



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2014 – 10:59 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 validation report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

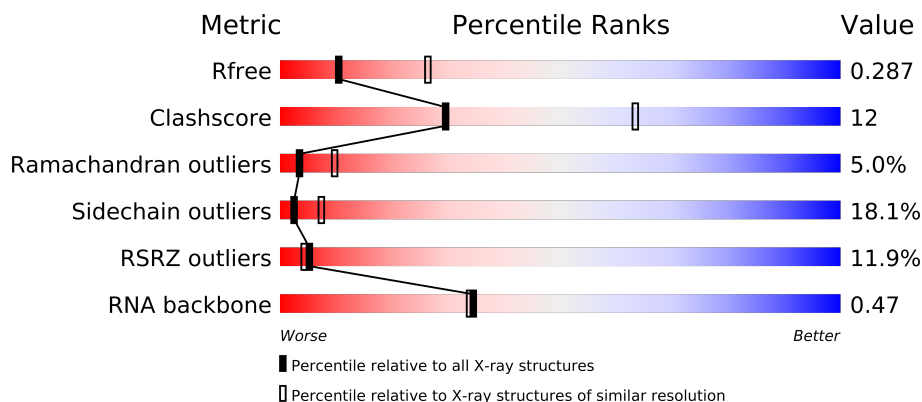
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable24037  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24037

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)
RNA backbone	1838	1076 (3.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
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	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	
81	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3401	-	X
85	MG	1	3402	-	X
85	MG	1	3404	-	X
85	MG	1	3405	-	X
85	MG	1	3408	-	X
85	MG	1	3409	-	X
85	MG	1	3410	-	X
85	MG	1	3412	-	X
85	MG	1	3413	-	X
85	MG	1	3417	-	X
85	MG	1	3418	-	X
85	MG	1	3419	-	X
85	MG	1	3423	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3429	-	X
85	MG	1	3431	-	X
85	MG	1	3439	-	X
85	MG	1	3444	-	X
85	MG	1	3447	-	X
85	MG	1	3450	-	X
85	MG	1	3451	-	X
85	MG	1	3454	-	X
85	MG	1	3456	-	X
85	MG	1	3458	-	X
85	MG	1	3460	-	X
85	MG	1	3462	-	X
85	MG	1	3463	-	X
85	MG	1	3466	-	X
85	MG	1	3469	-	X
85	MG	1	3470	-	X
85	MG	1	3471	-	X
85	MG	1	3472	-	X
85	MG	1	3474	-	X
85	MG	1	3475	-	X
85	MG	1	3479	-	X
85	MG	1	3481	-	X
85	MG	1	3482	-	X
85	MG	1	3484	-	X
85	MG	1	3485	-	X
85	MG	1	3487	-	X
85	MG	1	3493	-	X
85	MG	1	3494	-	X
85	MG	1	3495	-	X
85	MG	1	3496	-	X
85	MG	1	3502	-	X
85	MG	1	3504	-	X
85	MG	1	3505	-	X
85	MG	1	3506	-	X
85	MG	1	3507	-	X
85	MG	1	3508	-	X
85	MG	1	3509	-	X
85	MG	1	3510	-	X
85	MG	1	3512	-	X
85	MG	1	3513	-	X
85	MG	1	3515	-	X
85	MG	1	3516	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3517	-	X
85	MG	1	3518	-	X
85	MG	1	3519	-	X
85	MG	1	3521	-	X
85	MG	1	3522	-	X
85	MG	1	3523	-	X
85	MG	1	3525	-	X
85	MG	1	3526	-	X
85	MG	1	3527	-	X
85	MG	1	3528	-	X
85	MG	1	3529	-	X
85	MG	1	3530	-	X
85	MG	1	3531	-	X
85	MG	1	3532	-	X
85	MG	1	3533	-	X
85	MG	1	3535	-	X
85	MG	1	3536	-	X
85	MG	1	3537	-	X
85	MG	1	3538	-	X
85	MG	1	3539	-	X
85	MG	1	3540	-	X
85	MG	1	3541	-	X
85	MG	1	3542	-	X
85	MG	1	3543	-	X
85	MG	1	3544	-	X
85	MG	1	3545	-	X
85	MG	1	3546	-	X
85	MG	1	3548	-	X
85	MG	1	3549	-	X
85	MG	1	3550	-	X
85	MG	1	3551	-	X
85	MG	1	3552	-	X
85	MG	1	3556	-	X
85	MG	1	3559	-	X
85	MG	1	3560	-	X
85	MG	1	3561	-	X
85	MG	1	3562	-	X
85	MG	1	3566	-	X
85	MG	1	3568	-	X
85	MG	1	3569	-	X
85	MG	1	3571	-	X
85	MG	1	3572	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3573	-	X
