99.31	105.70
36	5	934	G	C5-C6-O6	-7.10	124.34	128.60
36	1	3275	U	C5-C6-N1	7.10	126.25	122.70
36	1	643	U	N3-C2-O2	7.10	127.17	122.20
36	1	3344	A	C8-N9-C4	-7.10	102.96	105.80
1	6	868	G	C5-C6-O6	-7.10	124.34	128.60
36	5	277	G	C5-C6-O6	7.10	132.86	128.60
36	5	1129	A	C2-N3-C4	7.09	114.15	110.60
36	1	634	C	N3-C2-O2	-7.09	116.94	121.90
36	5	1513	G	N9-C4-C5	7.09	108.23	105.40
1	6	1614	A	C5-N7-C8	-7.08	100.36	103.90
36	5	339	C	N3-C4-N4	-7.08	113.04	118.00
37	7	28	C	N1-C2-O2	-7.08	114.65	118.90
1	6	1514	U	N3-C4-O4	-7.08	114.44	119.40
36	5	891	G	C5-C6-O6	7.08	132.85	128.60
38	8	110	C	C6-N1-C2	-7.08	117.47	120.30
36	1	282	G	C8-N9-C4	-7.08	103.57	106.40
36	1	1409	G	N1-C6-O6	-7.08	115.66	119.90
1	6	987	G	C5-C6-O6	-7.08	124.36	128.60
36	5	2190	U	N1-C2-N3	7.08	119.14	114.90
38	8	6	U	O5'-P-OP2	-7.08	99.33	105.70
1	6	858	G	C4-C5-N7	7.07	113.63	110.80
36	5	2743	A	C5-N7-C8	7.07	107.44	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3259	U	C6-N1-C2	-7.07	116.76	121.00
38	8	51	G	C5-C6-O6	-7.07	124.36	128.60
36	1	304	G	C2-N3-C4	7.07	115.43	111.90
36	1	2400	G	C5-C6-O6	-7.07	124.36	128.60
1	2	1096	C	C6-N1-C1'	-7.07	112.32	120.80
36	5	2412	G	C5-C6-O6	7.07	132.84	128.60
1	6	308	C	N1-C2-N3	7.07	124.15	119.20
36	1	895	A	N3-C4-C5	7.06	131.75	126.80
15	C3	22	ALA	C-N-CD	-7.06	105.06	120.60
43	L6	31	ARG	NE-CZ-NH2	-7.06	116.77	120.30
36	1	3373	U	C6-N1-C2	7.06	125.24	121.00
1	6	609	U	N3-C4-O4	-7.06	114.46	119.40
1	6	1082	C	N3-C2-O2	-7.06	116.96	121.90
36	5	2725	U	C5-C4-O4	-7.06	121.66	125.90
64	n8	73	LEU	CA-CB-CG	7.06	131.54	115.30
36	1	2885	C	C5-C6-N1	-7.06	117.47	121.00
36	5	3374	U	C6-N1-C2	7.06	125.23	121.00
1	2	1761	U	P-O3'-C3'	7.05	128.16	119.70
44	17	229	PHE	CB-CG-CD1	7.05	125.74	120.80
1	6	315	A	C8-N9-C4	-7.05	102.98	105.80
1	6	993	A	O5'-P-OP2	-7.05	99.36	105.70
36	5	2872	A	N1-C6-N6	-7.05	114.37	118.60
36	5	2901	G	C5-C6-O6	-7.05	124.37	128.60
36	1	2808	A	C6-C5-N7	-7.04	127.37	132.30
36	5	2181	C	N1-C2-O2	-7.04	114.67	118.90
36	5	967	A	N9-C4-C5	7.04	108.62	105.80
36	5	2635	A	N1-C6-N6	-7.04	114.38	118.60
1	2	1611	A	C2-N3-C4	-7.04	107.08	110.60
36	5	73	C	N3-C4-C5	7.04	124.72	121.90
36	5	2794	G	C5-C6-O6	-7.04	124.38	128.60
1	6	321	C	N3-C2-O2	-7.03	116.98	121.90
36	5	44	U	N1-C2-O2	-7.03	117.88	122.80
36	1	708	G	O5'-P-OP1	-7.03	99.37	105.70
36	1	2983	C	N1-C2-N3	7.03	124.12	119.20
1	6	542	A	C4-N9-C1'	7.03	138.95	126.30
36	5	2160	G	N3-C2-N2	7.03	124.82	119.90
36	5	2369	G	N3-C4-N9	7.03	130.22	126.00
36	1	2242	A	C8-N9-C4	-7.03	102.99	105.80
1	6	1605	G	N1-C6-O6	-7.03	115.68	119.90
39	L2	191	LEU	CA-CB-CG	-7.02	99.14	115.30
1	2	1596	C	C6-N1-C2	-7.02	117.49	120.30
36	1	1902	G	N9-C4-C5	-7.02	102.59	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	875	G	N1-C6-O6	-7.02	115.69	119.90
36	5	1389	G	C5-C6-O6	-7.02	124.39	128.60
36	1	99	A	C5'-C4'-O4'	7.02	117.52	109.10
36	1	1142	G	C5-C6-O6	-7.01	124.39	128.60
36	1	1405	U	C6-N1-C2	7.01	125.21	121.00
36	1	1433	A	N1-C2-N3	-7.01	125.79	129.30
36	1	3178	A	N1-C6-N6	7.01	122.81	118.60
1	2	542	A	O4'-C1'-N9	7.01	113.81	108.20
36	1	2786	G	N9-C4-C5	7.01	108.20	105.40
36	1	777	U	O5'-P-OP2	-7.01	99.39	105.70
1	2	75	U	C2-N1-C1'	7.01	126.11	117.70
36	1	325	A	C5-C6-N1	7.01	121.20	117.70
36	1	2249	G	C5-C6-O6	7.00	132.80	128.60
36	1	3309	G	C6-C5-N7	-7.00	126.20	130.40
36	1	630	A	C2-N3-C4	7.00	114.10	110.60
1	6	400	A	N1-C6-N6	7.00	122.80	118.60
36	5	2299	A	C2-N3-C4	7.00	114.10	110.60
1	2	1654	G	C5-C6-N1	7.00	115.00	111.50
36	1	2957	G	O5'-P-OP2	7.00	119.10	110.70
1	2	959	U	N3-C2-O2	-7.00	117.30	122.20
1	6	1773	C	C6-N1-C2	-7.00	117.50	120.30
36	5	2211	U	C4-C5-C6	7.00	123.90	119.70
36	5	216	G	C5-C6-O6	-6.99	124.40	128.60
36	5	2375	G	C5-C6-O6	6.99	132.80	128.60
36	1	1364	C	N3-C4-C5	6.99	124.70	121.90
36	1	2830	G	N9-C4-C5	6.99	108.20	105.40
36	5	1152	G	C4-C5-C6	-6.99	114.61	118.80
36	5	189	G	C5-C6-O6	6.99	132.79	128.60
36	1	2368	A	N7-C8-N9	-6.98	110.31	113.80
36	5	282	G	C2'-C3'-O3'	6.98	124.87	113.70
68	O2	43	ARG	NE-CZ-NH1	6.97	123.79	120.30
36	1	329	U	C2-N1-C1'	-6.97	109.33	117.70
36	1	646	A	N7-C8-N9	6.97	117.29	113.80
36	5	1390	A	N1-C6-N6	-6.97	114.42	118.60
36	1	3055	U	C6-N1-C1'	-6.97	111.44	121.20
36	5	879	U	O5'-P-OP1	-6.97	99.43	105.70
36	5	2304	C	C6-N1-C2	-6.97	117.51	120.30
36	5	2908	G	C5-C6-O6	6.97	132.78	128.60
36	1	319	A	O5'-P-OP1	-6.96	99.43	105.70
36	5	427	C	OP2-P-O3'	6.96	120.52	105.20
36	5	1311	G	C2-N3-C4	6.96	115.38	111.90
36	5	3144	G	C8-N9-C4	-6.96	103.61	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	646	A	C8-N9-C4	-6.96	103.02	105.80
52	m6	94	ARG	NE-CZ-NH2	6.96	123.78	120.30
36	1	3318	G	N3-C4-C5	-6.96	125.12	128.60
1	6	638	U	N3-C2-O2	-6.96	117.33	122.20
36	5	1331	U	C5-C4-O4	-6.96	121.72	125.90
36	5	2142	A	O5'-P-OP2	6.96	119.05	110.70
36	5	935	U	C2-N3-C4	-6.95	122.83	127.00
36	1	3217	C	C2-N1-C1'	6.95	126.45	118.80
36	1	1170	A	N7-C8-N9	-6.95	110.33	113.80
1	6	10	G	C5-C6-O6	6.95	132.77	128.60
36	5	3047	U	C5-C6-N1	-6.95	119.23	122.70
1	2	728	U	C2-N1-C1'	6.94	126.03	117.70
36	5	2643	A	C5-N7-C8	-6.94	100.43	103.90
36	5	1064	A	C4-C5-N7	6.94	114.17	110.70
36	1	802	C	O5'-P-OP2	6.94	119.03	110.70
36	1	1200	A	O4'-C1'-N9	6.94	113.75	108.20
36	5	1481	A	P-O3'-C3'	6.94	128.03	119.70
36	5	1483	G	O4'-C1'-N9	6.94	113.75	108.20
36	1	2434	U	N3-C4-O4	-6.94	114.54	119.40
1	6	102	U	N1-C2-O2	-6.94	117.94	122.80
17	c5	36	LEU	CA-CB-CG	6.94	131.26	115.30
36	5	2287	C	C5-C6-N1	6.94	124.47	121.00
36	1	1307	G	N1-C6-O6	-6.93	115.74	119.90
1	6	1549	C	N3-C4-C5	-6.93	119.13	121.90
36	5	931	C	C6-N1-C2	6.93	123.07	120.30
36	5	2369	G	N9-C4-C5	-6.93	102.63	105.40
36	1	818	C	C6-N1-C2	-6.93	117.53	120.30
1	6	1389	C	N1-C2-O2	6.93	123.06	118.90
36	1	905	U	N1-C2-N3	6.93	119.06	114.90
36	1	959	C	N1-C2-O2	-6.92	114.75	118.90
36	1	203	G	N1-C6-O6	-6.92	115.75	119.90
1	2	795	U	N3-C2-O2	-6.92	117.36	122.20
36	1	591	G	C5-C6-O6	-6.92	124.45	128.60
36	1	1405	U	C2-N3-C4	-6.92	122.85	127.00
1	6	18	C	N3-C4-C5	-6.92	119.13	121.90
36	5	2141	U	OP2-P-O3'	6.92	120.42	105.20
36	1	643	U	N1-C2-O2	-6.92	117.96	122.80
36	1	1184	A	O5'-P-OP2	-6.92	99.48	105.70
1	6	163	G	C8-N9-C4	-6.92	103.63	106.40
36	5	2401	A	C2-N3-C4	6.92	114.06	110.60
36	1	1493	G	O5'-P-OP2	-6.92	99.48	105.70
36	5	857	G	C5-C6-O6	-6.91	124.45	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2374	C	C6-N1-C2	-6.91	117.54	120.30
37	3	86	U	C2-N3-C4	-6.91	122.86	127.00
36	5	3101	G	C5-C6-O6	6.91	132.75	128.60
37	7	40	C	N1-C2-O2	-6.91	114.76	118.90
36	1	1156	C	N1-C2-O2	6.91	123.04	118.90
38	4	73	U	N3-C4-O4	-6.91	114.57	119.40
36	1	652	G	N3-C2-N2	6.90	124.73	119.90
36	5	835	G	C5-C6-O6	-6.90	124.46	128.60
36	5	1163	A	O5'-P-OP2	-6.90	99.49	105.70
36	5	2308	C	N1-C2-O2	-6.90	114.76	118.90
36	1	782	U	N3-C4-O4	-6.90	114.57	119.40
1	2	453	U	N1-C2-O2	6.89	127.62	122.80
36	1	1496	C	C2-N1-C1'	6.89	126.38	118.80
36	5	2735	U	C5-C6-N1	6.89	126.15	122.70
36	5	590	G	C5-C6-O6	-6.89	124.47	128.60
36	5	2350	C	C2-N3-C4	-6.89	116.46	119.90
36	1	908	G	O4'-C1'-N9	-6.89	102.69	108.20
36	1	1495	U	C5-C4-O4	6.89	130.03	125.90
36	1	2725	U	C5-C6-N1	-6.88	119.26	122.70
36	1	968	G	N7-C8-N9	6.88	116.54	113.10
52	M6	110	PRO	C-N-CD	-6.88	105.47	120.60
36	5	950	G	C5-C6-O6	-6.88	124.47	128.60
36	1	33	G	N7-C8-N9	6.87	116.54	113.10
36	1	1489	A	N1-C6-N6	6.87	122.72	118.60
49	M3	35	ARG	NE-CZ-NH1	-6.87	116.86	120.30
36	1	1433	A	C2-N3-C4	6.87	114.03	110.60
36	1	2369	G	N3-C4-C5	-6.87	125.17	128.60
36	1	2134	G	N3-C2-N2	6.87	124.71	119.90
36	1	1586	G	O5'-P-OP2	-6.86	99.52	105.70
36	1	2899	C	N3-C4-N4	-6.86	113.19	118.00
76	Q0	127	LEU	CA-CB-CG	6.86	131.09	115.30
36	5	1855	U	C2-N3-C4	-6.86	122.88	127.00
36	1	359	U	C5-C6-N1	-6.86	119.27	122.70
36	5	3143	C	C6-N1-C2	6.86	123.05	120.30
1	2	1454	G	C5-C6-O6	6.86	132.72	128.60
1	6	778	G	N1-C6-O6	-6.86	115.78	119.90
12	C0	88	PRO	N-CA-CB	6.86	111.53	103.30
36	1	1832	C	N3-C2-O2	-6.86	117.10	121.90
36	1	2618	G	C2-N3-C4	6.86	115.33	111.90
36	5	2619	G	N1-C6-O6	6.86	124.01	119.90
1	2	1782	A	N9-C4-C5	6.85	108.54	105.80
36	5	770	G	O4'-C1'-N9	6.85	113.68	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	209	A	O5'-P-OP2	-6.85	99.53	105.70
36	1	1403	C	C2-N3-C4	-6.85	116.48	119.90
36	5	33	G	C5-C6-N1	6.85	114.92	111.50
36	5	3010	U	N3-C2-O2	-6.85	117.41	122.20
1	6	687	G	N9-C4-C5	6.85	108.14	105.40
36	5	3214	U	C5-C4-O4	6.85	130.01	125.90
36	1	1177	G	C5-C6-O6	-6.84	124.49	128.60
1	6	31	C	C6-N1-C2	-6.84	117.56	120.30
36	5	2376	G	N7-C8-N9	-6.84	109.68	113.10
36	1	2614	G	C5-C6-O6	6.84	132.71	128.60
36	5	878	G	C5-C6-O6	-6.84	124.50	128.60
36	5	909	G	C5-N7-C8	6.84	107.72	104.30
36	5	2113	A	C4-C5-C6	-6.84	113.58	117.00
36	5	3209	A	O4'-C1'-N9	6.84	113.67	108.20
36	1	280	U	N3-C4-O4	6.84	124.19	119.40
1	6	1796	C	C5-C6-N1	-6.84	117.58	121.00
36	5	28	C	C6-N1-C2	6.83	123.03	120.30
36	5	2726	C	N3-C4-N4	-6.83	113.22	118.00
37	7	101	G	N1-C6-O6	6.83	124.00	119.90
36	1	1425	U	C2-N3-C4	-6.83	122.90	127.00
36	5	2957	G	C8-N9-C4	6.83	109.13	106.40
36	1	890	C	C6-N1-C2	-6.83	117.57	120.30
36	1	2314	U	N1-C2-N3	-6.83	110.80	114.90
36	1	2362	C	N1-C2-O2	6.83	123.00	118.90
1	6	858	G	O4'-C1'-N9	6.83	113.66	108.20
36	5	1391	C	N1-C2-O2	-6.83	114.80	118.90
1	6	610	G	C8-N9-C1'	-6.83	118.13	127.00
36	1	2868	U	C5-C6-N1	-6.82	119.29	122.70
36	5	3050	U	N3-C4-O4	-6.82	114.62	119.40
1	2	142	G	N3-C4-C5	6.82	132.01	128.60
36	1	54	C	N3-C4-C5	6.82	124.63	121.90
1	6	144	U	C6-N1-C2	-6.82	116.91	121.00
1	2	158	U	P-O3'-C3'	6.82	127.88	119.70
36	1	324	A	C6-N1-C2	-6.82	114.51	118.60
36	1	2977	G	C5-N7-C8	6.82	107.71	104.30
36	1	272	G	N7-C8-N9	-6.82	109.69	113.10
36	1	2944	U	OP1-P-O3'	6.82	120.19	105.20
36	5	1481	A	N7-C8-N9	6.82	117.21	113.80
36	1	105	C	C2-N3-C4	-6.81	116.49	119.90
36	5	3120	C	C6-N1-C2	-6.81	117.57	120.30
1	2	1486	G	C8-N9-C4	-6.81	103.67	106.40
36	1	65	A	P-O3'-C3'	6.81	127.88	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	946	U	N1-C2-N3	6.81	118.99	114.90
36	5	987	U	O5'-P-OP1	-6.81	99.57	105.70
49	m3	47	ALA	C-N-CD	6.81	142.70	128.40
36	1	2148	U	N1-C2-O2	-6.81	118.03	122.80
36	5	1886	A	O5'-P-OP2	-6.81	99.57	105.70
1	2	142	G	N3-C4-N9	-6.81	121.92	126.00
36	1	272	G	C8-N9-C4	6.81	109.12	106.40
36	5	1605	A	O4'-C1'-N9	6.80	113.64	108.20
36	1	2393	G	C5-C6-O6	-6.80	124.52	128.60
36	1	2144	A	O4'-C1'-N9	6.80	113.64	108.20
36	5	1439	U	C2-N3-C4	-6.80	122.92	127.00
36	5	2314	U	N3-C4-O4	6.80	124.16	119.40
36	5	2633	U	N3-C4-O4	-6.80	114.64	119.40
36	5	1513	G	C2-N3-C4	6.80	115.30	111.90
36	5	1861	G	C8-N9-C4	-6.80	103.68	106.40
36	5	1469	C	C6-N1-C2	-6.79	117.58	120.30
36	1	2797	C	C5-C4-N4	-6.79	115.44	120.20
37	3	102	A	C8-N9-C4	6.79	108.52	105.80
36	5	2826	U	N1-C2-O2	6.79	127.56	122.80
36	1	875	G	O5'-P-OP2	-6.79	99.59	105.70
1	6	630	A	C2-N3-C4	-6.79	107.20	110.60
36	5	2643	A	N1-C6-N6	6.79	122.67	118.60
36	5	3245	A	N1-C2-N3	6.79	132.70	129.30
1	6	378	A	O5'-P-OP1	6.79	118.84	110.70
1	2	507	U	N1-C2-O2	6.78	127.55	122.80
36	1	1379	G	N3-C2-N2	6.78	124.65	119.90
36	1	521	A	C5-C6-N6	-6.78	118.28	123.70
36	1	672	A	N1-C6-N6	6.78	122.67	118.60
1	6	387	A	C2-N3-C4	6.78	113.99	110.60
1	6	1596	C	C5-C4-N4	6.78	124.95	120.20
36	5	1450	G	C6-C5-N7	6.78	134.47	130.40
36	1	1279	C	C6-N1-C2	-6.78	117.59	120.30
36	5	2231	C	O4'-C1'-N1	6.78	113.62	108.20
36	1	2952	G	C5-C6-O6	-6.78	124.53	128.60
36	5	96	G	O5'-P-OP1	6.78	118.83	110.70
36	1	2920	U	O5'-P-OP2	6.77	118.83	110.70
36	5	776	U	N3-C2-O2	-6.77	117.46	122.20
36	5	2211	U	C5-C4-O4	6.77	129.96	125.90
37	7	121	U	N1-C2-O2	6.77	127.54	122.80
36	1	1402	C	N3-C2-O2	-6.77	117.16	121.90
37	7	88	G	C5-C6-O6	6.77	132.66	128.60
36	1	806	A	O4'-C1'-N9	-6.77	102.78	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2830	G	N9-C4-C5	6.77	108.11	105.40
36	1	2434	U	C5-C6-N1	-6.77	119.32	122.70
36	5	883	A	N7-C8-N9	-6.77	110.42	113.80
36	5	2550	U	C5-C4-O4	6.77	129.96	125.90
36	1	1664	G	C5-C6-O6	6.77	132.66	128.60
1	2	553	G	C5-C6-N1	-6.76	108.12	111.50
36	1	421	G	N9-C4-C5	-6.76	102.70	105.40
36	5	1833	G	N1-C6-O6	-6.76	115.84	119.90
36	5	1546	A	O5'-P-OP1	-6.76	99.62	105.70
1	6	687	G	N1-C2-N2	6.76	122.28	116.20
36	1	3373	U	C5-C6-N1	-6.75	119.32	122.70
36	5	2119	A	C5-C6-N6	-6.75	118.30	123.70
36	1	424	G	N1-C6-O6	-6.75	115.85	119.90
36	1	2723	U	C5-C6-N1	-6.75	119.32	122.70
36	5	2808	A	N1-C6-N6	6.75	122.65	118.60
1	2	1096	C	N3-C2-O2	-6.75	117.17	121.90
36	1	1409	G	C5-C6-O6	6.75	132.65	128.60
1	6	389	G	C5-C6-O6	6.75	132.65	128.60
36	1	76	G	C5-C6-O6	-6.75	124.55	128.60
36	1	1847	A	OP1-P-OP2	6.75	129.72	119.60
36	5	2949	U	N3-C2-O2	-6.75	117.48	122.20
36	5	2343	C	N3-C4-N4	-6.75	113.28	118.00
36	1	288	C	C5-C4-N4	-6.74	115.48	120.20
36	5	1604	G	N3-C4-N9	6.74	130.05	126.00
36	5	2633	U	O5'-P-OP2	-6.74	99.63	105.70
36	1	2899	C	C5-C6-N1	-6.74	117.63	121.00
36	1	1931	U	N1-C2-O2	-6.74	118.08	122.80
36	1	2950	G	C5-N7-C8	-6.74	100.93	104.30
36	1	979	U	P-O3'-C3'	6.74	127.78	119.70
36	5	422	A	O5'-P-OP2	-6.74	99.64	105.70
36	5	1113	G	C2-N3-C4	-6.74	108.53	111.90
36	1	1054	A	O5'-P-OP2	-6.74	99.64	105.70
36	5	2796	G	C4-C5-N7	6.74	113.49	110.80
1	2	933	A	C8-N9-C4	-6.73	103.11	105.80
36	5	3374	U	N3-C4-C5	6.73	118.64	114.60
36	1	2936	A	O5'-P-OP1	-6.73	99.64	105.70
36	1	3207	U	C5-C4-O4	6.73	129.94	125.90
36	1	949	C	C4-C5-C6	6.73	120.76	117.40
36	1	689	U	N3-C2-O2	-6.72	117.49	122.20
36	5	2984	C	N3-C4-C5	6.72	124.59	121.90
36	5	643	U	N1-C2-O2	-6.72	118.09	122.80
36	1	895	A	N3-C4-N9	-6.72	122.02	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	647	G	N3-C4-N9	-6.72	121.97	126.00
37	3	47	C	O5'-P-OP2	-6.72	99.65	105.70
37	3	94	C	N1-C2-O2	-6.72	114.87	118.90
36	1	957	C	O5'-P-OP2	-6.72	99.66	105.70
36	1	2651	G	N7-C8-N9	-6.72	109.74	113.10
36	1	1653	G	N1-C6-O6	-6.71	115.87	119.90
36	1	1911	A	N1-C6-N6	6.71	122.63	118.60
36	1	2611	U	OP1-P-OP2	-6.71	109.53	119.60
36	5	1374	G	N7-C8-N9	-6.71	109.74	113.10
36	1	1902	G	N3-C2-N2	6.71	124.60	119.90
36	1	2422	C	N1-C2-O2	6.71	122.93	118.90
36	1	2993	G	C5-C6-N1	6.71	114.86	111.50
36	5	206	G	C5-C6-O6	-6.71	124.57	128.60
36	5	1115	G	N7-C8-N9	6.71	116.46	113.10
36	5	2797	C	N1-C2-O2	-6.71	114.87	118.90
36	5	3047	U	N3-C2-O2	-6.71	117.50	122.20
36	1	2395	G	C5-C6-O6	6.71	132.63	128.60
36	5	1176	C	C2-N3-C4	-6.71	116.55	119.90
36	1	2919	A	O5'-P-OP2	-6.71	99.66	105.70
36	1	2935	U	N1-C2-O2	6.71	127.50	122.80
1	6	610	G	C4-N9-C1'	6.71	135.22	126.50
1	6	1600	A	N1-C2-N3	6.71	132.65	129.30
36	5	793	C	C5-C6-N1	6.71	124.35	121.00
36	5	1083	G	O5'-P-OP1	-6.71	99.67	105.70
36	5	2403	G	N3-C4-C5	-6.71	125.25	128.60
36	5	427	C	N3-C4-C5	6.70	124.58	121.90
36	5	1354	G	O5'-P-OP2	-6.70	99.67	105.70
1	2	1514	U	O5'-P-OP1	-6.70	99.67	105.70
36	1	2983	C	O4'-C1'-N1	6.70	113.56	108.20
36	5	1547	G	N3-C4-C5	6.70	131.95	128.60
36	1	589	A	O5'-P-OP2	-6.70	99.67	105.70
36	1	1164	G	N1-C6-O6	-6.70	115.88	119.90
36	1	1911	A	C5-C6-N6	-6.70	118.34	123.70
36	1	2950	G	C5-C6-O6	-6.70	124.58	128.60
1	6	1361	U	C2-N1-C1'	6.70	125.74	117.70
36	1	709	A	N7-C8-N9	-6.70	110.45	113.80
36	5	3337	G	N1-C6-O6	-6.70	115.88	119.90
1	2	425	A	C8-N9-C4	-6.70	103.12	105.80
36	1	2169	G	N1-C6-O6	-6.70	115.88	119.90
36	1	2859	U	N1-C2-N3	6.69	118.92	114.90
36	1	407	A	C6-N1-C2	6.69	122.62	118.60
36	5	2979	U	N1-C2-O2	-6.69	118.11	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	830	U	N1-C2-O2	6.69	127.48	122.80
36	5	3098	G	C5-C6-O6	6.69	132.61	128.60
36	1	1639	C	O5'-P-OP2	-6.69	99.68	105.70
36	1	760	G	O4'-C1'-N9	6.69	113.55	108.20
36	1	2633	U	N1-C2-O2	6.69	127.48	122.80
36	1	271	C	N3-C2-O2	-6.68	117.22	121.90
36	1	2423	U	C5-C4-O4	-6.68	121.89	125.90
36	5	1331	U	N3-C4-C5	6.68	118.61	114.60
36	1	2426	U	N3-C4-C5	6.68	118.61	114.60
36	1	785	G	C2-N3-C4	6.68	115.24	111.90
36	5	2927	C	C6-N1-C2	-6.68	117.63	120.30
38	4	89	A	C8-N9-C4	6.68	108.47	105.80
36	5	3102	G	C5-C6-O6	6.68	132.61	128.60
36	5	3218	A	N1-C6-N6	6.68	122.61	118.60
68	o2	33	ARG	NE-CZ-NH1	6.68	123.64	120.30
36	1	2302	G	N1-C2-N2	-6.68	110.19	116.20
36	5	2429	G	C8-N9-C4	-6.68	103.73	106.40
36	1	2846	U	N1-C2-O2	6.67	127.47	122.80
36	5	938	C	C6-N1-C2	6.67	122.97	120.30
36	5	2169	G	N1-C6-O6	-6.67	115.90	119.90
36	1	229	G	N3-C2-N2	-6.67	115.23	119.90
36	1	722	G	O5'-P-OP1	-6.67	99.70	105.70
36	5	641	C	N1-C2-N3	6.67	123.87	119.20
36	5	2726	C	C4-C5-C6	6.67	120.73	117.40
36	1	360	G	C4-C5-N7	6.67	113.47	110.80
36	5	1547	G	O5'-P-OP1	-6.67	99.70	105.70
36	1	678	G	C5-C6-O6	-6.66	124.60	128.60
36	1	2786	G	O5'-P-OP2	-6.66	99.70	105.70
37	3	81	U	C6-N1-C2	6.66	125.00	121.00
36	1	641	C	C2-N1-C1'	-6.66	111.47	118.80
36	1	1494	U	N3-C4-O4	-6.66	114.74	119.40
36	5	908	G	O5'-P-OP1	6.66	118.69	110.70
78	Q2	87	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	6	1614	A	C4-C5-N7	6.66	114.03	110.70
36	5	908	G	N3-C4-N9	6.66	130.00	126.00
36	5	3137	C	N3-C4-N4	-6.66	113.34	118.00
36	5	3173	G	C5-C6-O6	-6.66	124.60	128.60
36	1	909	G	C5-N7-C8	6.66	107.63	104.30
36	5	217	U	OP1-P-O3'	6.66	119.85	105.20
36	1	344	A	N1-C6-N6	-6.66	114.61	118.60
36	1	1007	U	C5-C4-O4	-6.66	121.91	125.90
36	5	359	U	OP1-P-OP2	-6.66	109.62	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	346	C	C4-C5-C6	6.65	120.73	117.40
36	1	2846	U	N3-C4-O4	-6.65	114.74	119.40
1	6	113	U	N1-C2-O2	-6.65	118.14	122.80
1	6	1535	U	N3-C2-O2	-6.65	117.54	122.20
36	5	3009	G	O5'-P-OP1	-6.65	99.72	105.70
36	1	636	C	O5'-P-OP2	6.65	118.68	110.70
36	5	205	C	C6-N1-C2	-6.65	117.64	120.30
36	5	3003	G	N3-C4-N9	-6.65	122.01	126.00
36	1	1741	A	C2-N3-C4	-6.64	107.28	110.60
36	5	2400	G	N1-C6-O6	6.64	123.89	119.90
36	1	963	G	C8-N9-C4	6.64	109.06	106.40
1	2	1448	G	O5'-P-OP1	-6.64	99.72	105.70
36	1	2861	U	O5'-P-OP2	6.64	118.67	110.70
36	1	3344	A	C6-C5-N7	-6.64	127.65	132.30
1	6	144	U	N1-C2-N3	6.64	118.88	114.90
36	5	2188	A	C8-N9-C4	6.64	108.45	105.80
36	5	1547	G	C2-N3-C4	-6.64	108.58	111.90
36	5	3060	C	C5-C4-N4	-6.64	115.55	120.20
36	5	935	U	C5-C6-N1	-6.63	119.38	122.70
37	7	92	A	N1-C6-N6	6.63	122.58	118.60
37	3	86	U	N1-C2-O2	-6.63	118.16	122.80
36	1	3369	G	C5-C6-O6	-6.63	124.62	128.60
36	5	1192	C	N1-C2-O2	6.63	122.88	118.90
36	5	2192	C	O5'-P-OP2	-6.63	99.73	105.70
36	5	3086	A	OP1-P-OP2	-6.63	109.65	119.60
36	1	2805	G	N3-C2-N2	6.63	124.54	119.90
36	5	1284	C	P-O3'-C3'	6.63	127.65	119.70
1	6	1749	A	N1-C6-N6	6.62	122.58	118.60
37	7	101	G	C8-N9-C4	6.62	109.05	106.40
36	1	504	A	C5-N7-C8	6.62	107.21	103.90
36	5	1489	A	C5-C6-N6	-6.62	118.40	123.70
36	5	2905	U	N3-C4-C5	6.62	118.57	114.60
36	1	2384	A	C5-C6-N6	-6.62	118.41	123.70
36	1	2983	C	C2-N3-C4	-6.62	116.59	119.90
36	5	578	A	O5'-P-OP2	6.62	118.64	110.70
1	2	507	U	N3-C2-O2	-6.62	117.57	122.20
1	6	113	U	C2-N1-C1'	-6.62	109.76	117.70
36	5	2298	U	N3-C4-C5	6.61	118.57	114.60
6	s4	38	LEU	CA-CB-CG	6.61	130.51	115.30
36	5	2904	U	N1-C2-N3	6.61	118.87	114.90
36	1	283	G	O4'-C1'-N9	-6.61	102.91	108.20
36	1	1432	C	C5-C4-N4	-6.61	115.57	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3053	G	N1-C6-O6	-6.61	115.94	119.90
36	5	1461	A	N7-C8-N9	-6.61	110.50	113.80
1	6	767	U	N3-C2-O2	-6.60	117.58	122.20
37	7	90	U	C5-C4-O4	-6.60	121.94	125.90
36	1	206	G	N1-C6-O6	-6.60	115.94	119.90
1	6	308	C	C2-N1-C1'	-6.60	111.54	118.80
37	7	46	A	C8-N9-C4	-6.60	103.16	105.80
36	1	1859	A	C8-N9-C4	6.59	108.44	105.80
36	1	2137	U	O4'-C1'-N1	6.59	113.47	108.20
36	5	283	G	N1-C6-O6	6.59	123.86	119.90
36	1	1555	U	N1-C2-O2	-6.59	118.19	122.80
36	1	2572	C	C6-N1-C1'	-6.59	112.89	120.80
36	5	2803	A	O5'-P-OP2	-6.59	99.77	105.70
1	2	1585	U	O5'-P-OP2	-6.59	99.77	105.70
36	5	2920	U	C2-N3-C4	-6.59	123.05	127.00
36	5	2639	G	N3-C4-N9	6.59	129.95	126.00
1	6	430	G	O5'-P-OP1	-6.59	99.77	105.70
1	6	558	U	N1-C2-O2	6.59	127.41	122.80
36	5	1192	C	N3-C2-O2	-6.59	117.29	121.90
36	5	2968	G	C5-C6-O6	6.59	132.55	128.60
36	5	2935	U	O5'-P-OP2	-6.58	99.77	105.70
36	1	708	G	C5-C6-N1	6.58	114.79	111.50
1	6	782	U	N1-C2-O2	6.58	127.41	122.80
36	5	2968	G	C8-N9-C4	6.58	109.03	106.40
36	1	878	G	OP1-P-O3'	6.58	119.68	105.20
36	1	1144	U	C2-N3-C4	-6.58	123.05	127.00
36	5	1486	G	N1-C6-O6	-6.58	115.95	119.90
36	5	2130	G	N1-C6-O6	-6.58	115.95	119.90
37	7	51	A	C8-N9-C4	-6.58	103.17	105.80
1	2	1111	G	O5'-P-OP1	6.58	118.59	110.70
36	1	200	C	C2-N1-C1'	6.58	126.04	118.80
36	5	519	A	N1-C6-N6	6.58	122.55	118.60
36	1	972	A	C8-N9-C4	6.58	108.43	105.80
36	5	982	C	OP2-P-O3'	6.58	119.67	105.20
36	5	3018	C	O5'-P-OP1	6.58	118.59	110.70
36	5	3317	U	C5-C4-O4	6.58	129.84	125.90
36	1	1379	G	N1-C6-O6	-6.57	115.96	119.90
36	1	2514	U	O5'-P-OP2	-6.57	99.79	105.70
36	5	76	G	C8-N9-C4	6.57	109.03	106.40
36	1	2278	C	C5-C6-N1	6.57	124.28	121.00
36	5	2385	G	C5-C6-O6	-6.57	124.66	128.60
35	SM	167	PRO	N-CA-CB	6.57	111.18	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1148	G	N3-C2-N2	6.57	124.50	119.90
38	4	90	U	C6-N1-C2	6.57	124.94	121.00
36	5	682	U	C5-C4-O4	-6.57	121.96	125.90
36	1	1555	U	C6-N1-C1'	6.57	130.39	121.20
36	1	2356	A	C5-N7-C8	-6.57	100.62	103.90
36	1	2397	A	O5'-P-OP1	6.56	118.58	110.70
1	6	337	G	N1-C6-O6	6.56	123.84	119.90
36	1	186	U	OP1-P-OP2	-6.56	109.76	119.60
1	6	1560	U	C5-C4-O4	6.56	129.84	125.90
36	5	2395	G	C8-N9-C4	6.56	109.03	106.40
1	2	61	A	N7-C8-N9	6.56	117.08	113.80
36	1	2904	U	N3-C4-C5	6.56	118.53	114.60
75	O9	45	ARG	NE-CZ-NH2	-6.56	117.02	120.30
36	5	825	U	N1-C2-O2	6.56	127.39	122.80
36	1	2149	A	O5'-P-OP1	-6.56	99.80	105.70
36	5	1591	G	N1-C6-O6	-6.56	115.97	119.90
1	2	142	G	N1-C6-O6	6.55	123.83	119.90
36	1	634	C	N1-C2-O2	6.55	122.83	118.90
36	5	810	A	N1-C2-N3	-6.55	126.02	129.30
36	1	1434	G	C5-C6-O6	-6.55	124.67	128.60
36	1	2373	A	C8-N9-C4	-6.55	103.18	105.80
36	1	3318	G	C8-N9-C4	-6.55	103.78	106.40
1	6	101	U	N1-C2-O2	6.55	127.39	122.80
1	2	1339	C	OP1-P-O3'	6.55	119.61	105.20
36	1	2610	G	N1-C6-O6	-6.55	115.97	119.90
36	5	3212	C	N1-C2-O2	-6.55	114.97	118.90
36	1	980	A	N7-C8-N9	6.55	117.07	113.80
1	6	1126	G	C5-C6-O6	6.55	132.53	128.60
36	5	519	A	C8-N9-C4	6.55	108.42	105.80
36	5	974	G	N3-C4-C5	-6.55	125.33	128.60
36	5	2700	G	C8-N9-C4	-6.55	103.78	106.40
1	6	542	A	C8-N9-C4	-6.54	103.18	105.80
36	5	966	U	O5'-P-OP2	-6.54	99.81	105.70
36	5	1449	A	C5-C6-N1	-6.54	114.43	117.70
36	5	1931	U	C5-C6-N1	-6.54	119.43	122.70
36	1	2941	A	O4'-C1'-N9	-6.54	102.97	108.20
36	5	2148	U	N1-C2-O2	-6.54	118.22	122.80
36	1	423	A	C5-C6-N1	-6.54	114.43	117.70
36	1	2993	G	N9-C4-C5	-6.54	102.78	105.40
36	1	1918	C	C6-N1-C2	-6.54	117.69	120.30
36	1	1440	G	C5-C6-O6	6.53	132.52	128.60
36	1	3344	A	C4-C5-N7	6.53	113.97	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	3	102	A	N1-C2-N3	-6.53	126.03	129.30
36	5	1879	A	C6-C5-N7	-6.53	127.73	132.30
36	5	1208	U	C5-C6-N1	-6.53	119.43	122.70
36	1	631	U	C2-N3-C4	-6.53	123.08	127.00
36	1	1581	C	N3-C2-O2	-6.53	117.33	121.90
1	6	1119	G	C8-N9-C4	-6.53	103.79	106.40
36	5	2139	A	C5-C6-N1	-6.53	114.44	117.70
36	5	2139	A	C5-C6-N6	6.53	128.93	123.70
1	6	272	U	P-O3'-C3'	6.53	127.53	119.70
36	1	2924	U	C5-C6-N1	-6.53	119.44	122.70
36	5	1042	U	N3-C2-O2	-6.53	117.63	122.20
36	1	1127	G	C5-C6-O6	-6.53	124.69	128.60
36	5	2211	U	N3-C2-O2	-6.53	117.63	122.20
1	2	1241	G	C4-C5-N7	6.52	113.41	110.80
36	1	3309	G	C4-C5-N7	6.52	113.41	110.80
47	M0	24	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	6	1509	C	N3-C2-O2	-6.52	117.33	121.90
36	5	1395	G	C5-C6-O6	-6.52	124.69	128.60
36	5	2908	G	C4-C5-N7	-6.52	108.19	110.80
36	1	2905	U	N3-C2-O2	6.52	126.77	122.20
48	m1	112	LEU	CA-CB-CG	6.52	130.30	115.30
36	1	1822	C	C6-N1-C2	-6.52	117.69	120.30
36	5	2821	C	N1-C2-O2	-6.52	114.99	118.90
36	1	1548	C	N1-C2-O2	-6.52	114.99	118.90
36	5	2327	U	C2-N3-C4	-6.52	123.09	127.00
36	5	2901	G	N1-C6-O6	6.52	123.81	119.90
36	5	326	U	N3-C2-O2	6.51	126.76	122.20
52	m6	84	LEU	CB-CG-CD1	-6.51	99.93	111.00
36	1	817	A	OP1-P-O3'	6.51	119.52	105.20
36	5	2514	U	O5'-P-OP1	-6.51	99.84	105.70
36	5	3337	G	C5-C6-O6	6.51	132.50	128.60
36	1	2281	A	C8-N9-C4	6.51	108.40	105.80
25	d3	33	LEU	CA-CB-CG	-6.51	100.34	115.30
36	5	3050	U	C5-C4-O4	6.50	129.80	125.90
36	1	608	A	C6-C5-N7	-6.50	127.75	132.30
36	5	1331	U	O4'-C1'-N1	-6.50	103.00	108.20
1	2	704	C	N1-C2-O2	6.50	122.80	118.90
1	2	1486	G	C4-C5-N7	6.50	113.40	110.80
36	1	652	G	N1-C2-N2	-6.50	110.35	116.20
36	5	3012	A	N9-C4-C5	-6.50	103.20	105.80
36	1	894	G	OP1-P-O3'	6.49	119.49	105.20
36	5	950	G	C5-C6-N1	6.49	114.75	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	776	U	C2-N3-C4	-6.49	123.11	127.00
1	2	1200	G	N1-C2-N2	6.49	122.04	116.20
36	5	3123	A	N1-C2-N3	-6.49	126.06	129.30
1	6	868	G	C4-C5-N7	6.49	113.39	110.80
36	1	797	U	N3-C4-C5	6.49	118.49	114.60
36	5	2701	U	C5-C4-O4	-6.49	122.01	125.90
36	5	2843	U	N3-C2-O2	-6.49	117.66	122.20
36	5	3041	U	N3-C4-C5	6.49	118.49	114.60
49	m3	85	LEU	CA-CB-CG	6.49	130.22	115.30
36	1	69	C	O5'-P-OP2	-6.48	99.87	105.70
36	1	645	A	N3-C4-N9	6.48	132.59	127.40
38	4	30	C	C5-C4-N4	6.48	124.74	120.20
36	5	981	U	C5-C6-N1	6.48	125.94	122.70
38	4	32	C	N3-C2-O2	6.48	126.44	121.90
36	5	2337	C	N3-C4-C5	6.48	124.49	121.90
36	5	2920	U	C5-C4-O4	-6.48	122.01	125.90
1	2	1430	U	C5-C4-O4	6.48	129.79	125.90
36	1	716	A	N1-C6-N6	6.48	122.49	118.60
36	1	2897	A	C8-N9-C4	6.48	108.39	105.80
1	6	1082	C	C6-N1-C2	-6.48	117.71	120.30
36	1	988	U	C5-C6-N1	-6.48	119.46	122.70
36	5	1292	C	O5'-P-OP1	-6.48	99.87	105.70
36	1	898	U	C5-C4-O4	-6.47	122.02	125.90
38	4	96	A	O5'-P-OP1	-6.47	99.87	105.70
36	1	1113	G	C4-C5-N7	-6.47	108.21	110.80
36	1	1440	G	N3-C2-N2	6.47	124.43	119.90
36	1	2385	G	O5'-P-OP2	6.47	118.47	110.70
37	3	86	U	N3-C4-O4	6.47	123.93	119.40
36	5	116	A	O5'-P-OP1	-6.47	99.88	105.70
36	5	663	C	N1-C2-O2	-6.47	115.02	118.90
36	5	649	A	N7-C8-N9	6.47	117.04	113.80
36	5	1910	A	OP2-P-O3'	6.47	119.44	105.20
36	1	2632	G	N3-C2-N2	6.47	124.43	119.90
1	6	542	A	C4-C5-N7	6.47	113.94	110.70
36	5	1123	U	C5-C6-N1	-6.47	119.47	122.70
36	5	2654	C	OP2-P-O3'	6.47	119.43	105.20
1	2	737	A	O4'-C1'-N9	6.47	113.37	108.20
36	1	2361	A	C8-N9-C4	-6.46	103.21	105.80
36	5	3128	G	N9-C4-C5	-6.46	102.81	105.40
36	5	907	G	O5'-P-OP1	-6.46	99.89	105.70
36	5	1168	U	N3-C4-O4	-6.46	114.88	119.40
36	5	1389	G	C4-C5-N7	6.46	113.38	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	m8	178	ARG	NE-CZ-NH2	-6.46	117.07	120.30
36	1	2979	U	C2-N3-C4	-6.46	123.12	127.00
38	4	120	C	N1-C2-O2	-6.46	115.02	118.90
1	2	139	C	C6-N1-C2	-6.46	117.72	120.30
36	1	278	U	N1-C2-N3	6.46	118.77	114.90
36	1	1313	G	C5-C6-O6	-6.46	124.73	128.60
36	1	2339	C	C6-N1-C2	-6.46	117.72	120.30
36	5	361	A	N1-C6-N6	-6.46	114.73	118.60
36	5	1307	G	N3-C2-N2	6.46	124.42	119.90
36	5	2790	A	O5'-P-OP2	-6.46	99.89	105.70
36	1	649	A	OP1-P-OP2	-6.45	109.92	119.60
36	1	3002	C	N3-C4-C5	6.45	124.48	121.90
1	6	1637	C	C6-N1-C2	6.45	122.88	120.30
36	5	591	G	N1-C6-O6	6.45	123.77	119.90
36	5	1908	A	C8-N9-C4	-6.45	103.22	105.80
36	1	143	G	N1-C6-O6	-6.45	116.03	119.90
36	1	1331	U	O4'-C1'-N1	-6.45	103.04	108.20
1	6	17	C	C6-N1-C2	-6.45	117.72	120.30
36	5	200	C	OP2-P-O3'	6.45	119.38	105.20
36	5	2292	U	N3-C2-O2	-6.45	117.69	122.20
1	2	402	C	C6-N1-C2	6.45	122.88	120.30
36	5	1337	A	C8-N9-C4	-6.45	103.22	105.80
36	1	1604	G	C4-N9-C1'	6.44	134.88	126.50
36	1	645	A	N3-C4-C5	-6.44	122.29	126.80
36	1	2550	U	N3-C4-O4	-6.44	114.89	119.40
36	1	2798	C	C5-C4-N4	6.44	124.71	120.20
36	1	2802	A	N1-C6-N6	-6.44	114.73	118.60
1	6	57	G	O5'-P-OP1	6.44	118.43	110.70
36	1	1310	G	C4-C5-N7	6.44	113.38	110.80
36	1	2891	U	C5-C4-O4	-6.44	122.04	125.90
36	1	2952	G	N1-C6-O6	6.44	123.77	119.90
1	6	1634	C	N3-C2-O2	-6.44	117.39	121.90
36	5	2426	U	N3-C2-O2	-6.44	117.69	122.20
36	5	3185	U	OP1-P-O3'	6.44	119.37	105.20
36	1	637	C	C6-N1-C2	-6.44	117.72	120.30
36	5	1592	G	N3-C2-N2	6.44	124.41	119.90
1	6	1783	C	O5'-P-OP2	-6.44	99.91	105.70
36	5	2623	G	OP1-P-OP2	-6.44	109.94	119.60
36	1	936	A	C8-N9-C4	6.43	108.37	105.80
36	1	942	U	OP1-P-OP2	-6.43	109.95	119.60
36	5	1330	A	O5'-P-OP1	-6.43	99.91	105.70
36	1	2867	C	C5-C4-N4	6.43	124.70	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	L4	95	ARG	NE-CZ-NH1	6.43	123.52	120.30
36	5	93	C	N3-C4-C5	-6.43	119.33	121.90
36	5	2827	U	O4'-C1'-N1	6.43	113.35	108.20
36	1	637	C	P-O3'-C3'	6.43	127.42	119.70
36	1	1335	C	N3-C2-O2	-6.43	117.40	121.90
36	1	1931	U	C2-N1-C1'	-6.43	109.98	117.70
36	1	2305	G	C6-C5-N7	-6.43	126.54	130.40
36	1	3207	U	N1-C2-N3	6.43	118.76	114.90
64	N8	115	LYS	C-N-CA	-6.43	108.80	122.30
41	14	90	PHE	C-N-CA	-6.43	108.80	122.30
36	5	1115	G	C4-C5-N7	6.43	113.37	110.80
36	1	2679	A	N1-C6-N6	6.43	122.45	118.60
36	1	2870	C	C6-N1-C1'	6.43	128.51	120.80
36	5	645	A	N1-C2-N3	6.43	132.51	129.30
36	5	2650	U	C2-N3-C4	-6.43	123.14	127.00
1	2	499	U	C2-N1-C1'	6.42	125.41	117.70
36	1	2380	U	C5-C4-O4	-6.42	122.05	125.90
36	5	1006	A	O5'-P-OP2	-6.42	99.92	105.70
36	1	2988	C	N3-C4-N4	-6.42	113.51	118.00
36	5	200	C	C6-N1-C1'	-6.42	113.10	120.80
36	1	3278	C	C6-N1-C2	-6.42	117.73	120.30
36	5	3078	U	C2-N1-C1'	6.42	125.40	117.70
36	5	41	G	N1-C6-O6	6.42	123.75	119.90
36	5	2814	G	N3-C2-N2	6.42	124.39	119.90
56	N0	58	ILE	CG1-CB-CG2	-6.42	97.29	111.40
36	5	2376	G	C5-C6-O6	6.41	132.45	128.60
36	1	2338	C	N1-C2-O2	6.41	122.75	118.90
36	5	1751	G	O5'-P-OP2	-6.41	99.93	105.70
36	5	949	C	N1-C2-O2	-6.41	115.06	118.90
37	7	101	G	N9-C4-C5	-6.41	102.84	105.40
36	1	2278	C	N3-C4-N4	-6.41	113.52	118.00
36	5	386	A	N1-C6-N6	6.41	122.44	118.60
36	5	1452	A	N9-C4-C5	-6.41	103.24	105.80
36	5	2881	C	C2-N3-C4	-6.41	116.70	119.90
1	2	1432	U	C6-N1-C2	6.40	124.84	121.00
1	2	1462	G	C5-C6-O6	-6.40	124.76	128.60
1	2	1652	C	C5-C6-N1	6.40	124.20	121.00
36	1	2797	C	N3-C2-O2	6.40	126.38	121.90
36	1	2836	C	N3-C2-O2	-6.40	117.42	121.90
1	6	944	A	C8-N9-C4	-6.40	103.24	105.80
36	5	2911	A	OP1-P-O3'	6.40	119.29	105.20
36	1	1605	A	O4'-C1'-N9	6.40	113.32	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	844	G	C8-N9-C4	6.40	108.96	106.40
36	5	1300	G	C5-C6-O6	-6.40	124.76	128.60
36	5	2816	G	O4'-C1'-N9	6.40	113.32	108.20
36	1	1904	C	C6-N1-C2	-6.40	117.74	120.30
36	5	1159	A	O5'-P-OP1	-6.40	99.94	105.70
36	1	859	G	N1-C2-N2	-6.39	110.44	116.20
1	6	194	U	N1-C2-O2	6.39	127.28	122.80
1	6	1614	A	N1-C6-N6	6.39	122.44	118.60
1	6	1663	G	C8-N9-C4	-6.39	103.84	106.40
36	1	517	G	C8-N9-C4	-6.39	103.84	106.40
36	1	871	U	N1-C2-O2	-6.39	118.33	122.80
36	5	685	G	N1-C6-O6	-6.39	116.06	119.90
36	1	2879	C	N1-C2-O2	-6.39	115.06	118.90
36	5	2993	G	N3-C4-N9	6.39	129.83	126.00
36	1	1297	C	C5-C6-N1	-6.39	117.81	121.00
36	1	2996	U	C2-N1-C1'	6.39	125.37	117.70
36	5	1178	G	N1-C2-N2	6.39	121.95	116.20
1	2	4	C	O5'-P-OP1	-6.39	99.95	105.70
36	1	49	A	C5-C6-N1	-6.39	114.51	117.70
36	5	1208	U	N3-C2-O2	-6.39	117.73	122.20
1	6	1596	C	N3-C4-N4	-6.38	113.53	118.00
36	1	329	U	N1-C2-O2	-6.38	118.33	122.80
36	1	2188	A	N1-C6-N6	-6.38	114.77	118.60
36	1	2409	G	C8-N9-C4	-6.38	103.85	106.40
36	1	59	G	O5'-P-OP1	6.38	118.36	110.70
36	5	2245	C	C6-N1-C2	-6.38	117.75	120.30
36	5	2409	G	C5-C6-O6	6.38	132.43	128.60
36	1	665	A	N1-C6-N6	-6.38	114.77	118.60
36	5	3178	A	O5'-P-OP1	-6.38	99.96	105.70
38	4	63	G	C8-N9-C4	-6.38	103.85	106.40
36	5	1793	C	N3-C4-C5	-6.38	119.35	121.90
36	5	1841	A	C8-N9-C4	-6.38	103.25	105.80
1	2	1131	A	C8-N9-C4	6.38	108.35	105.80
36	1	2104	A	C8-N9-C4	6.37	108.35	105.80
36	1	2899	C	P-O3'-C3'	6.37	127.35	119.70
36	1	2314	U	C6-N1-C1'	-6.37	112.28	121.20
36	1	2412	G	N9-C4-C5	6.37	107.95	105.40
36	1	3054	U	C5-C6-N1	-6.37	119.52	122.70
36	5	810	A	C2-N3-C4	6.37	113.78	110.60
36	5	1371	G	C5-C6-N1	6.37	114.68	111.50
36	5	1588	A	C8-N9-C4	6.37	108.35	105.80
36	1	3344	A	C2-N3-C4	-6.37	107.42	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1568	C	P-O3'-C3'	6.37	127.34	119.70
36	1	2758	A	C5-C6-N1	6.37	120.88	117.70
36	5	811	U	C5-C4-O4	-6.37	122.08	125.90
36	5	819	U	C5-C6-N1	-6.37	119.52	122.70
36	5	957	C	C2-N3-C4	-6.37	116.72	119.90
36	1	1454	A	O5'-P-OP1	-6.36	99.97	105.70
36	1	1493	G	O4'-C1'-N9	6.36	113.29	108.20
36	5	1878	G	C4-N9-C1'	6.36	134.77	126.50
36	5	2655	U	C5-C4-O4	6.36	129.72	125.90
38	4	125	U	C2-N1-C1'	6.36	125.33	117.70
36	5	2403	G	O5'-P-OP2	-6.36	99.98	105.70
36	1	317	A	C8-N9-C4	-6.36	103.26	105.80
36	1	2392	C	C2-N3-C4	-6.36	116.72	119.90
36	1	2795	U	O5'-P-OP1	-6.36	99.98	105.70
1	6	1774	G	N1-C6-O6	-6.36	116.09	119.90
36	5	1340	G	N1-C6-O6	-6.36	116.08	119.90
36	5	2340	U	N3-C2-O2	-6.36	117.75	122.20
36	5	3196	U	C2-N1-C1'	-6.36	110.07	117.70
1	2	142	G	N3-C2-N2	-6.36	115.45	119.90
36	1	24	G	N3-C2-N2	-6.36	115.45	119.90
36	1	360	G	N1-C6-O6	6.36	123.71	119.90
36	5	2856	G	C4-C5-N7	6.35	113.34	110.80
36	5	3016	A	OP2-P-O3'	6.35	119.18	105.20
36	1	2986	U	C5-C6-N1	-6.35	119.52	122.70
36	1	1417	G	C8-N9-C4	6.35	108.94	106.40
36	1	3078	U	N3-C2-O2	-6.35	117.75	122.20
36	1	981	U	O5'-P-OP2	-6.35	99.99	105.70
36	1	1297	C	C6-N1-C2	6.35	122.84	120.30
36	5	775	A	N1-C6-N6	-6.34	114.80	118.60
36	5	2131	A	N1-C6-N6	6.34	122.40	118.60
1	2	1455	G	C4-C5-N7	-6.34	108.27	110.80
1	6	1082	C	N1-C2-O2	6.33	122.70	118.90
37	7	102	A	C8-N9-C4	6.33	108.33	105.80
1	2	1748	G	N9-C4-C5	6.33	107.93	105.40
36	1	1379	G	C5-C6-O6	6.33	132.40	128.60
36	1	3319	U	P-O3'-C3'	6.33	127.30	119.70
52	M6	84	LEU	CB-CG-CD2	-6.33	100.23	111.00
36	5	893	C	N3-C4-C5	-6.33	119.37	121.90
38	8	90	U	C6-N1-C2	6.33	124.80	121.00
1	2	137	U	N1-C2-O2	6.33	127.23	122.80
36	1	1175	C	C2-N3-C4	-6.33	116.73	119.90
36	5	437	G	N3-C2-N2	-6.33	115.47	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1136	A	C6-N1-C2	-6.33	114.80	118.60
1	6	114	C	N1-C2-O2	6.33	122.70	118.90
1	6	1473	U	C2-N1-C1'	6.33	125.29	117.70
36	5	2654	C	C5-C6-N1	-6.33	117.84	121.00
36	1	637	C	OP2-P-O3'	-6.33	91.28	105.20
36	5	1118	C	O5'-P-OP1	-6.33	100.01	105.70
36	5	3275	U	N3-C2-O2	-6.33	117.77	122.20
36	1	1175	C	O5'-P-OP2	6.32	118.29	110.70
36	5	1404	G	N1-C6-O6	-6.32	116.11	119.90
36	1	67	A	O5'-P-OP1	-6.32	100.01	105.70
38	4	45	C	O5'-P-OP2	-6.32	100.01	105.70
36	5	2341	A	N7-C8-N9	-6.32	110.64	113.80
36	5	3306	U	N3-C4-C5	6.32	118.39	114.60
59	n3	48	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	2	73	U	OP1-P-O3'	6.32	119.10	105.20
36	5	2326	A	C8-N9-C4	6.32	108.33	105.80
36	1	1118	C	C6-N1-C2	-6.32	117.77	120.30
36	5	3245	A	C5-C6-N1	-6.32	114.54	117.70
36	5	2248	C	C5-C6-N1	-6.32	117.84	121.00
36	5	2833	A	N1-C6-N6	-6.32	114.81	118.60
36	5	2899	C	C5-C6-N1	-6.32	117.84	121.00
1	6	539	G	N7-C8-N9	6.31	116.26	113.10
36	5	2202	C	N3-C4-N4	6.31	122.42	118.00
36	1	2328	U	N3-C4-O4	-6.31	114.98	119.40
1	2	765	G	C5-C6-O6	-6.31	124.81	128.60
36	1	362	U	N3-C4-O4	-6.31	114.98	119.40
36	1	1450	G	O5'-P-OP2	6.31	118.27	110.70
36	1	2395	G	N3-C2-N2	6.31	124.32	119.90
10	S8	29	LEU	CA-CB-CG	6.31	129.81	115.30
1	6	1473	U	C5-C4-O4	6.31	129.69	125.90
36	1	2827	U	N1-C2-O2	-6.31	118.39	122.80
36	5	1660	C	C6-N1-C2	-6.31	117.78	120.30
1	2	359	A	C8-N9-C4	6.30	108.32	105.80
1	2	408	C	N1-C2-O2	-6.30	115.12	118.90
36	1	364	G	O5'-P-OP1	-6.30	100.03	105.70
36	1	2986	U	N1-C2-N3	6.30	118.68	114.90
36	1	2719	U	C5-C6-N1	-6.30	119.55	122.70
36	5	856	G	N1-C6-O6	6.30	123.68	119.90
36	5	3043	C	N3-C4-N4	-6.30	113.59	118.00
36	5	3181	C	O5'-P-OP2	-6.30	100.03	105.70
36	1	416	A	N1-C6-N6	-6.30	114.82	118.60
36	1	2983	C	C2-N1-C1'	6.30	125.73	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3382	U	C2-N1-C1'	6.30	125.26	117.70
36	5	426	G	N1-C6-O6	-6.30	116.12	119.90
36	5	1193	A	C8-N9-C4	-6.30	103.28	105.80
36	1	1141	C	N3-C4-C5	-6.30	119.38	121.90
36	1	1364	C	N3-C4-N4	-6.30	113.59	118.00
36	5	41	G	C5-C6-O6	-6.30	124.82	128.60
36	5	672	A	C8-N9-C4	-6.30	103.28	105.80
1	2	607	G	N1-C6-O6	6.30	123.68	119.90
36	5	1847	A	N3-C4-C5	6.30	131.21	126.80
36	5	1925	U	C5-C4-O4	-6.30	122.12	125.90
36	1	112	U	N1-C1'-C2'	-6.30	105.07	112.00
36	1	582	G	O5'-P-OP2	-6.30	100.03	105.70
36	1	716	A	N9-C4-C5	-6.30	103.28	105.80
36	1	1919	G	C8-N9-C4	-6.30	103.88	106.40
1	6	609	U	C4-C5-C6	6.30	123.48	119.70
1	6	1000	C	C2-N3-C4	-6.30	116.75	119.90
36	5	959	C	N3-C4-C5	6.30	124.42	121.90
38	4	21	C	N1-C2-O2	-6.29	115.12	118.90
1	6	1735	U	O5'-P-OP2	-6.29	100.03	105.70
36	1	2986	U	N3-C4-O4	-6.29	114.99	119.40
36	5	1307	G	OP1-P-O3'	6.29	119.04	105.20
36	5	1380	G	O5'-P-OP1	6.29	118.25	110.70
36	5	2977	G	C8-N9-C4	6.29	108.92	106.40
1	2	934	C	C6-N1-C1'	-6.29	113.25	120.80
1	6	1058	U	OP1-P-O3'	6.29	119.04	105.20
36	5	1882	G	O5'-P-OP1	-6.29	100.04	105.70
1	2	1145	U	N3-C4-O4	6.29	123.80	119.40
36	1	2385	G	N3-C4-C5	6.29	131.75	128.60
36	1	3275	U	OP1-P-O3'	6.29	119.04	105.20
36	5	1421	G	N3-C4-N9	-6.29	122.23	126.00
36	1	2366	C	C5-C6-N1	6.29	124.14	121.00
36	5	1375	G	N1-C2-N3	-6.29	120.13	123.90
36	1	346	C	C2-N3-C4	-6.29	116.76	119.90
36	5	2408	U	N1-C2-N3	6.29	118.67	114.90
1	6	1498	G	N1-C6-O6	-6.28	116.13	119.90
1	6	314	C	N3-C2-O2	-6.28	117.50	121.90
1	6	101	U	N3-C2-O2	-6.28	117.80	122.20
12	c0	97	PRO	N-CA-CB	6.28	110.84	103.30
36	5	426	G	C5-N7-C8	6.28	107.44	104.30
36	1	333	G	C5-C6-O6	6.28	132.37	128.60
36	1	2278	C	C6-N1-C2	-6.28	117.79	120.30
36	1	2278	C	N3-C4-C5	6.28	124.41	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2339	C	C5-C6-N1	6.28	124.14	121.00
36	1	2369	G	N3-C4-N9	6.28	129.77	126.00
36	5	3154	C	C2-N1-C1'	6.28	125.70	118.80
36	5	2346	C	C2-N3-C4	-6.27	116.76	119.90
1	2	554	C	C2-N1-C1'	6.27	125.70	118.80
36	1	97	U	N1-C2-N3	6.27	118.66	114.90
36	1	2188	A	C5-C6-N6	6.27	128.72	123.70
36	1	592	A	O5'-P-OP1	-6.27	100.06	105.70
36	5	297	G	O4'-C1'-N9	6.27	113.22	108.20
36	5	2765	C	C6-N1-C2	-6.27	117.79	120.30
1	6	158	U	P-O3'-C3'	6.27	127.22	119.70
36	1	686	G	C5-C6-O6	6.27	132.36	128.60
36	1	3055	U	C2-N1-C1'	6.27	125.22	117.70
36	5	2980	U	N1-C2-N3	6.27	118.66	114.90
36	5	339	C	C5-C4-N4	6.27	124.59	120.20
36	1	2827	U	C5-C6-N1	-6.26	119.57	122.70
36	1	3213	A	C6-C5-N7	-6.26	127.92	132.30
36	5	3216	G	O5'-P-OP2	-6.26	100.06	105.70
36	1	2714	G	C4-C5-C6	-6.26	115.04	118.80
36	5	1389	G	N1-C6-O6	6.26	123.66	119.90
36	5	1390	A	C5-C6-N6	6.26	128.71	123.70
36	1	960	U	N3-C2-O2	6.26	126.58	122.20
36	5	200	C	N1-C2-O2	6.26	122.66	118.90
36	5	2878	G	N1-C6-O6	-6.26	116.14	119.90
36	5	2883	U	N1-C2-O2	6.26	127.18	122.80
36	5	3377	G	C5-C6-O6	-6.26	124.84	128.60
1	2	1768	G	C4-C5-N7	-6.26	108.30	110.80
36	1	2800	G	N7-C8-N9	-6.26	109.97	113.10
1	6	308	C	C6-N1-C1'	6.26	128.31	120.80
1	6	801	G	N1-C6-O6	-6.26	116.14	119.90
36	5	217	U	C2-N3-C4	-6.26	123.24	127.00
36	5	2694	A	C2-N3-C4	6.26	113.73	110.60
36	1	2714	G	C6-N1-C2	6.26	128.85	125.10
36	1	3304	U	O5'-P-OP1	-6.26	100.07	105.70
38	4	32	C	C2-N1-C1'	-6.26	111.92	118.80
43	L6	31	ARG	NE-CZ-NH1	6.26	123.43	120.30
36	5	3138	U	N1-C2-N3	6.26	118.65	114.90
36	1	2726	C	N1-C2-O2	6.25	122.65	118.90
36	5	909	G	N7-C8-N9	-6.25	109.97	113.10
36	5	1049	C	N3-C4-C5	6.25	124.40	121.90
36	5	1305	U	C5-C6-N1	-6.25	119.57	122.70
1	2	1273	G	O4'-C1'-N9	6.25	113.20	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1659	A	C2-N3-C4	-6.25	107.47	110.60
36	5	2290	C	O5'-P-OP2	-6.25	100.07	105.70
36	5	2635	A	C5-C6-N6	6.25	128.70	123.70
36	5	2948	C	C4-C5-C6	-6.25	114.27	117.40
36	1	948	C	N1-C2-O2	-6.25	115.15	118.90
36	1	2382	G	C5-C6-O6	6.25	132.35	128.60
61	N5	115	ARG	NE-CZ-NH1	6.25	123.43	120.30
36	5	1376	C	O5'-P-OP1	-6.25	100.07	105.70
36	5	2684	C	O5'-P-OP2	-6.25	100.07	105.70
1	2	1782	A	C8-N9-C4	-6.25	103.30	105.80
36	5	2290	C	C5-C6-N1	-6.25	117.88	121.00
1	2	1731	A	O5'-P-OP2	-6.25	100.08	105.70
36	1	949	C	N3-C4-N4	6.25	122.37	118.00
36	1	3010	U	N3-C2-O2	-6.25	117.83	122.20
36	5	2719	U	C6-N1-C1'	6.25	129.94	121.20
36	1	2830	G	C4-C5-N7	-6.25	108.30	110.80
36	5	3274	A	N1-C6-N6	-6.25	114.85	118.60
36	1	1858	A	O4'-C1'-N9	6.24	113.19	108.20
1	6	387	A	C4-C5-N7	-6.24	107.58	110.70
36	5	2798	C	O5'-P-OP2	6.24	118.19	110.70
36	5	2928	C	N3-C4-C5	-6.24	119.40	121.90
36	5	3368	U	OP1-P-O3'	6.24	118.93	105.20
36	1	2818	U	C4-C5-C6	-6.24	115.95	119.70
36	5	981	U	C6-N1-C2	-6.24	117.25	121.00
1	2	1129	U	N3-C4-C5	6.24	118.34	114.60
36	1	412	G	C8-N9-C4	-6.24	103.90	106.40
36	1	637	C	C2-N3-C4	-6.24	116.78	119.90
36	1	2786	G	C8-N9-C4	-6.24	103.90	106.40
36	1	2870	C	N3-C4-N4	-6.24	113.63	118.00
52	M6	69	GLY	N-CA-C	-6.24	97.50	113.10
36	5	3123	A	N7-C8-N9	-6.24	110.68	113.80
49	m3	46	ILE	CG1-CB-CG2	-6.24	97.67	111.40
1	6	858	G	C5-N7-C8	-6.24	101.18	104.30
36	5	943	U	N3-C4-C5	6.24	118.34	114.60
39	12	216	HIS	N-CA-C	-6.24	94.16	111.00
1	2	728	U	N1-C2-O2	6.24	127.17	122.80
1	6	1544	U	O5'-P-OP2	-6.24	100.09	105.70
36	5	506	U	C2-N3-C4	-6.24	123.26	127.00
1	2	532	U	O5'-P-OP1	-6.24	100.09	105.70
36	1	816	A	C2-N3-C4	6.24	113.72	110.60
36	1	2948	C	N3-C4-C5	6.23	124.39	121.90
36	1	3079	U	C5-C6-N1	-6.23	119.58	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	48	U	C5-C4-O4	-6.23	122.16	125.90
36	5	1113	G	O5'-P-OP1	-6.23	100.09	105.70
36	5	2772	C	N1-C2-O2	-6.23	115.16	118.90
36	1	910	G	C8-N9-C4	-6.23	103.91	106.40
36	5	2363	A	N9-C4-C5	6.23	108.29	105.80
36	1	365	A	N1-C6-N6	6.23	122.34	118.60
37	7	1	G	N3-C4-N9	6.22	129.74	126.00
36	1	1434	G	O5'-P-OP2	-6.22	100.10	105.70
36	1	3181	C	C4-C5-C6	6.22	120.51	117.40
36	5	1419	A	N1-C6-N6	-6.22	114.87	118.60
1	2	507	U	C2-N1-C1'	6.22	125.17	117.70
1	2	1748	G	C8-N9-C4	-6.22	103.91	106.40
36	1	3344	A	N1-C6-N6	6.22	122.33	118.60
1	6	874	C	C2-N1-C1'	6.22	125.64	118.80
36	5	2634	U	N1-C2-N3	6.22	118.63	114.90
36	1	2877	G	C5-C6-O6	6.22	132.33	128.60
36	5	1381	A	C8-N9-C4	6.22	108.29	105.80
36	5	3174	A	C5-N7-C8	-6.22	100.79	103.90
1	2	554	C	C5-C6-N1	6.21	124.11	121.00
1	2	811	A	C8-N9-C4	-6.21	103.31	105.80
1	2	966	A	C8-N9-C4	6.21	108.29	105.80
36	5	3097	C	C6-N1-C2	-6.21	117.81	120.30
36	1	2175	U	C5-C6-N1	-6.21	119.59	122.70
36	5	3091	A	N1-C6-N6	-6.21	114.87	118.60
36	1	1307	G	OP1-P-O3'	6.21	118.86	105.20
36	1	1394	A	OP2-P-O3'	6.21	118.86	105.20
1	6	174	U	O5'-P-OP2	-6.21	100.11	105.70
36	5	2919	A	C5-C6-N6	6.21	128.67	123.70
36	1	2244	A	C8-N9-C4	6.21	108.28	105.80
36	5	2412	G	N3-C4-C5	-6.21	125.50	128.60
36	5	2634	U	C5-C4-O4	-6.21	122.17	125.90
36	1	1807	G	C8-N9-C4	-6.21	103.92	106.40
36	5	908	G	C8-N9-C1'	-6.21	118.93	127.00
36	5	1589	A	O4'-C1'-N9	-6.21	103.23	108.20
1	2	1429	G	O5'-P-OP1	-6.21	100.11	105.70
36	1	215	G	N9-C4-C5	6.21	107.88	105.40
36	1	317	A	O5'-P-OP2	-6.21	100.11	105.70
36	1	2827	U	N3-C4-O4	-6.21	115.06	119.40
36	5	3060	C	N3-C4-N4	6.21	122.34	118.00
36	1	2600	C	N3-C2-O2	-6.20	117.56	121.90
36	5	3217	C	C6-N1-C2	6.20	122.78	120.30
36	5	1604	G	C8-N9-C1'	-6.20	118.94	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2714	G	C4-C5-N7	6.20	113.28	110.80
36	5	2348	A	C8-N9-C4	-6.20	103.32	105.80
36	5	2524	A	N9-C1'-C2'	6.20	122.06	114.00
36	5	1116	G	N3-C4-C5	-6.20	125.50	128.60
36	5	1327	C	N3-C4-C5	6.20	124.38	121.90
36	1	658	G	O5'-P-OP2	-6.20	100.12	105.70
36	1	2872	A	C2-N3-C4	6.20	113.70	110.60
36	5	412	G	C5-C6-O6	6.20	132.32	128.60
36	5	1170	A	C5-N7-C8	6.20	107.00	103.90
36	1	1305	U	C5-C6-N1	-6.19	119.60	122.70
36	1	874	U	C6-N1-C2	6.19	124.72	121.00
36	1	1581	C	N1-C2-O2	6.19	122.61	118.90
48	M1	112	LEU	CA-CB-CG	6.19	129.54	115.30
1	6	1539	G	N3-C4-C5	6.19	131.70	128.60
1	2	1560	U	N1-C2-N3	6.19	118.61	114.90
36	1	362	U	C2-N3-C4	-6.19	123.28	127.00
36	5	721	G	N1-C6-O6	-6.19	116.19	119.90
36	5	876	A	OP1-P-OP2	-6.19	110.31	119.60
36	1	324	A	N1-C2-N3	6.19	132.39	129.30
36	1	1447	G	O5'-P-OP2	-6.19	100.13	105.70
36	1	2868	U	C6-N1-C2	6.19	124.71	121.00
36	5	94	G	C2-N3-C4	6.19	114.99	111.90
36	5	1301	A	N1-C6-N6	6.19	122.31	118.60
36	1	910	G	N9-C4-C5	6.18	107.87	105.40
36	1	2818	U	C5'-C4'-O4'	-6.18	101.68	109.10
36	5	577	C	N1-C2-O2	-6.18	115.19	118.90
36	5	1314	C	C5-C4-N4	-6.18	115.87	120.20
36	5	1852	G	N1-C6-O6	-6.18	116.19	119.90
36	5	2663	G	C5-C6-O6	-6.18	124.89	128.60
1	2	1258	U	N3-C2-O2	-6.18	117.87	122.20
36	5	2531	C	N1-C2-O2	6.18	122.61	118.90
36	5	3317	U	N3-C2-O2	-6.18	117.87	122.20
36	1	2373	A	N7-C8-N9	6.18	116.89	113.80
36	5	2292	U	N1-C2-O2	6.18	127.13	122.80
36	1	1156	C	C5-C4-N4	6.18	124.53	120.20
36	5	2694	A	N9-C4-C5	6.18	108.27	105.80
36	5	1902	G	N3-C4-N9	6.18	129.71	126.00
36	5	107	A	N1-C6-N6	-6.18	114.89	118.60
36	5	150	A	C5-C6-N6	-6.18	118.76	123.70
36	1	694	C	N3-C4-C5	6.17	124.37	121.90
36	1	959	C	N3-C4-N4	6.17	122.32	118.00
36	5	2385	G	N9-C4-C5	-6.17	102.93	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2820	A	C8-N9-C4	-6.17	103.33	105.80
1	6	1634	C	C6-N1-C1'	-6.17	113.39	120.80
1	6	1456	C	N3-C2-O2	-6.17	117.58	121.90
36	1	2409	G	N9-C4-C5	6.17	107.87	105.40
36	1	186	U	N3-C4-C5	6.17	118.30	114.60
37	3	93	C	N3-C4-C5	6.17	124.37	121.90
36	5	2800	G	N3-C4-N9	-6.17	122.30	126.00
36	1	521	A	N9-C4-C5	-6.17	103.33	105.80
36	1	2649	A	N1-C2-N3	-6.17	126.22	129.30
36	5	645	A	C5-C6-N1	6.17	120.78	117.70
76	q0	102	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	2	75	U	N3-C2-O2	-6.16	117.89	122.20
36	5	921	A	OP1-P-OP2	-6.16	110.36	119.60
36	5	2935	U	C5-C4-O4	-6.16	122.20	125.90
1	2	1761	U	C5-C4-O4	6.16	129.60	125.90
36	1	1108	U	OP2-P-O3'	6.16	118.75	105.20
36	1	2887	A	O5'-P-OP2	-6.16	100.16	105.70
36	5	929	A	O5'-P-OP2	-6.16	100.16	105.70
36	5	2361	A	C8-N9-C4	-6.16	103.34	105.80
68	o2	33	ARG	NE-CZ-NH2	-6.16	117.22	120.30
36	1	641	C	N3-C4-C5	6.16	124.36	121.90
36	5	3197	G	C2-N3-C4	-6.16	108.82	111.90
36	1	2408	U	C2-N3-C4	-6.16	123.31	127.00
35	sM	167	PRO	N-CA-CB	6.16	110.69	103.30
36	5	801	A	O5'-P-OP2	-6.15	100.16	105.70
36	5	912	G	N1-C6-O6	-6.15	116.21	119.90
36	5	2234	G	N9-C4-C5	-6.15	102.94	105.40
1	2	144	U	N3-C2-O2	-6.15	117.89	122.20
36	1	2948	C	C6-N1-C2	6.15	122.76	120.30
1	6	970	A	P-O3'-C3'	6.15	127.08	119.70
36	5	1152	G	N1-C2-N3	6.15	127.59	123.90
36	1	1411	C	N3-C4-N4	-6.15	113.69	118.00
36	1	2366	C	O5'-P-OP1	6.15	118.08	110.70
36	1	2740	A	C8-N9-C4	-6.15	103.34	105.80
36	1	614	C	C6-N1-C2	6.15	122.76	120.30
36	1	2308	C	N1-C2-O2	-6.15	115.21	118.90
36	1	2645	G	N9-C4-C5	6.15	107.86	105.40
1	6	1082	C	O5'-P-OP2	-6.15	100.17	105.70
36	5	1113	G	N7-C8-N9	-6.15	110.03	113.10
36	5	2955	U	N3-C2-O2	-6.15	117.90	122.20
36	5	2400	G	C6-C5-N7	-6.14	126.71	130.40
36	5	2404	A	O5'-P-OP2	6.14	118.07	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2979	U	O4'-C1'-N1	-6.14	103.28	108.20
36	1	2719	U	N1-C2-N3	6.14	118.59	114.90
36	1	3147	G	N1-C6-O6	-6.14	116.21	119.90
36	5	2639	G	C6-C5-N7	-6.14	126.72	130.40
36	1	3181	C	C2-N3-C4	-6.14	116.83	119.90
1	6	400	A	OP2-P-O3'	6.14	118.71	105.20
36	5	1839	A	N1-C6-N6	-6.14	114.92	118.60
36	1	120	G	C8-N9-C4	6.14	108.86	106.40
1	6	754	A	N1-C6-N6	6.14	122.28	118.60
36	1	1371	G	N7-C8-N9	-6.14	110.03	113.10
36	5	942	U	O5'-P-OP1	6.14	118.07	110.70
36	5	1159	A	N1-C2-N3	-6.14	126.23	129.30
37	3	100	C	N3-C4-C5	-6.14	119.44	121.90
1	6	44	U	N1-C2-O2	-6.14	118.50	122.80
36	5	2289	U	C2-N1-C1'	6.14	125.06	117.70
36	1	32	U	C2-N3-C4	-6.13	123.32	127.00
36	1	329	U	C6-N1-C1'	6.13	129.79	121.20
36	5	820	A	C8-N9-C4	-6.13	103.35	105.80
36	5	1942	U	N1-C2-O2	-6.13	118.51	122.80
1	2	728	U	N3-C2-O2	-6.13	117.91	122.20
36	1	2302	G	N3-C2-N2	6.13	124.19	119.90
1	2	1572	G	C4-C5-N7	6.13	113.25	110.80
37	3	82	G	C5-C6-O6	6.13	132.28	128.60
1	6	315	A	N9-C4-C5	6.13	108.25	105.80
36	5	1130	A	C5-N7-C8	6.13	106.97	103.90
36	5	1290	A	OP2-P-O3'	6.13	118.69	105.20
56	n0	40	ARG	NE-CZ-NH1	6.13	123.37	120.30
36	1	1444	G	N9-C4-C5	-6.13	102.95	105.40
36	1	1656	A	C8-N9-C4	6.13	108.25	105.80
36	5	2630	C	C2-N3-C4	-6.13	116.83	119.90
36	5	2872	A	C5-C6-N6	6.13	128.60	123.70
36	1	882	A	O5'-P-OP1	-6.13	100.19	105.70
36	1	1843	C	O5'-P-OP2	-6.13	100.19	105.70
36	1	1852	G	C6-N1-C2	6.13	128.78	125.10
36	1	1931	U	C5-C6-N1	-6.13	119.64	122.70
36	1	3214	U	N3-C4-O4	-6.13	115.11	119.40
36	1	1536	G	O5'-P-OP2	-6.12	100.19	105.70
36	5	994	G	N1-C6-O6	-6.12	116.22	119.90
1	2	400	A	O4'-C1'-N9	6.12	113.10	108.20
1	2	1748	G	C5-C6-O6	6.12	132.27	128.60
1	6	380	U	N3-C2-O2	-6.12	117.91	122.20
36	5	3382	U	C2-N1-C1'	6.12	125.05	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	369	A	N9-C4-C5	6.12	108.25	105.80
36	1	3172	A	C8-N9-C4	6.12	108.25	105.80
36	5	640	U	OP1-P-OP2	-6.12	110.42	119.60
36	5	3217	C	C2-N1-C1'	-6.12	112.07	118.80
36	1	606	C	N3-C2-O2	-6.12	117.62	121.90
36	1	806	A	C5-C6-N6	-6.12	118.81	123.70
37	3	90	U	C5-C4-O4	-6.12	122.23	125.90
36	5	644	G	C8-N9-C4	-6.12	103.95	106.40
40	L3	186	GLY	N-CA-C	6.12	128.39	113.10
36	1	609	G	C4-C5-N7	6.12	113.25	110.80
36	1	650	C	N1-C2-O2	-6.12	115.23	118.90
36	1	970	A	C5-N7-C8	-6.12	100.84	103.90
36	1	2343	C	N3-C4-C5	6.12	124.35	121.90
36	1	2372	A	C2-N3-C4	6.12	113.66	110.60
36	5	1899	G	C8-N9-C4	-6.12	103.95	106.40
36	5	2295	A	N9-C4-C5	-6.11	103.36	105.80
36	5	2744	U	N3-C2-O2	-6.11	117.92	122.20
1	6	387	A	C5-N7-C8	6.11	106.96	103.90
36	5	1461	A	C8-N9-C4	6.11	108.25	105.80
1	2	553	G	N1-C2-N2	6.11	121.70	116.20
36	1	3143	C	O5'-P-OP2	-6.11	100.20	105.70
36	5	2151	C	C4-C5-C6	6.11	120.45	117.40
36	1	155	G	N3-C4-C5	-6.11	125.55	128.60
1	6	337	G	N9-C4-C5	-6.11	102.96	105.40
36	5	2281	A	C8-N9-C4	6.11	108.24	105.80
36	1	362	U	N3-C4-C5	6.11	118.26	114.60
36	1	1313	G	C4-C5-N7	6.11	113.24	110.80
36	1	1501	U	O5'-P-OP2	-6.11	100.20	105.70
36	1	2215	A	N9-C4-C5	-6.11	103.36	105.80
36	5	2290	C	C6-N1-C2	6.11	122.74	120.30
36	1	2604	U	N1-C2-O2	6.10	127.07	122.80
36	5	329	U	C2-N1-C1'	-6.10	110.38	117.70
36	1	1143	A	O5'-P-OP1	-6.10	100.21	105.70
36	1	1898	G	C5-C6-O6	-6.10	124.94	128.60
1	6	1121	C	C6-N1-C2	-6.10	117.86	120.30
36	1	284	A	O4'-C1'-N9	6.10	113.08	108.20
36	1	648	C	C6-N1-C2	-6.10	117.86	120.30
36	1	718	G	C4-C5-N7	6.10	113.24	110.80
36	1	1425	U	C5-C6-N1	-6.10	119.65	122.70
36	5	2366	C	C2-N1-C1'	6.10	125.51	118.80
36	5	2905	U	C2-N3-C4	-6.10	123.34	127.00
36	1	922	U	N3-C4-O4	-6.10	115.13	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2632	G	C5-C6-O6	6.10	132.26	128.60
1	6	314	C	O5'-P-OP1	-6.10	100.21	105.70
36	1	709	A	N9-C4-C5	-6.10	103.36	105.80
36	1	2159	U	O5'-P-OP1	-6.10	100.21	105.70
36	5	2118	C	N3-C2-O2	-6.10	117.63	121.90
36	1	1114	U	N1-C2-N3	-6.09	111.24	114.90
36	5	2385	G	C4-C5-N7	6.09	113.24	110.80
36	1	153	U	C6-N1-C2	-6.09	117.34	121.00
36	1	3309	G	C5-N7-C8	-6.09	101.25	104.30
36	5	951	A	O5'-P-OP2	-6.09	100.22	105.70
36	1	1294	A	O4'-C1'-N9	6.09	113.07	108.20
36	5	2838	A	O5'-P-OP1	6.09	118.01	110.70
36	1	971	G	C8-N9-C4	6.09	108.83	106.40
37	3	36	C	N3-C2-O2	-6.09	117.64	121.90
1	6	453	U	C5-C4-O4	6.09	129.55	125.90
36	5	2744	U	N1-C2-O2	6.09	127.06	122.80
1	6	1600	A	N9-C1'-C2'	6.08	121.91	114.00
36	5	640	U	C4-C5-C6	6.08	123.35	119.70
36	5	125	C	N3-C4-N4	-6.08	113.74	118.00
36	5	794	U	C6-N1-C2	-6.08	117.35	121.00
36	5	1421	G	N3-C4-C5	6.08	131.64	128.60
36	5	3195	U	P-O3'-C3'	6.08	127.00	119.70
36	1	1196	C	C2-N1-C1'	-6.08	112.11	118.80
36	1	2188	A	C5-N7-C8	6.08	106.94	103.90
36	1	1168	U	O5'-P-OP1	6.08	117.99	110.70
1	6	571	G	N3-C2-N2	-6.08	115.64	119.90
36	5	933	A	N1-C2-N3	6.08	132.34	129.30
36	5	2990	G	N3-C4-N9	6.08	129.65	126.00
36	5	2849	C	OP1-P-OP2	6.08	128.72	119.60
36	1	295	A	C8-N9-C4	-6.08	103.37	105.80
36	1	1405	U	C5-C6-N1	-6.08	119.66	122.70
36	1	2805	G	N1-C6-O6	-6.08	116.25	119.90
36	5	1388	U	N3-C4-C5	-6.08	110.95	114.60
36	5	2305	G	O4'-C1'-N9	6.08	113.06	108.20
36	1	2636	A	C8-N9-C4	-6.07	103.37	105.80
36	5	652	G	OP2-P-O3'	6.07	118.56	105.20
36	1	439	C	C5-C6-N1	6.07	124.04	121.00
37	3	83	U	C2-N3-C4	-6.07	123.36	127.00
38	4	39	G	N1-C6-O6	-6.07	116.26	119.90
36	5	767	U	O4'-C1'-N1	6.07	113.06	108.20
36	5	2341	A	C5-N7-C8	6.07	106.94	103.90
36	1	2699	G	O5'-P-OP2	-6.07	100.24	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2719	U	C2-N3-C4	-6.07	123.36	127.00
36	1	3375	A	C8-N9-C4	-6.07	103.37	105.80
36	5	339	C	C6-N1-C2	-6.07	117.87	120.30
36	1	63	A	C2-N3-C4	6.06	113.63	110.60
36	1	1192	C	C5-C6-N1	6.06	124.03	121.00
36	1	1919	G	N9-C4-C5	6.06	107.83	105.40
1	2	554	C	N1-C2-O2	6.06	122.54	118.90
36	1	1820	U	P-O3'-C3'	6.06	126.97	119.70
36	1	2846	U	N1-C2-N3	6.06	118.53	114.90
1	6	1781	A	C4-C5-C6	6.06	120.03	117.00
36	5	2340	U	C2-N3-C4	-6.06	123.36	127.00
1	2	18	C	C5-C6-N1	6.06	124.03	121.00
36	1	46	U	C5-C4-O4	6.06	129.53	125.90
36	1	859	G	C8-N9-C1'	-6.06	119.13	127.00
36	1	1192	C	C2-N1-C1'	6.06	125.46	118.80
1	6	647	G	N3-C4-N9	-6.06	122.36	126.00
36	5	2655	U	N3-C4-O4	-6.06	115.16	119.40
36	5	3128	G	N3-C4-N9	6.06	129.63	126.00
36	1	402	A	O5'-P-OP1	-6.06	100.25	105.70
36	1	2945	G	O5'-P-OP1	6.06	117.97	110.70
1	2	334	G	C2-N3-C4	-6.05	108.87	111.90
1	2	1291	G	N9-C4-C5	6.05	107.82	105.40
1	6	363	G	C5-C6-O6	-6.05	124.97	128.60
36	5	1894	U	OP1-P-OP2	6.05	128.68	119.60
36	5	2421	U	C5-C6-N1	-6.05	119.67	122.70
36	5	2697	A	O5'-P-OP1	-6.05	100.25	105.70
36	5	2865	U	C4-C5-C6	-6.05	116.07	119.70
1	6	2	A	O5'-P-OP1	-6.05	100.25	105.70
1	6	1726	G	OP2-P-O3'	6.05	118.51	105.20
36	5	2362	C	C6-N1-C2	-6.05	117.88	120.30
36	1	1411	C	N1-C2-O2	6.05	122.53	118.90
1	2	1200	G	C4-C5-C6	6.05	122.43	118.80
36	5	2361	A	N9-C4-C5	6.05	108.22	105.80
36	1	2653	C	N3-C2-O2	-6.05	117.67	121.90
36	1	3344	A	O4'-C1'-N9	6.05	113.04	108.20
37	3	88	G	C5-C6-O6	6.05	132.23	128.60
41	L4	206	LEU	CA-CB-CG	6.05	129.21	115.30
1	6	87	C	C6-N1-C2	-6.05	117.88	120.30
1	6	1514	U	N3-C2-O2	-6.05	117.97	122.20
36	5	2598	G	C5-C6-O6	-6.04	124.97	128.60
36	1	1869	C	N1-C2-O2	6.04	122.53	118.90
36	1	2817	A	OP1-P-OP2	-6.04	110.53	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2897	A	N7-C8-N9	-6.04	110.78	113.80
1	6	987	G	N1-C6-O6	6.04	123.53	119.90
36	5	1296	C	C6-N1-C2	-6.04	117.88	120.30
36	5	1430	U	C5-C6-N1	-6.04	119.68	122.70
1	2	1000	C	N3-C2-O2	-6.04	117.67	121.90
36	1	640	U	C4-C5-C6	6.04	123.33	119.70
1	6	558	U	C2-N1-C1'	6.04	124.95	117.70
36	1	1898	G	O4'-C1'-N9	6.04	113.03	108.20
36	1	2347	U	C4-C5-C6	-6.04	116.08	119.70
36	5	915	A	N3-C4-C5	-6.04	122.57	126.80
36	1	2679	A	N1-C2-N3	6.04	132.32	129.30
38	4	135	G	N9-C4-C5	6.04	107.81	105.40
36	5	960	U	N3-C2-O2	-6.04	117.97	122.20
36	1	1118	C	C4-C5-C6	6.03	120.42	117.40
36	1	2188	A	C4-C5-N7	-6.03	107.68	110.70
36	1	2397	A	O5'-P-OP2	-6.03	100.27	105.70
1	6	1631	A	C8-N9-C4	6.03	108.21	105.80
36	5	1308	A	N7-C8-N9	6.03	116.82	113.80
36	5	2176	U	N3-C2-O2	-6.03	117.98	122.20
36	5	2917	G	C5-C6-O6	-6.03	124.98	128.60
1	2	704	C	O4'-C1'-N1	6.03	113.02	108.20
36	1	407	A	O5'-P-OP1	6.03	117.94	110.70
36	5	633	C	C5-C6-N1	-6.03	117.98	121.00
36	1	2595	A	C4-C5-N7	6.03	113.72	110.70
1	6	1097	U	P-O3'-C3'	6.03	126.94	119.70
62	N6	57	LEU	CA-CB-CG	6.03	129.16	115.30
36	1	92	G	O5'-P-OP1	-6.03	100.28	105.70
36	5	953	G	O4'-C1'-N9	6.02	113.02	108.20
36	1	1838	G	OP1-P-O3'	6.02	118.45	105.20
36	1	2685	C	N3-C4-C5	-6.02	119.49	121.90
36	5	1113	G	N3-C4-C5	6.02	131.61	128.60
36	5	1544	G	N3-C2-N2	6.02	124.12	119.90
36	5	1884	A	C8-N9-C4	-6.02	103.39	105.80
36	1	153	U	N3-C4-C5	-6.02	110.99	114.60
36	1	143	G	N3-C4-C5	-6.02	125.59	128.60
36	1	818	C	N3-C2-O2	-6.02	117.69	121.90
36	1	974	G	N3-C4-C5	-6.02	125.59	128.60
36	1	1426	C	C5-C4-N4	6.02	124.41	120.20
36	5	1397	C	O5'-P-OP1	-6.02	100.28	105.70
36	5	2618	G	C5-C6-N1	6.02	114.51	111.50
36	5	386	A	C6-C5-N7	-6.02	128.09	132.30
36	5	2897	A	N1-C6-N6	-6.02	114.99	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	n9	18	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	2	1462	G	N9-C4-C5	-6.01	102.99	105.40
36	1	1325	U	N1-C2-O2	-6.01	118.59	122.80
36	1	2323	G	N3-C2-N2	6.01	124.11	119.90
36	1	2950	G	N7-C8-N9	6.01	116.11	113.10
36	1	1703	U	C5-C6-N1	6.01	125.71	122.70
36	1	2426	U	N3-C4-O4	-6.01	115.19	119.40
36	1	2899	C	C2-N3-C4	-6.01	116.89	119.90
1	6	1	U	N3-C2-O2	-6.01	117.99	122.20
1	6	542	A	C4-C5-C6	6.01	120.01	117.00
36	5	682	U	C6-N1-C2	6.01	124.61	121.00
1	2	1428	G	N3-C4-N9	-6.01	122.39	126.00
36	5	1908	A	N9-C4-C5	6.01	108.20	105.80
36	5	2234	G	C5-C6-O6	-6.01	124.99	128.60
36	1	93	C	C6-N1-C1'	6.01	128.01	120.80
36	1	2766	U	O5'-P-OP2	-6.01	100.29	105.70
36	1	2945	G	C5-C6-O6	-6.01	125.00	128.60
1	6	1129	U	N3-C4-O4	-6.01	115.19	119.40
36	5	1112	A	N1-C6-N6	6.01	122.20	118.60
36	5	1311	G	C5-C6-N1	6.01	114.50	111.50
36	5	1725	C	C5'-C4'-O4'	6.01	116.31	109.10
10	S8	172	ARG	NE-CZ-NH1	6.01	123.30	120.30
36	1	1095	U	C2-N1-C1'	-6.00	110.49	117.70
36	1	663	C	N1-C2-O2	-6.00	115.30	118.90
36	1	2307	G	C8-N9-C4	6.00	108.80	106.40
38	4	151	C	C5-C6-N1	6.00	124.00	121.00
36	1	2795	U	N3-C4-O4	-6.00	115.20	119.40
1	6	25	C	P-O3'-C3'	6.00	126.90	119.70
1	6	1568	C	C2-N1-C1'	6.00	125.40	118.80
36	5	872	U	N3-C4-C5	6.00	118.20	114.60
36	5	2371	G	C2-N3-C4	-6.00	108.90	111.90
36	5	2703	A	C8-N9-C4	-6.00	103.40	105.80
36	1	1412	G	N1-C6-O6	-6.00	116.30	119.90
1	2	543	C	N1-C2-O2	6.00	122.50	118.90
36	1	2756	C	C6-N1-C2	-6.00	117.90	120.30
36	5	1371	G	C4-C5-N7	-6.00	108.40	110.80
36	5	2400	G	C5-C6-O6	-6.00	125.00	128.60
36	5	3245	A	C8-N9-C4	-6.00	103.40	105.80
37	7	93	C	O5'-P-OP2	-6.00	100.30	105.70
36	5	793	C	C6-N1-C2	-6.00	117.90	120.30
36	5	915	A	N3-C4-N9	6.00	132.20	127.40
38	8	22	U	N3-C4-C5	6.00	118.20	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1891	A	C8-N9-C4	6.00	108.20	105.80
1	6	767	U	C5-C4-O4	6.00	129.50	125.90
1	6	1100	G	N3-C4-N9	6.00	129.60	126.00
36	5	2188	A	N7-C8-N9	-6.00	110.80	113.80
36	1	422	A	C2-N3-C4	5.99	113.60	110.60
1	6	10	G	C4-C5-N7	-5.99	108.40	110.80
1	6	595	G	O5'-P-OP2	-5.99	100.31	105.70
36	1	2291	A	OP1-P-O3'	5.99	118.38	105.20
36	5	1938	U	C5-C6-N1	-5.99	119.70	122.70
36	5	2979	U	OP1-P-O3'	5.99	118.38	105.20
36	5	1044	U	N3-C4-O4	-5.99	115.21	119.40
36	5	3105	U	N1-C2-O2	-5.99	118.61	122.80
37	7	48	U	C2-N3-C4	-5.99	123.41	127.00
1	2	767	U	N3-C2-O2	-5.99	118.01	122.20
36	1	1852	G	C8-N9-C4	5.99	108.80	106.40
36	1	69	C	C4-C5-C6	5.98	120.39	117.40
36	1	689	U	C2-N1-C1'	5.98	124.88	117.70
36	1	2314	U	N1-C2-O2	5.98	126.99	122.80
36	5	1802	C	N3-C4-N4	5.98	122.19	118.00
36	5	2800	G	N1-C2-N2	5.98	121.58	116.20
36	1	375	A	O5'-P-OP2	-5.98	100.31	105.70
36	1	1308	A	O5'-P-OP1	5.98	117.88	110.70
36	5	844	G	N7-C8-N9	-5.98	110.11	113.10
36	5	1115	G	C4-N9-C1'	5.98	134.28	126.50
36	5	2315	G	N3-C4-C5	5.98	131.59	128.60
37	7	96	U	OP2-P-O3'	5.98	118.36	105.20
36	1	2817	A	C6-N1-C2	-5.98	115.01	118.60
36	1	3210	A	N1-C6-N6	-5.98	115.01	118.60
36	1	2645	G	C4-C5-N7	-5.98	108.41	110.80
36	1	2280	A	N1-C6-N6	5.98	122.19	118.60
36	1	2298	U	C2-N3-C4	-5.98	123.41	127.00
1	6	75	U	O4'-C1'-N1	5.98	112.98	108.20
36	5	92	G	N3-C4-C5	-5.98	125.61	128.60
36	5	3009	G	C5-C6-O6	5.98	132.19	128.60
36	1	143	G	N9-C4-C5	5.98	107.79	105.40
36	1	1425	U	N1-C2-N3	5.98	118.49	114.90
20	c8	15	LEU	CA-CB-CG	5.98	129.04	115.30
36	5	2912	G	O5'-P-OP1	-5.98	100.32	105.70
36	5	3101	G	N3-C2-N2	5.98	124.08	119.90
36	1	702	C	C2-N3-C4	-5.97	116.91	119.90
36	1	1481	A	C6-C5-N7	-5.97	128.12	132.30
36	1	2877	G	N1-C6-O6	-5.97	116.31	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	740	G	N1-C6-O6	-5.97	116.31	119.90
36	5	1846	C	C5-C6-N1	-5.97	118.01	121.00
36	1	2392	C	C5-C4-N4	-5.97	116.02	120.20
36	5	2140	U	C5-C4-O4	5.97	129.48	125.90
1	6	14	C	C6-N1-C2	-5.97	117.91	120.30
36	5	3010	U	N1-C2-O2	5.97	126.98	122.80
36	5	971	G	OP2-P-O3'	5.97	118.33	105.20
36	1	789	A	N1-C2-N3	5.97	132.28	129.30
36	1	1841	A	C5-C6-N1	5.97	120.68	117.70
36	5	230	U	N1-C2-O2	-5.97	118.62	122.80
36	5	2260	U	O5'-P-OP1	-5.97	100.33	105.70
36	1	2370	G	O5'-P-OP2	-5.96	100.33	105.70
36	5	507	U	N1-C2-O2	5.96	126.97	122.80
36	5	2298	U	C2-N1-C1'	-5.96	110.54	117.70
36	5	2402	A	N1-C2-N3	5.96	132.28	129.30
36	5	2434	U	C5-C6-N1	-5.96	119.72	122.70
36	1	369	A	C2-N3-C4	5.96	113.58	110.60
1	6	355	G	OP2-P-O3'	5.96	118.32	105.20
36	5	1115	G	C6-C5-N7	-5.96	126.82	130.40
36	5	1604	G	C4-N9-C1'	5.96	134.25	126.50
1	6	322	G	O5'-P-OP1	-5.96	100.34	105.70
36	1	2851	A	C8-N9-C4	5.96	108.18	105.80
36	5	205	C	N3-C2-O2	-5.96	117.73	121.90
36	5	1883	A	N1-C6-N6	-5.96	115.03	118.60
36	1	1114	U	C4-C5-C6	-5.96	116.13	119.70
36	1	1797	A	O5'-P-OP1	-5.96	100.34	105.70
36	5	575	G	C8-N9-C4	-5.96	104.02	106.40
36	5	1496	C	C2-N1-C1'	5.96	125.35	118.80
36	5	1907	C	N3-C4-C5	-5.96	119.52	121.90
36	5	2364	G	N9-C4-C5	5.96	107.78	105.40
36	1	2871	G	C8-N9-C1'	5.96	134.74	127.00
36	5	412	G	C8-N9-C4	-5.96	104.02	106.40
36	5	1201	C	C6-N1-C1'	5.96	127.95	120.80
36	5	2968	G	C4-C5-N7	-5.96	108.42	110.80
1	2	1565	C	N1-C2-O2	-5.95	115.33	118.90
36	1	364	G	C5-C6-N1	5.95	114.48	111.50
36	1	922	U	C5-C6-N1	5.95	125.68	122.70
36	5	2857	C	C5-C4-N4	-5.95	116.03	120.20
36	1	406	G	N1-C6-O6	-5.95	116.33	119.90
36	1	1196	C	N1-C2-O2	-5.95	115.33	118.90
37	3	96	U	C6-N1-C2	5.95	124.57	121.00
1	6	359	A	C6-N1-C2	5.95	122.17	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3009	G	N1-C6-O6	-5.95	116.33	119.90
36	1	1520	G	C5-N7-C8	5.95	107.27	104.30
36	5	96	G	N3-C4-N9	-5.95	122.43	126.00
36	1	2165	G	C8-N9-C4	-5.95	104.02	106.40
41	L4	327	LEU	CA-CB-CG	5.95	128.97	115.30
36	5	2144	A	O4'-C1'-N9	5.95	112.96	108.20
41	14	98	ARG	NE-CZ-NH2	-5.95	117.33	120.30
36	1	2754	G	O5'-P-OP2	-5.94	100.35	105.70
1	6	687	G	C6-C5-N7	5.94	133.97	130.40
36	5	326	U	C5-C4-O4	-5.94	122.33	125.90
36	5	2724	U	N1-C2-N3	5.94	118.47	114.90
36	1	2608	G	N7-C8-N9	-5.94	110.13	113.10
36	5	416	A	N9-C4-C5	5.94	108.18	105.80
36	5	3214	U	N1-C2-N3	5.94	118.47	114.90
38	8	32	C	N1-C2-O2	-5.94	115.33	118.90
36	1	1940	G	N1-C6-O6	-5.94	116.34	119.90
36	1	2356	A	C4-C5-N7	5.94	113.67	110.70
36	1	2403	G	C2-N3-C4	5.94	114.87	111.90
36	5	2630	C	N1-C2-O2	-5.94	115.34	118.90
36	1	1392	G	N1-C6-O6	5.94	123.46	119.90
36	1	2871	G	C4-N9-C1'	-5.94	118.78	126.50
36	5	1159	A	N9-C4-C5	-5.94	103.42	105.80
36	5	1314	C	C6-N1-C1'	-5.94	113.67	120.80
36	5	3049	A	C6-N1-C2	5.94	122.16	118.60
36	5	1863	G	C5-C6-N1	5.94	114.47	111.50
1	2	736	C	C2-N1-C1'	5.93	125.33	118.80
36	1	278	U	C6-N1-C2	-5.93	117.44	121.00
36	1	2389	C	C5-C6-N1	-5.93	118.03	121.00
36	5	3047	U	N1-C2-O2	5.93	126.95	122.80
36	5	1448	U	C5-C6-N1	-5.93	119.73	122.70
1	6	402	C	C5-C4-N4	-5.93	116.05	120.20
36	5	2366	C	N3-C4-N4	5.93	122.15	118.00
1	2	416	A	O5'-P-OP1	-5.92	100.37	105.70
1	2	1119	G	N1-C6-O6	-5.92	116.35	119.90
36	1	971	G	C5-N7-C8	5.92	107.26	104.30
36	5	922	U	C6-N1-C1'	5.92	129.49	121.20
36	5	44	U	C2-N3-C4	-5.92	123.45	127.00
1	2	779	U	O4'-C1'-N1	5.92	112.94	108.20
36	5	2882	U	N1-C2-N3	5.92	118.45	114.90
36	1	2811	A	C5-C6-N1	5.92	120.66	117.70
36	1	2874	G	C5-C6-O6	5.92	132.15	128.60
36	5	2376	G	N1-C6-O6	-5.92	116.35	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	618	C	N1-C2-O2	-5.92	115.35	118.90
36	5	2874	G	O5'-P-OP2	5.92	117.80	110.70
36	5	945	C	N3-C4-C5	5.92	124.27	121.90
36	1	610	G	N9-C4-C5	-5.92	103.03	105.40
36	1	2798	C	N3-C4-C5	-5.91	119.53	121.90
36	5	3128	G	C5-C6-O6	-5.91	125.05	128.60
36	1	1507	G	C5-N7-C8	5.91	107.26	104.30
36	1	686	G	N1-C6-O6	-5.91	116.35	119.90
36	1	3269	U	N1-C2-N3	5.91	118.45	114.90
1	6	16	G	N1-C6-O6	-5.91	116.35	119.90
36	5	662	U	C5-C4-O4	5.91	129.45	125.90
36	1	25	U	N3-C4-O4	5.91	123.54	119.40
36	5	401	U	O5'-P-OP2	-5.91	100.38	105.70
36	5	3020	U	N3-C4-O4	5.91	123.54	119.40
36	1	962	A	C6-N1-C2	-5.91	115.06	118.60
36	1	2846	U	O5'-P-OP1	-5.91	100.38	105.70
36	1	1122	U	N3-C4-C5	5.91	118.14	114.60
36	1	2821	C	N1-C2-O2	-5.91	115.36	118.90
64	N8	66	ALA	N-CA-C	-5.91	95.06	111.00
1	6	901	G	C4-C5-N7	5.91	113.16	110.80
36	5	1192	C	N3-C4-C5	5.91	124.26	121.90
36	5	1907	C	N1-C2-O2	-5.91	115.36	118.90
36	1	2380	U	N3-C4-C5	5.90	118.14	114.60
36	1	2892	A	N1-C6-N6	-5.90	115.06	118.60
36	5	1189	C	C6-N1-C2	5.90	122.66	120.30
36	5	2621	G	N3-C2-N2	-5.90	115.77	119.90
36	5	2758	A	C2-N3-C4	5.90	113.55	110.60
36	1	1113	G	C5-N7-C8	5.90	107.25	104.30
36	1	1481	A	O4'-C1'-N9	5.90	112.92	108.20
36	1	2787	G	C8-N9-C4	-5.90	104.04	106.40
36	5	2899	C	N3-C4-N4	-5.90	113.87	118.00
36	1	641	C	OP1-P-O3'	5.90	118.18	105.20
37	3	28	C	C6-N1-C2	-5.90	117.94	120.30
1	6	1560	U	N1-C2-O2	5.90	126.93	122.80
36	5	861	C	O5'-P-OP1	5.90	117.78	110.70
36	5	1592	G	C4-C5-N7	5.90	113.16	110.80
36	5	3003	G	C5-N7-C8	-5.90	101.35	104.30
36	1	1115	G	N3-C4-N9	5.90	129.54	126.00
36	1	1304	A	O5'-P-OP1	-5.90	100.39	105.70
36	1	2701	U	C5-C6-N1	-5.90	119.75	122.70
36	1	3318	G	C4-N9-C1'	5.90	134.17	126.50
36	5	1305	U	C2-N3-C4	-5.90	123.46	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2899	C	C2-N3-C4	-5.90	116.95	119.90
38	8	111	A	O5'-P-OP1	5.90	117.78	110.70
36	1	3173	G	N7-C8-N9	5.90	116.05	113.10
25	d3	73	ARG	NE-CZ-NH1	-5.90	117.35	120.30
36	1	2870	C	O4'-C1'-N1	5.89	112.92	108.20
36	5	386	A	N9-C4-C5	-5.89	103.44	105.80
36	5	998	A	OP2-P-O3'	5.89	118.17	105.20
36	1	86	G	O5'-P-OP2	-5.89	100.40	105.70
36	1	1931	U	C6-N1-C2	5.89	124.54	121.00
12	c0	83	PRO	N-CA-CB	5.89	110.37	103.30
36	5	1152	G	C5-C6-N1	-5.89	108.55	111.50
36	5	1833	G	C5-C6-N1	5.89	114.45	111.50
36	5	1863	G	N9-C1'-C2'	-5.89	105.52	112.00
1	2	610	G	C5-C6-O6	-5.89	125.06	128.60
36	1	1387	G	C5-C6-O6	5.89	132.13	128.60
36	5	813	G	N3-C4-C5	-5.89	125.66	128.60
36	1	1909	A	C2-N3-C4	-5.89	107.66	110.60
1	6	523	G	C8-N9-C4	5.89	108.76	106.40
36	5	2363	A	C8-N9-C4	-5.89	103.44	105.80
36	5	3047	U	C2-N3-C4	-5.89	123.47	127.00
1	2	74	U	O5'-P-OP1	-5.89	100.40	105.70
36	1	971	G	C5-C6-N1	5.89	114.44	111.50
36	1	1167	U	N3-C4-O4	-5.89	115.28	119.40
36	1	3053	G	C5-C6-O6	5.89	132.13	128.60
1	6	1096	C	N3-C2-O2	-5.89	117.78	121.90
36	1	214	G	N9-C4-C5	5.89	107.75	105.40
36	1	1431	G	N1-C6-O6	-5.89	116.37	119.90
36	1	2365	C	N1-C2-O2	5.88	122.43	118.90
36	1	2403	G	C4-N9-C1'	5.88	134.15	126.50
54	M8	99	THR	N-CA-C	5.88	126.89	111.00
36	5	1120	A	C4-C5-N7	-5.88	107.76	110.70
36	5	1655	G	C8-N9-C4	-5.88	104.05	106.40
36	5	1902	G	C5-C6-N1	5.88	114.44	111.50
1	2	1535	U	C6-N1-C1'	-5.88	112.97	121.20
36	5	648	C	C6-N1-C2	-5.88	117.95	120.30
36	5	646	A	N7-C8-N9	5.88	116.74	113.80
1	2	1416	G	N1-C6-O6	5.88	123.43	119.90
36	1	61	A	N1-C6-N6	5.88	122.13	118.60
36	5	963	G	C5-C6-N1	5.88	114.44	111.50
36	5	1316	C	N1-C2-O2	-5.88	115.37	118.90
36	1	1433	A	C5-C6-N1	5.88	120.64	117.70
36	1	1546	A	C2-N3-C4	5.88	113.54	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1693	C	N1-C2-O2	-5.88	115.38	118.90
36	5	2244	A	O5'-P-OP1	5.88	117.75	110.70
36	5	2754	G	N3-C4-C5	-5.88	125.66	128.60
36	5	2814	G	C4-C5-N7	5.88	113.15	110.80
36	1	44	U	N3-C4-C5	5.88	118.12	114.60
36	1	979	U	N3-C2-O2	-5.88	118.09	122.20
36	5	661	G	C8-N9-C4	-5.88	104.05	106.40
36	1	1476	G	N1-C6-O6	-5.87	116.38	119.90
1	6	879	G	N1-C6-O6	-5.87	116.38	119.90
36	5	2393	G	O5'-P-OP1	5.87	117.75	110.70
36	1	2389	C	C2-N3-C4	-5.87	116.96	119.90
36	1	2821	C	N3-C2-O2	5.87	126.01	121.90
1	6	422	G	C8-N9-C4	-5.87	104.05	106.40
36	5	909	G	C5-C6-O6	5.87	132.12	128.60
36	1	1305	U	N1-C2-O2	5.87	126.91	122.80
36	1	2621	G	N9-C4-C5	5.87	107.75	105.40
36	1	2871	G	N3-C4-N9	-5.87	122.48	126.00
36	1	2944	U	N1-C2-O2	5.87	126.91	122.80
36	5	150	A	N1-C6-N6	5.87	122.12	118.60
36	5	1420	C	OP2-P-O3'	5.87	118.11	105.20
36	1	2305	G	N1-C6-O6	5.87	123.42	119.90
36	1	2996	U	C6-N1-C1'	-5.87	112.99	121.20
36	5	283	G	C4-C5-N7	5.87	113.15	110.80
1	2	1560	U	C6-N1-C2	-5.87	117.48	121.00
36	1	1392	G	C5-C6-O6	-5.87	125.08	128.60
36	1	2679	A	O4'-C1'-N9	5.87	112.89	108.20
1	6	306	U	C5-C6-N1	-5.87	119.77	122.70
36	5	3075	G	OP1-P-O3'	5.87	118.11	105.20
36	1	114	A	C4-C5-N7	5.86	113.63	110.70
36	1	2123	G	N7-C8-N9	-5.86	110.17	113.10
36	5	877	C	C4-C5-C6	-5.86	114.47	117.40
36	5	908	G	N7-C8-N9	5.86	116.03	113.10
36	5	3218	A	C5-C6-N1	-5.86	114.77	117.70
36	5	3309	G	N3-C4-C5	-5.86	125.67	128.60
1	2	1559	A	O4'-C1'-N9	5.86	112.89	108.20
36	1	304	G	N1-C2-N3	-5.86	120.38	123.90
36	1	944	C	C4-C5-C6	-5.86	114.47	117.40
62	N6	6	LEU	CA-CB-CG	-5.86	101.82	115.30
36	5	2598	G	N1-C6-O6	5.86	123.42	119.90
1	2	1339	C	C5-C6-N1	5.86	123.93	121.00
36	1	931	C	N3-C4-C5	5.86	124.24	121.90
36	1	2634	U	C5-C6-N1	-5.86	119.77	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1040	G	N1-C6-O6	-5.86	116.38	119.90
36	5	2376	G	C8-N9-C1'	-5.86	119.38	127.00
1	6	1656	U	OP2-P-O3'	5.86	118.09	105.20
36	5	1849	C	N1-C2-O2	5.86	122.42	118.90
36	1	1103	A	C5-C6-N1	5.86	120.63	117.70
36	1	1336	U	C5-C4-O4	5.86	129.41	125.90
36	1	1371	G	C8-N9-C4	5.86	108.74	106.40
36	5	779	G	O5'-P-OP2	-5.86	100.43	105.70
36	5	914	A	C8-N9-C4	5.86	108.14	105.80
36	1	946	U	C2-N3-C4	-5.86	123.49	127.00
36	1	1307	G	P-O3'-C3'	5.86	126.73	119.70
36	1	2862	U	N1-C2-O2	5.86	126.90	122.80
36	5	1450	G	N1-C6-O6	-5.86	116.39	119.90
36	5	3217	C	C5-C6-N1	-5.86	118.07	121.00
36	1	2298	U	O4'-C1'-N1	5.85	112.88	108.20
36	5	777	U	O5'-P-OP2	-5.85	100.43	105.70
36	5	1121	U	N1-C2-O2	-5.85	118.70	122.80
36	5	1124	U	C4-C5-C6	-5.85	116.19	119.70
36	5	2160	G	N1-C2-N2	-5.85	110.93	116.20
1	6	90	C	N3-C2-O2	-5.85	117.81	121.90
36	5	110	G	O5'-P-OP1	5.85	117.72	110.70
36	5	929	A	N7-C8-N9	-5.85	110.88	113.80
36	5	941	G	N1-C6-O6	-5.85	116.39	119.90
36	1	1396	C	N3-C4-C5	5.85	124.24	121.90
36	5	1202	A	N7-C8-N9	5.85	116.72	113.80
36	5	2245	C	N3-C4-C5	-5.85	119.56	121.90
36	5	2894	C	C6-N1-C2	-5.85	117.96	120.30
36	5	2964	G	N1-C6-O6	-5.85	116.39	119.90
36	1	3303	G	O4'-C1'-N9	5.85	112.88	108.20
16	c4	35	GLY	N-CA-C	5.85	127.72	113.10
36	5	659	G	C5-C6-N1	5.85	114.42	111.50
36	1	76	G	N3-C4-C5	-5.84	125.68	128.60
36	1	1451	C	C5-C6-N1	-5.84	118.08	121.00
36	1	2811	A	N9-C4-C5	5.84	108.14	105.80
36	1	3057	U	C5-C6-N1	-5.84	119.78	122.70
38	4	6	U	C5-C4-O4	-5.84	122.39	125.90
36	1	3213	A	N1-C6-N6	5.84	122.11	118.60
36	5	1047	A	O5'-P-OP1	-5.84	100.44	105.70
36	5	2990	G	C5-C6-O6	-5.84	125.09	128.60
1	2	1596	C	N1-C2-O2	5.84	122.41	118.90
36	1	59	G	N3-C2-N2	5.84	123.99	119.90
36	1	1440	G	C6-N1-C2	5.84	128.60	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1536	G	C5-C6-O6	-5.84	125.09	128.60
1	6	1048	G	N9-C4-C5	-5.84	103.06	105.40
36	5	1466	G	O5'-P-OP1	-5.84	100.44	105.70
36	5	1902	G	O5'-P-OP1	-5.84	100.44	105.70
36	5	2314	U	C5-C4-O4	-5.84	122.39	125.90
36	1	1326	A	N9-C4-C5	5.84	108.14	105.80
36	1	2305	G	C5-C6-O6	-5.84	125.10	128.60
36	1	2634	U	N1-C2-N3	5.84	118.40	114.90
36	5	2666	C	N1-C2-O2	-5.84	115.40	118.90
36	1	421	G	C5-C6-O6	-5.84	125.10	128.60
1	6	453	U	N1-C2-O2	5.84	126.89	122.80
36	5	2991	A	C8-N9-C4	-5.84	103.47	105.80
1	6	874	C	N1-C2-O2	5.84	122.40	118.90
1	6	1149	G	N1-C6-O6	-5.84	116.40	119.90
36	5	2634	U	C5-C6-N1	-5.84	119.78	122.70
1	6	48	G	O5'-P-OP2	-5.83	100.45	105.70
1	6	630	A	N1-C6-N6	5.83	122.10	118.60
38	8	22	U	O4'-C1'-N1	5.83	112.87	108.20
36	1	1440	G	N1-C2-N3	-5.83	120.40	123.90
36	1	2768	U	C5-C6-N1	-5.83	119.78	122.70
36	5	1495	U	N3-C4-C5	-5.83	111.10	114.60
1	6	1010	C	C6-N1-C2	-5.83	117.97	120.30
1	6	1028	C	O5'-P-OP1	-5.83	100.45	105.70
36	5	1931	U	C6-N1-C2	5.83	124.50	121.00
36	5	2858	U	C2-N1-C1'	5.83	124.70	117.70
36	5	3154	C	N3-C2-O2	-5.83	117.82	121.90
36	1	1366	A	N1-C2-N3	-5.83	126.39	129.30
36	1	2883	U	C4-C5-C6	-5.83	116.20	119.70
1	6	633	U	C6-N1-C2	5.83	124.50	121.00
36	5	2148	U	C2-N3-C4	-5.83	123.50	127.00
36	5	2377	G	C2-N3-C4	5.83	114.81	111.90
36	1	2123	G	C8-N9-C4	5.83	108.73	106.40
1	6	142	G	C8-N9-C1'	-5.83	119.42	127.00
36	5	110	G	O4'-C1'-N9	5.83	112.86	108.20
36	5	2747	A	N1-C6-N6	-5.83	115.10	118.60
36	5	2981	U	N3-C4-C5	5.83	118.10	114.60
36	1	339	C	C5-C4-N4	5.83	124.28	120.20
12	c0	88	PRO	N-CA-CB	5.83	110.29	103.30
36	1	43	A	N1-C2-N3	-5.83	126.39	129.30
36	1	282	G	C2'-C3'-O3'	5.83	123.02	113.70
36	1	968	G	C5-C6-O6	5.83	132.09	128.60
36	5	3173	G	N7-C8-N9	5.83	116.01	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3183	A	C8-N9-C4	-5.83	103.47	105.80
40	l3	232	ARG	NE-CZ-NH1	5.83	123.21	120.30
36	1	39	A	C5-N7-C8	-5.82	100.99	103.90
36	1	407	A	O5'-P-OP2	-5.82	100.46	105.70
36	1	1846	C	O5'-P-OP1	-5.82	100.46	105.70
36	1	3151	U	O5'-P-OP2	-5.82	100.46	105.70
1	6	1144	U	OP2-P-O3'	5.82	118.01	105.20
36	1	862	U	C5-C6-N1	5.82	125.61	122.70
36	1	1368	U	C5-C6-N1	-5.82	119.79	122.70
36	1	2184	U	N3-C4-O4	5.82	123.48	119.40
36	1	2187	G	N1-C6-O6	5.82	123.39	119.90
36	1	2986	U	C2-N3-C4	-5.82	123.51	127.00
1	6	390	G	N3-C4-C5	-5.82	125.69	128.60
1	6	597	G	O5'-P-OP2	-5.82	100.46	105.70
36	5	967	A	N1-C6-N6	-5.82	115.11	118.60
36	5	1847	A	C8-N9-C4	5.82	108.13	105.80
1	2	992	A	C2-N3-C4	-5.82	107.69	110.60
36	1	163	C	C6-N1-C2	-5.82	117.97	120.30
36	1	3078	U	C5-C4-O4	5.82	129.39	125.90
36	5	1888	U	C5-C6-N1	-5.82	119.79	122.70
36	5	911	C	N3-C4-N4	5.82	122.07	118.00
38	8	108	C	C6-N1-C2	-5.82	117.97	120.30
36	5	959	C	C5-C4-N4	-5.82	116.13	120.20
37	7	41	G	N9-C4-C5	-5.82	103.07	105.40
51	M5	105	ARG	NE-CZ-NH1	5.81	123.21	120.30
36	5	2302	G	C5-C6-O6	5.81	132.09	128.60
36	5	2377	G	N1-C6-O6	-5.81	116.41	119.90
36	1	2283	G	N1-C6-O6	5.81	123.39	119.90
36	1	2608	G	C8-N9-C4	5.81	108.72	106.40
45	L8	189	LEU	CA-CB-CG	5.81	128.66	115.30
1	6	144	U	O4'-C1'-N1	5.81	112.85	108.20
36	5	1872	C	C4-C5-C6	5.81	120.31	117.40
36	1	53	G	N3-C4-N9	5.81	129.49	126.00
36	1	645	A	C5-N7-C8	5.81	106.81	103.90
36	1	2323	G	N1-C6-O6	-5.81	116.41	119.90
36	5	1120	A	OP2-P-O3'	5.81	117.98	105.20
36	5	2800	G	C4-C5-N7	-5.81	108.48	110.80
36	5	2909	U	C5-C4-O4	-5.81	122.41	125.90
36	1	964	G	OP2-P-O3'	5.81	117.98	105.20
1	6	102	U	O5'-P-OP1	-5.81	100.47	105.70
1	6	194	U	N3-C2-O2	-5.81	118.14	122.20
36	5	2772	C	N3-C2-O2	5.81	125.97	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2141	U	N3-C2-O2	-5.81	118.14	122.20
36	1	2306	C	N1-C2-O2	-5.81	115.42	118.90
1	2	113	U	N1-C2-O2	-5.80	118.74	122.80
1	2	1241	G	C5-N7-C8	-5.80	101.40	104.30
36	5	2816	G	N9-C4-C5	5.80	107.72	105.40
36	5	2996	U	O5'-P-OP1	5.80	117.67	110.70
36	5	3339	A	N1-C6-N6	5.80	122.08	118.60
1	2	1324	G	N3-C2-N2	-5.80	115.84	119.90
36	1	346	C	OP2-P-O3'	5.80	117.97	105.20
36	1	49	A	N1-C6-N6	5.80	122.08	118.60
36	1	2727	A	O4'-C1'-N9	-5.80	103.56	108.20
1	6	1489	U	N3-C2-O2	-5.80	118.14	122.20
36	5	376	G	C5-C6-N1	5.80	114.40	111.50
36	1	1839	A	N1-C6-N6	-5.80	115.12	118.60
1	6	2	A	C8-N9-C4	5.80	108.12	105.80
36	5	692	A	O5'-P-OP1	-5.80	100.48	105.70
36	5	1044	U	C5-C6-N1	-5.80	119.80	122.70
38	8	112	U	C2-N1-C1'	-5.80	110.74	117.70
36	5	1303	A	O5'-P-OP1	-5.80	100.48	105.70
36	1	1319	G	N1-C6-O6	-5.80	116.42	119.90
36	1	2133	U	O4'-C1'-N1	5.80	112.84	108.20
36	1	2935	U	C2-N3-C4	5.80	130.48	127.00
36	5	2350	C	N1-C2-N3	5.80	123.26	119.20
36	1	885	U	C5-C6-N1	-5.79	119.80	122.70
36	1	2412	G	OP1-P-O3'	5.79	117.95	105.20
36	1	2800	G	C5-N7-C8	5.79	107.20	104.30
1	6	874	C	N3-C2-O2	-5.79	117.84	121.90
36	5	341	G	OP1-P-O3'	5.79	117.95	105.20
36	5	643	U	N3-C2-O2	5.79	126.26	122.20
36	5	2388	U	C5-C6-N1	-5.79	119.80	122.70