85	MG	1	3574	-	X
85	MG	1	3575	-	X
85	MG	1	3576	-	X
85	MG	1	3578	-	X
85	MG	1	3579	-	X
85	MG	1	3580	-	X
85	MG	1	3583	-	X
85	MG	1	3585	-	X
85	MG	1	3586	-	X
85	MG	1	3587	-	X
85	MG	1	3588	-	X
85	MG	1	3589	-	X
85	MG	1	3590	-	X
85	MG	1	3591	-	X
85	MG	1	3592	-	X
85	MG	1	3593	-	X
85	MG	1	3594	-	X
85	MG	1	3595	-	X
85	MG	1	3596	-	X
85	MG	1	3597	-	X
85	MG	1	3598	-	X
85	MG	1	3599	-	X
85	MG	1	3600	-	X
85	MG	1	3604	-	X
85	MG	1	3607	-	X
85	MG	1	3609	-	X
85	MG	1	3610	-	X
85	MG	1	3614	-	X
85	MG	1	3615	-	X
85	MG	1	3618	-	X
85	MG	1	3622	-	X
85	MG	1	3623	-	X
85	MG	1	3624	-	X
85	MG	1	3625	-	X
85	MG	1	3629	-	X
85	MG	1	3630	-	X
85	MG	1	3631	-	X
85	MG	1	3634	-	X
85	MG	1	3637	-	X
85	MG	1	3643	-	X
85	MG	1	3646	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3647	-	X
85	MG	1	3652	-	X
85	MG	1	3653	-	X
85	MG	1	3655	-	X
85	MG	1	3658	-	X
85	MG	1	3660	-	X
85	MG	1	3663	-	X
85	MG	1	3667	-	X
85	MG	1	3669	-	X
85	MG	1	3670	-	X
85	MG	1	3674	-	X
85	MG	1	3677	-	X
85	MG	1	3679	-	X
85	MG	1	3684	-	X
85	MG	1	3685	-	X
85	MG	1	3687	-	X
85	MG	1	3694	-	X
85	MG	1	3700	-	X
85	MG	1	3702	-	X
85	MG	1	3704	-	X
85	MG	1	3707	-	X
85	MG	1	3708	-	X
85	MG	1	3709	-	X
85	MG	1	3713	-	X
85	MG	1	3716	-	X
85	MG	1	3718	-	X
85	MG	1	3720	-	X
85	MG	1	3721	-	X
85	MG	1	3722	-	X
85	MG	1	3726	-	X
85	MG	1	3728	-	X
85	MG	1	3730	-	X
85	MG	1	3733	-	X
85	MG	1	3734	-	X
85	MG	1	3735	-	X
85	MG	1	3739	-	X
85	MG	1	3742	-	X
85	MG	1	3743	-	X
85	MG	1	3747	-	X
85	MG	1	3748	-	X
85	MG	1	3749	-	X
85	MG	1	3751	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3752	-	X
85	MG	1	3757	-	X
85	MG	1	3761	-	X
85	MG	1	3762	-	X
85	MG	1	3766	-	X
85	MG	1	3769	-	X
85	MG	1	3773	-	X
85	MG	1	3774	-	X
85	MG	1	3776	-	X
85	MG	1	3785	-	X
85	MG	1	3786	-	X
85	MG	1	3789	-	X
85	MG	1	3791	-	X
85	MG	1	3796	-	X
85	MG	1	3799	-	X
85	MG	1	3801	-	X
85	MG	1	3804	-	X
85	MG	1	3805	-	X
85	MG	1	3806	-	X
85	MG	1	3808	-	X
85	MG	1	3809	-	X
85	MG	1	3810	-	X
85	MG	1	3813	-	X
85	MG	1	3814	-	X
85	MG	1	3815	-	X
85	MG	1	3817	-	X
85	MG	1	3818	-	X
85	MG	1	3820	-	X
85	MG	1	3821	-	X
85	MG	1	3826	-	X
85	MG	1	3827	-	X
85	MG	1	3834	-	X
85	MG	1	3835	-	X
85	MG	1	3836	-	X
85	MG	1	3839	-	X
85	MG	1	3843	-	X
85	MG	1	3844	-	X
85	MG	1	3847	-	X
85	MG	1	3848	-	X
85	MG	1	3850	-	X
85	MG	1	3853	-	X
85	MG	1	3854	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3856	-	X
85	MG	1	3858	-	X
85	MG	1	3859	-	X
85	MG	1	3860	-	X
85	MG	1	3861	-	X
85	MG	1	3862	-	X
85	MG	1	3863	-	X
85	MG	1	3865	-	X
85	MG	1	4217	-	X
85	MG	1	4219	-	X
85	MG	1	4224	-	X