36	1	1437	C	C6-N1-C2	-5.79	117.98	120.30
36	1	2640	A	N1-C6-N6	-5.79	115.12	118.60
1	6	782	U	C2-N1-C1'	5.79	124.65	117.70
36	5	2889	C	N1-C2-O2	5.79	122.38	118.90
36	5	3094	A	N1-C6-N6	-5.79	115.12	118.60
1	2	1535	U	N1-C2-O2	5.79	126.86	122.80
38	4	32	C	C6-N1-C1'	5.79	127.75	120.80
1	2	1611	A	N1-C2-N3	5.79	132.19	129.30
36	1	2275	A	O5'-P-OP1	-5.79	100.49	105.70
36	1	2950	G	C5-C6-N1	5.79	114.39	111.50
69	O3	67	MET	CG-SD-CE	-5.79	90.94	100.20
1	6	1	U	N1-C2-O2	5.79	126.85	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1784	C	O5'-P-OP1	-5.79	100.49	105.70
36	5	437	G	C8-N9-C4	-5.79	104.08	106.40
36	5	878	G	N1-C6-O6	5.79	123.37	119.90
36	5	922	U	C2-N1-C1'	-5.79	110.75	117.70
36	5	1404	G	C5-C6-O6	5.79	132.07	128.60
38	4	17	A	OP1-P-OP2	-5.78	110.92	119.60
36	5	636	C	C2-N3-C4	-5.78	117.01	119.90
37	7	120	C	C5-C6-N1	-5.78	118.11	121.00
36	1	3270	U	O5'-P-OP1	-5.78	100.50	105.70
1	6	1082	C	C2-N1-C1'	5.78	125.16	118.80
36	5	908	G	N3-C4-C5	-5.78	125.71	128.60
36	1	2920	U	N3-C2-O2	-5.78	118.15	122.20
38	4	23	U	C5-C6-N1	-5.78	119.81	122.70
36	5	1426	C	N1-C2-O2	-5.78	115.43	118.90
36	5	2976	A	C5-C6-N1	5.78	120.59	117.70
36	1	189	G	N3-C2-N2	5.78	123.94	119.90
36	1	2376	G	C5-C6-N1	5.78	114.39	111.50
36	1	2732	G	N1-C2-N2	-5.78	111.00	116.20
1	6	1036	A	N9-C4-C5	5.78	108.11	105.80
36	5	1520	G	OP2-P-O3'	5.78	117.91	105.20
1	2	553	G	C4-C5-C6	5.78	122.27	118.80
1	2	1218	G	N1-C6-O6	5.78	123.37	119.90
36	1	24	G	C5-C6-O6	-5.78	125.13	128.60
36	1	424	G	C8-N9-C4	5.78	108.71	106.40
36	1	829	U	N3-C2-O2	-5.78	118.16	122.20
36	1	1132	C	N3-C2-O2	-5.78	117.86	121.90
36	5	1419	A	N7-C8-N9	-5.78	110.91	113.80
36	5	1607	U	N3-C4-O4	-5.78	115.36	119.40
36	5	2370	G	C5-C6-N1	5.78	114.39	111.50
36	1	1178	G	N1-C6-O6	-5.78	116.44	119.90
36	5	2190	U	N3-C2-O2	-5.78	118.16	122.20
1	2	1595	U	N1-C2-O2	-5.77	118.76	122.80
36	5	1855	U	C5-C6-N1	-5.77	119.81	122.70
1	6	1172	G	O5'-P-OP1	-5.77	100.51	105.70
1	2	1731	A	N1-C2-N3	-5.77	126.42	129.30
36	1	674	G	C4-C5-N7	-5.77	108.49	110.80
1	6	1584	G	OP1-P-O3'	5.77	117.89	105.20
36	5	1203	A	O5'-P-OP1	-5.77	100.51	105.70
36	5	2113	A	C4-N9-C1'	-5.77	115.92	126.30
36	5	2643	A	C4-C5-N7	5.77	113.58	110.70
36	1	826	G	O5'-P-OP1	-5.77	100.51	105.70
36	1	670	C	C2-N3-C4	-5.77	117.02	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2711	C	C6-N1-C2	-5.77	117.99	120.30
36	1	1724	U	O4'-C1'-N1	5.76	112.81	108.20
36	1	2314	U	C5-C4-O4	-5.76	122.44	125.90
36	1	2631	U	C5-C4-O4	5.76	129.36	125.90
38	4	90	U	C5-C6-N1	-5.76	119.82	122.70
1	6	297	U	N3-C4-O4	5.76	123.43	119.40
36	5	2421	U	N1-C2-N3	5.76	118.36	114.90
36	1	802	C	C4-C5-C6	5.76	120.28	117.40
38	4	47	C	O5'-P-OP1	5.76	117.61	110.70
1	6	402	C	N3-C4-C5	5.76	124.20	121.90
36	5	2880	U	C6-N1-C2	-5.76	117.55	121.00
1	2	1596	C	N3-C4-N4	-5.76	113.97	118.00
1	6	1101	G	C5-C6-O6	5.76	132.05	128.60
36	1	223	U	N1-C2-O2	-5.75	118.77	122.80
36	5	404	G	O5'-P-OP2	-5.75	100.52	105.70
36	5	989	A	OP2-P-O3'	5.75	117.86	105.20
36	1	806	A	O5'-P-OP1	-5.75	100.52	105.70
36	1	2945	G	N1-C6-O6	5.75	123.35	119.90
36	1	3092	C	C6-N1-C1'	5.75	127.70	120.80
36	5	1445	U	N3-C2-O2	5.75	126.23	122.20
36	5	2330	C	N1-C2-O2	-5.75	115.45	118.90
77	q1	9	ARG	NE-CZ-NH2	-5.75	117.42	120.30
36	1	972	A	N7-C8-N9	-5.75	110.92	113.80
1	6	1748	G	O5'-P-OP2	5.75	117.60	110.70
36	5	693	A	N1-C6-N6	-5.75	115.15	118.60
36	5	1188	U	C5-C4-O4	-5.75	122.45	125.90
36	5	1592	G	N1-C2-N2	-5.75	111.02	116.20
36	5	1848	G	N1-C6-O6	5.75	123.35	119.90
36	5	423	A	C2-N3-C4	5.75	113.47	110.60
36	1	271	C	N1-C2-O2	5.75	122.35	118.90
36	1	360	G	C6-C5-N7	-5.75	126.95	130.40
36	1	887	G	N1-C6-O6	5.75	123.35	119.90
36	1	2396	G	C4-C5-C6	5.75	122.25	118.80
36	1	2599	U	C6-N1-C2	-5.75	117.55	121.00
36	1	2624	G	C5-C6-O6	-5.75	125.15	128.60
36	1	2868	U	C2-N3-C4	-5.75	123.55	127.00
1	6	1000	C	C2-N1-C1'	5.75	125.12	118.80
36	5	1330	A	OP1-P-OP2	5.75	128.22	119.60
36	5	1387	G	O5'-P-OP1	-5.75	100.53	105.70
36	1	817	A	N9-C1'-C2'	5.75	121.47	114.00
38	4	109	A	C5-C6-N6	-5.75	119.10	123.70
36	5	2298	U	N3-C4-O4	-5.75	115.38	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2808	A	C4-C5-N7	5.75	113.57	110.70
36	1	648	C	O5'-P-OP1	-5.75	100.53	105.70
36	1	1167	U	N3-C4-C5	5.75	118.05	114.60
38	4	46	G	C4-C5-N7	-5.75	108.50	110.80
36	5	426	G	C8-N9-C4	5.75	108.70	106.40
36	1	916	G	C5-C6-O6	5.74	132.05	128.60
36	5	2777	G	C5-C6-O6	5.74	132.05	128.60
36	1	63	A	N1-C2-N3	-5.74	126.43	129.30
36	1	2142	A	O5'-P-OP2	5.74	117.59	110.70
1	6	431	C	O5'-P-OP1	-5.74	100.53	105.70
1	6	594	A	OP1-P-O3'	5.74	117.83	105.20
36	5	3016	A	OP1-P-O3'	-5.74	92.57	105.20
36	1	66	A	O5'-P-OP1	-5.74	100.53	105.70
36	1	186	U	N1-C2-O2	5.74	126.82	122.80
36	1	1450	G	N9-C4-C5	-5.74	103.11	105.40
36	1	2363	A	C5-C6-N6	5.74	128.29	123.70
36	1	2865	U	OP2-P-O3'	5.74	117.83	105.20
1	6	403	G	N9-C4-C5	-5.74	103.10	105.40
36	5	661	G	N1-C2-N3	-5.74	120.46	123.90
36	1	2227	C	P-O3'-C3'	5.74	126.58	119.70
37	7	5	G	N9-C4-C5	-5.74	103.11	105.40
6	S4	164	LEU	CA-CB-CG	5.74	128.49	115.30
18	C6	40	GLU	C-N-CA	5.74	146.09	122.00
36	1	620	U	N1-C1'-C2'	5.74	121.46	114.00
36	1	1122	U	C2-N3-C4	-5.74	123.56	127.00
36	1	1131	G	O5'-P-OP2	-5.74	100.54	105.70
36	1	2201	G	N3-C2-N2	5.74	123.91	119.90
36	5	895	A	C5'-C4'-O4'	5.74	115.98	109.10
36	5	3245	A	N3-C4-C5	5.74	130.82	126.80
52	m6	78	ARG	NE-CZ-NH2	-5.74	117.43	120.30
36	1	410	U	N1-C2-O2	-5.73	118.79	122.80
36	1	1305	U	N3-C4-C5	5.73	118.04	114.60
36	5	2335	G	C5-C6-O6	-5.73	125.16	128.60
41	14	300	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	2	720	G	OP1-P-O3'	5.73	117.81	105.20
36	1	1476	G	C8-N9-C4	5.73	108.69	106.40
1	6	308	C	N3-C2-O2	-5.73	117.89	121.90
36	5	61	A	C2-N3-C4	-5.73	107.73	110.60
36	5	1475	A	O5'-P-OP2	-5.73	100.54	105.70
36	5	2144	A	N1-C6-N6	5.73	122.04	118.60
36	5	1297	C	C2-N3-C4	-5.73	117.03	119.90
36	1	1552	G	C5-C6-O6	-5.73	125.16	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2870	C	N3-C4-C5	5.73	124.19	121.90
1	2	1517	U	O5'-P-OP2	-5.73	100.55	105.70
36	1	221	A	N1-C2-N3	5.73	132.16	129.30
36	1	304	G	N9-C4-C5	5.73	107.69	105.40
36	1	674	G	N9-C4-C5	5.73	107.69	105.40
36	1	1888	U	C2-N3-C4	-5.73	123.56	127.00
1	6	287	G	C5-C6-O6	-5.73	125.16	128.60
36	5	3138	U	N1-C2-O2	-5.73	118.79	122.80
36	1	609	G	N3-C4-N9	5.73	129.44	126.00
36	1	801	A	O5'-P-OP1	5.73	117.57	110.70
36	1	973	A	C8-N9-C4	-5.73	103.51	105.80
36	1	2281	A	N9-C4-C5	-5.73	103.51	105.80
1	2	810	G	C6-C5-N7	-5.72	126.97	130.40
1	2	1119	G	C5-C6-O6	5.72	132.03	128.60
36	1	2368	A	C8-N9-C4	5.72	108.09	105.80
36	5	1133	A	C5-N7-C8	5.72	106.76	103.90
36	5	1391	C	C5-C4-N4	-5.72	116.19	120.20
1	6	1078	C	N3-C4-N4	-5.72	114.00	118.00
36	5	37	U	C6-N1-C2	-5.72	117.57	121.00
1	2	810	G	C4-C5-N7	5.72	113.09	110.80
36	5	96	G	C5-C6-O6	5.72	132.03	128.60
36	5	186	U	N1-C2-O2	5.72	126.80	122.80
36	5	218	G	O5'-P-OP1	-5.72	100.55	105.70
36	5	1878	G	C8-N9-C1'	-5.72	119.56	127.00
36	5	2412	G	N1-C6-O6	-5.72	116.47	119.90
36	5	3115	C	C6-N1-C2	-5.72	118.01	120.30
36	5	1219	C	N3-C4-C5	5.72	124.19	121.90
36	1	1124	U	OP2-P-O3'	5.72	117.78	105.20
36	1	2434	U	N3-C2-O2	-5.72	118.20	122.20
41	L4	139	GLY	N-CA-C	-5.72	98.81	113.10
36	5	1107	C	OP2-P-O3'	5.72	117.78	105.20
36	5	2249	G	C8-N9-C4	-5.72	104.11	106.40
36	1	23	A	C5-C6-N6	-5.71	119.13	123.70
36	1	1123	U	C5-C6-N1	-5.71	119.84	122.70
1	6	1535	U	P-O3'-C3'	5.71	126.56	119.70
36	5	1154	A	C5-C6-N1	5.71	120.56	117.70
36	5	2250	G	N1-C6-O6	-5.71	116.47	119.90
36	1	371	G	N3-C2-N2	5.71	123.90	119.90
36	1	1664	G	N1-C6-O6	-5.71	116.47	119.90
36	1	2827	U	O4'-C1'-N1	5.71	112.77	108.20
1	6	554	C	N3-C2-O2	-5.71	117.90	121.90
36	5	2287	C	C4-C5-C6	-5.71	114.54	117.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2968	G	C6-C5-N7	5.71	133.83	130.40
1	2	1455	G	N3-C2-N2	-5.71	115.90	119.90
36	1	2893	C	OP1-P-OP2	5.71	128.17	119.60
37	3	96	U	C5-C6-N1	-5.71	119.84	122.70
1	6	362	G	N3-C4-N9	5.71	129.43	126.00
36	5	436	A	N7-C8-N9	5.71	116.66	113.80
36	1	1592	G	N3-C2-N2	5.71	123.90	119.90
36	1	2391	G	C5-C6-O6	5.71	132.03	128.60
36	5	1487	G	C8-N9-C4	-5.71	104.12	106.40
36	5	2593	A	P-O3'-C3'	5.71	126.55	119.70
36	1	975	C	OP1-P-OP2	5.71	128.16	119.60
36	1	1906	G	N3-C4-C5	-5.71	125.75	128.60
36	1	2813	A	C4-C5-N7	-5.71	107.85	110.70
36	5	775	A	C8-N9-C4	-5.71	103.52	105.80
36	5	953	G	C5-C6-O6	-5.71	125.18	128.60
1	2	380	U	N1-C2-O2	5.71	126.79	122.80
36	1	661	G	C4-N9-C1'	5.71	133.92	126.50
36	1	2800	G	C6-N1-C2	-5.71	121.68	125.10
36	1	2960	C	N3-C4-C5	5.71	124.18	121.90
1	6	174	U	C5-C4-O4	-5.71	122.48	125.90
37	3	102	A	N9-C4-C5	-5.70	103.52	105.80
1	6	66	U	P-O3'-C3'	5.70	126.54	119.70
36	5	1189	C	C5-C4-N4	-5.70	116.21	120.20
36	5	1487	G	N1-C6-O6	-5.70	116.48	119.90
1	2	1196	A	P-O3'-C3'	5.70	126.54	119.70
36	1	507	U	O5'-P-OP1	5.70	117.54	110.70
36	5	1481	A	C8-N9-C4	-5.70	103.52	105.80
38	4	125	U	N3-C2-O2	-5.70	118.21	122.20
1	6	425	A	O5'-P-OP1	5.70	117.54	110.70
36	5	1931	U	N3-C4-O4	-5.70	115.41	119.40
37	7	7	G	O5'-P-OP1	5.70	117.54	110.70
38	8	8	C	C6-N1-C2	-5.70	118.02	120.30
36	1	2621	G	N3-C2-N2	-5.70	115.91	119.90
36	5	213	A	O5'-P-OP2	-5.70	100.57	105.70
36	1	3271	G	N1-C6-O6	5.70	123.32	119.90
36	5	2402	A	OP2-P-O3'	5.70	117.73	105.20
36	5	2944	U	C2-N3-C4	-5.70	123.58	127.00
36	5	3062	G	C8-N9-C4	-5.70	104.12	106.40
36	1	2819	A	C2-N3-C4	5.70	113.45	110.60
36	1	3305	A	O5'-P-OP2	-5.70	100.58	105.70
1	6	1269	U	N3-C2-O2	-5.70	118.21	122.20
36	5	513	G	N1-C6-O6	-5.70	116.48	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	112	U	O4'-C1'-N1	5.69	112.75	108.20
36	1	1189	C	C2-N3-C4	-5.69	117.05	119.90
36	5	509	U	O5'-P-OP1	-5.69	100.58	105.70
36	1	297	G	O4'-C1'-N9	5.69	112.75	108.20
36	5	26	A	C8-N9-C4	5.69	108.08	105.80
36	5	2335	G	C6-N1-C2	-5.69	121.68	125.10
36	1	718	G	C4-C5-C6	-5.69	115.39	118.80
36	1	764	U	P-O3'-C3'	5.69	126.53	119.70
36	1	1365	G	N3-C2-N2	5.69	123.88	119.90
36	1	1389	G	N9-C4-C5	-5.69	103.12	105.40
36	1	1888	U	C5-C6-N1	-5.69	119.86	122.70
36	1	2305	G	N9-C4-C5	-5.69	103.12	105.40
36	5	518	G	O4'-C1'-N9	5.69	112.75	108.20
36	5	2836	C	C5-C6-N1	-5.69	118.16	121.00
36	5	3004	C	N1-C2-O2	-5.69	115.49	118.90
69	o3	73	ARG	NE-CZ-NH1	-5.69	117.45	120.30
36	1	53	G	C5-C6-N1	5.69	114.34	111.50
36	1	2362	C	O5'-P-OP2	-5.69	100.58	105.70
36	5	202	G	N1-C2-N2	-5.69	111.08	116.20
36	5	339	C	C2-N1-C1'	-5.69	112.54	118.80
36	5	1161	G	C5-C6-N1	5.69	114.34	111.50
36	1	1366	A	C6-N1-C2	5.69	122.01	118.60
36	1	1661	G	O5'-P-OP2	-5.69	100.58	105.70
36	1	2226	U	O5'-P-OP2	5.69	117.53	110.70
1	6	390	G	N3-C4-N9	5.69	129.41	126.00
1	6	1124	A	N9-C4-C5	-5.69	103.53	105.80
36	5	1048	A	OP1-P-O3'	5.69	117.71	105.20
36	5	2656	A	C8-N9-C4	-5.69	103.53	105.80
1	2	734	A	P-O3'-C3'	5.69	126.52	119.70
36	1	1841	A	N3-C4-C5	-5.69	122.82	126.80
36	1	2198	A	N7-C8-N9	-5.69	110.96	113.80
36	1	2651	G	N3-C4-N9	-5.69	122.59	126.00
1	6	65	A	C4-C5-N7	5.69	113.54	110.70
1	2	992	A	N3-C4-C5	5.68	130.78	126.80
36	1	143	G	C2-N3-C4	5.68	114.74	111.90
36	1	2790	A	N1-C6-N6	-5.68	115.19	118.60
36	1	3209	A	C4-C5-N7	5.68	113.54	110.70
36	1	2632	G	N1-C2-N2	-5.68	111.08	116.20
36	1	2818	U	O5'-P-OP2	-5.68	100.59	105.70
36	5	1186	G	C8-N9-C4	-5.68	104.13	106.40
36	5	2403	G	C5-C6-O6	5.68	132.01	128.60
36	5	2743	A	N7-C8-N9	-5.68	110.96	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	320	U	N3-C2-O2	5.68	126.18	122.20
36	5	437	G	C6-C5-N7	5.68	133.81	130.40
36	1	1513	G	C5-C6-N1	5.68	114.34	111.50
1	6	4	C	O5'-P-OP1	-5.68	100.59	105.70
1	6	542	A	P-O3'-C3'	5.68	126.52	119.70
36	5	780	A	N1-C2-N3	-5.68	126.46	129.30
36	5	903	U	N3-C4-C5	5.68	118.01	114.60
36	5	1833	G	C8-N9-C4	5.68	108.67	106.40
36	1	422	A	C5-C6-N1	5.68	120.54	117.70
36	1	903	U	N3-C2-O2	-5.68	118.23	122.20
1	6	321	C	N1-C2-O2	5.68	122.31	118.90
1	6	1620	C	C6-N1-C2	-5.68	118.03	120.30
36	1	1859	A	N7-C8-N9	-5.68	110.96	113.80
36	1	2867	C	C4-C5-C6	-5.68	114.56	117.40
36	5	778	U	N1-C2-O2	5.68	126.77	122.80
36	1	1420	C	C5-C4-N4	5.67	124.17	120.20
36	1	1857	C	N1-C2-O2	-5.67	115.50	118.90
36	5	1116	G	C5-C6-O6	5.67	132.00	128.60
36	5	2639	G	N3-C4-C5	-5.67	125.76	128.60
36	5	2913	C	N1-C2-O2	-5.67	115.50	118.90
36	1	2367	A	O5'-P-OP1	-5.67	100.59	105.70
36	1	3204	C	N3-C4-C5	5.67	124.17	121.90
1	6	313	U	C2-N3-C4	-5.67	123.60	127.00
36	1	420	G	O5'-P-OP2	-5.67	100.60	105.70
36	5	1412	G	C8-N9-C4	-5.67	104.13	106.40
36	1	765	C	C6-N1-C2	-5.67	118.03	120.30
38	4	9	A	C8-N9-C4	-5.67	103.53	105.80
36	5	926	A	C5-C6-N6	-5.67	119.17	123.70
36	5	2531	C	C6-N1-C1'	-5.67	114.00	120.80
36	5	2894	C	C5-C6-N1	5.67	123.83	121.00
1	2	432	G	C2-N3-C4	5.67	114.73	111.90
1	2	1634	C	C6-N1-C2	5.67	122.57	120.30
36	1	272	G	C5-N7-C8	5.67	107.13	104.30
36	1	2148	U	N3-C2-O2	5.67	126.17	122.20
36	1	2983	C	C5-C6-N1	-5.67	118.17	121.00
36	5	1302	A	OP2-P-O3'	5.67	117.66	105.20
36	1	963	G	O5'-P-OP1	5.67	117.50	110.70
36	5	3032	A	C2-N3-C4	5.67	113.43	110.60
36	1	2297	U	N3-C4-C5	5.66	118.00	114.60
38	4	25	G	O5'-P-OP1	5.66	117.50	110.70
36	5	2426	U	C5-C4-O4	5.66	129.30	125.90
36	1	204	A	C2-N3-C4	5.66	113.43	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2651	G	C6-C5-N7	5.66	133.80	130.40
36	5	3223	A	N1-C6-N6	-5.66	115.20	118.60
36	5	2127	U	O5'-P-OP1	-5.66	100.61	105.70
36	1	1442	U	C5-C6-N1	5.66	125.53	122.70
1	6	1781	A	C5-C6-N1	-5.66	114.87	117.70
36	5	887	G	N1-C2-N2	-5.66	111.11	116.20
36	5	2857	C	C6-N1-C2	5.66	122.56	120.30
37	7	5	G	C8-N9-C4	5.66	108.66	106.40
37	7	112	G	C8-N9-C4	-5.66	104.14	106.40
36	1	2180	G	N9-C4-C5	5.66	107.66	105.40
37	3	81	U	N1-C2-O2	5.66	126.76	122.80
1	6	163	G	N7-C8-N9	5.66	115.93	113.10
1	2	542	A	C4-N9-C1'	5.66	136.48	126.30
1	6	76	A	O4'-C1'-N9	5.66	112.72	108.20
36	5	216	G	C4-C5-N7	5.66	113.06	110.80
36	5	1065	A	O5'-P-OP1	-5.66	100.61	105.70
36	1	1476	G	N7-C8-N9	-5.65	110.27	113.10
36	1	2409	G	N3-C4-C5	-5.65	125.77	128.60
38	4	151	C	N3-C4-N4	5.65	121.96	118.00
1	2	1564	U	N1-C2-O2	-5.65	118.84	122.80
36	1	2160	G	N3-C2-N2	5.65	123.86	119.90
36	1	3136	G	N1-C6-O6	-5.65	116.51	119.90
36	5	1371	G	C6-C5-N7	5.65	133.79	130.40
36	5	2820	A	N9-C4-C5	5.65	108.06	105.80
38	8	38	U	N3-C4-O4	-5.65	115.44	119.40
36	5	2604	U	N3-C2-O2	-5.65	118.25	122.20
36	1	916	G	C5-C6-N1	-5.65	108.68	111.50
36	1	2827	U	C2-N3-C4	-5.65	123.61	127.00
54	M8	138	LEU	CA-CB-CG	5.65	128.29	115.30
36	5	629	U	C5-C4-O4	-5.65	122.51	125.90
36	5	931	C	C5-C4-N4	-5.65	116.25	120.20
36	5	2792	A	C8-N9-C4	-5.65	103.54	105.80
36	5	3218	A	P-O3'-C3'	5.65	126.48	119.70
1	2	1559	A	C2-N3-C4	-5.65	107.78	110.60
36	5	1178	G	C8-N9-C4	-5.65	104.14	106.40
1	2	320	U	C5-C4-O4	-5.64	122.51	125.90
36	1	124	U	N3-C2-O2	-5.64	118.25	122.20
36	1	2522	G	C4-N9-C1'	5.64	133.84	126.50
1	6	634	G	O5'-P-OP2	-5.64	100.62	105.70
36	5	516	A	N1-C6-N6	5.64	121.99	118.60
36	5	715	A	O4'-C1'-N9	5.64	112.72	108.20
36	5	1162	U	C2-N3-C4	-5.64	123.61	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3217	C	C6-N1-C1'	-5.64	114.03	120.80
1	6	144	U	C2-N1-C1'	5.64	124.47	117.70
36	5	35	A	C2-N3-C4	-5.64	107.78	110.60
36	5	2119	A	C6-C5-N7	-5.64	128.35	132.30
36	5	2994	A	N1-C6-N6	5.64	121.98	118.60
1	2	1361	U	N1-C2-O2	5.64	126.75	122.80
36	1	957	C	N3-C2-O2	5.64	125.85	121.90
36	1	2257	C	C6-N1-C2	-5.64	118.04	120.30
36	5	1323	G	N1-C6-O6	-5.64	116.52	119.90
36	5	2874	G	C5-C6-O6	5.64	131.98	128.60
36	5	946	U	C5-C4-O4	5.64	129.28	125.90
36	1	1114	U	N3-C4-O4	-5.64	115.45	119.40
1	6	795	U	OP1-P-OP2	-5.64	111.14	119.60
1	2	1432	U	C5-C4-O4	-5.63	122.52	125.90
36	1	2142	A	N1-C2-N3	5.63	132.12	129.30
36	1	3181	C	C5-C6-N1	-5.63	118.18	121.00
36	5	3076	C	N1-C2-O2	5.63	122.28	118.90
1	2	1675	C	N3-C2-O2	-5.63	117.96	121.90
36	5	202	G	N3-C2-N2	5.63	123.84	119.90
36	5	925	A	C2-N3-C4	5.63	113.42	110.60
36	1	890	C	O5'-P-OP2	-5.63	100.63	105.70
36	1	907	G	N3-C4-C5	-5.63	125.78	128.60
51	M5	38	ARG	NE-CZ-NH1	5.63	123.11	120.30
36	5	1879	A	O5'-P-OP2	-5.63	100.63	105.70
36	5	2398	A	N9-C4-C5	5.63	108.05	105.80
36	5	2966	G	C5-C6-O6	-5.63	125.22	128.60
36	1	995	U	C4-C5-C6	-5.63	116.32	119.70
36	1	2980	U	OP1-P-OP2	-5.63	111.16	119.60
36	5	301	G	C8-N9-C4	5.63	108.65	106.40
52	m6	160	ARG	NE-CZ-NH1	5.63	123.11	120.30
36	1	24	G	C6-N1-C2	-5.63	121.72	125.10
36	1	425	G	N1-C6-O6	-5.63	116.53	119.90
36	1	2423	U	C2-N1-C1'	5.63	124.45	117.70
36	5	1375	G	C2-N3-C4	5.63	114.71	111.90
36	5	1506	A	N9-C4-C5	5.63	108.05	105.80
36	5	2907	G	OP2-P-O3'	5.63	117.58	105.20
36	5	3302	U	C5-C4-O4	-5.63	122.52	125.90
36	1	1598	G	N1-C6-O6	-5.62	116.53	119.90
37	3	72	A	C8-N9-C4	-5.62	103.55	105.80
78	Q2	93	LEU	CA-CB-CG	5.62	128.24	115.30
36	5	1313	G	O5'-P-OP1	5.62	117.45	110.70
36	5	1446	A	C8-N9-C4	5.62	108.05	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2339	C	O4'-C1'-N1	-5.62	103.70	108.20
1	2	1441	C	C5-C6-N1	-5.62	118.19	121.00
36	1	192	C	O5'-P-OP1	-5.62	100.64	105.70
36	1	1419	A	C5'-C4'-O4'	5.62	115.85	109.10
36	5	1588	A	N9-C4-C5	-5.62	103.55	105.80
36	1	388	G	C8-N9-C4	-5.62	104.15	106.40
36	1	859	G	N9-C4-C5	-5.62	103.15	105.40
36	5	101	G	O4'-C1'-N9	5.62	112.70	108.20
36	5	2373	A	OP1-P-O3'	5.62	117.57	105.20
36	5	2949	U	N1-C2-O2	5.62	126.73	122.80
36	1	338	A	N9-C4-C5	5.62	108.05	105.80
36	1	967	A	C6-C5-N7	5.62	136.23	132.30
1	6	119	A	C2-N3-C4	-5.62	107.79	110.60
36	1	2612	U	O5'-P-OP1	-5.62	100.64	105.70
1	6	1257	U	N3-C2-O2	-5.62	118.27	122.20
1	6	1498	G	C5-C6-O6	5.62	131.97	128.60
64	n8	12	ARG	NE-CZ-NH2	-5.62	117.49	120.30
36	1	3278	C	C5-C4-N4	5.62	124.13	120.20
37	3	102	A	C4-C5-C6	-5.62	114.19	117.00
1	6	401	A	N1-C6-N6	5.62	121.97	118.60
1	6	1100	G	N3-C4-C5	-5.62	125.79	128.60
1	6	1749	A	C6-C5-N7	-5.62	128.37	132.30
36	5	682	U	C2-N3-C4	-5.62	123.63	127.00
36	5	3218	A	C5-N7-C8	-5.62	101.09	103.90
37	7	20	A	N1-C6-N6	5.62	121.97	118.60
36	1	210	U	N3-C2-O2	-5.61	118.27	122.20
1	2	1766	A	C8-N9-C4	5.61	108.05	105.80
36	1	1713	G	C8-N9-C4	5.61	108.64	106.40
36	5	2969	A	C8-N9-C4	5.61	108.05	105.80
36	1	226	C	C5-C4-N4	-5.61	116.27	120.20
36	1	420	G	N9-C4-C5	-5.61	103.16	105.40
36	1	2313	A	N1-C6-N6	5.61	121.97	118.60
36	5	437	G	C8-N9-C1'	5.61	134.29	127.00
36	5	1210	U	N1-C2-O2	5.61	126.73	122.80
36	5	1340	G	N3-C2-N2	5.61	123.83	119.90
73	o7	45	ARG	NE-CZ-NH2	-5.61	117.50	120.30
36	1	641	C	O4'-C1'-N1	5.61	112.69	108.20
36	1	895	A	C5-C6-N1	-5.61	114.89	117.70
38	4	81	U	N3-C2-O2	-5.61	118.27	122.20
1	6	17	C	N3-C2-O2	-5.61	117.97	121.90
1	6	1572	G	N3-C2-N2	-5.61	115.97	119.90
36	5	2963	C	OP2-P-O3'	5.61	117.54	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1539	G	N3-C4-N9	-5.61	122.64	126.00
36	5	2892	A	C6-N1-C2	5.61	121.96	118.60
36	5	1433	A	O4'-C1'-N9	-5.61	103.72	108.20
38	8	99	C	N3-C4-C5	5.61	124.14	121.90
1	2	992	A	N3-C4-N9	-5.60	122.92	127.40
36	1	1426	C	N3-C4-N4	-5.60	114.08	118.00
36	1	730	C	N3-C4-C5	5.60	124.14	121.90
36	1	1412	G	C5-C6-O6	5.60	131.96	128.60
36	1	2656	A	C2-N3-C4	5.60	113.40	110.60
36	5	93	C	C6-N1-C2	-5.60	118.06	120.30
1	6	542	A	C5-C6-N6	-5.60	119.22	123.70
36	5	1495	U	C6-N1-C2	-5.60	117.64	121.00
36	1	25	U	C2-N3-C4	-5.60	123.64	127.00
1	6	1745	G	C5-C6-O6	-5.60	125.24	128.60
25	d3	23	ARG	CG-CD-NE	5.60	123.56	111.80
36	5	819	U	OP2-P-O3'	5.60	117.52	105.20
36	1	2956	A	O5'-P-OP1	-5.60	100.66	105.70
36	5	1686	U	N1-C2-O2	-5.60	118.88	122.80
37	7	92	A	N9-C4-C5	-5.60	103.56	105.80
36	1	3057	U	N3-C2-O2	-5.60	118.28	122.20
36	1	3089	C	N3-C4-C5	5.60	124.14	121.90
37	7	48	U	N3-C4-C5	5.60	117.96	114.60
36	1	340	C	N3-C2-O2	-5.59	117.98	121.90
36	1	1536	G	N1-C6-O6	5.59	123.26	119.90
36	1	2642	A	C4-C5-C6	-5.59	114.20	117.00
36	1	2697	A	N9-C4-C5	5.59	108.04	105.80
1	2	720	G	P-O3'-C3'	5.59	126.41	119.70
24	D2	65	LEU	CA-CB-CG	5.59	128.16	115.30
36	1	386	A	C4-C5-C6	5.59	119.80	117.00
36	1	1329	U	C3'-C2'-C1'	5.59	105.97	101.50
36	1	2178	A	C5-C6-N6	5.59	128.17	123.70
1	6	93	A	N1-C6-N6	5.59	121.95	118.60
36	5	50	U	O5'-P-OP1	-5.59	100.67	105.70
1	2	1456	C	N3-C2-O2	-5.59	117.99	121.90
36	1	1379	G	N1-C2-N2	-5.59	111.17	116.20
36	5	629	U	N3-C4-C5	5.59	117.95	114.60
36	5	2651	G	OP2-P-O3'	5.59	117.50	105.20
36	5	3052	G	N9-C4-C5	5.59	107.64	105.40
1	2	610	G	C8-N9-C1'	-5.59	119.74	127.00
36	5	630	A	C5-C6-N1	-5.59	114.91	117.70
36	5	2157	G	C8-N9-C4	5.59	108.64	106.40
36	5	2352	A	C5-C6-N1	-5.59	114.91	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2618	G	C6-N1-C2	-5.59	121.75	125.10
1	2	1524	A	N9-C4-C5	5.59	108.03	105.80
36	1	374	A	O4'-C1'-N9	5.59	112.67	108.20
1	6	687	G	C8-N9-C1'	5.59	134.26	127.00
36	5	693	A	N9-C4-C5	5.59	108.03	105.80
36	5	1336	U	O5'-P-OP2	-5.59	100.67	105.70
36	5	1589	A	N1-C2-N3	-5.59	126.51	129.30
36	5	2371	G	N3-C4-C5	5.59	131.39	128.60
36	5	2830	G	C4-C5-N7	-5.59	108.56	110.80
36	1	2787	G	C2-N3-C4	5.58	114.69	111.90
36	1	2836	C	N3-C4-N4	-5.58	114.09	118.00
38	4	56	G	N3-C2-N2	5.58	123.81	119.90
36	5	2139	A	O4'-C1'-N9	-5.58	103.73	108.20
36	5	2153	U	C5-C6-N1	-5.58	119.91	122.70
36	1	123	A	C8-N9-C4	-5.58	103.57	105.80
36	1	212	G	O4'-C1'-N9	5.58	112.67	108.20
36	1	2639	G	OP2-P-O3'	5.58	117.49	105.20
36	5	1124	U	C6-N1-C2	5.58	124.35	121.00
36	1	3054	U	C2-N3-C4	-5.58	123.65	127.00
36	1	3090	U	O5'-P-OP2	-5.58	100.68	105.70
37	3	86	U	OP1-P-O3'	5.58	117.48	105.20
36	1	364	G	C5-C6-O6	-5.58	125.25	128.60
36	1	1178	G	N9-C4-C5	5.58	107.63	105.40
36	1	1342	C	C5-C4-N4	-5.58	116.29	120.20
36	5	1057	A	N1-C6-N6	5.58	121.95	118.60
36	5	3074	G	N3-C2-N2	5.58	123.81	119.90
36	1	2382	G	N3-C2-N2	5.58	123.80	119.90
1	6	1361	U	C6-N1-C1'	-5.58	113.39	121.20
36	5	2814	G	C6-C5-N7	-5.58	127.05	130.40
1	2	1365	C	C6-N1-C2	-5.58	118.07	120.30
1	2	1462	G	C8-N9-C4	5.58	108.63	106.40
36	5	2398	A	N7-C8-N9	5.58	116.59	113.80
36	5	2860	U	N3-C4-O4	5.58	123.30	119.40
1	2	704	C	C2-N1-C1'	5.57	124.93	118.80
36	1	369	A	N1-C6-N6	-5.57	115.26	118.60
36	5	1517	G	O5'-P-OP2	-5.57	100.69	105.70
38	4	85	G	N1-C6-O6	5.57	123.24	119.90
52	M6	189	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	6	782	U	N3-C2-O2	-5.57	118.30	122.20
36	5	2735	U	C6-N1-C2	-5.57	117.66	121.00
36	1	609	G	C5-C6-N1	5.57	114.28	111.50
36	1	862	U	C6-N1-C2	-5.57	117.66	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	920	A	OP1-P-O3'	5.57	117.45	105.20
38	4	100	U	N1-C2-O2	5.57	126.70	122.80
59	n3	45	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	2	75	U	C6-N1-C1'	-5.57	113.41	121.20
1	2	1455	G	C5-C6-N1	-5.57	108.72	111.50
36	1	110	G	C5'-C4'-O4'	5.57	115.78	109.10
36	1	344	A	C6-C5-N7	5.57	136.20	132.30
36	1	801	A	N7-C8-N9	5.57	116.58	113.80
36	1	967	A	C5-N7-C8	5.57	106.68	103.90
36	1	2305	G	N3-C4-N9	5.57	129.34	126.00
38	4	19	C	C5-C4-N4	5.57	124.10	120.20
38	4	23	U	N3-C2-O2	5.57	126.09	122.20
36	5	221	A	N9-C4-C5	-5.57	103.57	105.80
36	5	1370	G	N1-C6-O6	-5.57	116.56	119.90
1	6	542	A	O4'-C1'-N9	5.56	112.65	108.20
36	5	2725	U	O5'-P-OP1	-5.56	100.69	105.70
36	5	2990	G	N3-C4-C5	-5.56	125.82	128.60
18	C6	28	LEU	CA-CB-CG	5.56	128.09	115.30
36	1	1444	G	C8-N9-C4	5.56	108.62	106.40
36	1	2376	G	N9-C4-C5	-5.56	103.17	105.40
36	1	2619	G	OP1-P-OP2	5.56	127.94	119.60
38	4	15	G	C5-C6-O6	-5.56	125.26	128.60
36	5	532	A	C8-N9-C4	-5.56	103.58	105.80
36	5	2408	U	N3-C4-O4	-5.56	115.51	119.40
38	8	104	A	C8-N9-C4	5.56	108.03	105.80
36	1	186	U	N3-C2-O2	-5.56	118.31	122.20
36	1	410	U	C4-C5-C6	5.56	123.04	119.70
36	1	429	U	N1-C2-O2	5.56	126.69	122.80
36	1	2871	G	N3-C2-N2	-5.56	116.01	119.90
36	5	2637	A	N1-C6-N6	5.56	121.94	118.60
1	2	780	A	C2-N3-C4	-5.56	107.82	110.60
36	1	1180	A	OP1-P-O3'	5.56	117.43	105.20
36	1	1931	U	N3-C2-O2	5.56	126.09	122.20
1	6	1432	U	O4'-C1'-N1	5.56	112.65	108.20
1	2	554	C	C6-N1-C2	-5.56	118.08	120.30
1	2	1243	G	O4'-C1'-N9	5.56	112.64	108.20
1	2	1473	U	N3-C2-O2	-5.56	118.31	122.20
68	O2	43	ARG	NE-CZ-NH2	-5.56	117.52	120.30
36	5	625	G	N9-C4-C5	5.56	107.62	105.40
36	5	1337	A	N9-C4-C5	5.56	108.02	105.80
36	5	2808	A	C6-C5-N7	-5.56	128.41	132.30
36	5	3266	G	C5-C6-O6	5.56	131.94	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1047	A	C5-N7-C8	-5.56	101.12	103.90
40	13	19	ARG	CG-CD-NE	-5.56	100.13	111.80
36	1	3010	U	N1-C2-O2	5.55	126.69	122.80
36	5	1159	A	C4-C5-N7	5.55	113.48	110.70
37	7	104	A	N1-C6-N6	5.55	121.93	118.60
38	8	111	A	O5'-P-OP2	-5.55	100.70	105.70
1	2	1761	U	N3-C2-O2	-5.55	118.31	122.20
36	1	267	G	O4'-C1'-N9	-5.55	103.76	108.20
36	1	419	G	N3-C2-N2	5.55	123.78	119.90
1	6	331	A	C2-N3-C4	-5.55	107.82	110.60
1	6	623	A	O4'-C1'-N9	5.55	112.64	108.20
36	5	415	G	C5-N7-C8	5.55	107.08	104.30
36	5	2231	C	C6-N1-C1'	-5.55	114.14	120.80
36	5	2715	A	C2-N3-C4	5.55	113.38	110.60
36	5	2946	A	N1-C6-N6	-5.55	115.27	118.60
36	1	288	C	N1-C2-O2	-5.55	115.57	118.90
36	1	2376	G	C8-N9-C1'	-5.55	119.78	127.00
36	5	648	C	C5-C6-N1	5.55	123.78	121.00
36	5	2384	A	N1-C6-N6	5.55	121.93	118.60
36	1	959	C	N3-C2-O2	5.55	125.78	121.90
36	1	3259	U	N1-C2-O2	-5.55	118.92	122.80
36	5	1319	G	N1-C6-O6	-5.55	116.57	119.90
36	1	1411	C	C5-C4-N4	5.55	124.08	120.20
36	1	1665	C	N3-C4-C5	5.55	124.12	121.90
1	6	1269	U	N1-C2-N3	5.55	118.23	114.90
36	5	907	G	N3-C4-N9	5.55	129.33	126.00
36	5	1379	G	N3-C2-N2	5.55	123.78	119.90
36	5	2180	G	C8-N9-C4	5.55	108.62	106.40
1	6	1751	C	N1-C2-O2	5.54	122.23	118.90
36	5	301	G	N7-C8-N9	-5.54	110.33	113.10
36	5	1047	A	C5-C6-N6	-5.54	119.26	123.70
36	5	1489	A	N9-C4-C5	-5.54	103.58	105.80
36	5	2897	A	C4-C5-N7	-5.54	107.93	110.70
36	5	2917	G	C2-N3-C4	5.54	114.67	111.90
36	1	1005	G	N1-C6-O6	-5.54	116.57	119.90
36	1	1369	A	C5-N7-C8	5.54	106.67	103.90
1	6	260	U	C6-N1-C2	5.54	124.33	121.00
1	2	145	A	N9-C4-C5	5.54	108.02	105.80
1	2	380	U	O5'-P-OP1	-5.54	100.71	105.70
1	6	1573	A	P-O3'-C3'	5.54	126.35	119.70
36	5	1858	A	N7-C8-N9	5.54	116.57	113.80
36	5	2836	C	C4-C5-C6	5.54	120.17	117.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3052	G	C6-C5-N7	5.54	133.72	130.40
36	1	859	G	C6-C5-N7	-5.54	127.08	130.40
36	1	2513	U	N1-C1'-C2'	-5.54	105.91	112.00
36	5	997	A	OP2-P-O3'	5.54	117.38	105.20
36	5	2631	U	N1-C2-N3	5.54	118.22	114.90
36	1	321	C	C6-N1-C2	-5.54	118.08	120.30
37	7	75	G	C5-C6-N1	-5.54	108.73	111.50
1	2	142	G	C5-C6-N1	-5.54	108.73	111.50
36	1	66	A	O5'-P-OP2	5.54	117.34	110.70
36	1	1402	C	N3-C4-N4	-5.54	114.13	118.00
36	1	2198	A	C8-N9-C4	5.54	108.02	105.80
38	4	79	A	N7-C8-N9	5.54	116.57	113.80
36	5	2772	C	P-O3'-C3'	5.54	126.34	119.70
36	5	2831	G	C8-N9-C4	-5.54	104.19	106.40
36	5	3341	U	C6-N1-C2	-5.54	117.68	121.00
1	2	401	A	OP2-P-O3'	5.53	117.37	105.20
47	M0	4	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	6	1600	A	C5-N7-C8	-5.53	101.13	103.90
36	5	1482	A	O5'-P-OP2	-5.53	100.72	105.70
36	5	2349	U	N3-C4-O4	-5.53	115.53	119.40
36	5	3206	C	C6-N1-C1'	5.53	127.44	120.80
1	6	864	U	C2-N3-C4	-5.53	123.68	127.00
36	1	76	G	N3-C4-N9	5.53	129.32	126.00
36	1	1389	G	C5-C6-O6	-5.53	125.28	128.60
36	1	1482	A	C2-N3-C4	5.53	113.36	110.60
36	5	1141	C	N1-C2-O2	-5.53	115.58	118.90
36	1	1163	A	O5'-P-OP2	-5.53	100.72	105.70
38	4	30	C	O5'-P-OP1	-5.53	100.72	105.70
36	5	1192	C	C2-N3-C4	-5.53	117.14	119.90
36	1	945	C	N3-C4-C5	5.53	124.11	121.90
36	1	1858	A	N3-C4-C5	-5.53	122.93	126.80
36	1	3081	C	N3-C4-N4	-5.53	114.13	118.00
36	5	318	A	N1-C6-N6	5.53	121.92	118.60
36	5	1402	C	N1-C2-O2	5.53	122.22	118.90
36	5	2805	G	C5-C6-O6	-5.53	125.28	128.60
38	8	79	A	O5'-P-OP2	-5.53	100.73	105.70
36	1	2169	G	C6-C5-N7	5.53	133.72	130.40
51	M5	105	ARG	NE-CZ-NH2	-5.53	117.54	120.30
36	5	2654	C	C6-N1-C2	5.53	122.51	120.30
64	N8	116	GLY	N-CA-C	5.52	126.91	113.10
1	2	610	G	C4-N9-C1'	5.52	133.68	126.50
36	5	1049	C	C4-C5-C6	-5.52	114.64	117.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2323	G	C8-N9-C4	-5.52	104.19	106.40
36	5	2360	C	N3-C4-C5	-5.52	119.69	121.90
36	5	2966	G	C5-C6-N1	5.52	114.26	111.50
39	12	246	LEU	CA-CB-CG	5.52	128.00	115.30
36	1	2156	C	C5-C6-N1	-5.52	118.24	121.00
36	1	2227	C	C6-N1-C2	-5.52	118.09	120.30
1	6	1697	G	N3-C4-C5	-5.52	125.84	128.60
36	1	2817	A	OP2-P-O3'	5.52	117.34	105.20
36	5	313	A	C8-N9-C4	-5.52	103.59	105.80
36	5	1846	C	OP2-P-O3'	5.52	117.34	105.20
36	5	1942	U	N3-C4-O4	5.52	123.26	119.40
36	5	3137	C	C5-C4-N4	5.52	124.06	120.20
36	5	3228	C	N3-C2-O2	-5.52	118.04	121.90
1	2	73	U	N3-C2-O2	-5.52	118.34	122.20
1	2	1776	A	N1-C6-N6	-5.52	115.29	118.60
36	5	1116	G	C4-C5-N7	-5.52	108.59	110.80
36	5	2927	C	N3-C2-O2	-5.52	118.04	121.90
1	2	359	A	C4-C5-C6	-5.51	114.24	117.00
1	2	1490	C	OP1-P-O3'	5.51	117.33	105.20
36	1	341	G	C4-C5-N7	5.51	113.01	110.80
36	1	2131	A	N1-C6-N6	5.51	121.91	118.60
37	3	42	A	C2-N3-C4	-5.51	107.84	110.60
1	6	489	C	C2-N1-C1'	5.51	124.87	118.80
36	5	59	G	O5'-P-OP1	5.51	117.32	110.70
36	5	927	C	N3-C4-C5	5.51	124.11	121.90
36	5	995	U	C5-C6-N1	-5.51	119.94	122.70
36	5	1158	A	N1-C6-N6	5.51	121.91	118.60
36	5	1391	C	N3-C2-O2	5.51	125.76	121.90
36	5	2904	U	C5-C6-N1	-5.51	119.94	122.70
1	2	499	U	C6-N1-C1'	-5.51	113.48	121.20
50	M4	72	LEU	CA-CB-CG	5.51	127.97	115.30
36	5	437	G	C5-C6-O6	5.51	131.91	128.60
36	5	1592	G	C6-C5-N7	-5.51	127.09	130.40
36	5	2643	A	N1-C2-N3	-5.51	126.55	129.30
36	5	1655	G	O5'-P-OP1	-5.51	100.74	105.70
36	5	3317	U	C6-N1-C2	-5.51	117.69	121.00
36	5	2818	U	C5'-C4'-O4'	-5.51	102.49	109.10
36	5	2966	G	N3-C4-N9	5.51	129.31	126.00
36	5	2971	A	C2-N3-C4	5.51	113.35	110.60
1	2	536	C	C5-C6-N1	5.51	123.75	121.00
36	1	2171	G	N3-C4-N9	5.51	129.30	126.00
36	5	201	A	C5-C6-N1	-5.51	114.95	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	691	A	C8-N9-C4	-5.51	103.60	105.80
36	5	2643	A	O5'-P-OP2	-5.50	100.75	105.70
36	5	1159	A	N1-C6-N6	5.50	121.90	118.60
36	5	1873	U	N1-C2-N3	5.50	118.20	114.90
36	1	109	A	C8-N9-C4	-5.50	103.60	105.80
59	N3	70	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	6	103	A	N7-C8-N9	5.50	116.55	113.80
36	5	1169	A	C5-C6-N1	-5.50	114.95	117.70
36	5	2634	U	N3-C4-C5	5.50	117.90	114.60
36	1	1178	G	C5-C6-O6	5.50	131.90	128.60
36	1	930	U	C2-N3-C4	-5.50	123.70	127.00
36	1	1374	G	N3-C2-N2	5.50	123.75	119.90
36	1	2422	C	N3-C2-O2	-5.50	118.05	121.90
1	6	114	C	C2-N1-C1'	5.50	124.85	118.80
36	5	963	G	C8-N9-C4	5.50	108.60	106.40
36	5	2618	G	C2-N3-C4	5.50	114.65	111.90
1	6	638	U	N1-C2-O2	5.50	126.65	122.80
37	7	95	A	N1-C2-N3	-5.50	126.55	129.30
36	1	1646	G	O4'-C1'-N9	5.50	112.60	108.20
36	1	2551	U	N1-C2-N3	5.50	118.20	114.90
36	1	2585	G	N3-C4-N9	5.50	129.30	126.00
36	1	94	G	N1-C2-N3	-5.49	120.60	123.90
36	1	394	G	C5-C6-O6	5.49	131.90	128.60
1	6	1473	U	N1-C2-N3	5.49	118.20	114.90
36	5	972	A	OP2-P-O3'	5.49	117.28	105.20
36	1	835	G	C5-C6-O6	-5.49	125.31	128.60
1	6	1783	C	N1-C2-O2	5.49	122.19	118.90
36	5	1432	C	N3-C2-O2	-5.49	118.06	121.90
36	5	2908	G	N9-C4-C5	5.49	107.60	105.40
36	5	3101	G	N1-C2-N2	-5.49	111.26	116.20
1	2	398	G	C4-C5-N7	5.49	113.00	110.80
36	1	3369	G	N1-C6-O6	5.49	123.19	119.90
1	6	1	U	N1-C1'-C2'	5.49	121.14	114.00
36	5	51	A	N1-C6-N6	5.49	121.89	118.60
36	5	3369	G	C5-C6-O6	-5.49	125.31	128.60
1	2	1000	C	N3-C4-N4	-5.49	114.16	118.00
36	1	711	A	N1-C6-N6	-5.49	115.31	118.60
36	1	728	G	OP2-P-O3'	5.49	117.27	105.20
36	1	2317	A	O5'-P-OP1	-5.49	100.76	105.70
33	e1	100	LEU	CA-CB-CG	5.49	127.92	115.30
36	5	2798	C	C6-N1-C2	5.49	122.50	120.30
36	1	3175	U	C6-N1-C2	5.49	124.29	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2355	G	C4-C5-N7	5.49	112.99	110.80
36	5	3323	A	C2-N3-C4	-5.49	107.86	110.60
36	1	2340	U	C5-C4-O4	5.48	129.19	125.90
36	1	3079	U	C2-N1-C1'	-5.48	111.12	117.70
36	5	911	C	O5'-P-OP2	5.48	117.28	110.70
36	1	2139	A	N1-C6-N6	-5.48	115.31	118.60
36	1	2871	G	N3-C4-C5	5.48	131.34	128.60
1	6	542	A	C8-N9-C1'	-5.48	117.83	127.70
36	5	1308	A	O5'-P-OP1	5.48	117.28	110.70
36	5	1376	C	OP1-P-OP2	5.48	127.82	119.60
1	2	440	U	N3-C4-O4	-5.48	115.56	119.40
36	1	406	G	O5'-P-OP2	-5.48	100.77	105.70
36	1	645	A	C2-N3-C4	5.48	113.34	110.60
36	1	1555	U	O4'-C1'-N1	5.48	112.58	108.20
36	1	2777	G	C5-C6-O6	5.48	131.89	128.60
68	O2	82	LEU	CA-CB-CG	5.48	127.90	115.30
36	5	494	G	N3-C4-C5	-5.48	125.86	128.60
1	2	1441	C	C6-N1-C2	5.48	122.49	120.30
36	5	363	G	N9-C4-C5	5.48	107.59	105.40
36	1	1148	G	C8-N9-C4	5.48	108.59	106.40
1	6	53	G	N1-C6-O6	-5.48	116.61	119.90
1	6	1681	A	O4'-C1'-N9	5.48	112.58	108.20
14	c2	58	LEU	CA-CB-CG	5.48	127.90	115.30
36	5	92	G	O5'-P-OP2	5.48	117.27	110.70
36	5	2278	C	C5-C4-N4	5.48	124.03	120.20
36	5	3091	A	N9-C4-C5	5.48	107.99	105.80
36	5	413	U	C2-N3-C4	-5.48	123.71	127.00
36	1	2809	C	N3-C2-O2	-5.47	118.07	121.90
36	1	2907	G	OP2-P-O3'	5.47	117.25	105.20
38	4	53	A	N3-C4-C5	-5.47	122.97	126.80
36	5	795	G	N1-C2-N3	-5.47	120.62	123.90
36	1	209	A	C5-C6-N1	-5.47	114.96	117.70
36	1	908	G	C8-N9-C1'	-5.47	119.89	127.00
36	1	1144	U	N1-C2-N3	5.47	118.18	114.90
36	1	1437	C	C2-N1-C1'	5.47	124.82	118.80
9	s7	118	LEU	CA-CB-CG	5.47	127.89	115.30
36	5	1130	A	C4-C5-N7	-5.47	107.96	110.70
36	5	2993	G	C5-C6-O6	-5.47	125.32	128.60
36	1	412	G	N9-C4-C5	5.47	107.59	105.40
36	1	661	G	C8-N9-C4	-5.47	104.21	106.40
36	1	1323	G	N1-C6-O6	-5.47	116.62	119.90
36	1	1507	G	O4'-C1'-N9	-5.47	103.83	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	294	U	C5-C4-O4	-5.47	122.62	125.90
36	5	999	G	N1-C6-O6	-5.47	116.62	119.90
36	5	3062	G	N3-C4-C5	-5.47	125.86	128.60
36	1	3375	A	P-O3'-C3'	5.47	126.26	119.70
36	1	1201	C	C6-N1-C2	-5.47	118.11	120.30
38	4	113	U	N3-C4-O4	-5.47	115.57	119.40
36	5	522	A	O5'-P-OP1	-5.47	100.78	105.70
36	5	2271	A	N1-C6-N6	-5.47	115.32	118.60
36	5	2632	G	N3-C2-N2	5.47	123.73	119.90
36	1	295	A	N7-C8-N9	5.46	116.53	113.80
36	1	2622	C	C6-N1-C2	-5.46	118.11	120.30
36	1	2740	A	C2-N3-C4	5.46	113.33	110.60
1	6	421	A	N1-C6-N6	5.46	121.88	118.60
36	5	1083	G	OP1-P-OP2	5.46	127.80	119.60
36	5	1397	C	OP1-P-O3'	5.46	117.22	105.20
36	5	2945	G	C8-N9-C4	5.46	108.59	106.40
38	8	74	U	C5-C4-O4	-5.46	122.62	125.90
1	2	396	G	C5-C6-O6	-5.46	125.32	128.60
36	5	304	G	O4'-C1'-N9	-5.46	103.83	108.20
36	1	52	A	OP1-P-OP2	5.46	127.79	119.60
36	1	1201	C	N1-C2-O2	-5.46	115.62	118.90
36	1	3093	C	C6-N1-C2	5.46	122.48	120.30
1	6	387	A	N9-C4-C5	5.46	107.98	105.80
36	5	932	U	C5-C4-O4	-5.46	122.62	125.90
36	5	1847	A	C2-N3-C4	-5.46	107.87	110.60
36	1	949	C	N1-C2-O2	-5.46	115.62	118.90
36	1	2748	A	N1-C6-N6	5.46	121.88	118.60
38	4	56	G	N1-C2-N2	-5.46	111.29	116.20
1	6	696	C	O4'-C1'-N1	5.46	112.57	108.20
36	5	426	G	C4-C5-N7	-5.46	108.62	110.80
36	5	902	G	O5'-P-OP1	-5.46	100.79	105.70
36	5	982	C	N1-C2-O2	5.46	122.17	118.90
36	5	986	U	N1-C2-O2	5.46	126.62	122.80
36	5	1073	U	O5'-P-OP1	-5.46	100.79	105.70
36	5	1087	G	C5-C6-O6	-5.46	125.33	128.60
36	5	2402	A	C2-N3-C4	-5.46	107.87	110.60
1	2	385	A	C8-N9-C4	5.46	107.98	105.80
1	2	1052	U	C2-N1-C1'	5.46	124.25	117.70
1	2	1428	G	N3-C2-N2	-5.46	116.08	119.90
36	1	651	G	N1-C6-O6	-5.46	116.63	119.90
36	1	1556	C	C6-N1-C2	-5.46	118.12	120.30
36	1	3244	A	O4'-C1'-N9	-5.46	103.83	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1539	G	O4'-C1'-N9	-5.46	103.83	108.20
36	5	2142	A	C2-N3-C4	5.46	113.33	110.60
1	2	453	U	C6-N1-C1'	-5.46	113.56	121.20
36	1	2923	U	O5'-P-OP1	-5.46	100.79	105.70
37	3	36	C	N1-C2-O2	5.46	122.17	118.90
1	6	389	G	N1-C2-N2	-5.46	111.29	116.20
36	5	1014	U	C2-N1-C1'	5.46	124.25	117.70
36	1	405	U	C2-N3-C4	-5.45	123.73	127.00
36	1	868	C	N1-C2-O2	5.45	122.17	118.90
36	1	2125	A	C8-N9-C4	5.45	107.98	105.80
36	1	2192	C	O5'-P-OP2	-5.45	100.79	105.70
36	1	3112	G	C5-C6-O6	-5.45	125.33	128.60
36	5	193	C	OP1-P-O3'	5.45	117.20	105.20
36	5	345	G	N1-C2-N2	-5.45	111.29	116.20
36	5	2380	U	N1-C2-N3	5.45	118.17	114.90
1	2	18	C	C6-N1-C2	-5.45	118.12	120.30
1	2	570	A	C2-N3-C4	5.45	113.33	110.60
36	1	74	G	N1-C2-N3	5.45	127.17	123.90
36	1	817	A	C2-N3-C4	5.45	113.33	110.60
36	1	2550	U	C6-N1-C2	-5.45	117.73	121.00
38	4	26	U	N3-C4-O4	-5.45	115.58	119.40
1	6	466	U	C6-N1-C2	-5.45	117.73	121.00
36	5	1170	A	N7-C8-N9	-5.45	111.08	113.80
1	2	973	A	C2-N3-C4	-5.45	107.88	110.60
36	1	1507	G	N3-C4-C5	-5.45	125.88	128.60
36	1	2196	C	C6-N1-C2	-5.45	118.12	120.30
36	1	2747	A	N1-C6-N6	-5.45	115.33	118.60
36	5	57	A	OP2-P-O3'	5.45	117.19	105.20
36	5	2271	A	C2-N3-C4	5.45	113.32	110.60
36	5	3098	G	N3-C2-N2	5.45	123.71	119.90
1	6	433	C	N1-C2-O2	-5.45	115.63	118.90
36	5	2287	C	N3-C4-C5	5.45	124.08	121.90
36	1	53	G	N1-C6-O6	-5.45	116.63	119.90
36	1	218	G	N9-C4-C5	5.45	107.58	105.40
36	1	2522	G	C8-N9-C1'	-5.45	119.92	127.00
1	6	3	U	C6-N1-C2	5.45	124.27	121.00
36	5	3340	G	P-O3'-C3'	5.45	126.23	119.70
37	7	10	C	N1-C2-O2	5.45	122.17	118.90
36	1	1130	A	N1-C2-N3	-5.44	126.58	129.30
36	1	2551	U	N3-C2-O2	-5.44	118.39	122.20
36	1	3375	A	N9-C4-C5	5.44	107.98	105.80
36	5	197	G	C8-N9-C4	-5.44	104.22	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	581	U	C6-N1-C1'	-5.44	113.58	121.20
1	2	973	A	O5'-P-OP2	-5.44	100.80	105.70
36	1	1178	G	C2-N3-C4	5.44	114.62	111.90
36	5	718	G	OP2-P-O3'	5.44	117.17	105.20
36	5	2286	U	N3-C2-O2	-5.44	118.39	122.20
36	5	3046	A	C2-N3-C4	5.44	113.32	110.60
36	5	3120	C	C5-C6-N1	5.44	123.72	121.00
1	2	1573	A	P-O3'-C3'	5.44	126.23	119.70
36	1	642	U	C5-C4-O4	-5.44	122.64	125.90
36	1	2298	U	N1-C2-N3	5.44	118.17	114.90
36	1	2885	C	C6-N1-C2	5.44	122.48	120.30
36	5	715	A	C2-N3-C4	5.44	113.32	110.60
36	5	3012	A	N7-C8-N9	-5.44	111.08	113.80
36	5	3295	A	OP2-P-O3'	5.44	117.17	105.20
1	2	1399	C	C5-C6-N1	5.44	123.72	121.00
36	1	1890	U	C6-N1-C2	5.44	124.26	121.00
36	1	2389	C	OP2-P-O3'	5.44	117.17	105.20
1	6	308	C	C5-C4-N4	5.44	124.01	120.20
36	5	2404	A	OP1-P-OP2	-5.44	111.44	119.60
36	1	226	C	N3-C4-N4	5.44	121.81	118.00
36	1	861	C	O5'-P-OP1	5.44	117.22	110.70
36	1	1212	A	O5'-P-OP2	-5.44	100.81	105.70
36	1	2121	G	N1-C6-O6	-5.44	116.64	119.90
36	1	2811	A	N1-C6-N6	-5.44	115.34	118.60
36	5	2288	G	C5-C6-N1	5.44	114.22	111.50
36	5	2364	G	C8-N9-C4	-5.44	104.22	106.40
36	5	2365	C	OP1-P-OP2	5.44	127.76	119.60
36	5	2424	A	N1-C6-N6	5.44	121.86	118.60
36	5	2572	C	C6-N1-C2	-5.44	118.12	120.30
36	5	2599	U	N1-C2-O2	-5.44	118.99	122.80
36	5	3107	U	C2-N1-C1'	5.44	124.22	117.70
36	1	916	G	P-O3'-C3'	5.44	126.22	119.70
36	1	2615	G	C8-N9-C4	-5.44	104.23	106.40
36	1	702	C	N1-C2-O2	-5.43	115.64	118.90
36	1	2400	G	N3-C2-N2	-5.43	116.10	119.90
36	1	3112	G	N1-C6-O6	5.43	123.16	119.90
41	L4	194	TYR	CA-CB-CG	5.43	123.73	113.40
1	6	1299	G	N3-C4-C5	-5.43	125.88	128.60
36	5	673	U	C2-N3-C4	-5.43	123.74	127.00
36	5	1817	G	O4'-C1'-N9	5.43	112.55	108.20
36	5	3141	A	O4'-C1'-N9	-5.43	103.85	108.20
38	8	53	A	OP1-P-OP2	-5.43	111.45	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	m6	66	LYS	CD-CE-NZ	5.43	124.20	111.70
36	1	206	G	N1-C2-N3	-5.43	120.64	123.90
36	5	1487	G	C5-C6-O6	5.43	131.86	128.60
36	5	2246	G	OP1-P-OP2	-5.43	111.45	119.60
36	5	3196	U	O5'-P-OP1	-5.43	100.81	105.70
1	6	1101	G	N1-C6-O6	-5.43	116.64	119.90
36	5	569	A	C5-N7-C8	5.43	106.61	103.90
36	5	2167	A	C8-N9-C4	-5.43	103.63	105.80
1	2	1134	C	N3-C4-C5	5.43	124.07	121.90
36	1	101	G	O4'-C1'-N9	5.43	112.54	108.20
36	1	713	U	C2-N3-C4	-5.43	123.74	127.00
36	1	2214	A	C6-C5-N7	-5.43	128.50	132.30
1	6	455	C	N1-C2-O2	-5.43	115.64	118.90
1	6	1793	G	C4-C5-N7	-5.43	108.63	110.80
36	5	267	G	O4'-C1'-N9	-5.43	103.86	108.20
36	5	3210	A	C2-N3-C4	-5.43	107.89	110.60
36	5	3321	C	C4-C5-C6	5.43	120.11	117.40
1	6	39	A	O4'-C1'-N9	5.43	112.54	108.20
1	6	1109	G	O5'-P-OP2	-5.43	100.82	105.70
36	5	356	C	N3-C4-N4	5.43	121.80	118.00
36	5	1929	G	C2-N3-C4	-5.43	109.19	111.90
36	5	2404	A	C8-N9-C4	5.43	107.97	105.80
36	5	2896	A	N9-C4-C5	5.43	107.97	105.80
42	15	147	ASP	CB-CG-OD1	5.43	123.18	118.30
36	1	2554	A	P-O3'-C3'	5.42	126.21	119.70
1	6	1354	G	C8-N9-C4	-5.42	104.23	106.40
36	5	893	C	C2-N3-C4	5.42	122.61	119.90
36	5	908	G	C4-C5-N7	5.42	112.97	110.80
36	1	683	U	C5-C6-N1	-5.42	119.99	122.70
1	6	1596	C	N1-C2-N3	5.42	123.00	119.20
36	1	721	G	C4-C5-N7	5.42	112.97	110.80
36	1	1269	U	C2-N1-C1'	5.42	124.21	117.70
36	1	1937	U	N3-C4-C5	5.42	117.85	114.60
1	6	794	U	N3-C2-O2	-5.42	118.41	122.20
36	5	1466	G	O5'-P-OP2	5.42	117.21	110.70
36	5	1879	A	N7-C8-N9	5.42	116.51	113.80
36	5	2865	U	N3-C2-O2	-5.42	118.41	122.20
1	2	501	U	OP1-P-O3'	5.42	117.12	105.20
36	1	1119	C	N3-C4-C5	5.42	124.07	121.90
36	5	44	U	C5-C4-O4	-5.42	122.65	125.90
36	5	283	G	C6-C5-N7	-5.42	127.15	130.40
36	5	1655	G	N7-C8-N9	5.42	115.81	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2289	U	C6-N1-C1'	-5.42	113.61	121.20
36	1	515	C	C6-N1-C2	-5.42	118.13	120.30
36	1	680	G	OP1-P-OP2	5.42	127.73	119.60
36	1	2728	G	N3-C4-C5	-5.42	125.89	128.60
38	4	111	A	C8-N9-C4	-5.42	103.63	105.80
36	5	2719	U	C5-C6-N1	-5.42	119.99	122.70
1	2	1462	G	N1-C6-O6	5.42	123.15	119.90
36	1	3135	U	C2-N3-C4	-5.42	123.75	127.00
36	5	366	A	N1-C6-N6	5.42	121.85	118.60
36	5	1044	U	C5-C4-O4	5.42	129.15	125.90
36	5	2142	A	OP1-P-O3'	5.42	117.11	105.20
36	5	3288	G	C5-C6-N1	5.42	114.21	111.50
36	1	2305	G	C8-N9-C1'	-5.42	119.96	127.00
36	5	1322	U	N3-C4-C5	5.42	117.85	114.60
36	1	320	G	N3-C2-N2	-5.41	116.11	119.90
36	1	847	A	C6-C5-N7	-5.41	128.51	132.30
36	1	1141	C	N3-C4-N4	5.41	121.79	118.00
1	6	1428	G	C8-N9-C4	-5.41	104.23	106.40
36	5	1054	A	C8-N9-C4	5.41	107.97	105.80
36	5	2584	G	C5-C6-O6	-5.41	125.35	128.60
36	5	914	A	O5'-P-OP1	-5.41	100.83	105.70
36	5	1215	U	C5-C4-O4	-5.41	122.65	125.90
36	5	2369	G	C8-N9-C1'	-5.41	119.96	127.00
41	14	76	ARG	NE-CZ-NH2	-5.41	117.59	120.30
36	1	496	C	OP2-P-O3'	5.41	117.10	105.20
36	5	1888	U	C4-C5-C6	5.41	122.95	119.70
36	5	2856	G	C5-N7-C8	-5.41	101.59	104.30
36	5	2906	C	C6-N1-C2	-5.41	118.14	120.30
36	1	331	G	N9-C4-C5	5.41	107.56	105.40
36	1	410	U	N3-C4-O4	5.41	123.19	119.40
36	1	1117	G	C5-C6-O6	-5.41	125.36	128.60
36	1	1296	C	C6-N1-C2	-5.41	118.14	120.30
36	1	1349	G	N3-C4-C5	-5.41	125.90	128.60
36	1	2404	A	N9-C1'-C2'	-5.41	106.05	112.00
36	1	2756	C	C2-N1-C1'	5.41	124.75	118.80
36	1	2932	U	O5'-P-OP2	-5.41	100.83	105.70
36	1	2952	G	C4-C5-N7	5.41	112.96	110.80
36	1	3209	A	C6-C5-N7	-5.41	128.51	132.30
1	6	1171	A	C8-N9-C4	-5.41	103.64	105.80
36	5	989	A	N1-C6-N6	-5.41	115.36	118.60
36	5	1917	C	C2-N3-C4	-5.41	117.20	119.90
36	5	2190	U	C6-N1-C2	-5.41	117.75	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2874	G	N1-C6-O6	-5.41	116.66	119.90
36	1	917	A	C5-C6-N6	5.41	128.02	123.70
36	1	1904	C	C5-C6-N1	5.41	123.70	121.00
36	1	2984	C	C6-N1-C2	-5.41	118.14	120.30
1	6	577	G	N7-C8-N9	5.41	115.80	113.10
36	1	3147	G	C5-C6-O6	5.40	131.84	128.60
36	5	1297	C	C5-C6-N1	-5.40	118.30	121.00
1	2	17	C	O5'-P-OP2	-5.40	100.84	105.70
36	1	228	U	N3-C2-O2	-5.40	118.42	122.20
36	1	802	C	N3-C2-O2	-5.40	118.12	121.90
36	1	1596	C	N3-C4-N4	-5.40	114.22	118.00
1	6	333	A	N7-C8-N9	-5.40	111.10	113.80
1	6	1398	U	C2-N1-C1'	5.40	124.18	117.70
36	5	1172	G	C5-C6-O6	5.40	131.84	128.60
36	5	2178	A	C8-N9-C4	5.40	107.96	105.80
38	8	26	U	N3-C2-O2	-5.40	118.42	122.20
36	1	1158	A	C8-N9-C4	-5.40	103.64	105.80
1	6	1753	A	N9-C4-C5	5.40	107.96	105.80
36	5	3043	C	O5'-P-OP2	-5.40	100.84	105.70
36	5	3362	A	N3-C4-C5	5.40	130.58	126.80
36	1	1127	G	C4-C5-N7	5.40	112.96	110.80
37	7	10	C	O5'-P-OP2	-5.40	100.84	105.70
36	1	1157	G	OP2-P-O3'	5.40	117.07	105.20
36	1	2834	G	OP1-P-OP2	5.40	127.70	119.60
36	5	1201	C	N1-C2-O2	-5.40	115.66	118.90
36	5	1854	C	C5-C4-N4	5.40	123.98	120.20
36	5	2681	U	C5-C6-N1	-5.40	120.00	122.70
54	m8	66	ARG	NE-CZ-NH2	-5.40	117.60	120.30
36	1	682	U	C5-C4-O4	-5.40	122.66	125.90
36	1	2811	A	N1-C2-N3	5.40	132.00	129.30
36	1	2855	U	N3-C4-C5	5.39	117.84	114.60
36	5	960	U	N3-C4-O4	-5.39	115.62	119.40
36	5	3134	A	C8-N9-C4	-5.39	103.64	105.80
1	2	607	G	C4-C5-N7	5.39	112.96	110.80
36	1	2924	U	C2-N1-C1'	-5.39	111.23	117.70
36	5	2234	G	C8-N9-C4	5.39	108.56	106.40
36	1	428	A	OP2-P-O3'	5.39	117.06	105.20
36	1	612	U	C5-C4-O4	-5.39	122.67	125.90
36	1	993	G	O4'-C1'-N9	5.39	112.51	108.20
64	N8	14	HIS	C-N-CA	-5.39	108.23	121.70
36	5	3078	U	C6-N1-C1'	-5.39	113.66	121.20
36	1	406	G	N3-C2-N2	5.39	123.67	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3036	G	N3-C4-C5	-5.39	125.91	128.60
38	8	34	U	C5-C6-N1	-5.39	120.01	122.70
36	1	227	G	C5-C6-O6	-5.39	125.37	128.60
36	1	2959	C	N1-C2-O2	-5.39	115.67	118.90
1	6	754	A	C5-C6-N6	-5.39	119.39	123.70
36	5	1858	A	O4'-C1'-N9	5.39	112.51	108.20
36	5	2210	G	C5-C6-O6	-5.39	125.37	128.60
36	5	283	G	C5-C6-O6	-5.38	125.37	128.60
36	5	824	C	C6-N1-C2	-5.38	118.15	120.30
36	5	2637	A	N9-C4-C5	-5.38	103.65	105.80
36	1	3280	U	O4'-C1'-N1	5.38	112.51	108.20
36	1	2121	G	N3-C2-N2	5.38	123.67	119.90
36	1	2145	A	C2-N3-C4	5.38	113.29	110.60
36	1	3306	U	C5-C6-N1	-5.38	120.01	122.70
1	6	310	C	C4-C5-C6	5.38	120.09	117.40
7	s5	92	ARG	NE-CZ-NH1	5.38	122.99	120.30
36	5	191	U	C2-N1-C1'	-5.38	111.24	117.70
36	5	1157	G	N7-C8-N9	-5.38	110.41	113.10
36	5	1833	G	C2-N3-C4	5.38	114.59	111.90
36	5	2385	G	C2-N3-C4	-5.38	109.21	111.90
36	5	2912	G	C5-N7-C8	5.38	106.99	104.30
36	5	2988	C	N1-C2-O2	5.38	122.13	118.90
36	5	3115	C	N1-C2-N3	5.38	122.97	119.20
37	7	77	G	O5'-P-OP1	5.38	117.16	110.70
36	5	416	A	OP2-P-O3'	5.38	117.04	105.20
36	1	963	G	N7-C8-N9	-5.38	110.41	113.10
36	1	2382	G	N1-C6-O6	-5.38	116.67	119.90
36	1	2958	A	C5-C6-N1	5.38	120.39	117.70
36	1	2963	C	N1-C2-O2	5.38	122.13	118.90
1	6	114	C	C6-N1-C1'	-5.38	114.35	120.80
36	5	2753	G	N3-C2-N2	-5.38	116.14	119.90
36	1	1135	A	N1-C2-N3	-5.38	126.61	129.30
36	1	1329	U	O4'-C1'-N1	5.38	112.50	108.20
1	6	995	A	C8-N9-C4	-5.38	103.65	105.80
1	6	1196	A	P-O3'-C3'	5.38	126.15	119.70
1	6	1656	U	N1-C1'-C2'	-5.38	106.09	112.00
36	5	1302	A	C8-N9-C4	-5.38	103.65	105.80
36	5	2798	C	C2-N1-C1'	-5.38	112.89	118.80
36	1	2802	A	OP2-P-O3'	5.38	117.02	105.20
36	5	2245	C	N3-C2-O2	-5.38	118.14	121.90
36	5	2320	A	C5-C6-N1	-5.38	115.01	117.70
36	5	3127	A	C6-C5-N7	5.38	136.06	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	720	A	C8-N9-C4	-5.37	103.65	105.80
36	1	1305	U	N3-C2-O2	-5.37	118.44	122.20
1	6	362	G	C4-N9-C1'	5.37	133.48	126.50
36	5	57	A	N1-C6-N6	5.37	121.82	118.60
36	5	324	A	N9-C4-C5	5.37	107.95	105.80
36	5	867	G	N1-C6-O6	5.37	123.12	119.90
36	5	1603	A	N1-C2-N3	5.37	131.99	129.30
36	1	933	A	O5'-P-OP2	-5.37	100.87	105.70
36	1	1118	C	N3-C4-C5	-5.37	119.75	121.90
36	1	1420	C	OP2-P-O3'	5.37	117.02	105.20
56	N0	24	LEU	CA-CB-CG	5.37	127.65	115.30
36	5	282	G	P-O3'-C3'	5.37	126.14	119.70
36	5	341	G	C5-N7-C8	-5.37	101.61	104.30
36	5	2160	G	C5-C6-O6	5.37	131.82	128.60
36	5	2948	C	C5-C4-N4	5.37	123.96	120.20
36	1	2142	A	OP1-P-OP2	-5.37	111.55	119.60
36	1	3317	U	C5-C4-O4	5.37	129.12	125.90
36	5	1319	G	C5-C6-O6	5.37	131.82	128.60
36	5	2623	G	C8-N9-C4	5.37	108.55	106.40
1	2	1024	U	N1-C2-O2	5.37	126.56	122.80
36	1	25	U	N1-C2-O2	-5.37	119.04	122.80
36	1	280	U	N3-C2-O2	5.37	125.96	122.20
38	4	148	G	N1-C6-O6	-5.37	116.68	119.90
1	6	142	G	C4-N9-C1'	5.37	133.48	126.50
36	5	1520	G	C5-C6-N1	5.37	114.19	111.50
36	5	2672	G	C8-N9-C4	5.37	108.55	106.40
36	5	3090	U	C2-N3-C4	-5.37	123.78	127.00
38	8	51	G	N1-C6-O6	5.37	123.12	119.90
1	2	406	U	C6-N1-C2	5.37	124.22	121.00
36	1	1507	G	C4-C5-N7	-5.37	108.65	110.80
36	5	1157	G	C8-N9-C4	5.37	108.55	106.40
36	1	39	A	N3-C4-N9	-5.37	123.11	127.40
36	1	641	C	C6-N1-C1'	5.37	127.24	120.80
38	4	29	U	C2-N3-C4	-5.37	123.78	127.00
36	5	1430	U	C6-N1-C2	5.37	124.22	121.00
36	5	2346	C	N3-C4-C5	5.37	124.05	121.90
36	5	2704	A	OP1-P-OP2	5.37	127.65	119.60
38	8	3	A	N1-C6-N6	-5.37	115.38	118.60
1	2	355	G	N3-C4-C5	-5.36	125.92	128.60
36	1	631	U	N1-C2-N3	5.36	118.12	114.90
36	1	976	U	O5'-P-OP2	-5.36	100.87	105.70
36	1	3096	C	O5'-P-OP1	-5.36	100.87	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3264	G	N7-C8-N9	-5.36	110.42	113.10
1	6	1480	G	C8-N9-C4	-5.36	104.25	106.40
36	5	1724	U	O4'-C1'-N1	5.36	112.49	108.20
37	7	92	A	C4-C5-N7	5.36	113.38	110.70
38	8	25	G	C5-C6-O6	5.36	131.82	128.60
1	2	542	A	N7-C8-N9	5.36	116.48	113.80
38	4	64	U	N3-C4-O4	-5.36	115.65	119.40
65	N9	20	GLY	N-CA-C	5.36	126.50	113.10
36	5	1110	U	N1-C2-O2	5.36	126.55	122.80
36	1	2390	A	C8-N9-C4	5.36	107.94	105.80
36	1	2767	U	O5'-P-OP2	-5.36	100.88	105.70
1	6	328	A	O5'-P-OP2	-5.36	100.88	105.70
1	6	1638	G	N1-C6-O6	-5.36	116.68	119.90
36	5	221	A	C8-N9-C4	5.36	107.94	105.80
36	5	1892	G	N1-C6-O6	-5.36	116.68	119.90
36	1	677	A	C5-C6-N6	-5.36	119.41	123.70
36	1	970	A	N7-C8-N9	5.36	116.48	113.80
36	1	1403	C	N1-C2-O2	-5.36	115.69	118.90
36	1	1753	G	C5-C6-O6	-5.36	125.39	128.60
36	1	2787	G	C5-C6-N1	5.36	114.18	111.50
71	O5	69	LEU	CA-CB-CG	5.36	127.62	115.30
1	6	858	G	N7-C8-N9	5.36	115.78	113.10
36	5	1161	G	C8-N9-C4	5.36	108.54	106.40
36	5	2920	U	N1-C2-N3	5.36	118.11	114.90
36	5	2938	G	O5'-P-OP1	-5.36	100.88	105.70
36	5	2941	A	C6-N1-C2	-5.36	115.39	118.60
36	1	351	A	OP1-P-OP2	5.36	127.63	119.60
36	1	808	A	C4-C5-N7	-5.36	108.02	110.70
36	1	1513	G	C5-C6-O6	-5.36	125.39	128.60
36	1	2368	A	N1-C6-N6	-5.36	115.39	118.60
36	1	3000	A	C8-N9-C4	5.36	107.94	105.80
1	6	1657	U	C2-N1-C1'	5.36	124.13	117.70
36	5	103	G	C5-C6-O6	5.36	131.81	128.60
36	5	1183	C	N3-C4-N4	-5.36	114.25	118.00
36	5	1881	A	N1-C6-N6	5.36	121.81	118.60
36	5	2386	A	C8-N9-C4	-5.36	103.66	105.80
36	5	3276	G	OP1-P-O3'	5.36	116.98	105.20
36	1	1741	A	N1-C2-N3	5.35	131.98	129.30
36	1	2194	G	O5'-P-OP1	5.35	117.12	110.70
1	6	1782	A	O5'-P-OP1	-5.35	100.88	105.70
36	5	1087	G	N3-C2-N2	-5.35	116.15	119.90
36	1	2624	G	N1-C6-O6	5.35	123.11	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2797	C	N1-C2-O2	-5.35	115.69	118.90
1	6	163	G	C4-N9-C1'	-5.35	119.54	126.50
36	5	341	G	N1-C6-O6	5.35	123.11	119.90
36	5	1242	G	C4-N9-C1'	5.35	133.46	126.50
36	5	2131	A	N9-C1'-C2'	-5.35	106.11	112.00
36	5	2393	G	N1-C2-N2	5.35	121.02	116.20
65	n9	39	PHE	N-CA-CB	5.35	120.24	110.60
1	2	497	G	P-O3'-C3'	5.35	126.12	119.70
36	1	1445	U	N1-C2-O2	-5.35	119.05	122.80
36	1	2365	C	C5-C4-N4	5.35	123.95	120.20
36	1	608	A	N9-C4-C5	-5.35	103.66	105.80
36	1	1468	A	OP1-P-OP2	5.35	127.62	119.60
36	1	1483	G	O4'-C1'-N9	5.35	112.48	108.20
36	1	2300	G	OP2-P-O3'	5.35	116.97	105.20
36	5	307	A	N9-C4-C5	5.35	107.94	105.80
36	5	1725	C	O4'-C1'-N1	5.35	112.48	108.20
1	2	1297	G	C4-N9-C1'	-5.35	119.55	126.50
36	1	229	G	N1-C2-N2	5.35	121.01	116.20
36	1	1434	G	N3-C4-C5	-5.35	125.93	128.60
36	1	2283	G	N3-C2-N2	-5.35	116.16	119.90
38	4	9	A	N1-C6-N6	-5.35	115.39	118.60
36	5	2211	U	C6-N1-C2	-5.35	117.79	121.00
1	2	1796	C	C4-C5-C6	5.35	120.07	117.40
36	1	1795	U	C2-N3-C4	-5.35	123.79	127.00
36	5	92	G	N3-C2-N2	5.35	123.64	119.90
36	5	1396	C	OP2-P-O3'	5.35	116.96	105.20
36	1	963	G	N9-C4-C5	-5.34	103.26	105.40
36	1	1581	C	C6-N1-C2	-5.34	118.16	120.30
36	1	2977	G	C5-C6-N1	5.34	114.17	111.50
1	6	163	G	N1-C2-N3	5.34	127.11	123.90
36	5	3058	U	C2-N3-C4	-5.34	123.79	127.00
36	1	2282	U	N3-C4-C5	5.34	117.81	114.60
36	1	2613	U	C6-N1-C2	-5.34	117.79	121.00
36	5	2889	C	N3-C4-N4	-5.34	114.26	118.00
36	5	3218	A	C4-C5-N7	5.34	113.37	110.70
36	1	1435	A	C8-N9-C4	-5.34	103.66	105.80
36	5	423	A	OP2-P-O3'	5.34	116.95	105.20
36	5	2833	A	OP1-P-OP2	5.34	127.61	119.60
36	5	2878	G	C5-C6-N1	5.34	114.17	111.50
36	5	3151	U	C6-N1-C2	5.34	124.20	121.00
36	1	1181	U	O5'-P-OP1	-5.34	100.89	105.70
36	1	1395	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(°)
36	1	2990	G	C4-C5-N7	-5.34	108.66	110.80
59	N3	13	ILE	CG1-CB-CG2	-5.34	99.65	111.40
1	6	280	U	C2-N1-C1'	5.34	124.11	117.70
36	5	660	A	C2-N3-C4	-5.34	107.93	110.60
36	5	2868	U	N3-C4-C5	5.34	117.80	114.60
38	4	16	G	C8-N9-C4	5.34	108.53	106.40
36	5	3011	A	C2-N3-C4	5.34	113.27	110.60
1	2	1657	U	C5-C6-N1	-5.34	120.03	122.70
1	2	1658	G	N9-C4-C5	-5.34	103.27	105.40
36	1	401	U	N3-C4-O4	5.34	123.14	119.40
36	1	659	G	OP1-P-O3'	5.34	116.94	105.20
36	1	3143	C	N3-C2-O2	5.34	125.64	121.90
1	6	17	C	N1-C2-O2	5.34	122.10	118.90
1	6	402	C	C6-N1-C2	5.34	122.44	120.30
36	1	637	C	N3-C4-N4	-5.33	114.27	118.00
1	6	260	U	C5-C6-N1	-5.33	120.03	122.70
36	5	2147	A	N1-C6-N6	5.33	121.80	118.60
36	5	2392	C	N1-C2-O2	-5.33	115.70	118.90
36	1	333	G	N1-C6-O6	-5.33	116.70	119.90
36	1	2347	U	N3-C4-C5	5.33	117.80	114.60
36	1	2381	G	O5'-P-OP1	-5.33	100.90	105.70
1	6	536	C	N3-C4-C5	-5.33	119.77	121.90
36	5	439	C	C4-C5-C6	5.33	120.07	117.40
36	5	646	A	OP1-P-OP2	-5.33	111.60	119.60
36	5	1116	G	O5'-P-OP1	-5.33	100.90	105.70
36	5	2932	U	N3-C4-O4	-5.33	115.67	119.40
1	2	1138	A	O5'-P-OP1	-5.33	100.90	105.70
36	1	1313	G	C8-N9-C4	-5.33	104.27	106.40
36	1	1494	U	C5-C6-N1	-5.33	120.03	122.70
36	1	2628	A	C8-N9-C4	-5.33	103.67	105.80
1	6	957	G	N1-C6-O6	5.33	123.10	119.90
1	6	1031	U	N3-C4-C5	5.33	117.80	114.60
36	5	2981	U	C2-N3-C4	-5.33	123.80	127.00
1	6	31	C	C5-C4-N4	5.33	123.93	120.20
1	6	1022	C	O5'-P-OP2	5.33	117.10	110.70
36	5	204	A	N1-C6-N6	-5.33	115.40	118.60
36	5	2825	C	C5-C4-N4	-5.33	116.47	120.20
36	5	1487	G	N9-C4-C5	5.33	107.53	105.40
36	5	3228	C	C6-N1-C2	-5.33	118.17	120.30
36	1	716	A	C4-C5-N7	5.33	113.36	110.70
36	1	1556	C	N3-C2-O2	-5.33	118.17	121.90
36	1	2236	G	N1-C6-O6	5.33	123.10	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3140	G	N1-C6-O6	5.33	123.10	119.90
36	5	2141	U	OP1-P-O3'	-5.33	93.48	105.20
36	5	3309	G	N3-C4-N9	5.33	129.20	126.00
36	1	1507	G	C4-C5-C6	5.33	122.00	118.80
36	1	1815	U	P-O3'-C3'	5.33	126.09	119.70
36	1	3311	C	C6-N1-C2	5.33	122.43	120.30
38	4	23	U	N3-C4-C5	5.33	117.80	114.60
36	5	300	G	N3-C4-N9	-5.33	122.80	126.00
36	5	688	G	N3-C2-N2	-5.33	116.17	119.90
36	5	1115	G	P-O3'-C3'	5.33	126.09	119.70
36	5	1506	A	C8-N9-C4	-5.33	103.67	105.80
36	5	2996	U	C6-N1-C2	5.33	124.20	121.00
38	8	136	G	C5-C6-O6	5.33	131.79	128.60
1	2	18	C	N3-C4-C5	-5.32	119.77	121.90
1	2	1748	G	C4-C5-N7	-5.32	108.67	110.80
36	1	730	C	C2-N3-C4	-5.32	117.24	119.90
36	1	1119	C	N3-C4-N4	-5.32	114.27	118.00
36	1	1598	G	C5-C6-O6	5.32	131.79	128.60
36	1	2411	U	C4-C5-C6	-5.32	116.51	119.70
36	1	2883	U	C5-C4-O4	5.32	129.09	125.90
36	1	3218	A	N9-C4-C5	5.32	107.93	105.80
1	6	1762	A	N1-C2-N3	-5.32	126.64	129.30
36	5	999	G	OP1-P-OP2	-5.32	111.61	119.60
36	5	1839	A	N9-C4-C5	5.32	107.93	105.80
36	5	2247	G	N1-C6-O6	-5.32	116.70	119.90
36	1	3181	C	C6-N1-C2	-5.32	118.17	120.30
10	S8	172	ARG	NE-CZ-NH2	-5.32	117.64	120.30
36	1	2186	U	N1-C2-O2	5.32	126.52	122.80
36	5	1101	G	N3-C2-N2	5.32	123.62	119.90
36	1	620	U	C2-N1-C1'	-5.32	111.32	117.70
36	1	1340	G	N3-C2-N2	5.32	123.62	119.90
36	1	690	A	C2-N3-C4	5.32	113.26	110.60
36	1	2363	A	C6-C5-N7	5.32	136.02	132.30
36	1	2954	U	N3-C2-O2	5.32	125.92	122.20
1	6	65	A	N3-C4-C5	5.32	130.52	126.80
1	6	399	A	C8-N9-C4	5.32	107.93	105.80
36	5	583	G	C8-N9-C4	5.32	108.53	106.40
36	5	811	U	C2-N3-C4	-5.32	123.81	127.00
36	5	2119	A	N9-C4-C5	-5.32	103.67	105.80
36	5	2178	A	N1-C6-N6	5.32	121.79	118.60
1	2	1486	G	O4'-C1'-N9	5.32	112.45	108.20
36	1	332	C	O5'-P-OP1	-5.32	100.92	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1005	G	N1-C2-N2	-5.32	111.42	116.20
1	6	583	C	C2-N1-C1'	5.32	124.65	118.80
36	5	353	G	O4'-C1'-N9	5.32	112.45	108.20
36	5	2970	C	C2-N1-C1'	-5.32	112.95	118.80
36	1	155	G	N3-C4-N9	5.31	129.19	126.00
36	1	695	C	C5-C6-N1	-5.31	118.34	121.00
36	1	196	G	C5-C6-O6	-5.31	125.41	128.60
36	1	906	A	C5-C6-N1	5.31	120.36	117.70
36	1	2384	A	C6-C5-N7	-5.31	128.58	132.30
1	6	377	G	N1-C6-O6	-5.31	116.71	119.90
1	6	1122	G	N3-C4-C5	5.31	131.26	128.60
36	5	1370	G	C5-C6-O6	5.31	131.79	128.60
36	1	424	G	C5-C6-N1	5.31	114.16	111.50
37	3	81	U	N3-C4-C5	5.31	117.79	114.60
36	5	2930	A	N9-C4-C5	5.31	107.92	105.80
36	1	1852	G	C5-C6-N1	-5.31	108.84	111.50
36	1	2318	U	N1-C2-N3	5.31	118.09	114.90
36	1	3151	U	O5'-P-OP1	5.31	117.07	110.70
36	5	908	G	C5-N7-C8	-5.31	101.64	104.30
36	5	2641	U	N3-C2-O2	5.31	125.92	122.20
36	1	323	A	O5'-P-OP1	-5.31	100.92	105.70
36	1	439	C	N3-C2-O2	-5.31	118.19	121.90
36	1	635	G	C5-C6-O6	-5.31	125.42	128.60
1	6	362	G	C8-N9-C1'	-5.31	120.10	127.00
36	5	2207	A	O4'-C1'-N9	5.31	112.44	108.20
36	5	2680	A	OP2-P-O3'	5.31	116.88	105.20
36	5	2756	C	OP2-P-O3'	5.31	116.88	105.20
36	5	3058	U	N3-C4-C5	5.31	117.78	114.60
36	1	202	G	N1-C6-O6	-5.31	116.72	119.90
36	5	1180	A	C2-N3-C4	-5.31	107.95	110.60
1	2	1486	G	C6-C5-N7	-5.30	127.22	130.40
36	1	92	G	O5'-C5'-C4'	-5.30	101.62	111.70
36	1	401	U	C2-N3-C4	-5.30	123.82	127.00
36	1	944	C	N3-C4-N4	5.30	121.71	118.00
36	1	1430	U	N1-C2-O2	-5.30	119.09	122.80
36	1	1450	G	N7-C8-N9	-5.30	110.45	113.10
36	1	1604	G	C8-N9-C1'	-5.30	120.10	127.00
36	1	1671	C	C6-N1-C2	-5.30	118.18	120.30
36	1	1786	G	O5'-P-OP1	-5.30	100.93	105.70
36	1	2541	U	P-O3'-C3'	5.30	126.06	119.70
36	5	216	G	C6-C5-N7	-5.30	127.22	130.40
36	5	393	U	N1-C2-N3	5.30	118.08	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	652	G	N3-C4-C5	-5.30	125.95	128.60
36	5	1042	U	N1-C2-O2	5.30	126.51	122.80
36	5	2856	G	C5-C6-O6	-5.30	125.42	128.60
37	7	92	A	C5-C6-N6	-5.30	119.46	123.70
36	1	936	A	C5-C6-N6	-5.30	119.46	123.70
54	M8	12	ARG	NE-CZ-NH1	-5.30	117.65	120.30
36	1	630	A	N9-C4-C5	5.30	107.92	105.80
38	4	23	U	C6-N1-C2	5.30	124.18	121.00
1	6	453	U	C6-N1-C2	-5.30	117.82	121.00
1	6	639	U	O4'-C1'-N1	5.30	112.44	108.20
36	5	1419	A	C8-N9-C4	5.30	107.92	105.80
36	5	1656	A	O5'-P-OP2	-5.30	100.93	105.70
36	5	2600	C	O5'-P-OP1	-5.30	100.93	105.70
36	1	715	A	O4'-C1'-N9	5.30	112.44	108.20
36	1	2752	U	N3-C4-O4	-5.30	115.69	119.40
36	1	2797	C	O5'-P-OP1	-5.30	100.93	105.70
36	1	3175	U	C5-C6-N1	-5.30	120.05	122.70
1	6	1058	U	P-O3'-C3'	5.30	126.06	119.70
36	5	349	A	O5'-P-OP1	-5.30	100.93	105.70
36	5	718	G	O4'-C1'-N9	5.30	112.44	108.20
36	5	2375	G	N3-C2-N2	5.30	123.61	119.90
36	5	2833	A	C8-N9-C4	5.30	107.92	105.80
36	1	75	G	N3-C4-N9	5.30	129.18	126.00
36	5	878	G	C6-C5-N7	-5.30	127.22	130.40
36	5	3107	U	OP2-P-O3'	5.30	116.86	105.20
68	o2	39	ASP	CB-CG-OD1	-5.30	113.53	118.30
36	1	659	G	N3-C2-N2	5.30	123.61	119.90
3	s1	47	LEU	CA-CB-CG	5.30	127.48	115.30
36	5	1371	G	N7-C8-N9	-5.30	110.45	113.10
36	5	3032	A	N1-C2-N3	-5.30	126.65	129.30
36	1	674	G	C2-N3-C4	5.29	114.55	111.90
36	1	1163	A	OP1-P-OP2	5.29	127.54	119.60
36	5	2302	G	N1-C6-O6	-5.29	116.72	119.90
36	5	3181	C	O5'-P-OP1	5.29	117.05	110.70
36	1	1349	G	N3-C4-N9	5.29	129.18	126.00
1	6	95	G	C8-N9-C4	-5.29	104.28	106.40
1	6	102	U	N1-C2-N3	5.29	118.08	114.90
36	5	826	G	N3-C4-N9	-5.29	122.82	126.00
36	5	851	C	N1-C2-O2	-5.29	115.72	118.90
36	5	2369	G	C8-N9-C4	5.29	108.52	106.40
36	5	2658	G	N7-C8-N9	-5.29	110.45	113.10
36	1	3135	U	C5-C6-N1	-5.29	120.06	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	144	U	N1-C2-O2	5.29	126.50	122.80
36	5	2298	U	C5-C6-N1	-5.29	120.05	122.70
36	1	1395	G	N1-C2-N3	-5.29	120.73	123.90
1	6	864	U	O4'-C1'-N1	5.29	112.43	108.20
1	6	1773	C	N3-C2-O2	5.29	125.60	121.90
36	5	619	A	N1-C6-N6	-5.29	115.43	118.60
1	2	139	C	P-O3'-C3'	5.29	126.05	119.70
36	1	515	C	N3-C4-C5	-5.29	119.78	121.90
36	1	1859	A	N9-C4-C5	-5.29	103.69	105.80
36	1	2725	U	C6-N1-C2	5.29	124.17	121.00
36	5	26	A	N7-C8-N9	-5.29	111.16	113.80
36	5	1376	C	N1-C2-O2	5.29	122.07	118.90
40	13	47	LEU	CA-CB-CG	5.29	127.46	115.30
1	2	543	C	C4-C5-C6	5.29	120.04	117.40
36	1	2808	A	N9-C4-C5	-5.29	103.69	105.80
36	5	73	C	C5-C6-N1	-5.29	118.36	121.00
1	2	499	U	P-O3'-C3'	5.29	126.04	119.70
36	1	3269	U	N3-C2-O2	-5.29	118.50	122.20
1	6	609	U	N1-C2-N3	5.29	118.07	114.90
36	5	2145	A	C2-N3-C4	5.29	113.24	110.60
36	5	2817	A	OP2-P-O3'	5.29	116.83	105.20
36	5	3311	C	C5-C4-N4	5.29	123.90	120.20
36	1	124	U	N1-C2-O2	5.28	126.50	122.80
36	1	288	C	N3-C2-O2	5.28	125.60	121.90
36	1	791	A	N9-C4-C5	5.28	107.91	105.80
36	1	2129	U	N3-C4-C5	5.28	117.77	114.60
36	1	2811	A	C8-N9-C4	-5.28	103.69	105.80
36	5	60	A	O5'-P-OP2	-5.28	100.95	105.70
36	5	963	G	C4-C5-C6	-5.28	115.63	118.80
36	5	2869	U	N1-C2-N3	5.28	118.07	114.90
1	6	1535	U	C5-C6-N1	-5.28	120.06	122.70
36	5	363	G	OP1-P-O3'	5.28	116.82	105.20
1	2	1762	A	O5'-P-OP1	-5.28	100.95	105.70
15	C3	22	ALA	C-N-CA	5.28	144.18	122.00
36	1	143	G	C4-C5-N7	-5.28	108.69	110.80
36	1	372	A	N9-C4-C5	-5.28	103.69	105.80
36	1	418	A	C2-N3-C4	-5.28	107.96	110.60
36	1	2142	A	N3-C4-C5	-5.28	123.10	126.80
1	6	1279	C	C6-N1-C2	-5.28	118.19	120.30
36	5	2732	G	N3-C4-N9	5.28	129.17	126.00
36	5	2935	U	OP1-P-O3'	5.28	116.82	105.20
36	5	3033	A	C8-N9-C4	5.28	107.91	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1190	C	C6-N1-C2	5.28	122.41	120.30
36	1	3121	U	P-O3'-C3'	5.28	126.03	119.70
36	5	916	G	P-O3'-C3'	5.28	126.03	119.70
36	5	961	C	C6-N1-C1'	-5.28	114.47	120.80
1	2	402	C	N3-C2-O2	5.28	125.59	121.90
1	2	527	A	C8-N9-C4	-5.28	103.69	105.80
36	1	1546	A	C4-C5-N7	-5.28	108.06	110.70
36	1	2583	C	O5'-P-OP2	-5.28	100.95	105.70
1	6	543	C	C4-C5-C6	-5.28	114.76	117.40
1	6	795	U	N1-C2-O2	5.28	126.49	122.80
36	5	1452	A	C5-C6-N6	-5.28	119.48	123.70
36	5	2369	G	N3-C2-N2	5.28	123.59	119.90
36	5	2724	U	OP1-P-O3'	5.28	116.81	105.20
36	5	3311	C	N3-C4-N4	-5.28	114.31	118.00
1	6	470	A	C8-N9-C4	-5.28	103.69	105.80
36	5	1311	G	OP1-P-OP2	-5.28	111.69	119.60
36	5	1322	U	C6-N1-C2	5.28	124.17	121.00
36	5	1517	G	C5-C6-O6	5.28	131.76	128.60
36	5	2643	A	C5-C6-N6	-5.28	119.48	123.70
36	5	2747	A	N9-C4-C5	5.28	107.91	105.80
36	5	2855	U	N1-C2-N3	-5.28	111.73	114.90
38	8	38	U	C2-N3-C4	-5.28	123.83	127.00
36	1	345	G	C6-N1-C2	-5.27	121.94	125.10
36	1	609	G	N9-C4-C5	-5.27	103.29	105.40
36	1	895	A	C6-N1-C2	5.27	121.76	118.60
36	1	2417	U	N1-C2-N3	5.27	118.06	114.90
36	5	986	U	N3-C2-O2	-5.27	118.51	122.20
1	2	1524	A	N1-C6-N6	-5.27	115.44	118.60
36	1	109	A	N1-C6-N6	-5.27	115.44	118.60
36	1	765	C	C2-N1-C1'	5.27	124.60	118.80
36	1	1400	G	C5-C6-O6	5.27	131.76	128.60
36	1	1907	C	N3-C4-C5	-5.27	119.79	121.90
36	5	424	G	C5-C6-O6	-5.27	125.44	128.60
36	5	1113	G	C8-N9-C4	5.27	108.51	106.40
36	5	2130	G	N3-C2-N2	5.27	123.59	119.90
37	7	93	C	N3-C4-N4	-5.27	114.31	118.00
36	5	2641	U	N1-C2-O2	-5.27	119.11	122.80
36	1	648	C	OP1-P-O3'	5.27	116.79	105.20
36	1	652	G	N1-C6-O6	-5.27	116.74	119.90
36	1	1408	G	C5-C6-O6	5.27	131.76	128.60
36	1	1500	G	OP2-P-O3'	5.27	116.79	105.20
1	2	624	G	N1-C6-O6	-5.27	116.74	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	504	A	C4-C5-N7	-5.27	108.07	110.70
1	6	410	A	N1-C6-N6	-5.27	115.44	118.60
37	7	47	C	C2-N3-C4	-5.27	117.27	119.90
40	13	266	ARG	NE-CZ-NH1	5.27	122.93	120.30
36	5	21	G	N3-C2-N2	5.27	123.59	119.90
36	5	2611	U	C5-C6-N1	-5.27	120.07	122.70
36	1	2255	A	O5'-P-OP1	-5.26	100.96	105.70
36	5	2392	C	N3-C4-C5	5.26	124.00	121.90
37	7	115	G	C8-N9-C4	-5.26	104.29	106.40
36	5	671	U	C2-N3-C4	-5.26	123.84	127.00
36	5	1591	G	C8-N9-C4	-5.26	104.30	106.40
36	1	596	C	N3-C2-O2	-5.26	118.22	121.90
1	6	390	G	C4-N9-C1'	5.26	133.34	126.50
1	6	416	A	O5'-P-OP2	-5.26	100.97	105.70
36	5	937	G	N3-C4-C5	-5.26	125.97	128.60
36	5	2869	U	C5-C4-O4	5.26	129.06	125.90
36	1	31	C	C2-N3-C4	-5.26	117.27	119.90
36	1	39	A	O5'-P-OP2	-5.26	100.97	105.70
36	5	2409	G	C8-N9-C4	-5.26	104.30	106.40
36	5	3004	C	C5-C4-N4	-5.26	116.52	120.20
37	7	49	G	O4'-C1'-N9	5.26	112.41	108.20
36	1	664	U	C5-C4-O4	-5.26	122.75	125.90
1	6	1048	G	C8-N9-C4	5.26	108.50	106.40
36	5	393	U	C6-N1-C2	-5.26	117.84	121.00
36	5	2909	U	C2-N3-C4	-5.26	123.84	127.00
1	2	61	A	C5-N7-C8	-5.26	101.27	103.90
36	1	1169	A	OP2-P-O3'	5.26	116.77	105.20
36	1	2625	C	C2-N3-C4	-5.26	117.27	119.90
1	6	299	A	O5'-P-OP1	5.26	117.01	110.70
36	5	41	G	C5-N7-C8	-5.26	101.67	104.30
36	5	1242	G	N3-C4-C5	-5.26	125.97	128.60
36	5	1308	A	C5'-C4'-C3'	-5.26	107.59	116.00
36	5	2645	G	C5-C6-N1	5.26	114.13	111.50
36	1	857	G	N1-C6-O6	5.25	123.05	119.90
36	5	708	G	C4-C5-N7	5.25	112.90	110.80
36	5	2289	U	C5-C4-O4	5.25	129.05	125.90
36	5	3039	C	N1-C2-O2	5.25	122.05	118.90
1	2	647	G	N3-C2-N2	-5.25	116.22	119.90
36	1	94	G	N3-C2-N2	5.25	123.58	119.90
36	1	98	G	N1-C6-O6	-5.25	116.75	119.90
36	1	2613	U	C5-C6-N1	5.25	125.33	122.70
36	5	1552	G	C5-C6-O6	-5.25	125.45	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2970	C	C6-N1-C2	5.25	122.40	120.30
44	17	88	ARG	NE-CZ-NH2	-5.25	117.67	120.30
36	1	188	U	C5-C4-O4	5.25	129.05	125.90
36	1	1339	C	C4-C5-C6	5.25	120.03	117.40
36	5	509	U	C2-N3-C4	-5.25	123.85	127.00
36	5	1435	A	P-O3'-C3'	5.25	126.00	119.70
36	5	1901	A	C4-C5-C6	5.25	119.63	117.00
36	1	2242	A	N1-C2-N3	5.25	131.93	129.30
36	1	65	A	C8-N9-C4	-5.25	103.70	105.80
36	1	419	G	N1-C2-N2	-5.25	111.48	116.20
36	1	1474	A	OP2-P-O3'	5.25	116.75	105.20
1	6	416	A	N1-C6-N6	5.25	121.75	118.60
36	5	726	G	N1-C6-O6	5.25	123.05	119.90
36	5	802	C	C4-C5-C6	5.25	120.03	117.40
36	5	1921	A	OP2-P-O3'	5.25	116.75	105.20
36	1	347	G	N1-C6-O6	5.25	123.05	119.90
36	1	2813	A	N9-C4-C5	5.25	107.90	105.80
36	5	1149	G	O4'-C1'-N9	5.25	112.40	108.20
1	2	323	A	C8-N9-C4	-5.25	103.70	105.80
36	1	96	G	N3-C2-N2	5.25	123.57	119.90
36	1	349	A	N9-C4-C5	5.25	107.90	105.80
36	1	504	A	C5-C6-N6	5.25	127.90	123.70
36	1	1446	A	O5'-P-OP1	-5.25	100.98	105.70
54	M8	159	LYS	CD-CE-NZ	5.25	123.76	111.70
36	5	33	G	N1-C6-O6	-5.25	116.75	119.90
36	5	110	G	N1-C6-O6	-5.25	116.75	119.90
1	2	1200	G	C8-N9-C4	-5.24	104.30	106.40
36	1	304	G	C6-C5-N7	5.24	133.55	130.40
36	1	345	G	C2-N3-C4	5.24	114.52	111.90
36	1	1398	U	OP2-P-O3'	5.24	116.73	105.20
36	1	1405	U	C5-C4-O4	-5.24	122.75	125.90
36	1	2836	C	N1-C2-N3	5.24	122.87	119.20
36	5	911	C	C5-C4-N4	-5.24	116.53	120.20
36	5	1340	G	N1-C2-N2	-5.24	111.48	116.20
39	12	238	ILE	C-N-CA	-5.24	108.59	121.70
36	1	1788	C	C5-C4-N4	-5.24	116.53	120.20
1	2	403	G	N3-C4-N9	5.24	129.15	126.00
36	1	608	A	C4-C5-N7	5.24	113.32	110.70
36	1	1008	U	C2-N1-C1'	-5.24	111.41	117.70
36	1	2808	A	C4-C5-C6	5.24	119.62	117.00
38	4	23	U	C2-N1-C1'	-5.24	111.41	117.70
36	5	649	A	OP2-P-O3'	5.24	116.73	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	929	A	N1-C2-N3	-5.24	126.68	129.30
36	5	1408	G	C5-C6-O6	5.24	131.75	128.60
36	5	3076	C	N3-C2-O2	-5.24	118.23	121.90
36	5	3218	A	C6-C5-N7	-5.24	128.63	132.30
1	2	1196	A	C8-N9-C4	-5.24	103.70	105.80
1	6	607	G	N1-C6-O6	-5.24	116.76	119.90
36	5	1166	G	N3-C2-N2	5.24	123.57	119.90
1	2	580	A	C8-N9-C4	-5.24	103.70	105.80
36	1	1110	U	OP1-P-OP2	5.24	127.45	119.60
36	5	3007	U	N3-C2-O2	-5.24	118.53	122.20
36	5	3232	G	O5'-P-OP2	-5.24	100.99	105.70
36	1	630	A	C8-N9-C4	-5.24	103.71	105.80
36	1	1140	G	N3-C4-N9	5.24	129.14	126.00
36	1	1931	U	C2-N3-C4	-5.24	123.86	127.00
36	1	3055	U	OP1-P-OP2	5.24	127.45	119.60
36	5	1484	U	C5-C6-N1	-5.24	120.08	122.70
36	5	2572	C	C6-N1-C1'	-5.24	114.52	120.80
36	1	72	C	C2-N3-C4	-5.23	117.28	119.90
36	1	114	A	C6-C5-N7	-5.23	128.64	132.30
36	5	2661	G	OP1-P-O3'	5.23	116.72	105.20
1	2	1596	C	C5-C4-N4	5.23	123.86	120.20
36	1	2242	A	N7-C8-N9	5.23	116.42	113.80
37	3	103	A	OP2-P-O3'	5.23	116.71	105.20
1	6	1071	U	OP1-P-O3'	5.23	116.71	105.20
36	5	708	G	C8-N9-C4	-5.23	104.31	106.40
36	5	1890	U	C5-C6-N1	-5.23	120.08	122.70
36	5	2139	A	C6-N1-C2	5.23	121.74	118.60
36	1	1408	G	O5'-P-OP1	-5.23	100.99	105.70
69	O3	48	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	6	113	U	N3-C2-O2	5.23	125.86	122.20
36	5	590	G	O5'-P-OP2	5.23	116.98	110.70
36	5	2349	U	OP1-P-O3'	5.23	116.71	105.20
36	5	2609	A	N1-C6-N6	-5.23	115.46	118.60
36	5	2841	G	N3-C2-N2	5.23	123.56	119.90
36	5	2944	U	N3-C4-C5	5.23	117.74	114.60
36	1	1338	C	N3-C4-C5	-5.23	119.81	121.90
36	5	645	A	OP1-P-O3'	5.23	116.70	105.20
36	5	2334	U	O5'-P-OP2	-5.23	100.99	105.70
1	2	1773	C	C2-N1-C1'	5.23	124.55	118.80
36	1	206	G	C2-N3-C4	5.23	114.51	111.90
36	1	1307	G	OP2-P-O3'	-5.23	93.70	105.20
36	1	2906	C	N3-C2-O2	-5.23	118.24	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3090	U	N1-C2-O2	-5.23	119.14	122.80
1	6	429	G	C4-C5-N7	-5.23	108.71	110.80
2	s0	62	ARG	NE-CZ-NH1	5.23	122.91	120.30
36	5	121	A	C8-N9-C4	5.23	107.89	105.80
36	5	1538	G	O5'-P-OP1	-5.23	101.00	105.70
37	3	89	G	OP2-P-O3'	5.23	116.70	105.20
36	5	1308	A	N9-C4-C5	5.23	107.89	105.80
1	2	1671	A	C6-N1-C2	5.22	121.73	118.60
36	1	53	G	N3-C2-N2	5.22	123.56	119.90
36	1	334	A	C8-N9-C4	-5.22	103.71	105.80
36	1	416	A	C6-C5-N7	5.22	135.96	132.30
36	1	802	C	C2-N1-C1'	5.22	124.55	118.80
1	6	904	G	N3-C4-C5	-5.22	125.99	128.60
36	5	278	U	C5-C6-N1	5.22	125.31	122.70
36	5	1789	G	C4-N9-C1'	-5.22	119.71	126.50
36	5	2796	G	C5-C6-O6	-5.22	125.47	128.60
1	2	1324	G	N9-C4-C5	5.22	107.49	105.40
36	1	2879	C	N3-C4-C5	-5.22	119.81	121.90
1	6	945	U	N3-C2-O2	-5.22	118.55	122.20
1	2	1768	G	C5-C6-O6	5.22	131.73	128.60
56	N0	167	ARG	NE-CZ-NH1	5.22	122.91	120.30
36	5	2794	G	C5-C6-N1	5.22	114.11	111.50
36	5	2992	U	C6-N1-C1'	-5.22	113.89	121.20
35	SM	134	ASP	CB-CG-OD2	5.22	123.00	118.30
36	1	368	G	N1-C2-N3	5.22	127.03	123.90
36	1	421	G	C4-C5-N7	5.22	112.89	110.80
36	1	498	A	N1-C6-N6	-5.22	115.47	118.60
36	1	1653	G	C5-C6-O6	5.22	131.73	128.60
36	1	2403	G	N7-C8-N9	5.22	115.71	113.10
36	1	2728	G	C2-N3-C4	5.22	114.51	111.90
36	1	2889	C	C4-C5-C6	5.22	120.01	117.40
1	6	747	C	C2-N3-C4	-5.22	117.29	119.90
1	6	1150	G	C8-N9-C4	5.22	108.49	106.40
36	5	1918	C	C6-N1-C2	-5.22	118.21	120.30
36	5	2683	U	N1-C2-O2	5.22	126.45	122.80
36	5	3142	A	N1-C6-N6	5.22	121.73	118.60
36	1	859	G	C4-N9-C1'	5.22	133.28	126.50
36	1	2946	A	C6-N1-C2	5.22	121.73	118.60
1	6	4	C	N3-C2-O2	5.22	125.55	121.90
36	5	1514	G	C5-N7-C8	5.22	106.91	104.30
1	2	1733	C	N3-C4-C5	-5.22	119.81	121.90
36	1	794	U	N1-C2-N3	5.22	118.03	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	870	G	N1-C6-O6	5.22	123.03	119.90
36	1	3140	G	C5-C6-O6	-5.22	125.47	128.60
37	7	1	G	N1-C2-N2	-5.22	111.50	116.20
36	1	154	U	O4'-C1'-N1	5.21	112.37	108.20
36	1	2638	C	N1-C2-O2	-5.21	115.77	118.90
36	1	3040	A	C2-N3-C4	5.21	113.21	110.60
1	6	306	U	C6-N1-C2	5.21	124.13	121.00
36	5	2142	A	C5-C6-N6	-5.21	119.53	123.70
1	2	268	C	C6-N1-C2	-5.21	118.22	120.30
36	1	1871	U	OP2-P-O3'	5.21	116.67	105.20
36	1	2422	C	C5-C4-N4	5.21	123.85	120.20
36	1	2513	U	O4'-C1'-N1	5.21	112.37	108.20
36	5	994	G	N3-C2-N2	5.21	123.55	119.90
36	5	3197	G	N1-C6-O6	5.21	123.03	119.90
41	14	76	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	2	783	G	O4'-C1'-N9	5.21	112.37	108.20
1	2	1129	U	N3-C4-O4	-5.21	115.75	119.40
1	6	194	U	C5-C6-N1	5.21	125.31	122.70
1	6	945	U	N1-C2-O2	5.21	126.45	122.80
36	5	921	A	O4'-C1'-N9	-5.21	104.03	108.20
50	m4	72	LEU	CA-CB-CG	5.21	127.29	115.30
36	1	619	A	N9-C4-C5	-5.21	103.72	105.80
36	1	2283	G	C5-C6-O6	-5.21	125.47	128.60
36	1	2702	A	C8-N9-C4	-5.21	103.72	105.80
73	O7	65	ARG	NE-CZ-NH1	5.21	122.91	120.30
36	1	2355	G	N1-C6-O6	5.21	123.03	119.90
36	1	2682	C	O5'-P-OP2	-5.21	101.01	105.70
36	1	2832	C	OP2-P-O3'	5.21	116.66	105.20
36	1	2867	C	N3-C4-C5	5.21	123.98	121.90
36	1	2983	C	N1-C2-O2	5.21	122.03	118.90
1	6	1121	C	C5-C4-N4	5.21	123.85	120.20
36	5	2191	U	N3-C4-O4	-5.21	115.75	119.40
36	5	2869	U	C6-N1-C1'	5.21	128.49	121.20
36	5	2913	C	C2-N3-C4	-5.21	117.30	119.90
1	2	334	G	N1-C2-N2	-5.21	111.51	116.20
1	2	1658	G	C4-C5-N7	5.21	112.88	110.80
36	1	2188	A	N7-C8-N9	-5.21	111.20	113.80
36	1	2730	G	C2-N3-C4	-5.21	109.30	111.90
1	6	572	C	C5-C4-N4	-5.21	116.56	120.20
36	5	1307	G	C2'-C3'-O3'	5.21	122.03	113.70
36	5	2992	U	N1-C2-O2	5.21	126.44	122.80
36	5	2830	G	N1-C2-N3	5.21	127.02	123.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	213	A	N1-C2-N3	-5.20	126.70	129.30
36	1	517	G	N9-C4-C5	5.20	107.48	105.40
36	1	661	G	OP2-P-O3'	5.20	116.65	105.20
36	1	720	A	C2-N3-C4	5.20	113.20	110.60
36	5	1331	U	N1-C2-N3	-5.20	111.78	114.90
36	5	2300	G	N3-C2-N2	5.20	123.54	119.90
36	5	2614	G	C5-C6-O6	5.20	131.72	128.60
36	1	2949	U	N3-C4-O4	-5.20	115.76	119.40
36	1	3052	G	N9-C4-C5	5.20	107.48	105.40
1	6	359	A	C4-C5-C6	-5.20	114.40	117.00
36	5	3081	C	N3-C4-N4	-5.20	114.36	118.00
36	1	197	G	N3-C2-N2	-5.20	116.26	119.90
36	1	1718	G	N1-C2-N2	5.20	120.88	116.20
36	1	1902	G	N3-C4-N9	5.20	129.12	126.00
41	L4	197	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	6	337	G	C4-C5-C6	5.20	121.92	118.80
1	6	1120	U	C5-C4-O4	5.20	129.02	125.90
36	5	971	G	C6-C5-N7	5.20	133.52	130.40
36	5	1120	A	C6-C5-N7	5.20	135.94	132.30
36	5	1141	C	O5'-P-OP1	-5.20	101.02	105.70
36	5	1451	C	C6-N1-C2	5.20	122.38	120.30
36	5	2898	G	O4'-C1'-N9	-5.20	104.04	108.20
1	2	1762	A	C8-N9-C4	5.20	107.88	105.80
36	1	847	A	C5-C6-N6	-5.20	119.54	123.70
37	3	52	G	N1-C6-O6	-5.20	116.78	119.90
36	5	1436	U	C5-C4-O4	-5.20	122.78	125.90
36	5	2249	G	C2'-C3'-O3'	5.20	122.02	113.70
36	1	212	G	N3-C4-N9	5.20	129.12	126.00
36	1	504	A	N1-C6-N6	-5.20	115.48	118.60
36	1	643	U	C2-N1-C1'	-5.20	111.47	117.70
36	1	867	G	N3-C2-N2	-5.20	116.26	119.90
36	1	1005	G	C5-C6-O6	5.20	131.72	128.60
36	1	3085	G	N1-C6-O6	5.20	123.02	119.90
1	6	978	A	C8-N9-C4	-5.20	103.72	105.80
36	5	205	C	N1-C2-O2	5.20	122.02	118.90
36	5	2955	U	N1-C2-N3	5.20	118.02	114.90
36	5	2957	G	N7-C8-N9	-5.20	110.50	113.10
36	5	3006	A	N9-C4-C5	5.20	107.88	105.80
38	8	95	G	N3-C4-N9	-5.20	122.88	126.00
1	2	17	C	C6-N1-C2	-5.19	118.22	120.30
36	1	1484	U	N3-C2-O2	-5.19	118.56	122.20
36	1	2393	G	O5'-P-OP2	-5.19	101.03	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	o3	86	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	2	55	A	C8-N9-C4	-5.19	103.72	105.80
36	1	344	A	C4-C5-N7	-5.19	108.10	110.70
36	1	836	A	C5-C6-N6	-5.19	119.55	123.70
36	1	1881	A	C8-N9-C4	5.19	107.88	105.80
36	1	3377	G	C5-C6-O6	-5.19	125.48	128.60
1	6	557	G	C5-C6-O6	5.19	131.72	128.60
36	5	831	G	C5-C6-O6	-5.19	125.48	128.60
36	5	1942	U	N1-C2-N3	5.19	118.02	114.90
36	5	2584	G	OP2-P-O3'	5.19	116.62	105.20
36	5	2836	C	OP2-P-O3'	5.19	116.62	105.20
36	1	360	G	N3-C4-N9	5.19	129.11	126.00
36	1	1133	A	C8-N9-C4	5.19	107.88	105.80
36	5	295	A	O5'-P-OP1	-5.19	101.03	105.70
36	5	1901	A	C4-N9-C1'	5.19	135.64	126.30
36	5	2754	G	N3-C4-N9	5.19	129.12	126.00
36	5	2881	C	N3-C4-C5	5.19	123.98	121.90
36	5	3154	C	C5-C6-N1	5.19	123.59	121.00
40	l3	10	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	2	1537	C	C5-C4-N4	-5.19	116.57	120.20
36	1	103	G	N1-C6-O6	-5.19	116.79	119.90
36	1	2980	U	O5'-P-OP2	5.19	116.93	110.70
1	6	139	C	N3-C2-O2	-5.19	118.27	121.90
39	l2	241	ARG	NE-CZ-NH2	-5.19	117.71	120.30
36	1	2873	U	N1-C2-O2	5.19	126.43	122.80
36	1	2945	G	C8-N9-C4	5.19	108.47	106.40
36	1	3058	U	C2-N1-C1'	5.19	123.93	117.70
1	6	118	U	N3-C4-C5	5.19	117.71	114.60
36	5	385	A	N1-C6-N6	5.19	121.71	118.60
1	6	1354	G	N7-C8-N9	5.19	115.69	113.10
36	5	2992	U	C2-N1-C1'	5.19	123.92	117.70
1	2	794	U	P-O3'-C3'	5.18	125.92	119.70
1	2	934	C	N3-C4-N4	5.18	121.63	118.00
36	1	405	U	O5'-P-OP1	-5.18	101.03	105.70
36	1	1115	G	C8-N9-C1'	-5.18	120.26	127.00
36	1	3058	U	C6-N1-C1'	-5.18	113.94	121.20
36	5	1327	C	N1-C2-O2	5.18	122.01	118.90
36	5	2167	A	N9-C4-C5	5.18	107.87	105.80
36	5	2818	U	N3-C4-C5	5.18	117.71	114.60
36	5	2928	C	O5'-P-OP2	-5.18	101.03	105.70