85	MG	2	1901	-	X
85	MG	2	1903	-	X
85	MG	2	1904	-	X
85	MG	2	1905	-	X
85	MG	2	1906	-	X
85	MG	2	1907	-	X
85	MG	2	1909	-	X
85	MG	2	1910	-	X
85	MG	2	1911	-	X
85	MG	2	1913	-	X
85	MG	2	1914	-	X
85	MG	2	1915	-	X
85	MG	2	1917	-	X
85	MG	2	1918	-	X
85	MG	2	1919	-	X
85	MG	2	1921	-	X
85	MG	2	1923	-	X
85	MG	2	1924	-	X
85	MG	2	1925	-	X
85	MG	2	1926	-	X
85	MG	2	1928	-	X
85	MG	2	1929	-	X
85	MG	2	1930	-	X
85	MG	2	1931	-	X
85	MG	2	1932	-	X
85	MG	2	1933	-	X
85	MG	2	1934	-	X
85	MG	2	1935	-	X
85	MG	2	1936	-	X
85	MG	2	1937	-	X
85	MG	2	1938	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1939	-	X
85	MG	2	1943	-	X
85	MG	2	1944	-	X
85	MG	2	1946	-	X
85	MG	2	1950	-	X
85	MG	2	1951	-	X
85	MG	2	1952	-	X
85	MG	2	1953	-	X
85	MG	2	1955	-	X
85	MG	2	1957	-	X
85	MG	2	1958	-	X
85	MG	2	1959	-	X
85	MG	2	1960	-	X
85	MG	2	1961	-	X
85	MG	2	1962	-	X
85	MG	2	1963	-	X
85	MG	2	1965	-	X
85	MG	2	1967	-	X
85	MG	2	1968	-	X
85	MG	2	1969	-	X
85	MG	2	1971	-	X
85	MG	2	1972	-	X
85	MG	2	1974	-	X
85	MG	2	1975	-	X
85	MG	2	1977	-	X
85	MG	2	1978	-	X
85	MG	2	1979	-	X
85	MG	2	1981	-	X
85	MG	2	1983	-	X
85	MG	2	1984	-	X
85	MG	2	1986	-	X
85	MG	2	1989	-	X
85	MG	2	1990	-	X
85	MG	2	1995	-	X
85	MG	2	1997	-	X
85	MG	2	1998	-	X
85	MG	2	2003	-	X
85	MG	2	2007	-	X
85	MG	2	2008	-	X
85	MG	2	2009	-	X
85	MG	2	2010	-	X
85	MG	2	2011	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	2012	-	X
85	MG	2	2013	-	X
85	MG	2	2014	-	X
85	MG	2	2015	-	X
85	MG	2	2017	-	X
85	MG	2	2018	-	X
85	MG	2	2019	-	X
85	MG	2	2020	-	X
85	MG	2	2023	-	X
85	MG	2	2183	-	X
85	MG	3	201	-	X
85	MG	3	202	-	X
85	MG	3	203	-	X
85	MG	3	204	-	X
85	MG	3	205	-	X
85	MG	3	206	-	X
85	MG	3	207	-	X
85	MG	3	209	-	X
85	MG	3	210	-	X
85	MG	3	212	-	X
85	MG	3	213	-	X
85	MG	3	214	-	X
85	MG	4	203	-	X
85	MG	4	205	-	X
85	MG	4	206	-	X
85	MG	4	211	-	X
85	MG	4	214	-	X
85	MG	4	220	-	X
85	MG	4	221	-	X
85	MG	5	3401	-	X
85	MG	5	3403	-	X
85	MG	5	3409	-	X
85	MG	5	3410	-	X
85	MG	5	3411	-	X
85	MG	5	3412	-	X
85	MG	5	3413	-	X
85	MG	5	3415	-	X
85	MG	5	3416	-	X
85	MG	5	3419	-	X
85	MG	5	3422	-	X
85	MG	5	3423	-	X
85	MG	5	3424	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3426	-	X
85	MG	5	3427	-	X
85	MG	5	3429	-	X
85	MG	5	3431	-	X
85	MG	5	3432	-	X
85	MG	5	3433	-	X
85	MG	5	3438	-	X
85	MG	5	3439	-	X
85	MG	5	3441	-	X
85	MG	5	3442	-	X
85	MG	5	3443	-	X
85	MG	5	3445	-	X
85	MG	5	3446	-	X
85	MG	5	3448	-	X
85	MG	5	3449	-	X
85	MG	5	3453	-	X
85	MG	5	3456	-	X
85	MG	5	3457	-	X
85	MG	5	3458	-	X
85	MG	5	3462	-	X
85	MG	5	3463	-	X
85	MG	5	3465	-	X