38	8	3	A	C2-N3-C4	5.18	113.19	110.60
36	1	33	G	C5-N7-C8	-5.18	101.71	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	223	U	C2-N3-C4	-5.18	123.89	127.00
36	1	780	A	N1-C6-N6	-5.18	115.49	118.60
36	1	2830	G	N3-C2-N2	-5.18	116.27	119.90
36	1	3271	G	C8-N9-C4	5.18	108.47	106.40
38	4	47	C	OP2-P-O3'	5.18	116.60	105.20
1	6	394	C	C5-C6-N1	-5.18	118.41	121.00
36	5	611	A	O5'-P-OP1	5.18	116.92	110.70
36	5	2379	U	C2-N3-C4	-5.18	123.89	127.00
36	5	2724	U	C5-C4-O4	5.18	129.01	125.90
37	7	74	C	N1-C2-O2	-5.18	115.79	118.90
52	m6	49	ARG	NE-CZ-NH1	-5.18	117.71	120.30
36	1	1117	G	C8-N9-C4	5.18	108.47	106.40
1	6	31	C	N3-C4-C5	-5.18	119.83	121.90
36	5	37	U	N1-C2-N3	5.18	118.01	114.90
36	1	2585	G	N3-C4-C5	-5.18	126.01	128.60
1	2	1458	G	C8-N9-C1'	-5.18	120.27	127.00
36	1	96	G	C2-N3-C4	-5.18	109.31	111.90
36	1	158	G	N3-C4-N9	-5.18	122.89	126.00
36	1	1838	G	C5-C6-O6	-5.18	125.49	128.60
36	1	2145	A	C8-N9-C4	-5.18	103.73	105.80
36	1	2286	U	O5'-P-OP2	-5.18	101.04	105.70
52	M6	33	ILE	CG1-CB-CG2	-5.18	100.01	111.40
1	6	794	U	C2-N1-C1'	5.18	123.91	117.70
1	6	1661	U	N1-C2-O2	-5.18	119.18	122.80
8	s6	133	LEU	CA-CB-CG	5.18	127.20	115.30
36	5	1134	G	O5'-P-OP2	-5.18	101.04	105.70
36	5	1464	G	C8-N9-C4	5.18	108.47	106.40
36	5	2234	G	C4-C5-N7	5.18	112.87	110.80
36	5	2995	A	C8-N9-C4	5.18	107.87	105.80
1	2	1739	C	N3-C4-C5	5.17	123.97	121.90
36	5	1154	A	C2-N3-C4	5.17	113.19	110.60
36	5	1199	C	C2-N3-C4	-5.17	117.31	119.90
36	5	1858	A	C2-N3-C4	5.17	113.19	110.60
36	5	2924	U	O5'-P-OP1	-5.17	101.04	105.70
38	4	63	G	N9-C4-C5	5.17	107.47	105.40
40	L3	19	ARG	NE-CZ-NH2	-5.17	117.71	120.30
36	5	1889	G	C5-C6-O6	5.17	131.70	128.60
36	5	2202	C	C5-C4-N4	-5.17	116.58	120.20
36	5	2294	U	C2-N3-C4	-5.17	123.90	127.00
1	2	758	U	N3-C2-O2	-5.17	118.58	122.20
1	6	417	A	C6-C5-N7	-5.17	128.68	132.30
36	5	411	U	N1-C2-N3	5.17	118.00	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2371	G	C6-N1-C2	5.17	128.20	125.10
29	D7	29	ARG	NE-CZ-NH1	5.17	122.89	120.30
36	1	340	C	N3-C4-C5	5.17	123.97	121.90
36	1	3173	G	C6-N1-C2	-5.17	122.00	125.10
68	O2	33	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	2	1678	A	C8-N9-C4	-5.17	103.73	105.80
36	1	793	C	N1-C2-O2	-5.17	115.80	118.90
36	1	897	U	C5-C6-N1	5.17	125.28	122.70
36	1	1112	A	N1-C6-N6	5.17	121.70	118.60
36	1	2157	G	C2-N3-C4	5.17	114.48	111.90
1	6	1084	A	N1-C6-N6	-5.17	115.50	118.60
36	5	914	A	N7-C8-N9	-5.17	111.22	113.80
36	1	400	G	C5-C6-O6	-5.17	125.50	128.60
1	6	65	A	C5-N7-C8	-5.17	101.32	103.90
1	6	1031	U	C2-N1-C1'	-5.17	111.50	117.70
36	5	428	A	OP2-P-O3'	5.17	116.57	105.20
38	8	65	A	C5-C6-N6	-5.17	119.57	123.70
36	1	291	C	N1-C2-N3	5.16	122.81	119.20
36	1	2883	U	C6-N1-C2	-5.16	117.90	121.00
36	1	2958	A	N7-C8-N9	-5.16	111.22	113.80
36	1	3108	G	C2-N3-C4	5.16	114.48	111.90
36	5	1305	U	N3-C4-O4	5.16	123.01	119.40
36	5	1390	A	C8-N9-C4	-5.16	103.73	105.80
36	5	2955	U	C6-N1-C2	-5.16	117.90	121.00
1	2	1768	G	N9-C4-C5	5.16	107.47	105.40
36	1	1370	G	N1-C2-N2	-5.16	111.55	116.20
1	6	1101	G	N9-C4-C5	5.16	107.47	105.40
36	1	352	A	O4'-C1'-N9	5.16	112.33	108.20
36	1	1153	A	O5'-P-OP1	-5.16	101.06	105.70
1	6	320	U	O5'-P-OP2	5.16	116.89	110.70
1	6	697	C	N3-C2-O2	-5.16	118.29	121.90
1	6	1670	G	O5'-P-OP2	-5.16	101.06	105.70
36	5	649	A	C5-N7-C8	-5.16	101.32	103.90
36	5	1604	G	N3-C4-C5	-5.16	126.02	128.60
36	5	3358	U	N3-C2-O2	-5.16	118.59	122.20
1	2	73	U	P-O3'-C3'	5.16	125.89	119.70
1	2	1206	U	N3-C4-O4	5.16	123.01	119.40
36	1	885	U	N3-C4-O4	-5.16	115.79	119.40
36	1	963	G	C5-C6-O6	-5.16	125.50	128.60
36	1	1908	A	C8-N9-C4	5.16	107.86	105.80
36	1	2714	G	O5'-P-OP2	5.16	116.89	110.70
1	6	539	G	C8-N9-C4	-5.16	104.34	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1605	G	C5-C6-O6	5.16	131.69	128.60
36	5	2607	G	N9-C4-C5	5.16	107.46	105.40
36	5	2836	C	N1-C2-N3	5.16	122.81	119.20
36	5	2917	G	N3-C4-N9	5.16	129.09	126.00
59	n3	42	SER	N-CA-C	5.16	124.93	111.00
36	1	37	U	C5-C6-N1	-5.16	120.12	122.70
36	1	1125	U	OP2-P-O3'	5.16	116.55	105.20
1	2	1792	G	N9-C4-C5	-5.16	103.34	105.40
36	1	930	U	N3-C4-C5	5.16	117.69	114.60
36	1	2138	A	C2-N3-C4	-5.16	108.02	110.60
36	5	640	U	C5-C6-N1	-5.16	120.12	122.70
36	5	2260	U	OP2-P-O3'	5.16	116.54	105.20
36	1	72	C	N3-C4-C5	5.15	123.96	121.90
36	1	142	C	C6-N1-C2	-5.15	118.24	120.30
36	5	793	C	C4-C5-C6	-5.15	114.82	117.40
36	5	1679	A	N1-C6-N6	-5.15	115.51	118.60
36	5	2961	G	N1-C6-O6	-5.15	116.81	119.90
1	2	447	U	C6-N1-C2	-5.15	117.91	121.00
36	1	1310	G	N3-C2-N2	5.15	123.51	119.90
36	1	2853	A	C8-N9-C4	-5.15	103.74	105.80
1	6	1006	C	C6-N1-C2	-5.15	118.24	120.30
1	6	1697	G	N3-C4-N9	5.15	129.09	126.00
36	5	94	G	N1-C2-N3	-5.15	120.81	123.90
36	5	2378	C	C2-N3-C4	5.15	122.48	119.90
36	5	2630	C	N1-C2-N3	5.15	122.81	119.20
36	5	3310	A	N1-C6-N6	-5.15	115.51	118.60
1	2	61	A	O4'-C1'-N9	5.15	112.32	108.20
36	1	2695	A	O4'-C1'-N9	5.15	112.32	108.20
59	N3	87	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	6	448	C	OP1-P-O3'	5.15	116.53	105.20
36	5	708	G	C5-N7-C8	-5.15	101.72	104.30
36	5	722	G	N9-C4-C5	5.15	107.46	105.40
36	5	1208	U	C5-C4-O4	5.15	128.99	125.90
36	5	217	U	C5-C6-N1	-5.15	120.13	122.70
36	5	1146	C	C6-N1-C2	-5.15	118.24	120.30
36	1	349	A	N1-C6-N6	-5.15	115.51	118.60
36	1	1060	U	C6-N1-C2	5.15	124.09	121.00
36	5	1371	G	C5-N7-C8	5.15	106.87	104.30
36	5	1908	A	N3-C4-C5	-5.15	123.20	126.80
36	5	2366	C	C6-N1-C2	-5.15	118.24	120.30
36	5	2608	G	N1-C2-N2	-5.15	111.57	116.20
36	1	93	C	C2-N1-C1'	-5.15	113.14	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2314	U	C2-N1-C1'	5.15	123.88	117.70
36	1	3187	A	C2-N3-C4	5.15	113.17	110.60
1	2	938	G	OP2-P-O3'	5.14	116.52	105.20
1	2	1051	G	P-O3'-C3'	5.14	125.87	119.70
36	1	971	G	N1-C6-O6	-5.14	116.81	119.90
36	1	1082	U	C2-N1-C1'	5.14	123.87	117.70
36	1	2392	C	N3-C4-N4	5.14	121.60	118.00
36	5	640	U	N1-C2-N3	5.14	117.99	114.90
36	5	1382	G	N1-C6-O6	-5.14	116.81	119.90
36	5	1468	A	OP1-P-OP2	5.14	127.32	119.60
36	5	2180	G	N7-C8-N9	-5.14	110.53	113.10
36	5	3362	A	C4-C5-N7	5.14	113.27	110.70
36	1	1152	G	C4-C5-N7	5.14	112.86	110.80
36	1	2365	C	N3-C4-N4	-5.14	114.40	118.00
36	1	2402	A	C4-C5-C6	5.14	119.57	117.00
36	1	2627	C	O4'-C1'-N1	5.14	112.31	108.20
69	O3	29	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	6	1535	U	C4-C5-C6	5.14	122.79	119.70
36	5	906	A	N1-C6-N6	-5.14	115.51	118.60
36	5	3042	U	N3-C4-C5	5.14	117.69	114.60
36	5	348	A	N7-C8-N9	-5.14	111.23	113.80
36	5	1439	U	N3-C4-C5	5.14	117.69	114.60
36	1	2236	G	C5-C6-O6	-5.14	125.52	128.60
36	1	2343	C	N3-C2-O2	-5.14	118.30	121.90
36	1	3171	U	N1-C2-O2	-5.14	119.20	122.80
1	6	1149	G	C5-C6-O6	5.14	131.68	128.60
36	5	653	A	OP2-P-O3'	5.14	116.51	105.20
36	5	2965	U	N1-C2-O2	-5.14	119.20	122.80
36	5	3093	C	N1-C2-O2	-5.14	115.82	118.90
1	2	142	G	C2-N3-C4	-5.14	109.33	111.90
1	6	90	C	N3-C4-N4	-5.14	114.40	118.00
1	6	417	A	C4-C5-C6	5.14	119.57	117.00
1	6	1203	A	O5'-P-OP1	-5.14	101.08	105.70
36	5	1133	A	N9-C4-C5	5.14	107.86	105.80
36	5	1634	G	N1-C6-O6	5.14	122.98	119.90
36	5	2794	G	N9-C4-C5	-5.14	103.34	105.40
1	2	1490	C	C6-N1-C2	-5.14	118.25	120.30
36	1	518	G	O4'-C1'-N9	5.14	112.31	108.20
36	1	1124	U	C4-C5-C6	-5.14	116.62	119.70
36	1	1150	A	C2-N3-C4	-5.14	108.03	110.60
43	L6	64	LEU	CA-CB-CG	5.14	127.11	115.30
1	6	350	U	N1-C2-N3	5.14	117.98	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1681	A	C2-N3-C4	-5.14	108.03	110.60
36	5	288	C	C6-N1-C2	5.14	122.36	120.30
36	5	2524	A	C3'-C2'-C1'	-5.14	97.39	101.50
1	2	1516	A	N1-C6-N6	5.13	121.68	118.60
36	1	48	A	O4'-C1'-N9	5.13	112.31	108.20
36	1	416	A	C5-C6-N6	5.13	127.81	123.70
36	5	509	U	N1-C2-N3	5.13	117.98	114.90
36	5	1096	U	N1-C2-O2	-5.13	119.21	122.80
36	5	1168	U	C4-C5-C6	-5.13	116.62	119.70
36	1	1419	A	N9-C1'-C2'	-5.13	106.35	112.00
1	6	1781	A	C8-N9-C4	-5.13	103.75	105.80
36	1	645	A	C5-C6-N6	-5.13	119.59	123.70
36	1	2320	A	OP1-P-OP2	-5.13	111.90	119.60
36	1	3083	G	N3-C4-C5	-5.13	126.03	128.60
36	1	3219	G	N3-C4-N9	5.13	129.08	126.00
36	5	1211	U	N3-C4-O4	-5.13	115.81	119.40
36	5	2639	G	N1-C6-O6	5.13	122.98	119.90
36	5	2886	U	N1-C2-N3	5.13	117.98	114.90
36	5	3226	A	N9-C4-C5	-5.13	103.75	105.80
36	5	3378	C	C2-N3-C4	-5.13	117.33	119.90
36	1	2300	G	C5-C6-O6	5.13	131.68	128.60
1	6	1081	A	O4'-C1'-N9	5.13	112.30	108.20
36	5	1145	G	N9-C4-C5	5.13	107.45	105.40
36	1	962	A	C5-C6-N1	5.13	120.26	117.70
36	1	2444	C	C2-N1-C1'	5.13	124.44	118.80
36	1	3038	U	N3-C2-O2	-5.13	118.61	122.20
38	4	9	A	N9-C4-C5	5.13	107.85	105.80
36	5	66	A	C8-N9-C4	5.13	107.85	105.80
36	5	1108	U	O5'-P-OP2	-5.13	101.08	105.70
1	2	734	A	OP1-P-O3'	5.13	116.48	105.20
1	2	765	G	O4'-C1'-N9	-5.13	104.10	108.20
36	1	291	C	OP2-P-O3'	5.13	116.48	105.20
36	1	347	G	C4-C5-N7	5.13	112.85	110.80
36	1	2627	C	C6-N1-C2	5.13	122.35	120.30
36	1	2820	A	C2-N3-C4	5.13	113.16	110.60
1	6	1138	A	N1-C2-N3	-5.13	126.74	129.30
1	6	1396	U	C6-N1-C2	-5.13	117.92	121.00
36	5	191	U	N3-C2-O2	5.13	125.79	122.20
36	5	594	U	O5'-P-OP2	-5.13	101.09	105.70
36	5	2341	A	N9-C4-C5	-5.13	103.75	105.80
36	5	3188	G	N1-C6-O6	-5.13	116.82	119.90
44	17	88	ARG	NE-CZ-NH1	5.13	122.86	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3308	C	C6-N1-C2	5.12	122.35	120.30
1	6	1600	A	C4-C5-N7	5.12	113.26	110.70
36	5	908	G	C5-C6-O6	-5.12	125.53	128.60
36	5	1242	G	N3-C4-N9	5.12	129.07	126.00
36	1	351	A	C8-N9-C4	5.12	107.85	105.80
36	1	966	U	N3-C2-O2	-5.12	118.61	122.20
36	1	3083	G	C2-N3-C4	5.12	114.46	111.90
1	6	60	U	N1-C2-O2	5.12	126.39	122.80
1	6	151	G	N9-C4-C5	5.12	107.45	105.40
1	6	577	G	C5-N7-C8	-5.12	101.74	104.30
36	5	1201	C	C2-N1-C1'	-5.12	113.16	118.80
36	5	1942	U	C5-C4-O4	-5.12	122.83	125.90
1	2	1491	U	O5'-P-OP1	-5.12	101.09	105.70
36	1	709	A	N1-C6-N6	5.12	121.67	118.60
36	1	3228	C	P-O3'-C3'	5.12	125.85	119.70
36	1	3275	U	P-O3'-C3'	5.12	125.84	119.70
1	6	187	G	P-O3'-C3'	5.12	125.84	119.70
36	5	1313	G	C6-N1-C2	5.12	128.17	125.10
36	5	1481	A	C5-N7-C8	-5.12	101.34	103.90
36	5	2886	U	O4'-C1'-N1	5.12	112.30	108.20
36	5	3030	G	N7-C8-N9	-5.12	110.54	113.10
1	2	1458	G	C4-N9-C1'	5.12	133.16	126.50
36	1	959	C	C2-N3-C4	-5.12	117.34	119.90
36	1	1305	U	N3-C4-O4	-5.12	115.82	119.40
36	1	2952	G	C2-N3-C4	-5.12	109.34	111.90
36	5	2699	G	C2-N3-C4	5.12	114.46	111.90
36	5	2834	G	OP1-P-OP2	5.12	127.28	119.60
37	7	96	U	C2-N3-C4	-5.12	123.93	127.00
1	2	829	A	P-O3'-C3'	5.12	125.84	119.70
36	1	748	U	N3-C4-C5	5.12	117.67	114.60
36	5	1507	G	O4'-C1'-N9	-5.12	104.11	108.20
1	2	959	U	N1-C2-O2	5.12	126.38	122.80
36	5	112	U	O4'-C1'-N1	5.12	112.29	108.20
36	5	2112	U	O5'-P-OP2	-5.12	101.10	105.70
36	5	2610	G	O4'-C1'-N9	5.12	112.29	108.20
36	5	3003	G	N3-C4-C5	5.12	131.16	128.60
38	8	92	A	N1-C6-N6	5.12	121.67	118.60
36	5	437	G	C4-C5-N7	-5.11	108.75	110.80
36	5	629	U	C2-N3-C4	-5.11	123.93	127.00
36	5	1178	G	C5-C6-O6	-5.11	125.53	128.60
36	5	2222	A	OP2-P-O3'	5.11	116.45	105.20
36	5	2767	U	O5'-P-OP2	-5.11	101.10	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2936	A	N1-C6-N6	5.11	121.67	118.60
44	17	227	GLY	N-CA-C	5.11	125.89	113.10
36	5	3369	G	C6-N1-C2	-5.11	122.03	125.10
36	1	74	G	N1-C2-N2	-5.11	111.60	116.20
36	1	1116	G	O5'-P-OP1	-5.11	101.10	105.70
36	1	1177	G	N3-C2-N2	-5.11	116.32	119.90
36	1	1287	A	O5'-P-OP1	-5.11	101.10	105.70
36	1	1482	A	N1-C6-N6	-5.11	115.53	118.60
36	1	3275	U	C6-N1-C2	-5.11	117.93	121.00
38	4	113	U	C2-N1-C1'	-5.11	111.57	117.70
36	5	1112	A	O5'-P-OP1	-5.11	101.10	105.70
36	5	1606	U	OP1-P-OP2	5.11	127.27	119.60
36	5	2611	U	C4-C5-C6	5.11	122.77	119.70
36	5	2955	U	O5'-P-OP2	-5.11	101.10	105.70
36	1	814	U	O5'-P-OP2	5.11	116.83	110.70
36	5	688	G	N3-C4-N9	-5.11	122.94	126.00
37	7	13	A	C2-N3-C4	5.11	113.15	110.60
36	1	1418	A	O5'-P-OP1	5.11	116.83	110.70
36	1	2606	G	N3-C4-N9	5.11	129.06	126.00
36	1	2787	G	N3-C4-C5	-5.11	126.05	128.60
36	1	3041	U	N1-C2-O2	-5.11	119.22	122.80
39	L2	207	VAL	CB-CA-C	-5.11	101.70	111.40
36	5	2808	A	O5'-P-OP2	-5.11	101.10	105.70
36	5	2860	U	C6-N1-C2	5.11	124.06	121.00
36	5	2995	A	N7-C8-N9	-5.11	111.25	113.80
1	2	1654	G	O5'-P-OP2	-5.11	101.11	105.70
36	1	681	U	O5'-P-OP2	-5.11	101.11	105.70
36	1	2946	A	N1-C2-N3	-5.11	126.75	129.30
1	6	1698	G	P-O3'-C3'	5.11	125.83	119.70
36	5	798	G	OP1-P-OP2	-5.11	111.94	119.60
36	5	2257	C	C6-N1-C2	-5.11	118.26	120.30
36	5	3249	C	OP1-P-OP2	5.11	127.26	119.60
36	1	1161	G	N1-C6-O6	-5.10	116.84	119.90
36	1	2385	G	C2-N3-C4	-5.10	109.35	111.90
36	1	2993	G	N3-C4-N9	5.10	129.06	126.00
36	5	1555	U	O4'-C1'-N1	5.10	112.28	108.20
1	2	391	A	C4-C5-C6	-5.10	114.45	117.00
36	1	2338	C	N3-C2-O2	-5.10	118.33	121.90
1	6	1389	C	C2-N1-C1'	5.10	124.41	118.80
2	s0	62	ARG	NE-CZ-NH2	-5.10	117.75	120.30
36	5	646	A	C8-N9-C4	-5.10	103.76	105.80
36	5	659	G	N3-C2-N2	5.10	123.47	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1334	U	N3-C4-O4	5.10	122.97	119.40
39	12	214	GLY	N-CA-C	5.10	125.85	113.10
36	1	351	A	N7-C8-N9	-5.10	111.25	113.80
36	1	2870	C	C4-C5-C6	-5.10	114.85	117.40
36	1	3109	G	C2-N3-C4	5.10	114.45	111.90
1	6	550	A	O5'-P-OP2	-5.10	101.11	105.70
44	17	191	VAL	C-N-CA	-5.10	111.59	122.30
1	2	1145	U	N1-C2-O2	-5.10	119.23	122.80
1	2	1277	G	N3-C4-N9	-5.10	122.94	126.00
36	1	959	C	C6-N1-C2	5.10	122.34	120.30
1	6	980	G	N1-C6-O6	-5.10	116.84	119.90
36	5	1373	A	C5-N7-C8	5.10	106.45	103.90
36	5	2409	G	N9-C4-C5	5.10	107.44	105.40
1	2	1354	G	C8-N9-C4	-5.10	104.36	106.40
36	1	3190	C	N3-C4-C5	5.10	123.94	121.90
38	4	23	U	C2-N3-C4	-5.10	123.94	127.00
1	6	352	A	N1-C6-N6	-5.10	115.54	118.60
1	6	1436	A	C8-N9-C4	-5.10	103.76	105.80
36	5	2610	G	C5-C6-O6	5.10	131.66	128.60
36	1	804	C	N1-C2-O2	-5.10	115.84	118.90
36	5	2938	G	OP1-P-OP2	5.10	127.25	119.60
1	2	1776	A	N9-C4-C5	5.09	107.84	105.80
36	1	24	G	N1-C6-O6	5.09	122.96	119.90
36	1	1897	G	OP2-P-O3'	5.09	116.41	105.20
36	1	2376	G	C4-C5-N7	5.09	112.84	110.80
36	1	2883	U	N3-C4-O4	-5.09	115.83	119.40
1	6	879	G	C5-C6-O6	5.09	131.66	128.60
36	5	101	G	C8-N9-C1'	-5.09	120.38	127.00
36	5	874	U	O5'-P-OP1	-5.09	101.12	105.70
36	5	1445	U	C2-N3-C4	-5.09	123.94	127.00
36	5	2950	G	O4'-C1'-N9	5.09	112.28	108.20
36	5	3060	C	N1-C2-O2	-5.09	115.84	118.90
37	7	71	G	OP2-P-O3'	5.09	116.41	105.20
36	1	678	G	N1-C6-O6	5.09	122.96	119.90
36	5	1162	U	C5-C6-N1	-5.09	120.15	122.70
36	1	55	G	C8-N9-C4	5.09	108.44	106.40
36	1	371	G	N9-C1'-C2'	-5.09	106.40	112.00
36	1	582	G	C5-C6-N1	5.09	114.05	111.50
36	1	2413	A	N1-C6-N6	-5.09	115.55	118.60
1	6	1084	A	C5-C6-N6	5.09	127.77	123.70
36	5	3041	U	C5-C4-O4	-5.09	122.84	125.90
36	5	3095	U	N3-C4-C5	5.09	117.66	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	66	A	N1-C2-N3	-5.09	126.75	129.30
1	2	704	C	N3-C2-O2	-5.09	118.34	121.90
25	D3	111	GLY	N-CA-C	-5.09	100.37	113.10
36	1	1724	U	N3-C2-O2	-5.09	118.64	122.20
36	1	2123	G	C5-N7-C8	5.09	106.84	104.30
41	L4	198	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	6	1782	A	P-O3'-C3'	5.09	125.81	119.70
36	5	1181	U	C6-N1-C2	5.09	124.05	121.00
36	5	1429	G	N3-C2-N2	5.09	123.46	119.90
36	5	2333	C	OP2-P-O3'	5.09	116.40	105.20
36	5	3144	G	N9-C4-C5	5.09	107.44	105.40
36	1	1138	U	N3-C2-O2	-5.09	118.64	122.20
36	1	1720	U	N1-C2-N3	5.09	117.95	114.90
36	1	2396	G	C5-C6-N1	-5.09	108.96	111.50
1	2	1280	C	N3-C4-C5	-5.09	119.86	121.90
36	1	93	C	C6-N1-C2	-5.09	118.27	120.30
36	1	112	U	C5-C6-N1	5.09	125.24	122.70
38	4	142	C	C6-N1-C2	-5.09	118.27	120.30
1	6	313	U	C5-C6-N1	-5.09	120.16	122.70
36	5	914	A	N3-C4-C5	5.09	130.36	126.80
36	5	2912	G	N1-C6-O6	-5.09	116.85	119.90
36	5	3309	G	C4-N9-C1'	5.09	133.11	126.50
38	8	79	A	C8-N9-C4	-5.09	103.77	105.80
1	2	425	A	N7-C8-N9	5.08	116.34	113.80
1	2	1600	A	P-O3'-C3'	5.08	125.80	119.70
36	1	2550	U	C4-C5-C6	5.08	122.75	119.70
49	M3	63	VAL	CB-CA-C	-5.08	101.74	111.40
1	6	1048	G	C4-C5-N7	5.08	112.83	110.80
1	6	1796	C	N3-C4-N4	-5.08	114.44	118.00
36	5	1858	A	N3-C4-C5	-5.08	123.24	126.80
36	5	1863	G	C5-C6-O6	-5.08	125.55	128.60
1	2	934	C	C5-C6-N1	5.08	123.54	121.00
36	1	895	A	C6-C5-N7	-5.08	128.74	132.30
36	1	934	G	C8-N9-C4	5.08	108.43	106.40
36	1	1413	G	N1-C6-O6	-5.08	116.85	119.90
36	1	1807	G	N3-C4-C5	-5.08	126.06	128.60
36	1	2883	U	N1-C2-O2	5.08	126.36	122.80
36	5	883	A	C8-N9-C4	5.08	107.83	105.80
36	5	1305	U	N1-C2-O2	-5.08	119.24	122.80
36	5	2644	C	N1-C2-O2	-5.08	115.85	118.90
49	m3	55	ARG	CG-CD-NE	5.08	122.47	111.80
1	6	1101	G	C4-C5-N7	-5.08	108.77	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1730	A	OP1-P-O3'	5.08	116.38	105.20
36	5	1307	G	C5-C6-N1	5.08	114.04	111.50
1	2	736	C	C5-C6-N1	5.08	123.54	121.00
36	1	1467	A	C8-N9-C4	-5.08	103.77	105.80
36	1	2636	A	N9-C4-C5	5.08	107.83	105.80
36	5	775	A	C5-C6-N1	5.08	120.24	117.70
36	5	788	C	OP2-P-O3'	5.08	116.38	105.20
36	5	810	A	N1-C6-N6	-5.08	115.55	118.60
36	5	2160	G	N1-C6-O6	-5.08	116.85	119.90
36	5	708	G	N7-C8-N9	5.08	115.64	113.10
36	5	1014	U	C6-N1-C1'	-5.08	114.09	121.20
36	5	1147	G	OP2-P-O3'	5.08	116.37	105.20
36	5	2833	A	C2-N3-C4	5.08	113.14	110.60
37	7	15	C	N3-C4-C5	5.08	123.93	121.90
36	1	686	G	N9-C4-C5	5.08	107.43	105.40
36	1	1906	G	N3-C4-N9	5.08	129.05	126.00
37	3	95	A	C6-C5-N7	-5.08	128.75	132.30
59	N3	54	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	6	359	A	N1-C2-N3	-5.08	126.76	129.30
36	5	64	G	OP2-P-O3'	5.08	116.37	105.20
36	5	1064	A	O4'-C1'-N9	-5.08	104.14	108.20
36	5	1362	G	N1-C6-O6	-5.08	116.85	119.90
36	5	2362	C	N1-C2-O2	5.08	121.95	118.90
37	7	92	A	OP1-P-O3'	5.08	116.36	105.20
36	1	3178	A	C2-N3-C4	-5.07	108.06	110.60
41	L4	194	TYR	CB-CG-CD1	-5.07	117.96	121.00
36	5	2808	A	C2-N3-C4	-5.07	108.06	110.60
36	5	3049	A	N1-C2-N3	-5.07	126.76	129.30
36	5	3052	G	N7-C8-N9	-5.07	110.56	113.10
36	1	511	G	N1-C6-O6	-5.07	116.86	119.90
36	1	1004	U	N3-C2-O2	-5.07	118.65	122.20
36	1	1397	C	C6-N1-C2	5.07	122.33	120.30
36	1	1556	C	N1-C2-O2	5.07	121.94	118.90
36	1	2142	A	OP1-P-O3'	5.07	116.35	105.20
36	1	2314	U	C4-C5-C6	-5.07	116.66	119.70
36	1	2339	C	OP1-P-O3'	5.07	116.35	105.20
1	6	351	C	C4-C5-C6	5.07	119.94	117.40
36	5	286	U	OP2-P-O3'	5.07	116.36	105.20
36	5	386	A	C4-C5-N7	5.07	113.23	110.70
36	5	1445	U	N1-C2-O2	-5.07	119.25	122.80
36	5	2326	A	N7-C8-N9	-5.07	111.27	113.80
36	5	2420	C	C5-C4-N4	-5.07	116.65	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2817	A	C2-N3-C4	5.07	113.14	110.60
36	5	2853	A	OP1-P-OP2	-5.07	111.99	119.60
36	1	787	G	N1-C6-O6	-5.07	116.86	119.90
36	1	2388	U	N3-C2-O2	5.07	125.75	122.20
1	6	951	A	C2-N3-C4	-5.07	108.06	110.60
36	5	1863	G	N9-C4-C5	-5.07	103.37	105.40
36	1	721	G	N1-C6-O6	5.07	122.94	119.90
36	1	1893	A	N9-C4-C5	5.07	107.83	105.80
36	1	2979	U	C5-C6-N1	-5.07	120.17	122.70
36	5	3317	U	N3-C4-O4	-5.07	115.85	119.40
36	1	374	A	N1-C2-N3	-5.07	126.77	129.30
36	1	2180	G	C5-C6-O6	5.07	131.64	128.60
1	6	162	A	O5'-P-OP2	-5.07	101.14	105.70
1	6	1595	U	O4'-C1'-N1	5.07	112.25	108.20
36	5	1464	G	N3-C2-N2	5.07	123.45	119.90
36	5	3340	G	N9-C4-C5	5.07	107.43	105.40
36	1	1129	A	C5-C6-N6	-5.06	119.65	123.70
36	1	2945	G	OP1-P-OP2	-5.06	112.00	119.60
36	1	3092	C	C6-N1-C2	5.06	122.33	120.30
1	6	308	C	C4-C5-C6	5.06	119.93	117.40
36	5	2314	U	O5'-P-OP1	-5.06	101.14	105.70
48	m1	9	MET	N-CA-C	-5.06	97.33	111.00
36	1	2420	C	C2-N3-C4	-5.06	117.37	119.90
36	5	1130	A	N9-C4-C5	5.06	107.83	105.80
36	5	1876	U	C4-C5-C6	-5.06	116.66	119.70
36	5	362	U	N1-C2-N3	5.06	117.94	114.90
1	2	1782	A	C5-C6-N6	5.06	127.75	123.70
36	1	213	A	C6-N1-C2	5.06	121.64	118.60
36	1	1858	A	C4-N9-C1'	5.06	135.41	126.30
1	6	1121	C	N3-C2-O2	-5.06	118.36	121.90
36	5	2349	U	O5'-P-OP1	5.06	116.77	110.70
36	5	2404	A	N9-C4-C5	-5.06	103.78	105.80
36	5	2882	U	OP1-P-OP2	5.06	127.19	119.60
1	2	1654	G	C6-N1-C2	-5.06	122.06	125.10
36	1	1415	U	N3-C4-O4	-5.06	115.86	119.40
36	1	1870	C	C2-N3-C4	-5.06	117.37	119.90
38	4	13	A	C8-N9-C4	-5.06	103.78	105.80
1	6	1195	C	OP1-P-O3'	5.06	116.33	105.20
36	5	412	G	N1-C6-O6	-5.06	116.87	119.90
36	5	2113	A	N7-C8-N9	-5.06	111.27	113.80
36	5	2298	U	O4'-C1'-N1	5.06	112.25	108.20
36	5	2914	G	N1-C6-O6	-5.06	116.87	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3093	C	C4-C5-C6	5.06	119.93	117.40
36	1	46	U	N1-C2-N3	5.06	117.93	114.90
36	5	2841	G	OP1-P-O3'	5.06	116.32	105.20
36	5	3366	G	N1-C6-O6	-5.06	116.87	119.90
1	2	1585	U	C5-C4-O4	5.05	128.93	125.90
1	6	114	C	O5'-P-OP1	-5.05	101.15	105.70
36	5	111	C	C6-N1-C2	5.05	122.32	120.30
36	5	927	C	N1-C2-O2	-5.05	115.87	118.90
36	5	948	C	OP1-P-OP2	-5.05	112.02	119.60
36	5	2258	U	N1-C2-O2	5.05	126.34	122.80
36	5	2628	A	C6-N1-C2	-5.05	115.57	118.60
1	2	582	U	O5'-P-OP1	-5.05	101.15	105.70
36	1	2595	A	N1-C6-N6	5.05	121.63	118.60
36	5	1439	U	C6-N1-C2	5.05	124.03	121.00
36	5	2970	C	C5-C6-N1	-5.05	118.47	121.00
42	15	152	ARG	NE-CZ-NH1	5.05	122.83	120.30
36	1	687	U	OP2-P-O3'	5.05	116.31	105.20
36	1	2423	U	C6-N1-C1'	-5.05	114.13	121.20
36	5	94	G	C5-C6-N1	5.05	114.03	111.50
36	5	320	G	C4-C5-N7	-5.05	108.78	110.80
36	5	2805	G	N3-C4-N9	5.05	129.03	126.00
6	S4	38	LEU	CA-CB-CG	5.05	126.92	115.30
36	1	421	G	N3-C2-N2	5.05	123.43	119.90
1	6	1783	C	O5'-P-OP1	5.05	116.76	110.70
36	5	416	A	C8-N9-C4	-5.05	103.78	105.80
36	5	2385	G	C8-N9-C1'	5.05	133.56	127.00
36	5	2964	G	C2-N3-C4	5.05	114.42	111.90
36	5	3190	C	C6-N1-C2	-5.05	118.28	120.30
36	5	3318	G	C5-C6-O6	5.05	131.63	128.60
36	1	983	A	C8-N9-C4	5.05	107.82	105.80
36	1	1845	G	N1-C6-O6	-5.05	116.87	119.90
1	6	541	A	P-O3'-C3'	-5.05	113.64	119.70
36	5	1475	A	C8-N9-C4	-5.05	103.78	105.80
36	1	1456	A	OP1-P-O3'	5.05	116.30	105.20
36	1	2131	A	C5-C6-N1	-5.05	115.18	117.70
36	5	110	G	N3-C4-C5	-5.05	126.08	128.60
36	5	125	C	N3-C2-O2	-5.05	118.37	121.90
36	5	813	G	C8-N9-C4	-5.05	104.38	106.40
36	5	2350	C	O5'-P-OP2	-5.05	101.16	105.70
36	5	2821	C	N3-C2-O2	5.05	125.43	121.90
36	1	1310	G	N1-C2-N2	-5.04	111.66	116.20
36	5	2390	A	OP2-P-O3'	5.04	116.30	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3103	A	C5-C6-N1	5.04	120.22	117.70
36	1	312	C	C6-N1-C2	5.04	122.32	120.30
50	M4	135	LEU	CA-CB-CG	5.04	126.90	115.30
1	6	314	C	N1-C2-O2	5.04	121.93	118.90
36	5	895	A	OP2-P-O3'	5.04	116.30	105.20
36	5	1481	A	O5'-P-OP2	-5.04	101.16	105.70
36	5	2743	A	C4-C5-N7	-5.04	108.18	110.70
36	5	2872	A	C4-C5-N7	-5.04	108.18	110.70
36	5	2916	U	O5'-P-OP2	-5.04	101.16	105.70
36	1	112	U	C2-N1-C1'	5.04	123.75	117.70
36	1	340	C	C6-N1-C2	-5.04	118.28	120.30
36	1	608	A	N3-C4-N9	5.04	131.43	127.40
36	1	690	A	OP1-P-O3'	5.04	116.29	105.20
36	1	1155	C	C5-C6-N1	5.04	123.52	121.00
36	1	1323	G	OP2-P-O3'	5.04	116.29	105.20
36	1	1708	C	O5'-P-OP2	-5.04	101.16	105.70
36	1	2752	U	C5-C6-N1	-5.04	120.18	122.70
1	6	1783	C	N3-C2-O2	-5.04	118.37	121.90
36	5	2941	A	C4-C5-C6	5.04	119.52	117.00
1	2	570	A	N3-C4-C5	-5.04	123.27	126.80
1	2	1765	A	O4'-C1'-N9	5.04	112.23	108.20
36	1	2867	C	C5'-C4'-O4'	-5.04	103.05	109.10
1	6	1082	C	OP1-P-OP2	5.04	127.16	119.60
36	5	413	U	C5-C4-O4	-5.04	122.88	125.90
36	5	436	A	C5-N7-C8	-5.04	101.38	103.90
36	5	941	G	C4-C5-N7	-5.04	108.78	110.80
1	2	608	U	O5'-P-OP1	-5.04	101.17	105.70
36	1	829	U	N1-C2-N3	5.04	117.92	114.90
36	1	1151	U	N1-C2-N3	5.04	117.92	114.90
36	1	1395	G	C2-N3-C4	5.04	114.42	111.90
36	1	2537	U	P-O3'-C3'	5.04	125.75	119.70
36	1	3062	G	N1-C6-O6	-5.04	116.88	119.90
36	5	36	C	OP2-P-O3'	5.04	116.28	105.20
36	5	986	U	C4-C5-C6	-5.04	116.68	119.70
36	5	1450	G	OP2-P-O3'	5.04	116.28	105.20
36	1	2279	A	N9-C4-C5	-5.04	103.78	105.80
1	6	1119	G	N3-C4-C5	-5.04	126.08	128.60
36	5	900	G	C8-N9-C4	-5.04	104.39	106.40
38	8	87	G	O4'-C1'-N9	5.04	112.23	108.20
1	2	822	U	C5-C6-N1	5.04	125.22	122.70
36	1	806	A	N1-C6-N6	5.04	121.62	118.60
36	1	1492	G	C2-N3-C4	5.04	114.42	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2147	A	O5'-P-OP2	5.04	116.74	110.70
36	1	2813	A	C5-N7-C8	5.04	106.42	103.90
36	1	2819	A	N1-C2-N3	-5.04	126.78	129.30
36	1	2930	A	O4'-C1'-N9	5.04	112.23	108.20
71	O5	86	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	6	170	U	OP2-P-O3'	5.04	116.28	105.20
1	6	1200	G	C4-N9-C1'	-5.04	119.95	126.50
36	5	1131	G	N3-C2-N2	-5.04	116.38	119.90
36	5	2896	A	C6-C5-N7	5.04	135.82	132.30
36	5	2965	U	N3-C4-O4	5.04	122.92	119.40
36	5	3042	U	N3-C4-O4	-5.04	115.88	119.40
1	2	1057	U	C5-C6-N1	5.03	125.22	122.70
36	1	2786	G	C2-N3-C4	5.03	114.42	111.90
41	L4	190	GLY	N-CA-C	5.03	125.68	113.10
36	5	2790	A	C8-N9-C4	-5.03	103.79	105.80
1	2	1000	C	N1-C2-O2	5.03	121.92	118.90
38	8	95	G	N3-C4-C5	5.03	131.12	128.60
36	1	570	A	C8-N9-C4	-5.03	103.79	105.80
38	4	51	G	N1-C6-O6	5.03	122.92	119.90
41	L4	194	TYR	CB-CG-CD2	5.03	124.02	121.00
1	6	31	C	N3-C2-O2	-5.03	118.38	121.90
36	5	1115	G	C5-N7-C8	-5.03	101.78	104.30
36	5	2142	A	N3-C4-N9	5.03	131.42	127.40
36	5	2273	G	C4-C5-N7	-5.03	108.79	110.80
38	8	104	A	N9-C4-C5	-5.03	103.79	105.80
36	1	639	G	N9-C1'-C2'	-5.03	106.47	112.00
36	1	2920	U	C2-N3-C4	-5.03	123.98	127.00
36	5	301	G	C6-C5-N7	5.03	133.42	130.40
36	5	721	G	C5-C6-O6	5.03	131.62	128.60
36	1	835	G	C5-C6-N1	5.03	114.01	111.50
36	1	908	G	C4-N9-C1'	5.03	133.04	126.50
36	1	2444	C	O4'-C1'-N1	5.03	112.22	108.20
36	5	813	G	C4-N9-C1'	5.03	133.04	126.50
1	2	1782	A	N1-C6-N6	-5.03	115.58	118.60
36	1	515	C	N3-C4-N4	5.03	121.52	118.00
36	1	1695	U	C6-N1-C2	5.03	124.02	121.00
36	5	630	A	C5-C6-N6	5.03	127.72	123.70
36	5	1544	G	C5-C6-O6	5.03	131.62	128.60
36	5	2207	A	N1-C6-N6	5.03	121.61	118.60
36	5	2590	A	OP2-P-O3'	5.03	116.26	105.20
36	1	833	G	N1-C6-O6	-5.02	116.89	119.90
73	O7	73	ARG	NE-CZ-NH1	5.02	122.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1178	G	OP2-P-O3'	5.02	116.25	105.20
36	5	1908	A	N1-C6-N6	-5.02	115.59	118.60
36	5	2553	U	C5-C6-N1	-5.02	120.19	122.70
1	2	113	U	N3-C2-O2	5.02	125.72	122.20
1	2	1537	C	C5-C6-N1	5.02	123.51	121.00
36	1	44	U	C2-N3-C4	-5.02	123.99	127.00
36	1	94	G	N1-C6-O6	-5.02	116.89	119.90
36	1	676	G	N3-C4-C5	-5.02	126.09	128.60
36	1	1716	U	P-O3'-C3'	5.02	125.73	119.70
36	1	1940	G	C5-C6-O6	5.02	131.61	128.60
36	1	2340	U	N1-C2-O2	5.02	126.32	122.80
36	5	1379	G	C5-N7-C8	5.02	106.81	104.30
36	5	2879	C	N3-C4-C5	5.02	123.91	121.90
36	5	3006	A	N7-C8-N9	5.02	116.31	113.80
38	8	110	C	OP2-P-O3'	5.02	116.25	105.20
36	1	1000	C	C5-C4-N4	-5.02	116.69	120.20
36	1	1495	U	N3-C4-C5	-5.02	111.59	114.60
1	6	1542	G	N9-C4-C5	5.02	107.41	105.40
36	5	1223	A	O5'-P-OP1	-5.02	101.18	105.70
36	1	344	A	C5-C6-N6	5.02	127.72	123.70
36	1	586	C	N3-C4-N4	5.02	121.51	118.00
36	1	1146	C	OP1-P-O3'	5.02	116.24	105.20
36	1	1365	G	N3-C4-N9	5.02	129.01	126.00
36	1	2898	G	C5-C6-O6	-5.02	125.59	128.60
36	5	1064	A	C6-C5-N7	-5.02	128.79	132.30
36	5	1364	C	C6-N1-C2	5.02	122.31	120.30
36	5	2825	C	C2-N3-C4	-5.02	117.39	119.90
36	5	3345	G	N3-C2-N2	-5.02	116.39	119.90
36	1	394	G	O5'-P-OP2	-5.02	101.18	105.70
36	1	1906	G	OP1-P-O3'	5.02	116.24	105.20
36	1	2393	G	N1-C6-O6	5.02	122.91	119.90
1	6	362	G	N3-C4-C5	-5.02	126.09	128.60
1	6	1782	A	O5'-P-OP2	5.02	116.72	110.70
36	5	55	G	N3-C2-N2	5.02	123.41	119.90
1	2	795	U	O5'-P-OP1	-5.01	101.19	105.70
36	1	282	G	P-O3'-C3'	5.01	125.72	119.70
36	1	907	G	N3-C2-N2	5.01	123.41	119.90
36	1	1103	A	OP2-P-O3'	5.01	116.23	105.20
36	1	2600	C	N1-C2-O2	5.01	121.91	118.90
36	1	2889	C	N3-C2-O2	-5.01	118.39	121.90
36	5	326	U	N1-C2-O2	-5.01	119.29	122.80
36	5	1344	G	OP2-P-O3'	5.01	116.23	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2896	A	C4-C5-N7	-5.01	108.19	110.70
36	5	2964	G	N9-C1'-C2'	-5.01	106.48	112.00
36	1	1049	C	C4-C5-C6	-5.01	114.89	117.40
36	1	1661	G	N3-C4-N9	5.01	129.01	126.00
1	6	1257	U	N1-C2-O2	5.01	126.31	122.80
36	5	2299	A	N1-C2-N3	-5.01	126.79	129.30
36	1	1140	G	N3-C2-N2	5.01	123.41	119.90
36	1	2642	A	C6-N1-C2	5.01	121.61	118.60
1	6	1293	U	C5-C6-N1	-5.01	120.19	122.70
36	5	1365	G	N3-C2-N2	5.01	123.41	119.90
36	5	1373	A	N7-C8-N9	-5.01	111.29	113.80
36	5	2366	C	C2-N3-C4	5.01	122.41	119.90
36	5	2966	G	C4-C5-N7	5.01	112.80	110.80
36	5	3206	C	N3-C2-O2	-5.01	118.39	121.90
1	2	570	A	N3-C4-N9	5.01	131.41	127.40
1	2	605	A	C8-N9-C4	5.01	107.80	105.80
1	2	1773	C	C5-C6-N1	5.01	123.50	121.00
36	1	1426	C	N1-C2-O2	5.01	121.91	118.90
36	1	2193	U	OP2-P-O3'	5.01	116.22	105.20
36	5	2211	U	N3-C4-C5	-5.01	111.59	114.60
36	5	2732	G	N3-C2-N2	5.01	123.41	119.90
41	14	190	GLY	N-CA-C	5.01	125.62	113.10
1	2	1486	G	C4-N9-C1'	5.01	133.01	126.50
36	1	1140	G	N1-C2-N2	-5.01	111.69	116.20
36	5	1120	A	C5-N7-C8	5.01	106.40	103.90
36	5	3207	U	N1-C2-N3	5.01	117.91	114.90
38	8	6	U	C5-C4-O4	-5.01	122.89	125.90
38	8	77	A	C2-N3-C4	-5.01	108.10	110.60
36	1	1192	C	C6-N1-C2	-5.01	118.30	120.30
36	1	1313	G	N1-C6-O6	5.01	122.90	119.90
36	1	1796	G	C8-N9-C4	-5.01	104.40	106.40
36	1	2960	C	C6-N1-C2	5.01	122.30	120.30
36	1	2993	G	C8-N9-C4	5.01	108.40	106.40
1	6	314	C	C6-N1-C2	-5.01	118.30	120.30
1	6	815	G	N9-C4-C5	-5.01	103.40	105.40
1	6	1200	G	C8-N9-C1'	5.01	133.51	127.00
1	6	1463	C	C6-N1-C2	5.01	122.30	120.30
36	5	248	U	C2-N1-C1'	5.01	123.71	117.70
36	5	296	A	C8-N9-C4	-5.01	103.80	105.80
36	5	867	G	C5-C6-N1	-5.01	109.00	111.50
36	5	945	C	C5-C6-N1	-5.01	118.50	121.00
36	5	1117	G	N7-C8-N9	-5.01	110.60	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1545	A	O5'-P-OP2	-5.01	101.19	105.70
40	l3	184	ASN	C-N-CA	-5.01	111.79	122.30
59	n3	87	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	6	86	A	OP2-P-O3'	5.00	116.21	105.20
1	6	314	C	C5'-C4'-O4'	5.00	115.11	109.10
36	5	658	G	C5-C6-O6	-5.00	125.60	128.60
36	5	3167	A	C8-N9-C4	-5.00	103.80	105.80
36	5	3382	U	N1-C2-O2	5.00	126.30	122.80
36	1	1336	U	OP2-P-O3'	5.00	116.21	105.20
36	1	3078	U	C6-N1-C2	-5.00	118.00	121.00
36	5	1607	U	N3-C4-C5	5.00	117.60	114.60
38	8	21	C	O4'-C1'-N1	5.00	112.20	108.20
38	8	24	G	C8-N9-C4	5.00	108.40	106.40
1	2	1241	G	O4'-C1'-N9	5.00	112.20	108.20
36	1	2215	A	C4-C5-C6	-5.00	114.50	117.00
36	1	3132	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
25	D3	3	LYS	Peptide
27	D5	94	LYS	Peptide
28	D6	84	VAL	Peptide
28	D6	85	ARG	Peptide
28	D6	97	PRO	Peptide
33	E1	137	ASP	Peptide
39	L2	19	HIS	Peptide
41	L4	190	GLY	Peptide
41	L4	318	LEU	Peptide
42	L5	257	GLU	Peptide
44	L7	157	ASN	Peptide
51	M5	182	ASN	Peptide
52	M6	110	PRO	Peptide
52	M6	111	PRO	Peptide
53	M7	8	SER	Peptide
57	N1	16	GLN	Peptide
63	N7	3	LYS	Peptide
65	N9	19	ASN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
67	O1	5	LYS	Peptide
72	O6	2	THR	Peptide
2	S0	188	LEU	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	Peptide
34	SR	160	GLU	Mainchain
34	SR	161	LYS	Mainchain
17	c5	52	LYS	Peptide
22	d0	70	THR	Peptide
25	d3	44	GLY	Peptide
26	d4	29	HIS	Peptide
26	d4	50	ALA	Peptide
31	d9	17	GLY	Peptide
39	l2	143	GLU	Peptide
39	l2	171	GLY	Peptide
40	l3	139	GLN	Peptide
40	l3	185	GLY	Peptide
41	l4	91	GLY	Peptide
42	l5	270	LYS	Peptide
42	l5	271	LYS	Peptide
43	l6	51	ARG	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
52	m6	110	PRO	Peptide
53	m7	66	SER	Peptide
59	n3	41	GLY	Peptide
62	n6	111	LEU	Peptide
63	n7	6	LYS	Peptide
64	n8	66	ALA	Peptide
64	n8	75	LEU	Peptide
65	n9	19	ASN	Peptide
65	n9	23	LYS	Peptide
65	n9	24	PRO	Peptide
67	o1	64	VAL	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	154 (76%)	27 (13%)	23 (11%)	0	1
2	s0	204/251 (81%)	161 (79%)	27 (13%)	16 (8%)	1	2
3	S1	212/254 (84%)	152 (72%)	31 (15%)	29 (14%)	0	0
3	s1	214/254 (84%)	179 (84%)	23 (11%)	12 (6%)	2	5
4	S2	215/253 (85%)	181 (84%)	25 (12%)	9 (4%)	3	9
4	s2	215/253 (85%)	187 (87%)	16 (7%)	12 (6%)	2	5
5	S3	221/239 (92%)	198 (90%)	14 (6%)	9 (4%)	3	9
5	s3	221/239 (92%)	193 (87%)	15 (7%)	13 (6%)	1	4
6	S4	258/260 (99%)	219 (85%)	27 (10%)	12 (5%)	2	7
6	s4	258/260 (99%)	223 (86%)	23 (9%)	12 (5%)	2	7
7	S5	204/224 (91%)	162 (79%)	21 (10%)	21 (10%)	0	1
7	s5	204/224 (91%)	164 (80%)	23 (11%)	17 (8%)	1	2
8	S6	224/236 (95%)	195 (87%)	21 (9%)	8 (4%)	3	11
8	s6	216/236 (92%)	194 (90%)	14 (6%)	8 (4%)	3	11
9	S7	182/189 (96%)	143 (79%)	21 (12%)	18 (10%)	0	1
9	s7	184/189 (97%)	148 (80%)	22 (12%)	14 (8%)	1	2
10	S8	184/200 (92%)	159 (86%)	12 (6%)	13 (7%)	1	2
10	s8	184/200 (92%)	164 (89%)	11 (6%)	9 (5%)	2	7
11	S9	183/196 (93%)	159 (87%)	15 (8%)	9 (5%)	2	7
11	s9	183/196 (93%)	148 (81%)	23 (13%)	12 (7%)	1	3
12	C0	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	1	3
12	c0	92/105 (88%)	63 (68%)	16 (17%)	13 (14%)	0	0
13	C1	153/155 (99%)	125 (82%)	18 (12%)	10 (6%)	1	3
13	c1	144/155 (93%)	117 (81%)	18 (12%)	9 (6%)	1	3
14	C2	122/142 (86%)	70 (57%)	26 (21%)	26 (21%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	71 (58%)	29 (24%)	22 (18%)	0	0
15	C3	148/150 (99%)	132 (89%)	13 (9%)	3 (2%)	7	24
15	c3	148/150 (99%)	123 (83%)	16 (11%)	9 (6%)	1	4
16	C4	125/136 (92%)	97 (78%)	16 (13%)	12 (10%)	0	1
16	c4	126/136 (93%)	101 (80%)	15 (12%)	10 (8%)	1	2
17	C5	122/141 (86%)	95 (78%)	16 (13%)	11 (9%)	1	1
17	c5	133/141 (94%)	97 (73%)	16 (12%)	20 (15%)	0	0
18	C6	139/142 (98%)	121 (87%)	13 (9%)	5 (4%)	3	11
18	c6	140/142 (99%)	121 (86%)	11 (8%)	8 (6%)	1	5
19	C7	116/136 (85%)	87 (75%)	22 (19%)	7 (6%)	1	4
19	c7	113/136 (83%)	96 (85%)	11 (10%)	6 (5%)	2	6
20	C8	143/145 (99%)	121 (85%)	11 (8%)	11 (8%)	1	2
20	c8	143/145 (99%)	115 (80%)	21 (15%)	7 (5%)	2	7
21	C9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	3	12
21	c9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	3	12
22	D0	105/120 (88%)	88 (84%)	15 (14%)	2 (2%)	8	26
22	d0	108/120 (90%)	85 (79%)	15 (14%)	8 (7%)	1	2
23	D1	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	1	2
23	d1	85/87 (98%)	75 (88%)	5 (6%)	5 (6%)	1	4
24	D2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19	49
24	d2	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	19	49
25	D3	142/144 (99%)	117 (82%)	14 (10%)	11 (8%)	1	2
25	d3	142/144 (99%)	131 (92%)	10 (7%)	1 (1%)	22	53
26	D4	132/134 (98%)	110 (83%)	14 (11%)	8 (6%)	1	4
26	d4	132/134 (98%)	106 (80%)	15 (11%)	11 (8%)	1	2
27	D5	68/107 (64%)	51 (75%)	9 (13%)	8 (12%)	0	1
27	d5	67/107 (63%)	48 (72%)	13 (19%)	6 (9%)	1	1
28	D6	95/97 (98%)	69 (73%)	12 (13%)	14 (15%)	0	0
28	d6	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	1	2
29	D7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	1	3
29	d7	79/81 (98%)	60 (76%)	10 (13%)	9 (11%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/66 (92%)	51 (84%)	7 (12%)	3 (5%)	2	7
30	d8	61/66 (92%)	46 (75%)	10 (16%)	5 (8%)	1	2
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	1	4
31	d9	51/55 (93%)	42 (82%)	5 (10%)	4 (8%)	1	2
32	E0	58/60 (97%)	45 (78%)	12 (21%)	1 (2%)	9	29
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
33	e1	74/76 (97%)	38 (51%)	16 (22%)	20 (27%)	0	0
34	SR	316/318 (99%)	274 (87%)	29 (9%)	13 (4%)	3	9
34	sR	316/318 (99%)	268 (85%)	40 (13%)	8 (2%)	5	19
35	SM	155/273 (57%)	109 (70%)	26 (17%)	20 (13%)	0	1
35	sM	98/273 (36%)	61 (62%)	24 (24%)	13 (13%)	0	0
39	L2	250/253 (99%)	226 (90%)	20 (8%)	4 (2%)	9	31
39	l2	250/253 (99%)	214 (86%)	27 (11%)	9 (4%)	3	11
40	L3	384/386 (100%)	340 (88%)	31 (8%)	13 (3%)	3	13
40	l3	384/386 (100%)	350 (91%)	25 (6%)	9 (2%)	6	21
41	L4	359/361 (99%)	315 (88%)	23 (6%)	21 (6%)	1	4
41	l4	359/361 (99%)	308 (86%)	38 (11%)	13 (4%)	3	11
42	L5	294/296 (99%)	253 (86%)	23 (8%)	18 (6%)	1	4
42	l5	292/296 (99%)	262 (90%)	21 (7%)	9 (3%)	4	14
43	L6	152/175 (87%)	141 (93%)	8 (5%)	3 (2%)	7	24
43	l6	153/175 (87%)	132 (86%)	17 (11%)	4 (3%)	5	18
44	L7	220/243 (90%)	205 (93%)	6 (3%)	9 (4%)	3	9
44	l7	221/243 (91%)	203 (92%)	15 (7%)	3 (1%)	11	34
45	L8	231/255 (91%)	193 (84%)	30 (13%)	8 (4%)	3	12
45	l8	229/255 (90%)	184 (80%)	25 (11%)	20 (9%)	1	1
46	L9	189/191 (99%)	170 (90%)	14 (7%)	5 (3%)	5	18
46	l9	189/191 (99%)	173 (92%)	10 (5%)	6 (3%)	4	13
47	M0	207/220 (94%)	185 (89%)	17 (8%)	5 (2%)	6	20
47	m0	209/220 (95%)	181 (87%)	20 (10%)	8 (4%)	3	10
48	M1	167/173 (96%)	133 (80%)	20 (12%)	14 (8%)	1	2
48	m1	167/173 (96%)	146 (87%)	11 (7%)	10 (6%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	164 (86%)	19 (10%)	8 (4%)	3	9
49	m3	192/198 (97%)	164 (85%)	17 (9%)	11 (6%)	1	5
50	M4	134/137 (98%)	118 (88%)	11 (8%)	5 (4%)	3	11
50	m4	135/137 (98%)	127 (94%)	6 (4%)	2 (2%)	10	33
51	M5	201/203 (99%)	188 (94%)	7 (4%)	6 (3%)	4	15
51	m5	201/203 (99%)	180 (90%)	14 (7%)	7 (4%)	3	12
52	M6	195/198 (98%)	185 (95%)	6 (3%)	4 (2%)	7	23
52	m6	195/198 (98%)	185 (95%)	8 (4%)	2 (1%)	15	44
53	M7	181/183 (99%)	159 (88%)	16 (9%)	6 (3%)	4	13
53	m7	153/183 (84%)	140 (92%)	10 (6%)	3 (2%)	7	24
54	M8	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	6	22
54	m8	183/185 (99%)	165 (90%)	11 (6%)	7 (4%)	3	10
55	M9	186/188 (99%)	173 (93%)	12 (6%)	1 (0%)	29	61
55	m9	186/188 (99%)	175 (94%)	8 (4%)	3 (2%)	9	31
56	N0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	13	39
56	n0	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	8	28
57	N1	157/159 (99%)	138 (88%)	14 (9%)	5 (3%)	4	13
57	n1	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	5	19
58	N2	98/120 (82%)	79 (81%)	15 (15%)	4 (4%)	3	9
58	n2	96/120 (80%)	84 (88%)	9 (9%)	3 (3%)	4	14
59	N3	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	22	53
59	n3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	22	53
60	N4	96/155 (62%)	77 (80%)	14 (15%)	5 (5%)	2	6
60	n4	133/155 (86%)	113 (85%)	12 (9%)	8 (6%)	1	4
61	N5	119/141 (84%)	110 (92%)	8 (7%)	1 (1%)	19	49
61	n5	118/141 (84%)	100 (85%)	13 (11%)	5 (4%)	3	9
62	N6	124/126 (98%)	114 (92%)	6 (5%)	4 (3%)	4	13
62	n6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	3	9
63	N7	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	1	2
63	n7	133/135 (98%)	111 (84%)	14 (10%)	8 (6%)	1	4
64	N8	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	2	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	126 (86%)	16 (11%)	4 (3%)	5	17
65	N9	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	3	11
65	n9	56/58 (97%)	43 (77%)	9 (16%)	4 (7%)	1	2
66	O0	95/104 (91%)	87 (92%)	6 (6%)	2 (2%)	7	23
66	o0	98/104 (94%)	89 (91%)	7 (7%)	2 (2%)	7	24
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	7
67	o1	107/112 (96%)	98 (92%)	5 (5%)	4 (4%)	3	11
68	O2	125/129 (97%)	116 (93%)	8 (6%)	1 (1%)	19	49
68	o2	125/129 (97%)	111 (89%)	11 (9%)	3 (2%)	6	20
69	O3	104/106 (98%)	101 (97%)	2 (2%)	1 (1%)	15	44
69	o3	104/106 (98%)	92 (88%)	7 (7%)	5 (5%)	2	7
70	O4	110/119 (92%)	103 (94%)	4 (4%)	3 (3%)	5	17
70	o4	110/119 (92%)	100 (91%)	8 (7%)	2 (2%)	8	28
71	O5	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	3	13
71	o5	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	9	29
72	O6	97/99 (98%)	78 (80%)	11 (11%)	8 (8%)	1	2
72	o6	97/99 (98%)	81 (84%)	9 (9%)	7 (7%)	1	2
73	O7	85/87 (98%)	76 (89%)	6 (7%)	3 (4%)	3	12
73	o7	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	3	12
74	O8	75/77 (97%)	62 (83%)	10 (13%)	3 (4%)	3	9
74	o8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	3	9
75	O9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	7	23
76	Q0	50/52 (96%)	48 (96%)	0	2 (4%)	3	9
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	7	24
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	90 (87%)	10 (10%)	3 (3%)	4	15
78	q2	103/105 (98%)	92 (89%)	8 (8%)	3 (3%)	4	15
79	Q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	6	22
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	14	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	e0	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1	3
82	p0	139/311 (45%)	117 (84%)	19 (14%)	3 (2%)	6	22
All	All	22333/24141 (92%)	19119 (86%)	2092 (9%)	1122 (5%)	2	6

All (1122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	66	ALA
2	S0	103	THR
2	S0	158	VAL
2	S0	163	ASN
2	S0	191	ARG
2	S0	203	PHE
3	S1	49	ASN
3	S1	79	HIS
3	S1	117	TRP
3	S1	132	ASP
3	S1	148	ASN
3	S1	179	SER
3	S1	206	PRO
3	S1	221	PRO
4	S2	148	LEU
5	S3	62	ASN
5	S3	64	ARG
5	S3	65	ARG
5	S3	93	ASP
5	S3	216	PRO
5	S3	220	PRO
6	S4	104	ASP
6	S4	164	LEU
6	S4	195	ILE
6	S4	223	ASN
7	S5	26	ALA
7	S5	35	GLN
7	S5	39	GLU
7	S5	43	PHE
7	S5	58	LEU
7	S5	60	ASP
7	S5	63	GLN
7	S5	101	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	S6	122	GLU
8	S6	173	PRO
9	S7	32	PRO
9	S7	64	VAL
9	S7	111	LYS
9	S7	112	ARG
9	S7	116	ARG
9	S7	131	PHE
9	S7	133	THR
9	S7	134	GLU
9	S7	155	ASP
10	S8	22	ARG
10	S8	152	ILE
10	S8	153	GLU
11	S9	98	ALA
11	S9	121	SER
11	S9	134	ILE
11	S9	150	LEU
12	C0	60	SER
12	C0	87	VAL
12	C0	88	PRO
13	C1	7	VAL
13	C1	29	LYS
14	C2	25	GLU
14	C2	93	ASP
14	C2	101	ALA
14	C2	119	SER
14	C2	127	GLY
15	C3	22	ALA
16	C4	50	ALA
16	C4	124	ASP
16	C4	125	SER
16	C4	126	THR
17	C5	54	ALA
17	C5	125	PRO
17	C5	130	ARG
18	C6	39	VAL
18	C6	58	ASP
18	C6	97	VAL
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	C7	124	VAL
20	C8	14	ILE
20	C8	61	LEU
20	C8	83	ALA
20	C8	91	ASP
20	C8	92	ILE
21	C9	53	TRP
22	D0	17	GLN
24	D2	83	ILE
25	D3	3	LYS
25	D3	92	CYS
25	D3	109	ARG
25	D3	144	ARG
26	D4	6	THR
27	D5	39	ALA
27	D5	43	ASP
27	D5	44	GLN
27	D5	71	ILE
28	D6	45	VAL
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
29	D7	62	ILE
31	D9	8	PHE
32	E0	47	VAL
33	E1	102	VAL
33	E1	103	LEU
33	E1	106	TYR
33	E1	128	ALA
33	E1	138	ARG
34	SR	160	GLU
35	SM	52	PRO
35	SM	86	ASN
35	SM	87	THR
35	SM	102	THR
35	SM	140	ASP
35	SM	166	VAL
35	SM	167	PRO
40	L3	3	HIS
40	L3	4	ARG
40	L3	5	LYS
40	L3	139	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	L3	140	ASP
40	L3	174	LYS
40	L3	186	GLY
41	L4	4	PRO
41	L4	292	SER
41	L4	293	SER
41	L4	311	HIS
41	L4	317	PRO
41	L4	320	ASN
42	L5	57	ASN
42	L5	233	ALA
42	L5	234	ASP
42	L5	258	LYS
43	L6	6	ALA
43	L6	98	VAL
44	L7	26	VAL
44	L7	160	ARG
45	L8	25	PRO
45	L8	39	ALA
46	L9	190	ASP
47	M0	189	GLU
47	M0	219	ALA
48	M1	8	PRO
48	M1	9	MET
48	M1	11	ASP
48	M1	94	ARG
48	M1	115	LYS
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
49	M3	134	GLU
50	M4	8	LYS
50	M4	9	ALA
51	M5	74	PRO
51	M5	144	ARG
52	M6	16	VAL
52	M6	111	PRO
53	M7	157	VAL
53	M7	182	ILE
54	M8	98	LYS
54	M8	99	THR
56	N0	2	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	N0	167	ARG
57	N1	124	VAL
57	N1	159	PHE
58	N2	31	ALA
60	N4	80	ARG
60	N4	81	PRO
60	N4	97	LYS
62	N6	52	ARG
62	N6	53	ASP
62	N6	84	LYS
63	N7	35	SER
64	N8	29	PRO
64	N8	76	ASP
64	N8	96	LYS
67	O1	5	LYS
67	O1	6	ASP
67	O1	84	ASP
68	O2	127	ALA
71	O5	119	LYS
72	O6	33	ALA
72	O6	34	SER
74	O8	33	LYS
76	Q0	78	ILE
78	Q2	15	LYS
78	Q2	100	LYS
2	s0	4	PRO
2	s0	44	GLY
2	s0	103	THR
2	s0	158	VAL
2	s0	164	ASN
2	s0	186	GLY
2	s0	189	VAL
2	s0	206	ASP
3	s1	62	LYS
3	s1	63	GLY
3	s1	81	PHE
3	s1	82	ARG
3	s1	147	ALA
3	s1	206	PRO
3	s1	223	PHE
4	s2	91	ARG
4	s2	92	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	s2	163	GLY
5	s3	61	GLU
5	s3	90	ARG
5	s3	115	ILE
5	s3	216	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	104	ASP
6	s4	163	ASP
6	s4	164	LEU
7	s5	184	PHE
8	s6	153	VAL
8	s6	154	ARG
8	s6	173	PRO
8	s6	174	LYS
9	s7	10	SER
9	s7	64	VAL
9	s7	66	SER
9	s7	74	GLN
9	s7	116	ARG
9	s7	131	PHE
9	s7	163	ASP
9	s7	185	ILE
10	s8	115	ALA
10	s8	116	HIS
12	c0	32	HIS
12	c0	82	LEU
12	c0	83	PRO
12	c0	88	PRO
12	c0	92	ILE
12	c0	97	PRO
13	c1	114	ALA
13	c1	133	LYS
13	c1	144	ALA
14	c2	22	VAL
14	c2	89	ILE
15	c3	19	SER
15	c3	66	ILE
15	c3	87	ASP
15	c3	137	PRO
15	c3	139	TRP
16	c4	35	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	c4	126	THR
16	c4	132	ARG
17	c5	11	VAL
17	c5	51	SER
17	c5	52	LYS
17	c5	125	PRO
17	c5	126	VAL
17	c5	127	ARG
18	c6	42	GLU
18	c6	116	LEU
19	c7	67	ARG
19	c7	88	VAL
19	c7	99	VAL
19	c7	116	LYS
20	c8	92	ILE
20	c8	145	ARG
21	c9	28	LEU
21	c9	29	GLU
21	c9	33	TYR
22	d0	15	GLN
22	d0	49	ASN
22	d0	52	LYS
26	d4	30	PRO
26	d4	78	SER
27	d5	85	LYS
27	d5	104	ALA
29	d7	38	PRO
29	d7	60	SER
29	d7	62	ILE
29	d7	63	LEU
30	d8	33	LEU
30	d8	61	ARG
31	d9	6	VAL
80	e0	47	VAL
80	e0	60	PRO
33	e1	83	LYS
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	103	LEU
33	e1	106	TYR
34	sR	4	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	sR	163	ASP
34	sR	165	ASP
34	sR	250	TYR
35	sM	47	ALA
35	sM	50	ASN
35	sM	64	LYS
35	sM	65	THR
39	l2	15	ILE
40	l3	3	HIS
40	l3	139	GLN
40	l3	293	ASN
40	l3	347	SER
41	l4	90	PHE
41	l4	272	VAL
41	l4	311	HIS
41	l4	329	PRO
41	l4	339	LEU
42	l5	260	PHE
43	l6	98	VAL
45	l8	25	PRO
45	l8	34	PHE
45	l8	117	ALA
45	l8	122	LYS
46	l9	144	ILE
46	l9	188	THR
47	m0	220	GLN
48	m1	8	PRO
48	m1	10	ARG
48	m1	94	ARG
49	m3	47	ALA
49	m3	51	LEU
49	m3	134	GLU
51	m5	48	ALA
51	m5	49	ARG
51	m5	76	PRO
52	m6	16	VAL
52	m6	110	PRO
53	m7	67	ILE
54	m8	98	LYS
54	m8	99	THR
56	n0	2	ALA
57	n1	122	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	n1	136	ARG
60	n4	76	VAL
61	n5	24	LEU
61	n5	25	LYS
61	n5	44	PRO
61	n5	45	LYS
62	n6	83	ASP
62	n6	84	LYS
62	n6	126	LEU
63	n7	5	LEU
63	n7	7	ALA
63	n7	125	GLY
64	n8	76	ASP
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
66	o0	100	ILE
67	o1	83	GLU
67	o1	86	LYS
69	o3	88	ASN
71	o5	119	LYS
72	o6	33	ALA
72	o6	63	ASN
72	o6	98	ARG
73	o7	85	LYS
74	o8	18	ALA
82	p0	93	LEU
2	S0	5	ALA
2	S0	27	ARG
2	S0	30	GLN
2	S0	94	GLY
2	S0	95	ALA
2	S0	139	VAL
2	S0	185	ARG
2	S0	189	VAL
2	S0	192	THR
2	S0	194	PRO
2	S0	195	TRP
3	S1	35	PRO
3	S1	51	SER
3	S1	63	GLY
3	S1	93	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	S1	116	LYS
3	S1	213	ARG
3	S1	223	PHE
4	S2	145	GLY
5	S3	218	LEU
6	S4	12	LEU
6	S4	26	CYS
6	S4	222	LEU
7	S5	156	ARG
7	S5	204	GLY
7	S5	206	SER
8	S6	154	ARG
8	S6	174	LYS
9	S7	30	SER
9	S7	31	SER
9	S7	73	VAL
9	S7	85	PHE
9	S7	98	ILE
9	S7	156	SER
10	S8	59	ARG
10	S8	105	ASP
10	S8	120	THR
11	S9	169	PRO
12	C0	86	ILE
13	C1	4	GLU
13	C1	145	ALA
13	C1	154	ALA
14	C2	55	GLY
14	C2	91	VAL
14	C2	115	VAL
14	C2	125	ASN
14	C2	130	THR
15	C3	12	SER
16	C4	42	VAL
16	C4	51	ASP
16	C4	123	SER
17	C5	48	GLY
17	C5	101	ALA
18	C6	113	ASP
20	C8	7	GLU
20	C8	8	GLN
20	C8	82	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	C8	139	LYS
21	C9	69	LYS
23	D1	49	GLU
25	D3	8	GLY
25	D3	41	SER
25	D3	114	LYS
25	D3	131	SER
26	D4	4	ALA
26	D4	36	SER
26	D4	60	PHE
28	D6	18	VAL
28	D6	63	ALA
28	D6	86	VAL
28	D6	97	PRO
29	D7	60	SER
29	D7	75	GLU
30	D8	36	THR
33	E1	84	VAL
33	E1	85	TYR
33	E1	98	VAL
33	E1	127	GLY
34	SR	98	GLU
34	SR	318	ALA
35	SM	82	THR
35	SM	88	ARG
35	SM	139	GLU
39	L2	250	GLN
39	L2	251	LYS
40	L3	351	LEU
41	L4	15	ALA
41	L4	190	GLY
41	L4	232	SER
41	L4	270	SER
41	L4	318	LEU
41	L4	339	LEU
42	L5	6	ASP
42	L5	137	ASP
42	L5	187	THR
42	L5	253	PHE
42	L5	260	PHE
42	L5	295	GLY
44	L7	24	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	L7	164	SER
44	L7	175	LYS
45	L8	157	VAL
47	M0	24	ARG
47	M0	194	GLY
48	M1	24	GLY
48	M1	167	TYR
51	M5	184	LYS
52	M6	182	ASN
53	M7	67	ILE
53	M7	160	ALA
53	M7	161	ALA
58	N2	11	ILE
59	N3	82	ALA
60	N4	64	THR
62	N6	126	LEU
63	N7	17	ARG
63	N7	18	TYR
64	N8	47	LYS
64	N8	66	ALA
67	O1	83	GLU
70	O4	77	GLY
70	O4	82	ALA
71	O5	90	ARG
71	O5	91	ALA
72	O6	28	TYR
73	O7	79	GLN
78	Q2	94	GLY
79	Q3	51	ALA
2	s0	30	GLN
2	s0	94	GLY
2	s0	95	ALA
2	s0	185	ARG
3	s1	93	GLY
4	s2	107	SER
4	s2	164	SER
4	s2	228	ASN
6	s4	12	LEU
6	s4	24	SER
6	s4	195	ILE
6	s4	196	VAL
7	s5	28	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	s5	36	ALA
7	s5	43	PHE
7	s5	54	LYS
7	s5	151	GLY
8	s6	68	LEU
8	s6	122	GLU
10	s8	62	THR
10	s8	101	ILE
11	s9	110	GLN
11	s9	134	ILE
11	s9	183	ALA
12	c0	23	ALA
12	c0	31	LYS
12	c0	35	ILE
13	c1	55	ASP
14	c2	58	LEU
14	c2	101	ALA
14	c2	119	SER
14	c2	131	ASP
15	c3	140	LYS
16	c4	50	ALA
16	c4	51	ASP
16	c4	124	ASP
16	c4	131	GLY
17	c5	17	TYR
17	c5	132	GLY
19	c7	113	LEU
20	c8	61	LEU
20	c8	135	GLY
22	d0	17	GLN
23	d1	4	ASP
23	d1	77	GLY
25	d3	131	SER
26	d4	33	ALA
26	d4	35	VAL
26	d4	53	ASP
27	d5	38	HIS
27	d5	83	LEU
28	d6	62	TYR
29	d7	20	LYS
29	d7	50	ALA
29	d7	75	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	d9	7	TRP
31	d9	19	ARG
80	e0	61	SER
33	e1	84	VAL
33	e1	97	LYS
33	e1	102	VAL
33	e1	127	GLY
39	l2	215	ASN
39	l2	238	ILE
39	l2	249	SER
40	l3	138	ALA
41	l4	302	ALA
42	l5	135	VAL
42	l5	258	LYS
42	l5	270	LYS
43	l6	97	ASN
45	l8	39	ALA
45	l8	79	GLN
45	l8	114	ALA
45	l8	121	SER
45	l8	188	THR
45	l8	190	VAL
45	l8	203	VAL
47	m0	204	GLY
47	m0	207	GLU
48	m1	7	ASN
49	m3	129	ASN
49	m3	141	ALA
50	m4	3	THR
50	m4	135	LEU
51	m5	183	THR
51	m5	184	LYS
54	m8	41	ASP
54	m8	167	SER
54	m8	171	LYS
55	m9	35	ALA
55	m9	155	LEU
55	m9	156	ASN
56	n0	50	LYS
57	n1	127	GLN
58	n2	51	GLY
60	n4	63	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
60	n4	71	ARG
60	n4	77	LYS
62	n6	92	GLY
62	n6	125	LYS
63	n7	16	GLY
64	n8	47	LYS
64	n8	129	PHE
67	o1	84	ASP
68	o2	124	GLY
70	o4	77	GLY
72	o6	12	ASN
72	o6	64	SER
74	o8	15	THR
82	p0	47	GLY
3	S1	26	ARG
3	S1	58	SER
3	S1	78	ASP
3	S1	147	ALA
4	S2	79	GLU
4	S2	91	ARG
4	S2	107	SER
4	S2	235	LEU
4	S2	248	SER
6	S4	77	ARG
6	S4	245	LYS
7	S5	127	GLN
7	S5	150	GLY
8	S6	70	PRO
8	S6	152	ASP
9	S7	84	LYS
10	S8	9	HIS
10	S8	40	ALA
10	S8	149	SER
10	S8	199	LYS
11	S9	118	LEU
11	S9	164	PHE
12	C0	94	GLU
13	C1	3	THR
13	C1	55	ASP
13	C1	153	PHE
14	C2	21	GLU
14	C2	22	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	C2	39	ASP
16	C4	40	ALA
16	C4	75	GLY
17	C5	51	SER
17	C5	69	GLU
17	C5	126	VAL
19	C7	120	SER
20	C8	60	GLU
25	D3	112	LYS
26	D4	34	ASN
26	D4	58	PHE
26	D4	133	ASN
28	D6	10	ARG
28	D6	62	TYR
28	D6	65	PRO
29	D7	38	PRO
33	E1	83	LYS
33	E1	86	THR
33	E1	87	THR
33	E1	118	ARG
34	SR	50	ASP
34	SR	161	LYS
34	SR	228	LYS
35	SM	53	ARG
35	SM	89	ARG
35	SM	153	ASP
35	SM	174	LEU
40	L3	155	ALA
40	L3	300	ARG
41	L4	5	GLN
41	L4	16	THR
42	L5	58	LYS
42	L5	188	GLU
42	L5	252	ALA
42	L5	259	LYS
44	L7	25	GLN
44	L7	212	GLY
45	L8	117	ALA
45	L8	255	SER
46	L9	2	LYS
47	M0	211	ARG
48	M1	7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	M3	76	THR
49	M3	130	GLY
49	M3	131	LYS
50	M4	28	SER
50	M4	136	ALA
53	M7	164	LYS
54	M8	183	GLY
57	N1	125	ALA
58	N2	91	ASP
63	N7	33	SER
63	N7	78	ASN
65	N9	57	ALA
72	O6	3	VAL
72	O6	21	THR
72	O6	95	ALA
72	O6	98	ARG
73	O7	85	LYS
2	s0	68	PRO
2	s0	102	PHE
3	s1	26	ARG
3	s1	154	SER
4	s2	238	SER
5	s3	93	ASP
6	s4	57	ASN
6	s4	245	LYS
7	s5	100	ASN
7	s5	127	GLN
7	s5	153	GLY
10	s8	199	LYS
11	s9	5	PRO
11	s9	105	LEU
11	s9	147	MET
12	c0	30	ALA
13	c1	61	THR
13	c1	132	SER
13	c1	146	ALA
14	c2	26	ASP
14	c2	59	LEU
14	c2	87	PRO
14	c2	103	LEU
14	c2	106	ILE
14	c2	107	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	c2	108	ARG
14	c2	118	ALA
16	c4	12	GLN
16	c4	92	LYS
17	c5	8	LYS
17	c5	49	MET
17	c5	68	PRO
17	c5	80	MET
17	c5	128	HIS
17	c5	129	GLY
18	c6	39	VAL
18	c6	97	VAL
18	c6	142	TYR
19	c7	120	SER
20	c8	91	ASP
23	d1	44	ARG
23	d1	78	LEU
24	d2	68	ARG
26	d4	51	GLU
26	d4	58	PHE
28	d6	46	GLU
28	d6	63	ALA
29	d7	3	LEU
30	d8	62	GLU
80	e0	54	ARG
33	e1	81	LYS
33	e1	110	ALA
33	e1	128	ALA
33	e1	148	TYR
34	sR	146	GLY
34	sR	161	LYS
35	sM	48	ARG
35	sM	66	ALA
35	sM	78	ASP
35	sM	167	PRO
39	l2	96	LEU
39	l2	142	ASP
41	l4	145	ILE
43	l6	32	ALA
45	l8	26	LEU
45	l8	120	LYS
45	l8	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	l8	124	ASP
45	l8	133	LYS
45	l8	237	ILE
46	l9	107	ASP
47	m0	3	ARG
47	m0	195	ALA
47	m0	219	ALA
48	m1	95	ASN
48	m1	173	ASP
49	m3	19	GLN
49	m3	135	ALA
53	m7	66	SER
54	m8	91	ALA
56	n0	138	GLN
57	n1	135	PRO
60	n4	83	THR
60	n4	127	LYS
61	n5	47	ALA
63	n7	127	ASN
64	n8	78	LEU
68	o2	6	HIS
69	o3	91	ALA
69	o3	92	LYS
70	o4	82	ALA
71	o5	40	SER
72	o6	34	SER
73	o7	86	ALA
74	o8	17	ARG
75	o9	3	ALA
76	q0	78	ILE
2	S0	4	PRO
2	S0	36	TYR
3	S1	54	LEU
3	S1	55	LYS
3	S1	82	ARG
3	S1	158	SER
3	S1	209	ASN
4	S2	150	GLN
5	S3	217	ILE
6	S4	157	ASN
6	S4	193	GLY
7	S5	21	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	S5	45	LYS
7	S5	64	VAL
7	S5	79	ASN
7	S5	154	ALA
8	S6	165	GLY
10	S8	10	LYS
10	S8	52	ASN
12	C0	34	GLU
14	C2	89	ILE
14	C2	106	ILE
14	C2	107	ASP
14	C2	108	ARG
14	C2	112	ALA
14	C2	131	ASP
15	C3	106	ARG
16	C4	18	ARG
16	C4	86	THR
16	C4	114	ARG
17	C5	24	LYS
17	C5	52	LYS
18	C6	41	PRO
21	C9	29	GLU
21	C9	130	ARG
23	D1	10	GLU
23	D1	28	ASP
23	D1	81	ASN
25	D3	40	SER
26	D4	5	VAL
27	D5	41	ILE
28	D6	36	ILE
28	D6	64	LEU
29	D7	63	LEU
30	D8	61	ARG
31	D9	34	TYR
33	E1	94	LYS
33	E1	100	LEU
33	E1	137	ASP
33	E1	148	TYR
34	SR	51	ASP
34	SR	117	LYS
34	SR	163	ASP
34	SR	237	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	SM	97	THR
35	SM	172	VAL
35	SM	173	GLU
40	L3	385	LYS
41	L4	182	LEU
41	L4	233	LEU
42	L5	7	ALA
42	L5	115	LEU
42	L5	125	VAL
43	L6	5	LYS
45	L8	120	LYS
46	L9	66	ALA
46	L9	189	GLU
48	M1	64	LYS
48	M1	114	ILE
49	M3	136	GLU
51	M5	75	VAL
54	M8	162	ALA
55	M9	53	LYS
60	N4	76	VAL
64	N8	94	ALA
73	O7	86	ALA
4	s2	235	LEU
6	s4	90	ILE
7	s5	29	ILE
7	s5	39	GLU
7	s5	60	ASP
7	s5	125	THR
9	s7	11	GLN
9	s7	133	THR
10	s8	52	ASN
11	s9	3	ARG
11	s9	65	LYS
11	s9	168	ARG
14	c2	54	ARG
14	c2	115	VAL
15	c3	29	SER
15	c3	60	VAL
16	c4	114	ARG
17	c5	14	THR
17	c5	69	GLU
17	c5	130	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	c6	115	THR
20	c8	60	GLU
22	d0	51	VAL
22	d0	118	VAL
23	d1	21	ASN
27	d5	53	GLU
28	d6	11	ASN
28	d6	59	TYR
29	d7	59	CYS
33	e1	100	LEU
33	e1	131	PHE
33	e1	144	CYS
34	sR	149	ASP
34	sR	317	THR
35	sM	63	ASP
35	sM	120	GLU
39	l2	24	GLN
39	l2	56	ALA
40	l3	155	ALA
40	l3	333	LYS
41	l4	305	ALA
41	l4	330	TYR
42	l5	44	TYR
42	l5	158	ARG
43	l6	10	TYR
44	l7	191	VAL
45	l8	240	ASN
46	l9	62	ARG
46	l9	167	VAL
48	m1	117	ASP
48	m1	167	TYR
49	m3	93	ILE
49	m3	101	ARG
53	m7	75	GLU
58	n2	49	ASN
58	n2	50	LEU
59	n3	46	LEU
60	n4	72	SER
60	n4	132	GLY
63	n7	103	GLN
68	o2	5	PRO
73	o7	84	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	q2	32	LYS
2	S0	81	PHE
2	S0	164	ASN
2	S0	205	ARG
3	S1	81	PHE
5	S3	196	ARG
7	S5	51	VAL
7	S5	65	ARG
11	S9	99	LEU
11	S9	163	PRO
14	C2	66	VAL
14	C2	87	PRO
14	C2	129	GLU
17	C5	22	LEU
19	C7	115	LEU
20	C8	144	ARG
22	D0	21	LYS
23	D1	12	TYR
27	D5	38	HIS
27	D5	42	LEU
33	E1	93	HIS
35	SM	12	VAL
35	SM	64	LYS
39	L2	143	GLU
40	L3	317	ILE
41	L4	14	GLU
41	L4	130	ALA
44	L7	158	LYS
45	L8	36	ILE
45	L8	78	PHE
48	M1	151	SER
49	M3	153	ASP
50	M4	6	ILE
57	N1	18	ASP
57	N1	123	GLY
58	N2	10	LYS
61	N5	50	ALA
63	N7	36	HIS
63	N7	102	GLU
63	N7	103	GLN
64	N8	117	ARG
66	O0	71	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	O1	7	VAL
69	O3	59	VAL
70	O4	3	GLN
71	O5	75	TYR
76	Q0	79	GLU
79	Q3	7	LYS
2	s0	10	THR
4	s2	106	ASP
4	s2	150	GLN
5	s3	145	ALA
5	s3	179	GLN
5	s3	196	ARG
5	s3	219	ALA
7	s5	71	ALA
9	s7	67	LEU
10	s8	136	SER
10	s8	148	ALA
11	s9	91	LYS
11	s9	146	PHE
12	c0	24	LYS
12	c0	95	ARG
13	c1	129	ARG
14	c2	82	PRO
14	c2	92	ALA
15	c3	22	ALA
17	c5	6	ASN
17	c5	131	ALA
18	c6	40	GLU
26	d4	34	ASN
26	d4	50	ALA
28	d6	8	ASN
28	d6	35	ALA
28	d6	60	PRO
30	d8	64	ARG
31	d9	11	PRO
35	sM	43	ASP
35	sM	83	LYS
39	l2	247	ARG
40	l3	37	ARG
40	l3	187	SER
41	l4	5	GLN
41	l4	146	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	l4	233	LEU
42	l5	125	VAL
42	l5	216	GLU
44	l7	229	PHE
45	l8	81	THR
45	l8	115	ALA
47	m0	193	ASP
48	m1	114	ILE
48	m1	115	LYS
49	m3	50	PRO
49	m3	76	THR
51	m5	68	ARG
51	m5	81	TYR
63	n7	28	PRO
63	n7	134	LEU
65	n9	25	LYS
78	q2	33	ALA
82	p0	33	VAL
3	S1	210	ILE
4	S2	106	ASP
6	S4	233	LYS
8	S6	146	GLY
9	S7	36	ALA
10	S8	147	ALA
13	C1	5	LEU
13	C1	6	THR
14	C2	126	TRP
19	C7	24	LEU
21	C9	35	ASP
27	D5	88	ILE
28	D6	59	TYR
30	D8	34	GLU
33	E1	111	GLU
34	SR	105	GLY
39	L2	13	GLY
40	L3	299	ASP
42	L5	221	GLU
44	L7	178	ILE
48	M1	117	ASP
48	M1	138	VAL
51	M5	94	TYR
63	N7	125	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
64	N8	97	GLU
65	N9	21	ILE
72	O6	78	GLY
74	O8	35	GLY
2	s0	139	VAL
3	s1	21	VAL
3	s1	22	ASP
5	s3	180	GLY
6	s4	30	ARG
6	s4	168	LYS
7	s5	21	THR
7	s5	59	VAL
10	s8	78	ILE
11	s9	126	ARG
12	c0	3	MET
14	c2	25	GLU
14	c2	66	VAL
21	c9	66	TYR
26	d4	52	LYS
27	d5	87	GLY
30	d8	32	PHE
33	e1	145	HIS
41	l4	328	ASN
42	l5	215	ASP
69	o3	59	VAL
72	o6	3	VAL
78	q2	31	GLY
79	q3	51	ALA
9	S7	13	PRO
14	C2	117	GLY
34	SR	15	GLY
34	SR	188	ILE
63	N7	16	GLY
4	s2	93	GLY
7	s5	33	VAL
9	s7	13	PRO
22	d0	96	PRO
26	d4	129	VAL
33	e1	124	PRO
47	m0	117	GLY
66	o0	10	ILE
14	C2	40	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	L4	328	ASN
4	s2	83	ILE
8	s6	69	LEU
8	s6	70	PRO
9	s7	32	PRO
13	c1	7	VAL
69	o3	61	GLY
3	S1	48	VAL
7	S5	153	GLY
14	C2	81	ASP
23	D1	6	GLY
41	L4	131	VAL
41	L4	146	PRO
46	L9	13	PRO
66	O0	100	ILE
74	O8	37	PRO
9	s7	73	VAL
18	c6	4	VAL
20	c8	14	ILE
21	c9	3	GLY
22	d0	97	VAL
33	e1	112	GLY
44	l7	178	ILE
3	S1	21	VAL
25	D3	108	GLY
31	D9	6	VAL
35	SM	17	VAL
51	M5	89	VAL
52	M6	110	PRO
5	s3	203	PRO
14	c2	91	VAL
14	c2	121	VAL
17	c5	48	GLY
35	sM	172	VAL
67	o1	45	GLY
3	S1	22	ASP
46	l9	187	ILE
54	m8	84	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	134 (82%)	30 (18%)	1	5
2	s0	165/209 (79%)	131 (79%)	34 (21%)	1	3
3	S1	191/223 (86%)	162 (85%)	29 (15%)	3	8
3	s1	192/223 (86%)	162 (84%)	30 (16%)	2	8
4	S2	176/204 (86%)	137 (78%)	39 (22%)	1	2
4	s2	176/204 (86%)	139 (79%)	37 (21%)	1	3
5	S3	182/194 (94%)	149 (82%)	33 (18%)	1	5
5	s3	182/194 (94%)	149 (82%)	33 (18%)	1	5
6	S4	221/221 (100%)	182 (82%)	39 (18%)	2	5
6	s4	221/221 (100%)	187 (85%)	34 (15%)	2	8
7	S5	173/190 (91%)	140 (81%)	33 (19%)	1	4
7	s5	173/190 (91%)	138 (80%)	35 (20%)	1	4
8	S6	188/201 (94%)	155 (82%)	33 (18%)	2	5
8	s6	187/201 (93%)	152 (81%)	35 (19%)	1	5
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3	8
9	s7	165/169 (98%)	134 (81%)	31 (19%)	1	5
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	9
10	s8	150/161 (93%)	129 (86%)	21 (14%)	3	11
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	2
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	4
12	C0	77/98 (79%)	58 (75%)	19 (25%)	0	2
12	c0	73/98 (74%)	61 (84%)	12 (16%)	2	7
13	C1	129/136 (95%)	104 (81%)	25 (19%)	1	4
13	c1	129/136 (95%)	107 (83%)	22 (17%)	2	6
14	C2	88/118 (75%)	68 (77%)	20 (23%)	1	2
14	c2	88/118 (75%)	65 (74%)	23 (26%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	3
15	c3	127/127 (100%)	105 (83%)	22 (17%)	2	6
16	C4	81/104 (78%)	61 (75%)	20 (25%)	0	2
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	2
17	C5	101/117 (86%)	86 (85%)	15 (15%)	3	9
17	c5	103/117 (88%)	83 (81%)	20 (19%)	1	4
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	4
18	c6	118/118 (100%)	98 (83%)	20 (17%)	2	6
19	C7	94/124 (76%)	70 (74%)	24 (26%)	0	1
19	c7	92/124 (74%)	76 (83%)	16 (17%)	2	6
20	C8	128/128 (100%)	102 (80%)	26 (20%)	1	4
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	3
21	C9	115/115 (100%)	93 (81%)	22 (19%)	1	4
21	c9	115/115 (100%)	95 (83%)	20 (17%)	2	6
22	D0	100/113 (88%)	74 (74%)	26 (26%)	0	1
22	d0	103/113 (91%)	80 (78%)	23 (22%)	1	2
23	D1	74/74 (100%)	60 (81%)	14 (19%)	1	5
23	d1	74/74 (100%)	57 (77%)	17 (23%)	1	2
24	D2	110/110 (100%)	94 (86%)	16 (14%)	3	9
24	d2	110/110 (100%)	96 (87%)	14 (13%)	4	14
25	D3	119/119 (100%)	97 (82%)	22 (18%)	1	5
25	d3	119/119 (100%)	104 (87%)	15 (13%)	4	14
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	6
26	d4	112/112 (100%)	99 (88%)	13 (12%)	5	17
27	D5	61/88 (69%)	43 (70%)	18 (30%)	0	1
27	d5	61/88 (69%)	54 (88%)	7 (12%)	5	17
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	3
28	d6	83/83 (100%)	69 (83%)	14 (17%)	2	6
29	D7	70/70 (100%)	57 (81%)	13 (19%)	1	5
29	d7	70/70 (100%)	59 (84%)	11 (16%)	2	8
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d8	56/59 (95%)	48 (86%)	8 (14%)	3	10
31	D9	47/48 (98%)	38 (81%)	9 (19%)	1	4
31	d9	47/48 (98%)	39 (83%)	8 (17%)	2	6
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1	4
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0	2
33	e1	66/66 (100%)	48 (73%)	18 (27%)	0	1
34	SR	260/261 (100%)	237 (91%)	23 (9%)	10	29
34	sR	260/261 (100%)	232 (89%)	28 (11%)	6	19
35	SM	97/228 (42%)	79 (81%)	18 (19%)	1	5
35	sM	54/228 (24%)	47 (87%)	7 (13%)	4	13
39	L2	193/195 (99%)	157 (81%)	36 (19%)	1	5
39	l2	192/195 (98%)	155 (81%)	37 (19%)	1	4
40	L3	321/322 (100%)	258 (80%)	63 (20%)	1	4
40	l3	320/322 (99%)	255 (80%)	65 (20%)	1	4
41	L4	288/288 (100%)	239 (83%)	49 (17%)	2	6
41	l4	288/288 (100%)	235 (82%)	53 (18%)	1	5
42	L5	244/244 (100%)	194 (80%)	50 (20%)	1	3
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	3
43	L6	134/152 (88%)	115 (86%)	19 (14%)	3	10
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	5
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	13
44	l7	187/204 (92%)	159 (85%)	28 (15%)	3	9
45	L8	187/207 (90%)	154 (82%)	33 (18%)	2	5
45	l8	177/207 (86%)	143 (81%)	34 (19%)	1	4
46	L9	171/171 (100%)	139 (81%)	32 (19%)	1	5
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	4
47	M0	177/186 (95%)	144 (81%)	33 (19%)	1	5
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	3
48	M1	147/150 (98%)	119 (81%)	28 (19%)	1	4
48	m1	147/150 (98%)	125 (85%)	22 (15%)	3	9
49	M3	154/158 (98%)	126 (82%)	28 (18%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	m3	154/158 (98%)	130 (84%)	24 (16%)	2	8
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1	4
50	m4	108/108 (100%)	90 (83%)	18 (17%)	2	6
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2	7
51	m5	175/175 (100%)	148 (85%)	27 (15%)	2	8
52	M6	160/161 (99%)	137 (86%)	23 (14%)	3	10
52	m6	160/161 (99%)	132 (82%)	28 (18%)	2	6
53	M7	140/145 (97%)	113 (81%)	27 (19%)	1	4
53	m7	125/145 (86%)	108 (86%)	17 (14%)	3	11
54	M8	150/150 (100%)	125 (83%)	25 (17%)	2	6
54	m8	150/150 (100%)	122 (81%)	28 (19%)	1	5
55	M9	153/153 (100%)	133 (87%)	20 (13%)	4	12
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	2
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	5
56	n0	156/156 (100%)	132 (85%)	24 (15%)	2	8
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	3
57	n1	136/136 (100%)	116 (85%)	20 (15%)	3	9
58	N2	87/106 (82%)	76 (87%)	11 (13%)	4	14
58	n2	85/106 (80%)	73 (86%)	12 (14%)	3	10
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	11
59	n3	104/104 (100%)	95 (91%)	9 (9%)	10	30
60	N4	57/129 (44%)	52 (91%)	5 (9%)	10	29
60	n4	100/129 (78%)	88 (88%)	12 (12%)	5	15
61	N5	104/117 (89%)	79 (76%)	25 (24%)	0	2
61	n5	104/117 (89%)	80 (77%)	24 (23%)	1	2
62	N6	109/109 (100%)	88 (81%)	21 (19%)	1	4
62	n6	109/109 (100%)	84 (77%)	25 (23%)	1	2
63	N7	115/115 (100%)	91 (79%)	24 (21%)	1	3
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1	4
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	5
64	n8	118/118 (100%)	95 (80%)	23 (20%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	6
65	n9	46/46 (100%)	35 (76%)	11 (24%)	0	2
66	O0	81/87 (93%)	66 (82%)	15 (18%)	1	5
66	o0	84/87 (97%)	68 (81%)	16 (19%)	1	4
67	O1	92/96 (96%)	72 (78%)	20 (22%)	1	3
67	o1	94/96 (98%)	77 (82%)	17 (18%)	1	5
68	O2	109/110 (99%)	94 (86%)	15 (14%)	3	11
68	o2	109/110 (99%)	92 (84%)	17 (16%)	2	8
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2	8
69	o3	90/90 (100%)	82 (91%)	8 (9%)	9	28
70	O4	95/101 (94%)	78 (82%)	17 (18%)	2	5
70	o4	95/101 (94%)	81 (85%)	14 (15%)	3	9
71	O5	104/104 (100%)	83 (80%)	21 (20%)	1	4
71	o5	103/104 (99%)	76 (74%)	27 (26%)	0	1
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0	1
72	o6	80/81 (99%)	52 (65%)	28 (35%)	0	0
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	6
73	o7	70/70 (100%)	59 (84%)	11 (16%)	2	8
74	O8	68/68 (100%)	55 (81%)	13 (19%)	1	4
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	5
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	4
75	o9	45/45 (100%)	35 (78%)	10 (22%)	1	2
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	9
76	q0	47/47 (100%)	40 (85%)	7 (15%)	3	9
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	76 (84%)	14 (16%)	2	8
78	q2	90/90 (100%)	73 (81%)	17 (19%)	1	5
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	10
79	q3	71/71 (100%)	58 (82%)	13 (18%)	1	5
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	p0	105/253 (42%)	84 (80%)	21 (20%)	1	4
All	All	18729/20239 (92%)	15348 (82%)	3381 (18%)	1	5

All (3381) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	24	LEU
2	S0	27	ARG
2	S0	34	GLU
2	S0	37	VAL
2	S0	43	ASP
2	S0	50	VAL
2	S0	62	ARG
2	S0	80	THR
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	93	THR
2	S0	96	THR
2	S0	101	ARG
2	S0	111	ILE
2	S0	114	SER
2	S0	119	ARG
2	S0	131	GLN
2	S0	135	GLU
2	S0	154	GLU
2	S0	156	VAL
2	S0	157	ASP
2	S0	169	SER
2	S0	170	ILE
2	S0	172	LEU
2	S0	177	LEU
2	S0	184	LEU
2	S0	185	ARG
2	S0	196	SER
2	S0	198	MET
3	S1	21	VAL
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	46	THR
3	S1	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	S1	70	LEU
3	S1	74	GLN
3	S1	79	HIS
3	S1	81	PHE
3	S1	89	ASP
3	S1	97	LEU
3	S1	105	PHE
3	S1	111	ARG
3	S1	135	LEU
3	S1	137	ILE
3	S1	144	ARG
3	S1	154	SER
3	S1	169	SER
3	S1	170	GLU
3	S1	174	LYS
3	S1	180	THR
3	S1	181	LEU
3	S1	198	GLU
3	S1	214	LYS
3	S1	218	LEU
3	S1	219	LYS
3	S1	220	GLN
3	S1	223	PHE
4	S2	41	LEU
4	S2	53	ILE
4	S2	55	GLU
4	S2	58	LEU
4	S2	64	LYS
4	S2	69	ILE
4	S2	71	THR
4	S2	76	LEU
4	S2	77	GLN
4	S2	80	VAL
4	S2	89	GLN
4	S2	90	THR
4	S2	91	ARG
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	117	THR
4	S2	130	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	S2	134	LEU
4	S2	137	ILE
4	S2	139	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	166	THR
4	S2	181	SER
4	S2	195	ASP
4	S2	206	THR
4	S2	207	LEU
4	S2	208	GLU
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	235	LEU
4	S2	242	ILE
4	S2	245	ASP
4	S2	246	GLU
5	S3	4	LEU
5	S3	10	LYS
5	S3	21	LEU
5	S3	23	GLU
5	S3	39	VAL
5	S3	41	VAL
5	S3	65	ARG
5	S3	67	ASN
5	S3	76	ARG
5	S3	81	PRO
5	S3	84	ILE
5	S3	92	GLN
5	S3	93	ASP
5	S3	105	MET
5	S3	111	ASN
5	S3	117	ARG
5	S3	127	MET
5	S3	134	CYS
5	S3	142	LEU
5	S3	151	LYS
5	S3	158	ILE
5	S3	172	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S3	176	LEU
5	S3	178	ARG
5	S3	179	GLN
5	S3	181	VAL
5	S3	182	LEU
5	S3	202	LEU
5	S3	204	ASP
5	S3	209	ILE
5	S3	215	GLU
5	S3	222	VAL
5	S3	223	LYS
6	S4	6	LYS
6	S4	7	LYS
6	S4	9	LEU
6	S4	12	LEU
6	S4	21	ASP
6	S4	23	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	45	ILE
6	S4	48	LEU
6	S4	62	LYS
6	S4	65	LEU
6	S4	67	GLN
6	S4	70	VAL
6	S4	72	VAL
6	S4	77	ARG
6	S4	92	LEU
6	S4	102	VAL
6	S4	105	VAL
6	S4	115	THR
6	S4	116	ASP
6	S4	123	LEU
6	S4	126	VAL
6	S4	131	LEU
6	S4	133	LYS
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	197	HIS
6	S4	198	LYS
6	S4	211	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	S4	215	ASP
6	S4	221	ARG
6	S4	222	LEU
6	S4	227	VAL
6	S4	240	LYS
6	S4	242	LYS
6	S4	248	ILE
6	S4	258	GLN
7	S5	23	VAL
7	S5	25	LEU
7	S5	38	THR
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	53	VAL
7	S5	65	ARG
7	S5	76	ARG
7	S5	79	ASN
7	S5	84	LYS
7	S5	88	PRO
7	S5	89	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	99	MET
7	S5	112	ARG
7	S5	119	ASP
7	S5	124	LEU
7	S5	139	ASN
7	S5	146	THR
7	S5	147	THR
7	S5	148	ARG
7	S5	149	VAL
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	162	VAL
7	S5	185	ARG
7	S5	190	ILE
7	S5	193	THR
7	S5	194	LEU
7	S5	225	ARG
8	S6	9	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	S6	13	GLN
8	S6	21	GLU
8	S6	25	ARG
8	S6	30	LYS
8	S6	65	GLN
8	S6	67	VAL
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	80	ASN
8	S6	82	SER
8	S6	97	VAL
8	S6	98	ARG
8	S6	120	GLU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	132	ARG
8	S6	133	LEU
8	S6	137	ARG
8	S6	143	LYS
8	S6	154	ARG
8	S6	155	ASP
8	S6	158	ILE
8	S6	169	TYR
8	S6	175	ILE
8	S6	176	GLN
8	S6	179	VAL
8	S6	182	GLN
8	S6	211	LEU
8	S6	212	LEU
8	S6	223	LYS
9	S7	14	THR
9	S7	15	GLU
9	S7	25	VAL
9	S7	37	GLU
9	S7	38	LEU
9	S7	46	ILE
9	S7	50	ASP
9	S7	51	VAL
9	S7	67	LEU
9	S7	70	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	S7	75	THR
9	S7	77	LEU
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	104	ARG
9	S7	105	THR
9	S7	109	VAL
9	S7	114	ARG
9	S7	116	ARG
9	S7	126	LEU
9	S7	136	VAL
9	S7	143	LEU
9	S7	144	VAL
9	S7	185	ILE
10	S8	17	LYS
10	S8	20	GLN
10	S8	21	PHE
10	S8	25	ARG
10	S8	28	GLU
10	S8	29	LEU
10	S8	32	GLN
10	S8	36	THR
10	S8	58	LEU
10	S8	60	ILE
10	S8	73	SER
10	S8	82	VAL
10	S8	110	ARG
10	S8	135	LYS
10	S8	138	ASN
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	164	ARG
10	S8	184	LEU
10	S8	185	GLU
10	S8	196	LEU
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	10	LYS
11	S9	14	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	S9	22	SER
11	S9	28	LEU
11	S9	39	LYS
11	S9	40	LYS
11	S9	49	LEU
11	S9	60	LEU
11	S9	78	ARG
11	S9	82	ARG
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	97	LEU
11	S9	101	VAL
11	S9	105	LEU
11	S9	109	LEU
11	S9	110	GLN
11	S9	111	THR
11	S9	113	VAL
11	S9	122	VAL
11	S9	133	HIS
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG
11	S9	151	ASP
11	S9	161	THR
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	182	GLU
12	C0	1	MET
12	C0	5	LYS
12	C0	7	ASP
12	C0	8	ARG
12	C0	11	ILE
12	C0	20	VAL
12	C0	29	GLN
12	C0	32	HIS
12	C0	40	LEU
12	C0	46	LEU
12	C0	50	THR
12	C0	55	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	C0	56	LYS
12	C0	67	THR
12	C0	71	GLU
12	C0	76	LEU
12	C0	78	GLU
12	C0	81	ASN
12	C0	82	LEU
13	C1	7	VAL
13	C1	21	ASN
13	C1	27	THR
13	C1	29	LYS
13	C1	37	ASN
13	C1	40	LEU
13	C1	43	LYS
13	C1	44	THR
13	C1	56	LYS
13	C1	67	ARG
13	C1	74	THR
13	C1	76	VAL
13	C1	79	LYS
13	C1	83	THR
13	C1	94	ILE
13	C1	99	ARG
13	C1	109	VAL
13	C1	118	GLN
13	C1	123	VAL
13	C1	131	ILE
13	C1	136	ARG
13	C1	138	ASN
13	C1	140	VAL
13	C1	141	LYS
13	C1	143	SER
14	C2	28	LEU
14	C2	33	ARG
14	C2	43	ARG
14	C2	46	ARG
14	C2	50	LYS
14	C2	54	ARG
14	C2	59	LEU
14	C2	66	VAL
14	C2	71	ILE
14	C2	73	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	C2	74	LEU
14	C2	86	VAL
14	C2	89	ILE
14	C2	97	LEU
14	C2	103	LEU
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
14	C2	140	PHE
15	C3	3	ARG
15	C3	9	LYS
15	C3	11	ILE
15	C3	16	ILE
15	C3	27	LYS
15	C3	32	SER
15	C3	39	LYS
15	C3	42	ARG
15	C3	45	LEU
15	C3	56	ASP
15	C3	64	ARG
15	C3	66	ILE
15	C3	76	LYS
15	C3	77	SER
15	C3	83	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	127	ARG
15	C3	134	VAL
15	C3	141	TYR
15	C3	143	SER
15	C3	145	THR
15	C3	149	LEU
16	C4	13	VAL
16	C4	14	PHE
16	C4	16	VAL
16	C4	20	TYR
16	C4	29	HIS
16	C4	30	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	C4	31	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	51	ASP
16	C4	55	SER
16	C4	56	SER
16	C4	92	LYS
16	C4	102	LEU
16	C4	103	ARG
16	C4	107	ARG
16	C4	123	SER
16	C4	132	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	13	LYS
17	C5	21	ASP
17	C5	22	LEU
17	C5	28	MET
17	C5	31	GLU
17	C5	35	LYS
17	C5	36	LEU
17	C5	43	ARG
17	C5	44	ARG
17	C5	47	ARG
17	C5	52	LYS
17	C5	92	SER
17	C5	110	GLU
17	C5	124	THR
18	C6	12	LYS
18	C6	14	LYS
18	C6	17	THR
18	C6	26	LYS
18	C6	28	LEU
18	C6	29	ILE
18	C6	39	VAL
18	C6	45	ARG
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	66	ARG
18	C6	68	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	C6	69	VAL
18	C6	98	ASP
18	C6	101	SER
18	C6	114	ARG
18	C6	116	LEU
18	C6	118	ILE
18	C6	123	ARG
18	C6	128	LYS
18	C6	137	ARG
18	C6	143	ARG
19	C7	5	ARG
19	C7	7	LYS
19	C7	8	THR
19	C7	29	GLN
19	C7	30	THR
19	C7	34	LEU
19	C7	36	ASP
19	C7	38	ILE
19	C7	46	LEU
19	C7	49	LYS
19	C7	54	THR
19	C7	61	ILE
19	C7	62	GLN
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	88	VAL
19	C7	105	GLN
19	C7	107	SER
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	8	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	18	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	C8	20	THR
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	40	ARG
20	C8	57	ARG
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN
20	C8	77	THR
20	C8	80	LYS
20	C8	92	ILE
20	C8	107	SER
20	C8	110	ARG
20	C8	116	LEU
20	C8	132	ARG
20	C8	136	GLN
20	C8	143	ARG
21	C9	4	VAL
21	C9	22	LEU
21	C9	28	LEU
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	53	TRP
21	C9	57	ARG
21	C9	63	ARG
21	C9	67	MET
21	C9	68	ARG
21	C9	84	LYS
21	C9	86	ARG
21	C9	88	VAL
21	C9	94	ILE
21	C9	117	SER
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	134	ARG
21	C9	144	GLU
22	D0	15	GLN
22	D0	17	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	D0	18	GLN
22	D0	23	ARG
22	D0	27	THR
22	D0	30	LYS
22	D0	34	LEU
22	D0	46	GLU
22	D0	47	GLN
22	D0	51	VAL
22	D0	57	ARG
22	D0	60	THR
22	D0	64	LYS
22	D0	66	SER
22	D0	67	THR
22	D0	72	ASN
22	D0	74	GLU
22	D0	76	SER
22	D0	77	LYS
22	D0	81	THR
22	D0	88	LYS
22	D0	89	ARG
22	D0	99	ILE
22	D0	103	ILE
22	D0	117	VAL
22	D0	121	ASN
23	D1	1	MET
23	D1	7	GLN
23	D1	9	VAL
23	D1	11	LEU
23	D1	25	LYS
23	D1	32	VAL
23	D1	34	ILE
23	D1	39	VAL
23	D1	41	GLU
23	D1	52	THR
23	D1	62	ARG
23	D1	69	LEU
23	D1	78	LEU
23	D1	80	LYS
24	D2	3	ARG
24	D2	4	SER
24	D2	7	LEU
24	D2	12	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	D2	22	LYS
24	D2	24	GLN
24	D2	25	VAL
24	D2	29	PRO
24	D2	49	GLU
24	D2	53	ILE
24	D2	65	LEU
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	105	THR
24	D2	129	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	14	LYS
25	D3	19	ARG
25	D3	26	GLU
25	D3	28	ASN
25	D3	60	GLU
25	D3	73	ARG
25	D3	82	LYS
25	D3	83	VAL
25	D3	84	THR
25	D3	101	GLU
25	D3	103	LEU
25	D3	107	PHE
25	D3	109	ARG
25	D3	110	LYS
25	D3	114	LYS
25	D3	117	ILE
25	D3	131	SER
25	D3	132	LEU
25	D3	139	LYS
25	D3	144	ARG
26	D4	10	ARG
26	D4	17	LEU
26	D4	32	ARG
26	D4	34	ASN
26	D4	36	SER
26	D4	51	GLU
26	D4	57	VAL
26	D4	61	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	D4	62	THR
26	D4	75	VAL
26	D4	84	LYS
26	D4	88	THR
26	D4	99	LYS
26	D4	102	LYS
26	D4	121	THR
26	D4	124	ARG
26	D4	127	LYS
26	D4	128	LYS
26	D4	133	ASN
27	D5	42	LEU
27	D5	49	ARG
27	D5	50	ILE
27	D5	58	ARG
27	D5	59	TYR
27	D5	60	VAL
27	D5	63	SER
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	78	ILE
27	D5	85	LYS
27	D5	92	ILE
27	D5	95	HIS
27	D5	97	LYS
27	D5	98	GLN
27	D5	100	ILE
27	D5	102	THR
28	D6	10	ARG
28	D6	15	ARG
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	45	VAL
28	D6	50	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	67	THR
28	D6	68	TYR
28	D6	69	ASN
28	D6	71	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	D6	83	ILE
28	D6	84	VAL
28	D6	85	ARG
28	D6	90	GLU
29	D7	2	VAL
29	D7	3	LEU
29	D7	20	LYS
29	D7	29	ARG
29	D7	33	LEU
29	D7	42	ASN
29	D7	43	ILE
29	D7	55	THR
29	D7	60	SER
29	D7	62	ILE
29	D7	67	THR
29	D7	72	LYS
29	D7	73	LEU
30	D8	14	LYS
30	D8	19	THR
30	D8	28	VAL
30	D8	35	ASP
30	D8	36	THR
30	D8	39	THR
30	D8	44	VAL
30	D8	49	ARG
30	D8	52	ASP
30	D8	59	SER
30	D8	64	ARG
30	D8	65	ARG
31	D9	5	ASN
31	D9	6	VAL
31	D9	12	ARG
31	D9	19	ARG
31	D9	22	ARG
31	D9	28	THR
31	D9	30	LEU
31	D9	32	ARG
31	D9	39	CYS
32	E0	3	LYS
32	E0	21	VAL
32	E0	25	GLU
32	E0	28	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	E0	29	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	43	ARG
32	E0	47	VAL
32	E0	49	LEU
33	E1	84	VAL
33	E1	86	THR
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	102	VAL
33	E1	108	VAL
33	E1	109	ASP
33	E1	113	LYS
33	E1	118	ARG
33	E1	120	GLU
33	E1	130	VAL
33	E1	146	SER
33	E1	151	ASN
34	SR	6	VAL
34	SR	7	LEU
34	SR	10	ARG
34	SR	29	GLN
34	SR	52	GLN
34	SR	59	ARG
34	SR	76	ASP
34	SR	96	THR
34	SR	117	LYS
34	SR	129	LYS
34	SR	136	ILE
34	SR	137	LYS
34	SR	165	ASP
34	SR	166	SER
34	SR	191	ASP
34	SR	196	ASN
34	SR	199	ILE
34	SR	238	ASP
34	SR	266	ASP
34	SR	268	GLN
34	SR	300	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	SR	316	MET
34	SR	317	THR
35	SM	25	ILE
35	SM	33	LYS
35	SM	34	LYS
35	SM	51	ARG
35	SM	53	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	68	ARG
35	SM	79	SER
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	94	HIS
35	SM	97	THR
35	SM	100	THR
35	SM	102	THR
35	SM	103	LYS
35	SM	139	GLU
39	L2	10	LYS
39	L2	20	THR
39	L2	23	ARG
39	L2	32	LEU
39	L2	36	GLU
39	L2	44	ILE
39	L2	45	VAL
39	L2	48	ILE
39	L2	62	VAL
39	L2	70	ARG
39	L2	74	GLU
39	L2	96	LEU
39	L2	101	VAL
39	L2	112	ILE
39	L2	116	VAL
39	L2	128	ARG
39	L2	134	VAL
39	L2	137	ILE
39	L2	141	PRO
39	L2	142	ASP
39	L2	143	GLU
39	L2	147	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	L2	157	VAL
39	L2	158	ILE
39	L2	165	VAL
39	L2	169	ILE
39	L2	177	LYS
39	L2	179	LEU
39	L2	181	LYS
39	L2	190	ARG
39	L2	191	LEU
39	L2	204	MET
39	L2	207	VAL
39	L2	227	ARG
39	L2	230	VAL
39	L2	247	ARG
40	L3	3	HIS
40	L3	7	GLU
40	L3	10	ARG
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	37	ARG
40	L3	39	LYS
40	L3	43	LEU
40	L3	47	LEU
40	L3	56	ILE
40	L3	70	ARG
40	L3	73	VAL
40	L3	79	VAL
40	L3	84	VAL
40	L3	85	VAL
40	L3	103	THR
40	L3	110	LEU
40	L3	111	SER
40	L3	114	VAL
40	L3	116	ARG
40	L3	121	ASN
40	L3	134	SER
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	156	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	L3	157	VAL
40	L3	169	THR
40	L3	173	GLN
40	L3	183	LEU
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	200	GLU
40	L3	202	THR
40	L3	205	VAL
40	L3	210	GLU
40	L3	229	VAL
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	238	LEU
40	L3	242	THR
40	L3	244	ARG
40	L3	252	ILE
40	L3	284	ARG
40	L3	296	THR
40	L3	305	ILE
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	331	ASN
40	L3	332	ARG
40	L3	338	LEU
40	L3	344	THR
40	L3	346	THR
40	L3	347	SER
40	L3	355	SER
40	L3	361	THR
40	L3	364	LYS
40	L3	380	MET
41	L4	4	PRO
41	L4	22	LEU
41	L4	25	VAL
41	L4	40	THR
41	L4	52	VAL
41	L4	53	SER
41	L4	60	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	L4	69	ARG
41	L4	71	VAL
41	L4	74	ILE
41	L4	93	MET
41	L4	118	LYS
41	L4	122	THR
41	L4	136	LEU
41	L4	138	ARG
41	L4	144	LYS
41	L4	148	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	156	LEU
41	L4	170	LYS
41	L4	172	VAL
41	L4	176	SER
41	L4	177	ASP
41	L4	179	LEU
41	L4	182	LEU
41	L4	185	LYS
41	L4	188	ARG
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL
41	L4	246	ARG
41	L4	258	LEU
41	L4	283	THR
41	L4	306	THR
41	L4	307	GLN
41	L4	313	LEU
41	L4	323	VAL
41	L4	327	LEU
41	L4	346	LYS
41	L4	349	THR
41	L4	354	VAL
41	L4	358	THR
41	L4	359	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	L5	5	LYS
42	L5	10	SER
42	L5	23	ARG
42	L5	35	ARG
42	L5	41	LYS
42	L5	64	ILE
42	L5	68	THR
42	L5	69	ILE
42	L5	75	LEU
42	L5	92	LEU
42	L5	101	THR
42	L5	105	ILE
42	L5	109	THR
42	L5	112	LYS
42	L5	113	LEU
42	L5	115	LEU
42	L5	118	THR
42	L5	122	VAL
42	L5	128	GLU
42	L5	131	LEU
42	L5	137	ASP
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
42	L5	152	ARG
42	L5	155	THR
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	194	LEU
42	L5	196	ARG
42	L5	205	SER
42	L5	216	GLU
42	L5	217	GLU
42	L5	222	LEU
42	L5	232	ASP
42	L5	234	ASP
42	L5	236	LEU
42	L5	254	LYS
42	L5	257	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	L5	259	LYS
42	L5	261	THR
42	L5	263	GLU
42	L5	273	ARG
42	L5	275	THR
42	L5	279	LYS
42	L5	290	ILE
42	L5	293	LEU
43	L6	2	SER
43	L6	5	LYS
43	L6	8	LYS
43	L6	12	SER
43	L6	21	THR
43	L6	52	VAL
43	L6	59	GLU
43	L6	65	ILE
43	L6	70	LYS
43	L6	78	ARG
43	L6	79	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	93	VAL
43	L6	94	GLU
43	L6	129	GLU
43	L6	134	ARG
43	L6	152	THR
43	L6	155	LEU
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	38	LYS
44	L7	45	LEU
44	L7	60	ARG
44	L7	82	LYS
44	L7	83	LEU
44	L7	92	ILE
44	L7	98	LYS
44	L7	100	ARG
44	L7	110	ARG
44	L7	121	LYS
44	L7	124	LEU
44	L7	143	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	L7	157	ASN
44	L7	158	LYS
44	L7	164	SER
44	L7	175	LYS
44	L7	179	LEU
44	L7	184	LEU
44	L7	229	PHE
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	47	SER
45	L8	50	VAL
45	L8	61	GLN
45	L8	63	LYS
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	84	ARG
45	L8	95	ASN
45	L8	110	THR
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	150	LEU
45	L8	156	ASP
45	L8	160	ILE
45	L8	163	VAL
45	L8	169	LEU
45	L8	172	LYS
45	L8	173	MET
45	L8	185	ARG
45	L8	189	LEU
45	L8	203	VAL
45	L8	204	ARG
45	L8	219	ASP
45	L8	238	LEU
45	L8	246	MET
45	L8	248	LYS
45	L8	251	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	L9	4	ILE
46	L9	5	GLN
46	L9	9	GLN
46	L9	14	GLU
46	L9	18	VAL
46	L9	22	SER
46	L9	33	THR
46	L9	41	ILE
46	L9	48	VAL
46	L9	52	LEU
46	L9	62	ARG
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	80	THR
46	L9	82	VAL
46	L9	124	ARG
46	L9	132	VAL
46	L9	135	GLU
46	L9	137	SER
46	L9	138	THR
46	L9	139	ASN
46	L9	150	SER
46	L9	151	VAL
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	173	ARG
46	L9	177	ASP
46	L9	188	THR
46	L9	189	GLU
46	L9	190	ASP
47	M0	18	PRO
47	M0	24	ARG
47	M0	26	VAL
47	M0	30	LYS
47	M0	31	ILE
47	M0	32	ARG
47	M0	33	ILE
47	M0	36	LEU
47	M0	39	LYS
47	M0	40	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	63	GLU
47	M0	74	LYS
47	M0	76	MET
47	M0	77	THR
47	M0	78	THR
47	M0	87	LEU
47	M0	99	ILE
47	M0	129	VAL
47	M0	130	ASP
47	M0	139	ARG
47	M0	140	THR
47	M0	143	SER
47	M0	163	GLN
47	M0	165	ILE
47	M0	169	LYS
47	M0	174	THR
47	M0	178	ARG
47	M0	185	ARG
47	M0	197	VAL
47	M0	203	LYS
48	M1	6	GLN
48	M1	9	MET
48	M1	10	ARG
48	M1	12	LEU
48	M1	13	LYS
48	M1	16	LYS
48	M1	23	VAL
48	M1	31	THR
48	M1	40	LEU
48	M1	44	THR
48	M1	46	VAL
48	M1	61	ARG
48	M1	65	ILE
48	M1	70	THR
48	M1	80	LEU
48	M1	94	ARG
48	M1	95	ASN
48	M1	106	ILE
48	M1	107	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	M1	112	LEU
48	M1	120	ILE
48	M1	130	VAL
48	M1	138	VAL
48	M1	140	ARG
48	M1	142	LYS
48	M1	158	ASP
48	M1	161	SER
48	M1	166	LYS
49	M3	5	LYS
49	M3	23	LYS
49	M3	34	SER
49	M3	42	ARG
49	M3	46	ILE
49	M3	54	LEU
49	M3	55	ARG
49	M3	58	VAL
49	M3	59	ARG
49	M3	63	VAL
49	M3	67	ARG
49	M3	69	VAL
49	M3	85	LEU
49	M3	93	ILE
49	M3	107	GLU
49	M3	114	GLN
49	M3	122	LYS
49	M3	124	ILE
49	M3	128	ARG
49	M3	131	LYS
49	M3	144	THR
49	M3	164	GLU
49	M3	165	SER
49	M3	171	ARG
49	M3	180	ARG
49	M3	182	ILE
49	M3	190	LYS
49	M3	194	GLU
50	M4	8	LYS
50	M4	20	VAL
50	M4	27	GLN
50	M4	42	LYS
50	M4	43	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	M4	50	LYS
50	M4	53	VAL
50	M4	55	ARG
50	M4	59	ASN
50	M4	64	VAL
50	M4	66	THR
50	M4	72	LEU
50	M4	90	VAL
50	M4	92	GLU
50	M4	102	LYS
50	M4	105	GLN
50	M4	108	ARG
50	M4	113	THR
50	M4	125	LYS
50	M4	126	GLN
50	M4	130	THR
51	M5	10	LEU
51	M5	15	GLN
51	M5	20	ARG
51	M5	22	LEU
51	M5	38	ARG
51	M5	49	ARG
51	M5	50	ARG
51	M5	56	LYS
51	M5	68	ARG
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR
51	M5	92	LEU
51	M5	96	ARG
51	M5	97	SER
51	M5	98	LEU
51	M5	105	ARG
51	M5	106	VAL
51	M5	109	ARG
51	M5	113	LEU
51	M5	133	ILE
51	M5	134	LEU
51	M5	138	GLN
51	M5	151	ILE
51	M5	155	VAL
51	M5	182	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	M5	183	THR
51	M5	187	ARG
51	M5	190	THR
52	M6	25	LYS
52	M6	33	ILE
52	M6	34	VAL
52	M6	41	LEU
52	M6	46	GLU
52	M6	66	LYS
52	M6	67	THR
52	M6	78	ARG
52	M6	82	LYS
52	M6	84	LEU
52	M6	85	ARG
52	M6	106	GLU
52	M6	115	LYS
52	M6	116	LYS
52	M6	117	ARG
52	M6	124	LEU
52	M6	126	VAL
52	M6	128	ARG
52	M6	160	ARG
52	M6	166	GLU
52	M6	180	SER
52	M6	189	ASP
52	M6	190	VAL
53	M7	9	THR
53	M7	23	ARG
53	M7	24	VAL
53	M7	29	THR
53	M7	32	THR
53	M7	36	ILE
53	M7	52	LEU
53	M7	53	ASP
53	M7	56	ARG
53	M7	65	SER
53	M7	69	ARG
53	M7	74	LYS
53	M7	94	LEU
53	M7	107	LEU
53	M7	112	LEU
53	M7	114	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	M7	117	ILE
53	M7	126	ARG
53	M7	127	ARG
53	M7	128	ARG
53	M7	136	ILE
53	M7	144	SER
53	M7	153	LYS
53	M7	157	VAL
53	M7	169	THR
53	M7	180	LYS
53	M7	181	ARG
54	M8	3	ILE
54	M8	8	LYS
54	M8	17	THR
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	34	THR
54	M8	41	ASP
54	M8	49	LEU
54	M8	50	LYS
54	M8	57	ILE
54	M8	66	ARG
54	M8	69	ARG
54	M8	74	GLU
54	M8	80	THR
54	M8	81	VAL
54	M8	95	GLU
54	M8	111	ARG
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	147	ARG
54	M8	150	VAL
54	M8	168	THR
54	M8	180	ARG
55	M9	22	VAL
55	M9	29	THR
55	M9	30	SER
55	M9	31	GLU
55	M9	41	ILE
55	M9	44	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	M9	53	LYS
55	M9	60	LYS
55	M9	74	ARG
55	M9	98	ARG
55	M9	99	LEU
55	M9	100	ARG
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	115	ILE
55	M9	116	ASP
55	M9	138	LEU
55	M9	160	GLU
55	M9	175	GLN
56	N0	1	MET
56	N0	8	GLN
56	N0	32	SER
56	N0	45	LEU
56	N0	49	HIS
56	N0	51	VAL
56	N0	57	GLU
56	N0	61	ILE
56	N0	64	ILE
56	N0	80	ARG
56	N0	87	THR
56	N0	97	VAL
56	N0	100	VAL
56	N0	104	GLU
56	N0	105	THR
56	N0	115	ARG
56	N0	117	ARG
56	N0	130	GLU
56	N0	132	THR
56	N0	137	ARG
56	N0	138	GLN
56	N0	142	GLN
56	N0	145	THR
56	N0	155	ARG
56	N0	157	GLN
56	N0	167	ARG
56	N0	171	PHE
56	N0	172	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	43	LYS
57	N1	55	LYS
57	N1	68	THR
57	N1	71	SER
57	N1	78	LYS
57	N1	79	MET
57	N1	83	ARG
57	N1	88	ARG
57	N1	96	ILE
57	N1	102	ARG
57	N1	104	GLU
57	N1	106	LEU
57	N1	118	GLU
57	N1	124	VAL
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	139	ARG
57	N1	141	VAL
57	N1	143	THR
57	N1	146	ASN
57	N1	149	GLN
57	N1	158	THR
57	N1	159	PHE
57	N1	160	ILE
58	N2	10	LYS
58	N2	39	ASP
58	N2	43	VAL
58	N2	52	ASN
58	N2	54	VAL
58	N2	61	THR
58	N2	66	VAL
58	N2	87	ASN
58	N2	88	GLN
58	N2	93	ILE
58	N2	100	THR
59	N3	9	THR
59	N3	13	ILE
59	N3	32	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	N3	48	ARG
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	74	MET
59	N3	83	LYS
59	N3	102	ILE
59	N3	115	THR
59	N3	120	LYS
59	N3	133	SER
59	N3	137	VAL
60	N4	5	ILE
60	N4	17	ARG
60	N4	26	SER
60	N4	39	LEU
60	N4	64	THR
61	N5	25	LYS
61	N5	27	ARG
61	N5	36	LYS
61	N5	37	THR
61	N5	39	LYS
61	N5	40	LEU
61	N5	45	LYS
61	N5	48	SER
61	N5	63	ILE
61	N5	71	THR
61	N5	73	MET
61	N5	77	GLU
61	N5	86	VAL
61	N5	104	GLU
61	N5	105	VAL
61	N5	106	ASP
61	N5	108	LEU
61	N5	109	LYS
61	N5	115	ARG
61	N5	125	ARG
61	N5	133	LEU
61	N5	135	ILE
61	N5	138	ARG
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	N6	5	SER
62	N6	8	VAL
62	N6	13	ARG
62	N6	26	GLN
62	N6	37	LYS
62	N6	42	GLN
62	N6	45	ILE
62	N6	50	ILE
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	70	ILE
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	88	GLU
62	N6	94	SER
62	N6	105	VAL
62	N6	126	LEU
62	N6	127	GLU
63	N7	14	VAL
63	N7	15	ARG
63	N7	17	ARG
63	N7	24	VAL
63	N7	26	VAL
63	N7	30	ASP
63	N7	34	LYS
63	N7	42	LEU
63	N7	46	ILE
63	N7	52	LYS
63	N7	54	THR
63	N7	64	LYS
63	N7	73	LYS
63	N7	75	VAL
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	87	LEU
63	N7	102	GLU
63	N7	108	GLU
63	N7	121	ARG
63	N7	132	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	N7	134	LEU
63	N7	135	ARG
64	N8	4	ARG
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	16	SER
64	N8	29	PRO
64	N8	42	ARG
64	N8	47	LYS
64	N8	58	MET
64	N8	60	TYR
64	N8	76	ASP
64	N8	78	LEU
64	N8	84	GLU
64	N8	85	ASP
64	N8	92	LYS
64	N8	115	LYS
64	N8	118	ILE
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	144	VAL
65	N9	4	SER
65	N9	18	ARG
65	N9	22	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	40	ARG
65	N9	50	THR
65	N9	59	LYS
66	O0	9	SER
66	O0	16	LEU
66	O0	18	ILE
66	O0	20	SER
66	O0	22	LYS
66	O0	30	THR
66	O0	34	LEU
66	O0	48	THR
66	O0	61	MET
66	O0	66	LYS
66	O0	83	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	O0	87	VAL
66	O0	97	ASP
66	O0	100	ILE
66	O0	101	LEU
67	O1	8	VAL
67	O1	13	THR
67	O1	16	LEU
67	O1	28	ARG
67	O1	31	ARG
67	O1	42	LEU
67	O1	46	THR
67	O1	47	ASP
67	O1	55	LEU
67	O1	64	VAL
67	O1	68	GLU
67	O1	79	ARG
67	O1	81	GLU
67	O1	82	GLU
67	O1	84	ASP
67	O1	89	LEU
67	O1	96	VAL
67	O1	102	LYS
67	O1	106	THR
67	O1	110	GLU
68	O2	8	LYS
68	O2	15	LYS
68	O2	18	LYS
68	O2	19	ARG
68	O2	31	ASN
68	O2	33	ARG
68	O2	62	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	76	VAL
68	O2	82	LEU
68	O2	87	MET
68	O2	109	LEU
68	O2	125	ARG
68	O2	128	LEU
69	O3	3	GLU
69	O3	20	LYS
69	O3	21	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
69	O3	31	LYS
69	O3	48	ARG
69	O3	49	ILE
69	O3	59	VAL
69	O3	60	ARG
69	O3	62	SER
69	O3	80	VAL
69	O3	81	VAL
69	O3	86	ARG
69	O3	98	VAL
69	O3	106	ASN
70	O4	5	VAL
70	O4	8	ARG
70	O4	20	ILE
70	O4	23	VAL
70	O4	24	LYS
70	O4	29	ILE
70	O4	31	ARG
70	O4	49	SER
70	O4	51	LEU
70	O4	56	THR
70	O4	58	ARG
70	O4	66	SER
70	O4	71	THR
70	O4	72	VAL
70	O4	81	CYS
70	O4	86	LYS
70	O4	104	VAL
71	O5	5	LYS
71	O5	15	GLU
71	O5	21	LEU
71	O5	28	LEU
71	O5	31	LEU
71	O5	43	LYS
71	O5	46	THR
71	O5	49	LYS
71	O5	50	SER
71	O5	62	GLN
71	O5	71	LYS
71	O5	73	LYS
71	O5	74	LYS
71	O5	84	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
71	O5	85	THR
71	O5	90	ARG
71	O5	94	LYS
71	O5	100	VAL
71	O5	101	THR
71	O5	107	LYS
71	O5	119	LYS
72	O6	11	LEU
72	O6	17	VAL
72	O6	18	THR
72	O6	21	THR
72	O6	26	ILE
72	O6	36	ARG
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	64	SER
72	O6	68	ARG
72	O6	70	ARG
72	O6	72	VAL
72	O6	75	LYS
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
72	O6	89	GLU
72	O6	90	MET
72	O6	99	ARG
73	O7	5	THR
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	45	ARG
73	O7	55	ARG
73	O7	58	THR
73	O7	59	THR
73	O7	67	LEU
73	O7	82	SER
73	O7	84	SER
74	O8	5	ILE
74	O8	8	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
74	O8	24	THR
74	O8	32	ASN
74	O8	45	VAL
74	O8	46	ARG
74	O8	48	SER
74	O8	53	THR
74	O8	61	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	77	ARG
74	O8	78	LEU
75	O9	4	GLN
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	30	ARG
75	O9	34	THR
75	O9	36	ARG
75	O9	45	ARG
75	O9	51	ILE
76	Q0	78	ILE
76	Q0	83	LYS
76	Q0	85	LEU
76	Q0	106	ARG
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	114	LYS
77	Q1	6	ARG
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	13	LEU
77	Q1	15	ARG
77	Q1	19	LYS
77	Q1	21	ARG
78	Q2	3	ASN
78	Q2	4	VAL
78	Q2	8	ARG
78	Q2	29	LYS
78	Q2	35	LEU
78	Q2	47	GLN
78	Q2	60	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	Q2	78	LYS
78	Q2	79	THR
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	93	LEU
78	Q2	104	LEU
79	Q3	11	THR
79	Q3	25	GLN
79	Q3	45	LYS
79	Q3	46	THR
79	Q3	48	LYS
79	Q3	49	ARG
79	Q3	56	THR
79	Q3	60	CYS
79	Q3	78	THR
79	Q3	80	ARG
2	s0	6	THR
2	s0	10	THR
2	s0	12	GLU
2	s0	21	ASN
2	s0	28	ASN
2	s0	30	GLN
2	s0	31	VAL
2	s0	41	ARG
2	s0	43	ASP
2	s0	45	VAL
2	s0	59	LEU
2	s0	62	ARG
2	s0	72	ASP
2	s0	87	LEU
2	s0	96	THR
2	s0	101	ARG
2	s0	106	SER
2	s0	111	ILE
2	s0	112	THR
2	s0	124	THR
2	s0	144	ILE
2	s0	146	LEU
2	s0	153	SER
2	s0	157	ASP
2	s0	167	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	s0	168	HIS
2	s0	172	LEU
2	s0	179	ARG
2	s0	183	ARG
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	191	ARG
2	s0	198	MET
3	s1	21	VAL
3	s1	25	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	61	LEU
3	s1	70	LEU
3	s1	73	LEU
3	s1	76	SER
3	s1	80	SER
3	s1	81	PHE
3	s1	89	ASP
3	s1	96	LEU
3	s1	105	PHE
3	s1	126	THR
3	s1	173	THR
3	s1	177	GLN
3	s1	180	THR
3	s1	184	LEU
3	s1	192	VAL
3	s1	193	ILE
3	s1	195	LYS
3	s1	202	LYS
3	s1	203	ASP
3	s1	204	ILE
3	s1	212	VAL
3	s1	222	LYS
3	s1	223	PHE
3	s1	225	VAL
3	s1	228	LEU
4	s2	41	LEU
4	s2	53	ILE
4	s2	55	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	s2	58	LEU
4	s2	69	ILE
4	s2	70	ASP
4	s2	71	THR
4	s2	72	LEU
4	s2	76	LEU
4	s2	80	VAL
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	94	GLN
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR
4	s2	140	ARG
4	s2	141	ARG
4	s2	146	THR
4	s2	159	THR
4	s2	185	LYS
4	s2	200	SER
4	s2	205	ARG
4	s2	206	THR
4	s2	207	LEU
4	s2	218	ILE
4	s2	222	TYR
4	s2	225	LEU
4	s2	233	GLN
4	s2	242	ILE
4	s2	245	ASP
4	s2	246	GLU
5	s3	4	LEU
5	s3	7	LYS
5	s3	9	ARG
5	s3	10	LYS
5	s3	37	VAL
5	s3	39	VAL
5	s3	40	ARG
5	s3	59	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	s3	66	ILE
5	s3	69	LEU
5	s3	84	ILE
5	s3	89	GLU
5	s3	90	ARG
5	s3	92	GLN
5	s3	93	ASP
5	s3	94	ARG
5	s3	111	ASN
5	s3	115	ILE
5	s3	117	ARG
5	s3	128	GLU
5	s3	132	LYS
5	s3	142	LEU
5	s3	143	ARG
5	s3	146	ARG
5	s3	158	ILE
5	s3	162	GLN
5	s3	164	VAL
5	s3	169	ASP
5	s3	172	THR
5	s3	181	VAL
5	s3	202	LEU
5	s3	212	LYS
5	s3	225	TYR
6	s4	7	LYS
6	s4	9	LEU
6	s4	23	LEU
6	s4	30	ARG
6	s4	38	LEU
6	s4	42	LEU
6	s4	48	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	67	GLN
6	s4	70	VAL
6	s4	78	THR
6	s4	91	THR
6	s4	95	THR
6	s4	102	VAL
6	s4	113	ARG
6	s4	116	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	s4	123	LEU
6	s4	126	VAL
6	s4	127	LYS
6	s4	129	VAL
6	s4	131	LEU
6	s4	147	ILE
6	s4	148	ARG
6	s4	160	VAL
6	s4	180	LEU
6	s4	182	TYR
6	s4	187	ARG
6	s4	192	ILE
6	s4	221	ARG
6	s4	222	LEU
6	s4	227	VAL
6	s4	237	SER
6	s4	254	ARG
7	s5	23	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	32	GLU
7	s5	38	THR
7	s5	39	GLU
7	s5	45	LYS
7	s5	59	VAL
7	s5	63	GLN
7	s5	64	VAL
7	s5	68	ILE
7	s5	76	ARG
7	s5	79	ASN
7	s5	83	ARG
7	s5	84	LYS
7	s5	89	ILE
7	s5	92	ARG
7	s5	93	LEU
7	s5	99	MET
7	s5	109	LYS
7	s5	114	ILE
7	s5	119	ASP
7	s5	125	THR
7	s5	146	THR
7	s5	147	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	s5	148	ARG
7	s5	149	VAL
7	s5	157	ARG
7	s5	163	SER
7	s5	167	ARG
7	s5	187	ILE
7	s5	194	LEU
7	s5	203	LYS
7	s5	216	GLU
7	s5	225	ARG
8	s6	5	ILE
8	s6	17	GLU
8	s6	25	ARG
8	s6	30	LYS
8	s6	31	ARG
8	s6	43	ASP
8	s6	44	GLU
8	s6	76	LEU
8	s6	78	THR
8	s6	88	ARG
8	s6	98	ARG
8	s6	108	VAL
8	s6	109	LEU
8	s6	112	VAL
8	s6	115	LYS
8	s6	120	GLU
8	s6	121	LEU
8	s6	125	THR
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR
8	s6	129	VAL
8	s6	143	LYS
8	s6	150	GLU
8	s6	151	ASP
8	s6	154	ARG
8	s6	155	ASP
8	s6	168	THR
8	s6	170	THR
8	s6	171	LYS
8	s6	177	ARG
8	s6	179	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	s6	193	LEU
8	s6	215	ARG
8	s6	217	SER
9	s7	5	GLN
9	s7	8	ILE
9	s7	26	GLU
9	s7	28	GLU
9	s7	33	GLU
9	s7	49	ILE
9	s7	50	ASP
9	s7	55	LYS
9	s7	67	LEU
9	s7	77	LEU
9	s7	79	ARG
9	s7	80	GLU
9	s7	86	GLN
9	s7	97	ARG
9	s7	101	LYS
9	s7	105	THR
9	s7	110	GLN
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	126	LEU
9	s7	136	VAL
9	s7	143	LEU
9	s7	144	VAL
9	s7	148	LYS
9	s7	156	SER
9	s7	159	VAL
9	s7	166	LEU
9	s7	175	LYS
9	s7	185	ILE
10	s8	20	GLN
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	46	VAL
10	s8	60	ILE
10	s8	61	GLU
10	s8	74	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	s8	76	THR
10	s8	77	ARG
10	s8	89	GLU
10	s8	110	ARG
10	s8	119	GLN
10	s8	121	LEU
10	s8	123	LYS
10	s8	138	ASN
10	s8	155	SER
10	s8	158	SER
10	s8	183	ILE
10	s8	184	LEU
10	s8	199	LYS
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	10	LYS
11	s9	28	LEU
11	s9	33	GLU
11	s9	39	LYS
11	s9	49	LEU
11	s9	82	ARG
11	s9	93	LEU
11	s9	96	VAL
11	s9	99	LEU
11	s9	101	VAL
11	s9	105	LEU
11	s9	109	LEU
11	s9	110	GLN
11	s9	111	THR
11	s9	113	VAL
11	s9	118	LEU
11	s9	130	THR
11	s9	134	ILE
11	s9	140	ILE
11	s9	149	ARG
11	s9	154	LYS
11	s9	161	THR
11	s9	168	ARG
11	s9	172	VAL
11	s9	175	ARG
11	s9	180	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	s9	182	GLU
12	c0	2	LEU
12	c0	5	LYS
12	c0	15	LEU
12	c0	20	VAL
12	c0	21	VAL
12	c0	27	PHE
12	c0	33	GLU
12	c0	36	ASP
12	c0	55	VAL
12	c0	57	THR
12	c0	67	THR
12	c0	71	GLU
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	26	LYS
13	c1	27	THR
13	c1	30	ARG
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	56	LYS
13	c1	60	PHE
13	c1	67	ARG
13	c1	74	THR
13	c1	80	MET
13	c1	83	THR
13	c1	109	VAL
13	c1	123	VAL
13	c1	129	ARG
13	c1	140	VAL
13	c1	143	SER
14	c2	28	LEU
14	c2	37	VAL
14	c2	43	ARG
14	c2	45	LEU
14	c2	53	THR
14	c2	58	LEU
14	c2	59	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	c2	61	VAL
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	86	VAL
14	c2	89	ILE
14	c2	103	LEU
14	c2	116	VAL
14	c2	120	VAL
14	c2	121	VAL
14	c2	132	GLU
14	c2	137	MET
14	c2	138	GLU
14	c2	140	PHE
15	c3	12	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	21	ASN
15	c3	39	LYS
15	c3	53	LEU
15	c3	64	ARG
15	c3	66	ILE
15	c3	67	THR
15	c3	70	LYS
15	c3	80	LEU
15	c3	87	ASP
15	c3	88	LEU
15	c3	93	LYS
15	c3	104	ARG
15	c3	114	ARG
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	138	ASN
15	c3	147	SER
15	c3	150	VAL
16	c4	18	ARG
16	c4	20	TYR
16	c4	26	THR
16	c4	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	c4	49	LYS
16	c4	51	ASP
16	c4	61	MET
16	c4	70	LYS
16	c4	79	VAL
16	c4	81	VAL
16	c4	92	LYS
16	c4	102	LEU
16	c4	111	ARG
16	c4	114	ARG
16	c4	119	THR
16	c4	124	ASP
16	c4	125	SER
16	c4	127	ARG
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	10	ARG
17	c5	12	PHE
17	c5	22	LEU
17	c5	24	LYS
17	c5	27	GLU
17	c5	36	LEU
17	c5	43	ARG
17	c5	44	ARG
17	c5	52	LYS
17	c5	64	LYS
17	c5	69	GLU
17	c5	71	GLU
17	c5	72	LYS
17	c5	77	ARG
17	c5	92	SER
17	c5	107	ILE
17	c5	110	GLU
17	c5	122	THR
17	c5	124	THR
17	c5	125	PRO
18	c6	7	VAL
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	c6	37	THR
18	c6	40	GLU
18	c6	43	ILE
18	c6	48	VAL
18	c6	53	LEU
18	c6	54	LEU
18	c6	57	LEU
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	81	ILE
18	c6	90	VAL
18	c6	110	THR
18	c6	113	ASP
18	c6	114	ARG
18	c6	137	ARG
19	c7	3	ARG
19	c7	8	THR
19	c7	14	LYS
19	c7	33	ARG
19	c7	34	LEU
19	c7	38	ILE
19	c7	45	ARG
19	c7	46	LEU
19	c7	60	ARG
19	c7	72	LYS
19	c7	74	GLN
19	c7	83	GLN
19	c7	85	VAL
19	c7	104	ASN
19	c7	110	VAL
19	c7	113	LEU
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	12	GLN
20	c8	13	HIS
20	c8	16	ARG
20	c8	27	LYS
20	c8	28	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	c8	34	THR
20	c8	36	LYS
20	c8	40	ARG
20	c8	57	ARG
20	c8	61	LEU
20	c8	63	GLN
20	c8	68	ARG
20	c8	88	ARG
20	c8	92	ILE
20	c8	100	THR
20	c8	110	ARG
20	c8	116	LEU
20	c8	119	ILE
20	c8	136	GLN
20	c8	138	THR
20	c8	143	ARG
20	c8	145	ARG
21	c9	6	VAL
21	c9	13	ASP
21	c9	25	GLN
21	c9	28	LEU
21	c9	34	VAL
21	c9	36	ILE
21	c9	37	VAL
21	c9	57	ARG
21	c9	68	ARG
21	c9	71	VAL
21	c9	75	LYS
21	c9	86	ARG
21	c9	88	VAL
21	c9	111	ILE
21	c9	123	ARG
21	c9	131	ASP
21	c9	135	ILE
21	c9	140	LEU
21	c9	142	GLU
21	c9	144	GLU
22	d0	12	GLN
22	d0	20	ILE
22	d0	23	ARG
22	d0	27	THR
22	d0	30	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	d0	44	ASN
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	67	THR
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	81	THR
22	d0	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	107	THR
22	d0	108	ILE
22	d0	118	VAL
23	d1	1	MET
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	25	LYS
23	d1	32	VAL
23	d1	41	GLU
23	d1	49	GLU
23	d1	52	THR
23	d1	62	ARG
23	d1	68	SER
23	d1	69	LEU
23	d1	74	GLN
23	d1	76	ASP
23	d1	79	LEU
24	d2	6	VAL
24	d2	7	LEU
24	d2	22	LYS
24	d2	23	ARG
24	d2	25	VAL
24	d2	26	LEU
24	d2	43	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	d2	65	LEU
24	d2	74	VAL
24	d2	88	LYS
24	d2	93	LEU
24	d2	103	ILE
24	d2	105	THR
24	d2	129	VAL
25	d3	9	LEU
25	d3	16	ARG
25	d3	19	ARG
25	d3	23	ARG
25	d3	40	SER
25	d3	69	ARG
25	d3	73	ARG
25	d3	83	VAL
25	d3	84	THR
25	d3	98	GLU
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	114	LYS
25	d3	131	SER
26	d4	13	ILE
26	d4	36	SER
26	d4	42	GLU
26	d4	43	LYS
26	d4	46	GLU
26	d4	49	LYS
26	d4	51	GLU
26	d4	61	ARG
26	d4	62	THR
26	d4	88	THR
26	d4	100	VAL
26	d4	105	ARG
26	d4	116	LYS
27	d5	43	ASP
27	d5	46	LYS
27	d5	51	LEU
27	d5	57	TYR
27	d5	60	VAL
27	d5	68	ARG
27	d5	81	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	d6	10	ARG
28	d6	11	ASN
28	d6	18	VAL
28	d6	24	VAL
28	d6	26	CYS
28	d6	34	LYS
28	d6	41	ILE
28	d6	44	ILE
28	d6	53	LEU
28	d6	55	GLU
28	d6	82	ARG
28	d6	83	ILE
28	d6	85	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	40	CYS
29	d7	41	LEU
29	d7	43	ILE
29	d7	44	THR
29	d7	52	THR
29	d7	61	THR
29	d7	63	LEU
29	d7	72	LYS
29	d7	77	THR
29	d7	81	ARG
30	d8	8	THR
30	d8	22	ARG
30	d8	32	PHE
30	d8	33	LEU
30	d8	36	THR
30	d8	48	VAL
30	d8	49	ARG
30	d8	54	LEU
31	d9	16	LYS
31	d9	28	THR
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	38	ILE
31	d9	53	ASN
31	d9	54	LYS
80	e0	4	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	e0	13	LYS
80	e0	22	GLU
80	e0	23	LYS
80	e0	26	LYS
80	e0	29	LYS
80	e0	36	LYS
80	e0	38	LEU
80	e0	44	PHE
80	e0	46	ASN
80	e0	54	ARG
80	e0	55	ARG
33	e1	80	ARG
33	e1	84	VAL
33	e1	86	THR
33	e1	90	LYS
33	e1	96	LYS
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	113	LYS
33	e1	119	ARG
33	e1	121	CYS
33	e1	125	THR
33	e1	130	VAL
33	e1	135	HIS
33	e1	137	ASP
33	e1	146	SER
33	e1	148	TYR
33	e1	150	VAL
34	sR	8	VAL
34	sR	21	THR
34	sR	25	THR
34	sR	29	GLN
34	sR	58	VAL
34	sR	65	SER
34	sR	66	HIS
34	sR	76	ASP
34	sR	96	THR
34	sR	118	LYS
34	sR	136	ILE
34	sR	145	LEU
34	sR	149	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	sR	153	GLN
34	sR	159	ASN
34	sR	166	SER
34	sR	168	THR
34	sR	184	ASN
34	sR	199	ILE
34	sR	202	LEU
34	sR	228	LYS
34	sR	252	LEU
34	sR	266	ASP
34	sR	275	ARG
34	sR	297	ASP
34	sR	309	VAL
34	sR	314	GLN
34	sR	317	THR
35	sM	23	LYS
35	sM	33	LYS
35	sM	43	ASP
35	sM	45	SER
35	sM	64	LYS
35	sM	74	LYS
35	sM	75	ASP
39	l2	15	ILE
39	l2	23	ARG
39	l2	32	LEU
39	l2	41	ILE
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	48	ILE
39	l2	61	VAL
39	l2	62	VAL
39	l2	70	ARG
39	l2	71	LEU
39	l2	74	GLU
39	l2	101	VAL
39	l2	112	ILE
39	l2	116	VAL
39	l2	119	LYS
39	l2	137	ILE
39	l2	142	ASP
39	l2	155	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	12	157	VAL
39	12	158	ILE
39	12	165	VAL
39	12	179	LEU
39	12	180	LEU
39	12	181	LYS
39	12	193	ARG
39	12	194	ASN
39	12	202	VAL
39	12	207	VAL
39	12	215	ASN
39	12	224	THR
39	12	225	ILE
39	12	230	VAL
39	12	241	ARG
39	12	246	LEU
39	12	249	SER
40	13	3	HIS
40	13	4	ARG
40	13	10	ARG
40	13	17	LEU
40	13	19	ARG
40	13	21	ARG
40	13	30	LYS
40	13	39	LYS
40	13	47	LEU
40	13	50	LYS
40	13	56	ILE
40	13	77	THR
40	13	79	VAL
40	13	81	THR
40	13	84	VAL
40	13	103	THR
40	13	114	VAL
40	13	120	LYS
40	13	124	LYS
40	13	134	SER
40	13	145	GLU
40	13	146	ARG
40	13	148	LEU
40	13	150	ARG
40	13	157	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	l3	160	VAL
40	l3	169	THR
40	l3	183	LEU
40	l3	187	SER
40	l3	188	ILE
40	l3	196	ARG
40	l3	202	THR
40	l3	205	VAL
40	l3	221	THR
40	l3	229	VAL
40	l3	232	ARG
40	l3	235	THR
40	l3	236	LYS
40	l3	238	LEU
40	l3	242	THR
40	l3	244	ARG
40	l3	248	LYS
40	l3	249	VAL
40	l3	252	ILE
40	l3	261	MET
40	l3	264	VAL
40	l3	284	ARG
40	l3	296	THR
40	l3	302	LYS
40	l3	308	MET
40	l3	317	ILE
40	l3	324	VAL
40	l3	328	ILE
40	l3	332	ARG
40	l3	335	ILE
40	l3	338	LEU
40	l3	340	LYS
40	l3	346	THR
40	l3	347	SER
40	l3	348	ARG
40	l3	349	LYS
40	l3	355	SER
40	l3	361	THR
40	l3	369	ARG
40	l3	382	THR
41	l4	2	SER
41	l4	14	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	14	25	VAL
41	14	52	VAL
41	14	60	THR
41	14	67	THR
41	14	93	MET
41	14	112	LYS
41	14	120	TYR
41	14	122	THR
41	14	143	GLU
41	14	144	LYS
41	14	145	ILE
41	14	150	LEU
41	14	156	LEU
41	14	160	GLN
41	14	161	LYS
41	14	172	VAL
41	14	176	SER
41	14	179	LEU
41	14	186	LYS
41	14	187	LEU
41	14	188	ARG
41	14	191	LYS
41	14	198	ARG
41	14	200	THR
41	14	203	ARG
41	14	206	LEU
41	14	217	LYS
41	14	220	ARG
41	14	222	VAL
41	14	226	GLU
41	14	229	ASN
41	14	230	VAL
41	14	246	ARG
41	14	258	LEU
41	14	267	VAL
41	14	283	THR
41	14	284	SER
41	14	287	THR
41	14	295	ILE
41	14	300	ARG
41	14	306	THR
41	14	307	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	14	313	LEU
41	14	319	LYS
41	14	323	VAL
41	14	327	LEU
41	14	342	LYS
41	14	345	GLU
41	14	358	THR
41	14	359	LEU
41	14	360	LYS
42	15	4	GLN
42	15	5	LYS
42	15	15	ARG
42	15	34	LYS
42	15	41	LYS
42	15	51	LEU
42	15	58	LYS
42	15	61	ILE
42	15	65	ILE
42	15	68	THR
42	15	70	THR
42	15	73	VAL
42	15	74	VAL
42	15	75	LEU
42	15	89	THR
42	15	93	THR
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	115	LEU
42	15	118	THR
42	15	120	LYS
42	15	124	GLU
42	15	131	LEU
42	15	132	THR
42	15	133	GLU
42	15	135	VAL
42	15	136	GLU
42	15	140	ARG
42	15	146	LEU
42	15	148	ILE
42	15	152	ARG
42	15	155	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	15	185	PHE
42	15	187	THR
42	15	190	ILE
42	15	194	LEU
42	15	210	GLU
42	15	211	LEU
42	15	218	ARG
42	15	220	SER
42	15	227	LEU
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	268	GLU
42	15	269	SER
42	15	273	ARG
42	15	275	THR
42	15	282	ARG
42	15	293	LEU
43	16	8	LYS
43	16	12	SER
43	16	20	LYS
43	16	21	THR
43	16	31	ARG
43	16	46	ARG
43	16	50	LYS
43	16	52	VAL
43	16	64	LEU
43	16	65	ILE
43	16	78	ARG
43	16	79	VAL
43	16	89	THR
43	16	91	VAL
43	16	93	VAL
43	16	98	VAL
43	16	99	GLU
43	16	109	GLU
43	16	131	LYS
43	16	133	GLU
43	16	143	LYS
43	16	152	THR
43	16	155	LEU
43	16	175	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	17	22	THR
44	17	26	VAL
44	17	30	ARG
44	17	41	ARG
44	17	54	GLU
44	17	60	ARG
44	17	77	VAL
44	17	83	LEU
44	17	88	ARG
44	17	93	ASN
44	17	98	LYS
44	17	100	ARG
44	17	110	ARG
44	17	121	LYS
44	17	124	LEU
44	17	130	ILE
44	17	156	ILE
44	17	158	LYS
44	17	173	LEU
44	17	175	LYS
44	17	178	ILE
44	17	179	LEU
44	17	184	LEU
44	17	193	PRO
44	17	219	LYS
44	17	228	SER
44	17	229	PHE
44	17	239	LEU
45	18	33	ASN
45	18	41	GLN
45	18	50	VAL
45	18	65	LEU
45	18	66	SER
45	18	67	ILE
45	18	69	LEU
45	18	71	VAL
45	18	74	THR
45	18	79	GLN
45	18	81	THR
45	18	89	GLU
45	18	90	THR
45	18	95	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	18	128	LYS
45	18	136	LEU
45	18	145	ASN
45	18	146	LYS
45	18	149	LYS
45	18	150	LEU
45	18	160	ILE
45	18	163	VAL
45	18	164	VAL
45	18	166	LEU
45	18	169	LEU
45	18	172	LYS
45	18	211	LEU
45	18	214	LEU
45	18	217	THR
45	18	230	LYS
45	18	231	LYS
45	18	238	LEU
45	18	241	LYS
45	18	248	LYS
46	19	2	LYS
46	19	4	ILE
46	19	5	GLN
46	19	6	THR
46	19	18	VAL
46	19	19	SER
46	19	20	ILE
46	19	31	ARG
46	19	33	THR
46	19	39	LYS
46	19	43	VAL
46	19	44	THR
46	19	52	LEU
46	19	55	VAL
46	19	62	ARG
46	19	68	LEU
46	19	69	ARG
46	19	70	THR
46	19	80	THR
46	19	82	VAL
46	19	105	GLU
46	19	106	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	l9	120	ASP
46	l9	130	ASP
46	l9	133	THR
46	l9	151	VAL
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	168	ARG
46	l9	169	ASN
46	l9	177	ASP
46	l9	179	ILE
46	l9	191	LEU
47	m0	3	ARG
47	m0	4	ARG
47	m0	24	ARG
47	m0	28	ASP
47	m0	31	ILE
47	m0	32	ARG
47	m0	36	LEU
47	m0	42	THR
47	m0	48	LEU
47	m0	52	LEU
47	m0	57	LEU
47	m0	74	LYS
47	m0	76	MET
47	m0	77	THR
47	m0	78	THR
47	m0	82	ARG
47	m0	87	LEU
47	m0	99	ILE
47	m0	101	LYS
47	m0	116	ARG
47	m0	129	VAL
47	m0	130	ASP
47	m0	139	ARG
47	m0	140	THR
47	m0	143	SER
47	m0	145	LYS
47	m0	163	GLN
47	m0	166	ILE
47	m0	167	LEU
47	m0	169	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	m0	182	LEU
47	m0	185	ARG
47	m0	197	VAL
47	m0	205	SER
47	m0	211	ARG
47	m0	212	GLU
47	m0	215	GLU
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	30	LEU
48	m1	31	THR
48	m1	44	THR
48	m1	54	VAL
48	m1	55	ARG
48	m1	71	VAL
48	m1	80	LEU
48	m1	85	LYS
48	m1	101	ASN
48	m1	107	ASP
48	m1	112	LEU
48	m1	129	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	153	LYS
48	m1	159	THR
48	m1	161	SER
48	m1	174	LYS
49	m3	13	HIS
49	m3	54	LEU
49	m3	55	ARG
49	m3	57	VAL
49	m3	59	ARG
49	m3	63	VAL
49	m3	67	ARG
49	m3	68	LYS
49	m3	69	VAL
49	m3	73	ARG
49	m3	85	LEU
49	m3	107	GLU
49	m3	114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	m3	115	ARG
49	m3	118	GLU
49	m3	122	LYS
49	m3	124	ILE
49	m3	128	ARG
49	m3	131	LYS
49	m3	164	GLU
49	m3	165	SER
49	m3	184	GLU
49	m3	190	LYS
49	m3	194	GLU
50	m4	3	THR
50	m4	13	ARG
50	m4	20	VAL
50	m4	27	GLN
50	m4	42	LYS
50	m4	50	LYS
50	m4	53	VAL
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	72	LEU
50	m4	80	THR
50	m4	82	SER
50	m4	105	GLN
50	m4	113	THR
50	m4	130	THR
50	m4	133	LYS
50	m4	135	LEU
51	m5	5	LYS
51	m5	10	LEU
51	m5	12	ARG
51	m5	22	LEU
51	m5	24	ARG
51	m5	49	ARG
51	m5	68	ARG
51	m5	76	PRO
51	m5	80	THR
51	m5	83	LYS
51	m5	85	THR
51	m5	92	LEU
51	m5	96	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	m5	97	SER
51	m5	98	LEU
51	m5	105	ARG
51	m5	106	VAL
51	m5	125	SER
51	m5	138	GLN
51	m5	153	ASP
51	m5	155	VAL
51	m5	159	ARG
51	m5	170	LYS
51	m5	188	ARG
51	m5	190	THR
51	m5	194	GLN
51	m5	196	THR
52	m6	12	LYS
52	m6	22	VAL
52	m6	25	LYS
52	m6	41	LEU
52	m6	58	LEU
52	m6	60	LYS
52	m6	67	THR
52	m6	68	ARG
52	m6	74	ARG
52	m6	78	ARG
52	m6	84	LEU
52	m6	85	ARG
52	m6	89	SER
52	m6	100	GLU
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	117	ARG
52	m6	124	LEU
52	m6	130	LYS
52	m6	152	VAL
52	m6	160	ARG
52	m6	167	TYR
52	m6	171	LYS
52	m6	175	THR
52	m6	182	ASN
52	m6	184	THR
52	m6	197	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	m7	9	THR
53	m7	23	ARG
53	m7	24	VAL
53	m7	31	GLU
53	m7	32	THR
53	m7	41	LEU
53	m7	52	LEU
53	m7	56	ARG
53	m7	78	VAL
53	m7	79	THR
53	m7	89	LYS
53	m7	94	LEU
53	m7	112	LEU
53	m7	114	VAL
53	m7	126	ARG
53	m7	128	ARG
53	m7	144	SER
54	m8	7	SER
54	m8	17	THR
54	m8	24	VAL
54	m8	26	LEU
54	m8	32	LEU
54	m8	34	THR
54	m8	41	ASP
54	m8	46	LYS
54	m8	49	LEU
54	m8	59	ARG
54	m8	63	SER
54	m8	66	ARG
54	m8	69	ARG
54	m8	80	THR
54	m8	81	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	95	GLU
54	m8	100	THR
54	m8	111	ARG
54	m8	127	LEU
54	m8	135	GLN
54	m8	144	ARG
54	m8	147	ARG
54	m8	150	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	m8	161	LYS
54	m8	170	ARG
54	m8	180	ARG
55	m9	5	ARG
55	m9	7	GLN
55	m9	10	LEU
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	36	ASN
55	m9	39	ASN
55	m9	43	LYS
55	m9	49	THR
55	m9	52	LYS
55	m9	55	VAL
55	m9	56	THR
55	m9	60	LYS
55	m9	63	THR
55	m9	71	ARG
55	m9	74	ARG
55	m9	76	SER
55	m9	88	ARG
55	m9	99	LEU
55	m9	106	LEU
55	m9	117	LYS
55	m9	126	GLU
55	m9	128	LYS
55	m9	134	HIS
55	m9	138	LEU
55	m9	150	GLN
55	m9	152	GLU
55	m9	153	LYS
55	m9	156	ASN
55	m9	158	GLU
55	m9	164	LEU
55	m9	170	ARG
55	m9	173	ARG
56	n0	1	MET
56	n0	13	ARG
56	n0	21	GLU
56	n0	60	SER
56	n0	61	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	n0	71	LYS
56	n0	73	LYS
56	n0	87	THR
56	n0	100	VAL
56	n0	105	THR
56	n0	106	LEU
56	n0	115	ARG
56	n0	117	ARG
56	n0	120	SER
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	138	GLN
56	n0	148	LEU
56	n0	149	LYS
56	n0	155	ARG
56	n0	161	LYS
56	n0	162	THR
56	n0	172	TYR
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	52	MET
57	n1	68	THR
57	n1	78	LYS
57	n1	83	ARG
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	102	ARG
57	n1	104	GLU
57	n1	122	GLN
57	n1	126	VAL
57	n1	135	PRO
57	n1	139	ARG
57	n1	141	VAL
57	n1	143	THR
57	n1	150	THR
58	n2	11	ILE
58	n2	21	SER
58	n2	27	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	n2	37	LEU
58	n2	43	VAL
58	n2	54	VAL
58	n2	63	VAL
58	n2	68	THR
58	n2	74	LYS
58	n2	90	ARG
58	n2	98	THR
58	n2	105	LEU
59	n3	13	ILE
59	n3	14	SER
59	n3	45	ARG
59	n3	48	ARG
59	n3	73	VAL
59	n3	91	VAL
59	n3	110	LYS
59	n3	115	THR
59	n3	120	LYS
60	n4	1	MET
60	n4	2	LYS
60	n4	5	ILE
60	n4	26	SER
60	n4	39	LEU
60	n4	43	ARG
60	n4	54	LEU
60	n4	63	ILE
60	n4	96	LEU
60	n4	99	GLU
60	n4	100	VAL
60	n4	127	LYS
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	38	LEU
61	n5	39	LYS
61	n5	45	LYS
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	64	GLU
61	n5	65	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
61	n5	71	THR
61	n5	86	VAL
61	n5	87	SER
61	n5	106	ASP
61	n5	108	LEU
61	n5	109	LYS
61	n5	115	ARG
61	n5	125	ARG
61	n5	133	LEU
61	n5	135	ILE
61	n5	137	ASN
61	n5	142	ILE
62	n6	12	ARG
62	n6	13	ARG
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	51	ARG
62	n6	55	GLU
62	n6	56	VAL
62	n6	57	LEU
62	n6	62	SER
62	n6	66	GLN
62	n6	71	SER
62	n6	74	TYR
62	n6	76	LEU
62	n6	80	VAL
62	n6	83	ASP
62	n6	94	SER
62	n6	97	ILE
62	n6	108	LYS
62	n6	113	LYS
62	n6	115	ARG
62	n6	120	GLN
62	n6	127	GLU
63	n7	3	LYS
63	n7	14	VAL
63	n7	17	ARG
63	n7	24	VAL
63	n7	26	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	n7	33	SER
63	n7	46	ILE
63	n7	52	LYS
63	n7	55	LYS
63	n7	64	LYS
63	n7	72	ILE
63	n7	73	LYS
63	n7	75	VAL
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR
63	n7	94	SER
63	n7	103	GLN
63	n7	111	LYS
63	n7	121	ARG
63	n7	126	LYS
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	9	ARG
64	n8	10	LYS
64	n8	12	ARG
64	n8	16	SER
64	n8	24	LYS
64	n8	26	ARG
64	n8	27	LYS
64	n8	47	LYS
64	n8	60	TYR
64	n8	70	LYS
64	n8	78	LEU
64	n8	85	ASP
64	n8	91	LEU
64	n8	95	SER
64	n8	98	THR
64	n8	115	LYS
64	n8	128	ARG
64	n8	130	VAL
64	n8	132	LYS
64	n8	133	LEU
65	n9	12	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
65	n9	14	ARG
65	n9	22	LYS
65	n9	26	THR
65	n9	31	SER
65	n9	33	LYS
65	n9	38	LYS
65	n9	50	THR
65	n9	52	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	8	GLU
66	o0	9	SER
66	o0	18	ILE
66	o0	33	SER
66	o0	34	LEU
66	o0	40	LYS
66	o0	41	LEU
66	o0	61	MET
66	o0	66	LYS
66	o0	68	TYR
66	o0	81	VAL
66	o0	86	ARG
66	o0	87	VAL
66	o0	97	ASP
66	o0	101	LEU
66	o0	103	THR
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	47	ASP
67	o1	50	ARG
67	o1	64	VAL
67	o1	83	GLU
67	o1	90	PHE
67	o1	96	VAL
67	o1	102	LYS
67	o1	106	THR
67	o1	107	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	o1	110	GLU
68	o2	4	LEU
68	o2	5	PRO
68	o2	16	LYS
68	o2	18	LYS
68	o2	19	ARG
68	o2	27	ARG
68	o2	31	ASN
68	o2	33	ARG
68	o2	34	LYS
68	o2	41	VAL
68	o2	50	ILE
68	o2	54	LYS
68	o2	73	THR
68	o2	75	LEU
68	o2	76	VAL
68	o2	82	LEU
68	o2	106	VAL
69	o3	10	LYS
69	o3	20	LYS
69	o3	31	LYS
69	o3	49	ILE
69	o3	70	LYS
69	o3	81	VAL
69	o3	92	LYS
69	o3	98	VAL
70	o4	5	VAL
70	o4	16	ARG
70	o4	19	LYS
70	o4	20	ILE
70	o4	24	LYS
70	o4	29	ILE
70	o4	30	LEU
70	o4	58	ARG
70	o4	64	THR
70	o4	65	VAL
70	o4	68	THR
70	o4	88	ARG
70	o4	98	GLN
70	o4	110	GLU
71	o5	20	GLN
71	o5	21	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
71	o5	28	LEU
71	o5	31	LEU
71	o5	38	ARG
71	o5	43	LYS
71	o5	45	LYS
71	o5	47	VAL
71	o5	48	ARG
71	o5	62	GLN
71	o5	68	GLN
71	o5	69	LEU
71	o5	73	LYS
71	o5	79	ASP
71	o5	81	ARG
71	o5	84	LYS
71	o5	85	THR
71	o5	86	ARG
71	o5	89	ARG
71	o5	90	ARG
71	o5	94	LYS
71	o5	98	SER
71	o5	100	VAL
71	o5	101	THR
71	o5	104	GLN
71	o5	107	LYS
71	o5	119	LYS
72	o6	3	VAL
72	o6	4	LYS
72	o6	7	ILE
72	o6	9	ILE
72	o6	11	LEU
72	o6	21	THR
72	o6	25	LYS
72	o6	26	ILE
72	o6	29	LYS
72	o6	34	SER
72	o6	36	ARG
72	o6	37	THR
72	o6	38	LYS
72	o6	43	LEU
72	o6	45	ARG
72	o6	58	ILE
72	o6	59	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
72	o6	60	LEU
72	o6	64	SER
72	o6	68	ARG
72	o6	74	LYS
72	o6	75	LYS
72	o6	76	ARG
72	o6	80	PHE
72	o6	81	THR
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
73	o7	17	THR
73	o7	24	ARG
73	o7	25	ARG
73	o7	33	THR
73	o7	36	SER
73	o7	44	THR
73	o7	55	ARG
73	o7	58	THR
73	o7	67	LEU
73	o7	68	LYS
73	o7	80	THR
74	o8	5	ILE
74	o8	12	LEU
74	o8	17	ARG
74	o8	31	LEU
74	o8	41	THR
74	o8	46	ARG
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	68	SER
74	o8	72	THR
75	o9	4	GLN
75	o9	15	LYS
75	o9	17	LYS
75	o9	19	GLN
75	o9	21	ARG
75	o9	23	LEU
75	o9	29	LEU
75	o9	45	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	o9	48	LYS
75	o9	51	ILE
76	q0	78	ILE
76	q0	85	LEU
76	q0	93	LYS
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
77	q1	6	ARG
77	q1	9	ARG
77	q1	10	THR
77	q1	13	LEU
77	q1	14	LYS
77	q1	16	LYS
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
78	q2	7	THR
78	q2	8	ARG
78	q2	16	THR
78	q2	22	GLN
78	q2	46	LYS
78	q2	47	GLN
78	q2	48	SER
78	q2	61	LYS
78	q2	71	ARG
78	q2	78	LYS
78	q2	79	THR
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	93	LEU
78	q2	100	LYS
78	q2	104	LEU
79	q3	3	LYS
79	q3	5	THR
79	q3	10	ILE
79	q3	22	LEU
79	q3	33	GLN
79	q3	42	CYS
79	q3	48	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	62	LYS
79	q3	78	THR
79	q3	90	VAL
82	p0	4	ILE
82	p0	5	ARG
82	p0	10	GLU
82	p0	25	LEU
82	p0	42	ARG
82	p0	43	LYS
82	p0	44	GLU
82	p0	48	ARG
82	p0	52	LEU
82	p0	55	LYS
82	p0	69	ASP
82	p0	70	LEU
82	p0	72	ASP
82	p0	76	LEU
82	p0	91	GLU
82	p0	93	LEU
82	p0	94	THR
82	p0	96	ILE
82	p0	97	LYS
82	p0	103	ASN
82	p0	104	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
2	S0	163	ASN
2	S0	168	HIS
3	S1	79	HIS
5	S3	159	HIS
7	S5	103	ASN
9	S7	71	HIS
11	S9	110	GLN
13	C1	110	HIS
15	C3	105	ASN
20	C8	6	GLN
23	D1	74	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	D2	70	ASN
26	D4	63	GLN
27	D5	44	GLN
27	D5	95	HIS
39	L2	83	HIS
39	L2	209	HIS
40	L3	121	ASN
42	L5	40	HIS
42	L5	81	HIS
44	L7	244	ASN
48	M1	95	ASN
53	M7	125	GLN
54	M8	73	GLN
59	N3	81	GLN
59	N3	98	ASN
61	N5	80	ASN
68	O2	104	ASN
69	O3	42	GLN
2	s0	140	ASN
9	s7	71	HIS
11	s9	110	GLN
12	c0	29	GLN
12	c0	32	HIS
15	c3	49	GLN
15	c3	62	GLN
23	d1	21	ASN
24	d2	56	HIS
26	d4	22	GLN
33	e1	93	HIS
34	sR	184	ASN
42	l5	264	GLN
45	l8	33	ASN
56	n0	108	GLN
61	n5	111	ASN
62	n6	120	GLN
64	n8	28	HIS
75	o9	19	GLN

5.3.3 RNA ⓘ

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	449 (25%)	63 (3%)
1	6	1794/1800 (99%)	430 (23%)	59 (3%)
36	1	3145/3396 (92%)	609 (19%)	99 (3%)
36	5	3145/3396 (92%)	613 (19%)	101 (3%)
37	3	120/121 (99%)	17 (14%)	2 (1%)
37	7	120/121 (99%)	15 (12%)	1 (0%)
38	4	157/158 (99%)	35 (22%)	3 (1%)
38	8	157/158 (99%)	37 (23%)	2 (1%)
All	All	10385/10950 (94%)	2205 (21%)	330 (3%)

All (2205) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	57	G
1	2	60	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	100	A
1	2	103	A
1	2	104	A
1	2	114	C
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	158	U
1	2	159	U
1	2	175	G
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	250	C
1	2	251	A
1	2	260	U
1	2	261	U
1	2	265	A
1	2	266	A
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	309	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	320	U
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	390	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	418	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	434	G
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	460	A
1	2	470	A
1	2	477	A
1	2	480	G
1	2	484	C
1	2	485	A
1	2	486	G
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	512	A
1	2	513	U
1	2	515	A
1	2	516	G
1	2	527	A
1	2	528	U
1	2	532	U
1	2	536	C
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	543	C
1	2	544	A
1	2	548	G
1	2	555	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	570	A
1	2	578	U
1	2	579	A
1	2	580	A
1	2	582	U
1	2	585	A
1	2	594	A
1	2	595	G
1	2	609	U
1	2	611	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	639	U
1	2	640	U
1	2	645	C
1	2	650	U
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	693	U
1	2	694	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	758	U
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	779	U
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	794	U
1	2	795	U
1	2	811	A
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	837	G
1	2	840	U
1	2	846	G
1	2	856	A
1	2	860	U
1	2	862	A
1	2	863	A
1	2	864	U
1	2	876	G
1	2	886	U
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	916	U
1	2	933	A
1	2	935	U
1	2	942	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	959	U
1	2	960	U
1	2	961	U
1	2	966	A
1	2	974	A
1	2	992	A
1	2	993	A
1	2	995	A
1	2	997	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	1031	U
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1074	G
1	2	1079	U
1	2	1080	U
1	2	1082	C
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1111	G
1	2	1138	A
1	2	1139	A
1	2	1146	G
1	2	1151	A
1	2	1155	G
1	2	1157	A
1	2	1158	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1160	A
1	2	1161	C
1	2	1167	G
1	2	1176	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1203	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1219	A
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1235	C
1	2	1241	G
1	2	1242	A
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1257	U
1	2	1258	U
1	2	1260	U
1	2	1286	U
1	2	1310	U
1	2	1314	U
1	2	1315	U
1	2	1320	U
1	2	1321	A
1	2	1337	A
1	2	1339	C
1	2	1340	U
1	2	1341	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1344	A
1	2	1345	A
1	2	1354	G
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1446	A
1	2	1448	G
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1462	G
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1477	G
1	2	1478	G
1	2	1482	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1506	G
1	2	1514	U
1	2	1515	A
1	2	1516	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1540	G
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1573	A
1	2	1574	G
1	2	1584	G
1	2	1590	G
1	2	1601	G
1	2	1616	G
1	2	1631	A
1	2	1657	U
1	2	1658	G
1	2	1663	G
1	2	1681	A
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1731	A
1	2	1751	C
1	2	1756	A
1	2	1759	C
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1796	C
36	1	13	A
36	1	14	U
36	1	18	G
36	1	26	A
36	1	40	A
36	1	43	A
36	1	44	U
36	1	49	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	75	G
36	1	77	A
36	1	92	G
36	1	99	A
36	1	109	A
36	1	110	G
36	1	113	C
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	142	C
36	1	156	G
36	1	157	A
36	1	163	C
36	1	166	C
36	1	169	U
36	1	170	G
36	1	173	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	210	U
36	1	218	G
36	1	219	A
36	1	224	C
36	1	234	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	238	A
36	1	240	U
36	1	241	G
36	1	243	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	256	G
36	1	269	G
36	1	282	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	305	U
36	1	323	A
36	1	329	U
36	1	344	A
36	1	349	A
36	1	350	C
36	1	352	A
36	1	375	A
36	1	376	G
36	1	395	A
36	1	398	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	417	A
36	1	421	G
36	1	422	A
36	1	438	A
36	1	440	A
36	1	495	G
36	1	520	U
36	1	521	A
36	1	535	G
36	1	544	C
36	1	546	C
36	1	547	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	548	G
36	1	551	A
36	1	552	G
36	1	555	U
36	1	557	A
36	1	559	A
36	1	578	A
36	1	579	G
36	1	588	G
36	1	589	A
36	1	592	A
36	1	604	G
36	1	609	G
36	1	611	A
36	1	620	U
36	1	621	A
36	1	622	A
36	1	636	C
36	1	637	C
36	1	638	C
36	1	649	A
36	1	654	C
36	1	656	A
36	1	660	A
36	1	677	A
36	1	681	U
36	1	691	A
36	1	705	A
36	1	708	G
36	1	712	G
36	1	715	A
36	1	716	A
36	1	763	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	806	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	817	A
36	1	830	A
36	1	849	C
36	1	861	C
36	1	870	G
36	1	874	U
36	1	879	U
36	1	883	A
36	1	889	U
36	1	890	C
36	1	896	A
36	1	897	U
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	924	G
36	1	937	G
36	1	943	U
36	1	944	C
36	1	959	C
36	1	960	U
36	1	961	C
36	1	962	A
36	1	966	U
36	1	974	G
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	994	G
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1013	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1024	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1064	A
36	1	1065	A
36	1	1071	U
36	1	1072	G
36	1	1079	A
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1121	U
36	1	1131	G
36	1	1153	A
36	1	1159	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1191	U
36	1	1192	C
36	1	1201	C
36	1	1202	A
36	1	1209	G
36	1	1217	A
36	1	1218	U
36	1	1222	G
36	1	1225	A
36	1	1226	G
36	1	1227	C
36	1	1232	C
36	1	1233	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1239	C
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1274	A
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1287	A
36	1	1292	C
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1329	U
36	1	1330	A
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1380	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	1386	A
36	1	1399	A
36	1	1400	G
36	1	1419	A
36	1	1422	G
36	1	1434	G
36	1	1437	C
36	1	1445	U
36	1	1446	A
36	1	1449	A
36	1	1450	G
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1489	A
36	1	1496	C
36	1	1503	A
36	1	1508	C
36	1	1526	U
36	1	1527	C
36	1	1555	U
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1576	G
36	1	1578	C
36	1	1579	C
36	1	1580	A
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1605	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	1607	U
36	1	1608	C
36	1	1612	A
36	1	1620	U
36	1	1629	U
36	1	1633	C
36	1	1643	A
36	1	1657	C
36	1	1658	G
36	1	1683	A
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C
36	1	1741	A
36	1	1742	U
36	1	1750	A
36	1	1751	G
36	1	1760	A
36	1	1761	C
36	1	1762	C
36	1	1764	U
36	1	1765	U
36	1	1767	C
36	1	1768	U
36	1	1770	G
36	1	1780	G
36	1	1781	C
36	1	1797	A
36	1	1809	A
36	1	1810	A
36	1	1812	G
36	1	1814	A
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	1846	C
36	1	1849	C
36	1	1855	U
36	1	1879	A
36	1	1880	U
36	1	1901	A
36	1	1906	G
36	1	1951	C
36	1	1952	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2106	A
36	1	2107	A
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2121	G
36	1	2122	G
36	1	2125	A
36	1	2130	G
36	1	2131	A
36	1	2140	U
36	1	2158	A
36	1	2169	G
36	1	2201	G
36	1	2205	U
36	1	2208	A
36	1	2210	G
36	1	2223	A
36	1	2228	A
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2255	A
36	1	2256	A
36	1	2272	G
36	1	2273	G
36	1	2279	A
36	1	2281	A
36	1	2282	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	2284	C
36	1	2288	G
36	1	2298	U
36	1	2299	A
36	1	2307	G
36	1	2308	C
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2319	U
36	1	2334	U
36	1	2336	U
36	1	2366	C
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2388	U
36	1	2393	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2405	C
36	1	2411	U
36	1	2412	G
36	1	2418	G
36	1	2419	A
36	1	2435	G
36	1	2437	G
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2513	U
36	1	2514	U
36	1	2515	A
36	1	2519	A
36	1	2522	G
36	1	2523	A
36	1	2529	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	2532	U
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2544	U
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2585	G
36	1	2586	G
36	1	2591	A
36	1	2593	A
36	1	2594	C
36	1	2600	C
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2617	U
36	1	2637	A
36	1	2652	U
36	1	2656	A
36	1	2672	G
36	1	2674	A
36	1	2677	G
36	1	2681	U
36	1	2689	A
36	1	2690	G
36	1	2691	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	2694	A
36	1	2709	C
36	1	2712	U
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2752	U
36	1	2753	G
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2777	G
36	1	2778	G
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2803	A
36	1	2810	C
36	1	2817	A
36	1	2818	U
36	1	2819	A
36	1	2830	G
36	1	2838	A
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2849	C
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2873	U
36	1	2874	G
36	1	2875	U
36	1	2887	A
36	1	2896	A
36	1	2897	A
36	1	2898	G
36	1	2899	C
36	1	2900	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	2902	A
36	1	2914	G
36	1	2923	U
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2945	G
36	1	2947	G
36	1	2957	G
36	1	2971	A
36	1	2974	U
36	1	2980	U
36	1	2983	C
36	1	2990	G
36	1	2996	U
36	1	2997	G
36	1	3012	A
36	1	3049	A
36	1	3056	U
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3086	A
36	1	3092	C
36	1	3113	A
36	1	3122	A
36	1	3128	G
36	1	3130	A
36	1	3131	U
36	1	3134	A
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3158	G
36	1	3164	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	3165	A
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3180	A
36	1	3181	C
36	1	3187	A
36	1	3196	U
36	1	3198	U
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3229	G
36	1	3235	C
36	1	3243	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3270	U
36	1	3272	C
36	1	3273	A
36	1	3276	G
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G
36	1	3289	G
36	1	3292	A
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	3320	A
36	1	3330	A
36	1	3335	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3350	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3377	G
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
37	3	7	G
37	3	13	A
37	3	14	U
37	3	22	A
37	3	42	A
37	3	50	U
37	3	51	A
37	3	54	U
37	3	59	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	95	A
37	3	102	A
37	3	110	G
37	3	112	G
37	3	121	U
38	4	2	A
38	4	11	C
38	4	22	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	4	34	U
38	4	35	C
38	4	52	A
38	4	53	A
38	4	59	A
38	4	62	C
38	4	63	G
38	4	79	A
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	96	A
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	142	C
38	4	152	G
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	13	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	42	G
1	6	44	U
1	6	46	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	47	A
1	6	49	C
1	6	50	C
1	6	57	G
1	6	60	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	78	A
1	6	100	A
1	6	104	A
1	6	114	C
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	146	U
1	6	153	G
1	6	158	U
1	6	159	U
1	6	166	C
1	6	178	U
1	6	179	A
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	195	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	261	U
1	6	262	U
1	6	265	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	275	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	299	A
1	6	308	C
1	6	314	C
1	6	316	A
1	6	319	U
1	6	321	C
1	6	322	G
1	6	337	G
1	6	338	C
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	370	A
1	6	393	C
1	6	400	A
1	6	401	A
1	6	402	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	404	G
1	6	416	A
1	6	417	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	445	A
1	6	448	C
1	6	454	U
1	6	469	C
1	6	470	A
1	6	475	A
1	6	477	A
1	6	484	C
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	495	C
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	507	U
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	514	G
1	6	519	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	527	A
1	6	534	A
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	565	C
1	6	570	A
1	6	574	G
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	606	A
1	6	609	U
1	6	610	G
1	6	617	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	630	A
1	6	637	C
1	6	639	U
1	6	640	U
1	6	652	G
1	6	653	C
1	6	658	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	668	C
1	6	670	U
1	6	676	G
1	6	679	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	687	G
1	6	689	G
1	6	691	C
1	6	696	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	730	G
1	6	733	A
1	6	742	U
1	6	753	A
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	789	A
1	6	793	A
1	6	794	U
1	6	795	U
1	6	806	A
1	6	807	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	811	A
1	6	812	A
1	6	815	G
1	6	821	U
1	6	823	G
1	6	825	U
1	6	826	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	856	A
1	6	863	A
1	6	864	U
1	6	873	U
1	6	898	A
1	6	906	A
1	6	910	C
1	6	912	U
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	991	G
1	6	992	A
1	6	993	A
1	6	996	U
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1026	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1046	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1075	C
1	6	1082	C
1	6	1091	A
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1101	G
1	6	1109	G
1	6	1138	A
1	6	1146	G
1	6	1150	G
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1162	C
1	6	1167	G
1	6	1185	U
1	6	1194	A
1	6	1196	A
1	6	1197	C
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1203	A
1	6	1208	A
1	6	1212	G
1	6	1217	A
1	6	1218	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	1219	A
1	6	1220	C
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1231	U
1	6	1239	U
1	6	1241	G
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1259	U
1	6	1284	C
1	6	1285	U
1	6	1286	U
1	6	1288	G
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1330	G
1	6	1338	C
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1361	U
1	6	1363	U
1	6	1364	G
1	6	1370	U
1	6	1371	A
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	1402	G
1	6	1412	G
1	6	1413	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1433	G
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1461	C
1	6	1471	A
1	6	1481	C
1	6	1482	C
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1494	C
1	6	1496	U
1	6	1497	U
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1539	G
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1573	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	1574	G
1	6	1575	G
1	6	1577	A
1	6	1584	G
1	6	1601	G
1	6	1616	G
1	6	1621	U
1	6	1634	C
1	6	1639	C
1	6	1657	U
1	6	1658	G
1	6	1683	C
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1703	C
1	6	1710	U
1	6	1712	A
1	6	1716	C
1	6	1717	G
1	6	1731	A
1	6	1742	U
1	6	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	11	A
36	5	15	C
36	5	26	A
36	5	38	U
36	5	40	A
36	5	49	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	76	G
36	5	99	A
36	5	110	G
36	5	113	C
36	5	116	A
36	5	121	A
36	5	122	A
36	5	131	C
36	5	133	U
36	5	134	U
36	5	136	G
36	5	139	G
36	5	150	A
36	5	156	G
36	5	157	A
36	5	165	A
36	5	171	G
36	5	172	G
36	5	173	G
36	5	174	C
36	5	180	C
36	5	182	U
36	5	184	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	193	C
36	5	204	A
36	5	210	U
36	5	218	G
36	5	219	A
36	5	221	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	236	G
36	5	237	G
36	5	238	A
36	5	239	G
36	5	240	U
36	5	244	G
36	5	247	C
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	259	C
36	5	269	G
36	5	282	G
36	5	283	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	298	U
36	5	311	C
36	5	322	U
36	5	323	A
36	5	329	U
36	5	349	A
36	5	350	C
36	5	352	A
36	5	376	G
36	5	397	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	438	A
36	5	439	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	440	A
36	5	441	U
36	5	442	G
36	5	443	G
36	5	492	U
36	5	495	G
36	5	520	U
36	5	521	A
36	5	535	G
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	555	U
36	5	557	A
36	5	559	A
36	5	560	G
36	5	578	A
36	5	579	G
36	5	592	A
36	5	600	G
36	5	604	G
36	5	609	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	630	A
36	5	636	C
36	5	649	A
36	5	660	A
36	5	677	A
36	5	681	U
36	5	683	U
36	5	684	G
36	5	705	A
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	719	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	720	A
36	5	725	G
36	5	726	G
36	5	735	A
36	5	736	A
36	5	758	C
36	5	766	U
36	5	767	U
36	5	768	C
36	5	774	G
36	5	776	U
36	5	777	U
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	830	A
36	5	861	C
36	5	874	U
36	5	876	A
36	5	879	U
36	5	891	G
36	5	895	A
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	937	G
36	5	944	C
36	5	959	C
36	5	960	U
36	5	963	G
36	5	974	G
36	5	979	U
36	5	980	A
36	5	983	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	994	G
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1010	G
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1034	U
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1075	A
36	5	1081	U
36	5	1082	U
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1131	G
36	5	1144	U
36	5	1153	A
36	5	1159	A
36	5	1166	G
36	5	1180	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	1181	U
36	5	1182	A
36	5	1192	C
36	5	1193	A
36	5	1196	C
36	5	1201	C
36	5	1202	A
36	5	1222	G
36	5	1232	C
36	5	1235	U
36	5	1236	G
36	5	1237	G
36	5	1238	C
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1245	A
36	5	1246	G
36	5	1254	C
36	5	1258	U
36	5	1259	A
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1285	G
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1312	C
36	5	1314	C
36	5	1329	U
36	5	1330	A
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1428	A
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1481	A
36	5	1482	A
36	5	1490	A
36	5	1500	G
36	5	1502	C
36	5	1503	A
36	5	1508	C
36	5	1522	U
36	5	1536	G
36	5	1553	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1564	U
36	5	1565	G
36	5	1566	A
36	5	1567	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1605	A
36	5	1620	U
36	5	1629	U
36	5	1638	A
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1655	G
36	5	1657	C
36	5	1658	G
36	5	1683	A
36	5	1685	C
36	5	1686	U
36	5	1687	U
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1741	A
36	5	1750	A
36	5	1751	G
36	5	1762	C
36	5	1765	U
36	5	1766	G
36	5	1770	G
36	5	1779	C
36	5	1780	G
36	5	1797	A
36	5	1810	A
36	5	1814	A
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1821	U
36	5	1839	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1847	A
36	5	1849	C
36	5	1850	A
36	5	1876	U
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1893	A
36	5	1906	G
36	5	1935	G
36	5	1940	G
36	5	1952	G
36	5	1953	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2158	A
36	5	2169	G
36	5	2170	U
36	5	2179	C
36	5	2201	G
36	5	2205	U
36	5	2206	G
36	5	2210	G
36	5	2223	A
36	5	2228	A
36	5	2244	A
36	5	2250	G
36	5	2251	G
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	2269	U
36	5	2273	G
36	5	2279	A
36	5	2281	A
36	5	2288	G
36	5	2306	C
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2360	C
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2393	G
36	5	2394	G
36	5	2396	G
36	5	2397	A
36	5	2398	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2436	U
36	5	2438	A
36	5	2439	A
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U
36	5	2506	U
36	5	2507	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
36	5	2514	U
36	5	2515	A
36	5	2518	C
36	5	2523	A
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2534	G
36	5	2536	A
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G
36	5	2550	U
36	5	2552	C
36	5	2555	G
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2610	G
36	5	2614	G
36	5	2622	C
36	5	2637	A
36	5	2639	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	2652	U
36	5	2656	A
36	5	2674	A
36	5	2677	G
36	5	2678	A
36	5	2681	U
36	5	2689	A
36	5	2690	G
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2714	G
36	5	2728	G
36	5	2729	U
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2810	C
36	5	2817	A
36	5	2818	U
36	5	2819	A
36	5	2822	U
36	5	2843	U
36	5	2845	A
36	5	2853	A
36	5	2871	G
36	5	2872	A
36	5	2874	G
36	5	2875	U
36	5	2887	A
36	5	2896	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	2897	A
36	5	2899	C
36	5	2902	A
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2945	G
36	5	2947	G
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2992	U
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3033	A
36	5	3049	A
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3080	G
36	5	3084	C
36	5	3086	A
36	5	3092	C
36	5	3119	U
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3159	C
36	5	3164	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	3165	A
36	5	3166	C
36	5	3167	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3179	U
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3206	C
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3233	C
36	5	3239	G
36	5	3243	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3265	C
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3281	U
36	5	3282	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3349	C
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3356	G
36	5	3358	U
36	5	3369	G
36	5	3378	C
36	5	3381	U
36	5	3382	U
36	5	3389	U
36	5	3390	G
36	5	3393	U
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	33	U
37	7	54	U
37	7	55	A
37	7	60	G
37	7	65	G
37	7	73	C
37	7	76	A
37	7	91	G
37	7	93	C
37	7	102	A
37	7	103	A
37	7	104	A
37	7	112	G
38	8	25	G
38	8	34	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	8	35	C
38	8	49	G
38	8	51	G
38	8	52	A
38	8	53	A
38	8	58	G
38	8	59	A
38	8	62	C
38	8	63	G
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	86	U
38	8	87	G
38	8	90	U
38	8	95	G
38	8	96	A
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	122	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A
38	8	152	G
38	8	155	A
38	8	156	U
38	8	157	U
38	8	158	U

All (330) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	73	U
1	2	74	U
1	2	93	A
1	2	103	A
1	2	130	C
1	2	131	C
1	2	132	U
1	2	139	C
1	2	144	U
1	2	158	U
1	2	218	A
1	2	240	U
1	2	278	U
1	2	280	U
1	2	352	A
1	2	400	A
1	2	417	A
1	2	468	A
1	2	497	G
1	2	498	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	510	G
1	2	512	A
1	2	558	U
1	2	582	U
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	782	U
1	2	794	U
1	2	811	A
1	2	829	A
1	2	1051	G
1	2	1058	U
1	2	1081	A
1	2	1137	A
1	2	1157	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1196	A
1	2	1207	C
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	1490	C
1	2	1568	C
1	2	1572	G
1	2	1573	A
1	2	1600	A
1	2	1615	C
1	2	1657	U
1	2	1761	U
36	1	43	A
36	1	65	A
36	1	99	A
36	1	169	U
36	1	210	U
36	1	217	U
36	1	223	U
36	1	239	G
36	1	282	G
36	1	397	A
36	1	398	A
36	1	547	G
36	1	588	G
36	1	594	U
36	1	620	U
36	1	637	C
36	1	647	A
36	1	715	A
36	1	719	U
36	1	763	G
36	1	764	U
36	1	816	A
36	1	873	C
36	1	896	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	916	G
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1317	A
36	1	1329	U
36	1	1352	A
36	1	1355	A
36	1	1481	A
36	1	1484	U
36	1	1507	G
36	1	1514	G
36	1	1554	U
36	1	1562	C
36	1	1607	U
36	1	1643	A
36	1	1716	U
36	1	1751	G
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	1849	C
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2227	C
36	1	2249	G
36	1	2281	A
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2385	G
36	1	2403	G
36	1	2418	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	2513	U
36	1	2522	G
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2677	G
36	1	2689	A
36	1	2728	G
36	1	2752	U
36	1	2801	A
36	1	2817	A
36	1	2818	U
36	1	2867	C
36	1	2896	A
36	1	2996	U
36	1	3056	U
36	1	3078	U
36	1	3121	U
36	1	3157	U
36	1	3195	U
36	1	3217	C
36	1	3218	A
36	1	3228	C
36	1	3242	G
36	1	3269	U
36	1	3275	U
36	1	3316	A
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	13	A
37	3	49	G
38	4	85	G
38	4	111	A
38	4	125	U
1	6	1	U
1	6	25	C
1	6	66	U
1	6	103	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	114	C
1	6	136	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	249	U
1	6	272	U
1	6	277	U
1	6	352	A
1	6	400	A
1	6	417	A
1	6	434	G
1	6	468	A
1	6	512	A
1	6	541	A
1	6	542	A
1	6	557	G
1	6	558	U
1	6	651	G
1	6	667	U
1	6	678	A
1	6	717	C
1	6	755	A
1	6	794	U
1	6	815	G
1	6	829	A
1	6	834	G
1	6	1004	U
1	6	1051	G
1	6	1058	U
1	6	1081	A
1	6	1097	U
1	6	1098	U
1	6	1137	A
1	6	1196	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1481	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1535	U
1	6	1568	C
1	6	1572	G
1	6	1573	A
1	6	1584	G
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
36	5	43	A
36	5	65	A
36	5	110	G
36	5	183	G
36	5	210	U
36	5	217	U
36	5	221	A
36	5	238	A
36	5	282	G
36	5	397	A
36	5	588	G
36	5	594	U
36	5	647	A
36	5	715	A
36	5	719	U
36	5	726	G
36	5	735	A
36	5	765	C
36	5	786	A
36	5	816	A
36	5	873	C
36	5	895	A
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	1181	U
36	5	1192	C
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1317	A
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1434	G
36	5	1481	A
36	5	1507	G
36	5	1514	G
36	5	1554	U
36	5	1560	G
36	5	1589	A
36	5	1716	U
36	5	1725	C
36	5	1815	U
36	5	1816	A
36	5	1841	A
36	5	1846	C
36	5	1849	C
36	5	2101	C
36	5	2112	U
36	5	2116	G
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2385	G
36	5	2398	A
36	5	2440	G
36	5	2507	C
36	5	2513	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	2531	C
36	5	2539	C
36	5	2584	G
36	5	2585	G
36	5	2593	A
36	5	2704	A
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2817	A
36	5	2818	U
36	5	2887	A
36	5	2896	A
36	5	2971	A
36	5	3049	A
36	5	3056	U
36	5	3078	U
36	5	3121	U
36	5	3154	C
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3242	G
36	5	3259	U
36	5	3275	U
36	5	3289	G
36	5	3317	U
36	5	3340	G
36	5	3341	U
36	5	3357	U
37	7	49	G
38	8	59	A
38	8	111	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 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	$\# Z > 2$
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	s4	301	-	0,6,6	0.00	-	-		
86	OHX	M5	304	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	o2	201	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	1	3870	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	C1	201	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	n9	3803	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	l3	403	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	C3	202	-	0,6,6	0.00	-	-		
86	OHX	1	4215	-	0,6,6	0.00	-	-		
86	OHX	5	3898	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	5	4250	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	1	3869	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	2	2032	86	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	1	4210	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	1	3957	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	4	223	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	O7	103	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	m8	201	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	15	306	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	5	4232	86	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	o4	203	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	5	3900	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	3	226	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	1	4209	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	15	304	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	M6	202	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	M9	202	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	2	2181	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2047	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
88	3H3	1	4216	-	33,34,34	1.01	3 (9%)	34,45,45	1.65	7 (20%)
86	OHX	m0	301	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	3	225	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	c8	203	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	M0	303	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	s9	201	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	7	217	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	8	215	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	O2	201	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	5	4248	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	8	214	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	m1	203	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	19	600	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	o7	502	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
88	3H3	5	4251	-	33,34,34	0.97	2 (6%)	34,45,45	1.42	4 (11%)
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	5	3901	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	5	3942	86	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	O9	101	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	L6	202	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	l3	402	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	2	2147	86	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	7	216	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	M7	207	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	5	3899	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	M7	208	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	c1	202	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	1	4213	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	4	222	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	Q2	503	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	O3	202	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	5	4249	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	o3	203	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	2	2180	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	L3	403	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	8	216	-	0,6,6	0.00	-	-		
86	OHX	d4	201	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	n3	203	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	1	4214	-	0,6,6	0.00	-	-		
86	OHX	1	4211	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	1	4200	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	m6	202	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	m4	202	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	M5	303	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	m5	302	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	15	305	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	13	404	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	2	2144	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	1	4212	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	L4	404	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	m7	206	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		

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
88	3H3	1	4216	-	-	7/39/51/51	0/1/2/2
88	3H3	5	4251	-	-	7/39/51/51	0/1/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4216	3H3	C3-C2	3.57	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4251	3H3	C14-C16	3.36	1.56	1.53
88	5	4251	3H3	C15-C14	-2.77	1.50	1.54
88	1	4216	3H3	C15-C14	-2.77	1.50	1.54
88	1	4216	3H3	C14-C13	2.16	1.54	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	4251	3H3	C15-C14-C16	4.81	116.50	109.19
88	1	4216	3H3	C15-C14-C16	4.77	116.44	109.19
88	1	4216	3H3	C1-C11-C12	4.38	122.64	113.89
88	5	4251	3H3	C1-C11-C12	3.40	120.67	113.89
88	1	4216	3H3	C-C1-C2	-3.30	102.02	109.99
88	1	4216	3H3	O1-C11-C12	-2.71	103.55	109.60
88	1	4216	3H3	C6-C7-C8	-2.27	106.97	112.92
88	5	4251	3H3	O2-C16-C17	2.21	124.38	121.41
88	1	4216	3H3	O2-C16-C17	2.15	124.30	121.41
88	5	4251	3H3	C6-C7-C8	-2.14	107.32	112.92
88	1	4216	3H3	C8-C9-C10	-2.13	117.49	122.92

There are no chirality outliers.

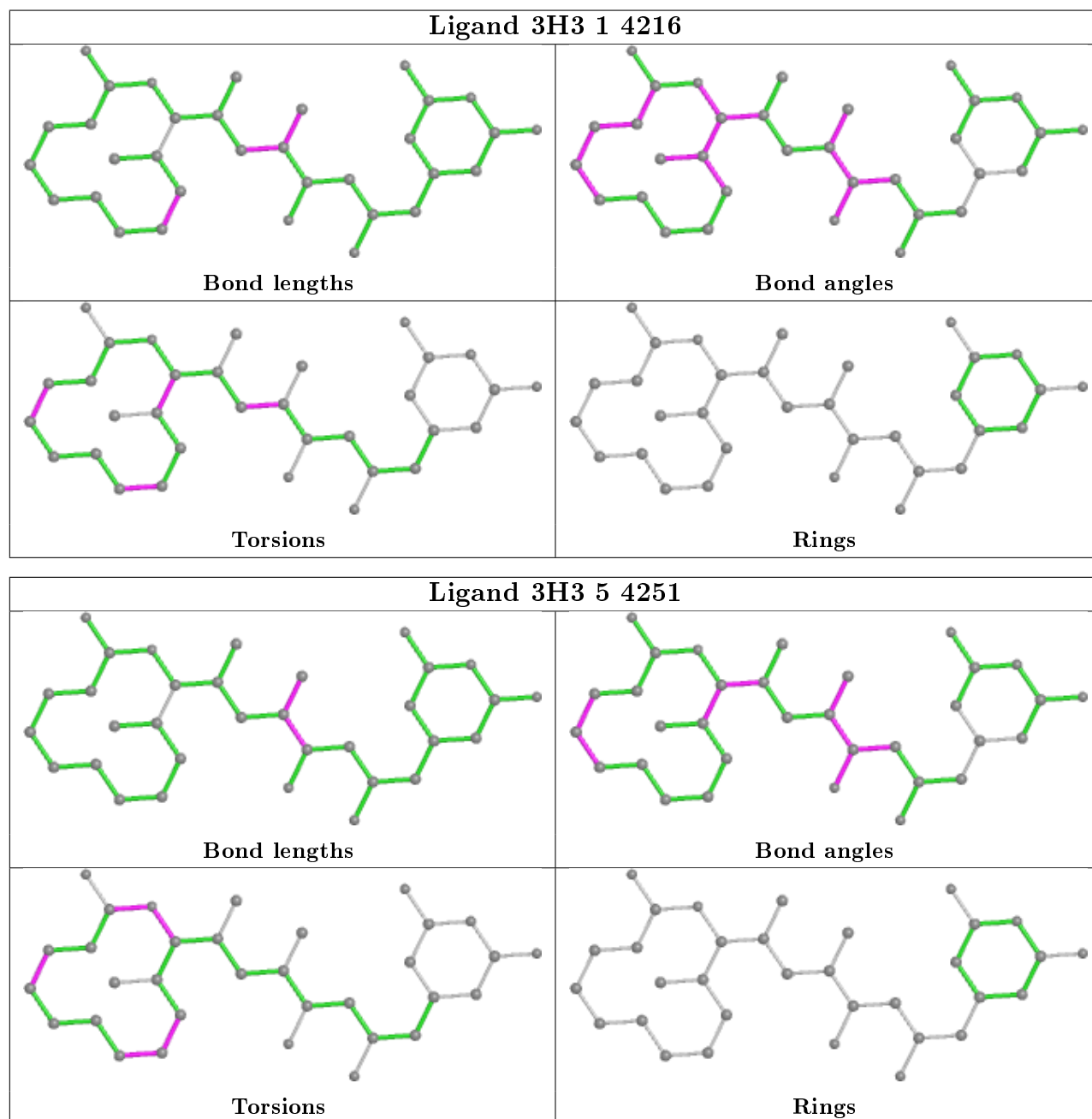
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	1	4216	3H3	C2-C1-C11-O1
88	1	4216	3H3	C2-C1-C11-C12
88	1	4216	3H3	C-C1-C11-O1
88	1	4216	3H3	C-C1-C11-C12
88	1	4216	3H3	C12-C13-C14-C16
88	5	4251	3H3	C12-C11-O1-C10
88	5	4251	3H3	C1-C11-O1-C10
88	5	4251	3H3	C1-C2-C3-C4
88	5	4251	3H3	C9-C10-O1-C11
88	1	4216	3H3	C2-C3-C4-C5
88	5	4251	3H3	O-C10-O1-C11
88	5	4251	3H3	C6-C7-C8-C9
88	5	4251	3H3	C2-C3-C4-C5
88	1	4216	3H3	C6-C7-C8-C9

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
34	SR	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SR	161:LYS	C	162:ALA	N	0.66
1	SR	160:GLU	C	161:LYS	N	0.45

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.