85	MG	5	3466	-	X
85	MG	5	3467	-	X
85	MG	5	3468	-	X
85	MG	5	3469	-	X
85	MG	5	3470	-	X
85	MG	5	3472	-	X
85	MG	5	3473	-	X
85	MG	5	3474	-	X
85	MG	5	3475	-	X
85	MG	5	3476	-	X
85	MG	5	3477	-	X
85	MG	5	3479	-	X
85	MG	5	3481	-	X
85	MG	5	3482	-	X
85	MG	5	3490	-	X
85	MG	5	3498	-	X
85	MG	5	3499	-	X
85	MG	5	3502	-	X
85	MG	5	3503	-	X
85	MG	5	3505	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3506	-	X
85	MG	5	3507	-	X
85	MG	5	3508	-	X
85	MG	5	3511	-	X
85	MG	5	3512	-	X
85	MG	5	3514	-	X
85	MG	5	3515	-	X
85	MG	5	3516	-	X
85	MG	5	3517	-	X
85	MG	5	3518	-	X
85	MG	5	3519	-	X
85	MG	5	3520	-	X
85	MG	5	3521	-	X
85	MG	5	3522	-	X
85	MG	5	3523	-	X
85	MG	5	3524	-	X
85	MG	5	3525	-	X
85	MG	5	3526	-	X
85	MG	5	3528	-	X
85	MG	5	3529	-	X
85	MG	5	3530	-	X
85	MG	5	3531	-	X
85	MG	5	3533	-	X
85	MG	5	3534	-	X
85	MG	5	3535	-	X
85	MG	5	3537	-	X
85	MG	5	3538	-	X
85	MG	5	3539	-	X
85	MG	5	3540	-	X
85	MG	5	3541	-	X
85	MG	5	3542	-	X
85	MG	5	3544	-	X
85	MG	5	3546	-	X
85	MG	5	3547	-	X
85	MG	5	3548	-	X
85	MG	5	3549	-	X
85	MG	5	3551	-	X
85	MG	5	3553	-	X
85	MG	5	3555	-	X
85	MG	5	3557	-	X
85	MG	5	3558	-	X
85	MG	5	3559	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3560	-	X
85	MG	5	3561	-	X
85	MG	5	3562	-	X
85	MG	5	3563	-	X
85	MG	5	3564	-	X
85	MG	5	3565	-	X
85	MG	5	3566	-	X
85	MG	5	3567	-	X
85	MG	5	3568	-	X
85	MG	5	3569	-	X
85	MG	5	3570	-	X
85	MG	5	3571	-	X
85	MG	5	3572	-	X
85	MG	5	3573	-	X
85	MG	5	3574	-	X
85	MG	5	3575	-	X
85	MG	5	3576	-	X
85	MG	5	3577	-	X
85	MG	5	3578	-	X
85	MG	5	3579	-	X
85	MG	5	3580	-	X
85	MG	5	3581	-	X
85	MG	5	3582	-	X
85	MG	5	3583	-	X
85	MG	5	3584	-	X
85	MG	5	3585	-	X
85	MG	5	3586	-	X
85	MG	5	3587	-	X
85	MG	5	3588	-	X
85	MG	5	3590	-	X
85	MG	5	3591	-	X
85	MG	5	3592	-	X
85	MG	5	3593	-	X
85	MG	5	3594	-	X
85	MG	5	3595	-	X
85	MG	5	3596	-	X
85	MG	5	3598	-	X
85	MG	5	3605	-	X
85	MG	5	3606	-	X
85	MG	5	3610	-	X
85	MG	5	3612	-	X
85	MG	5	3613	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3618	-	X
85	MG	5	3619	-	X
85	MG	5	3622	-	X
85	MG	5	3623	-	X
85	MG	5	3626	-	X
85	MG	5	3629	-	X
85	MG	5	3630	-	X
85	MG	5	3633	-	X
85	MG	5	3634	-	X
85	MG	5	3638	-	X
85	MG	5	3639	-	X
85	MG	5	3643	-	X
85	MG	5	3644	-	X
85	MG	5	3646	-	X
85	MG	5	3647	-	X
85	MG	5	3648	-	X
85	MG	5	3649	-	X
85	MG	5	3652	-	X
85	MG	5	3655	-	X
85	MG	5	3659	-	X
85	MG	5	3661	-	X
85	MG	5	3662	-	X
85	MG	5	3665	-	X
85	MG	5	3667	-	X
85	MG	5	3670	-	X
85	MG	5	3671	-	X
85	MG	5	3672	-	X
85	MG	5	3673	-	X
85	MG	5	3676	-	X
85	MG	5	3677	-	X
85	MG	5	3680	-	X
85	MG	5	3681	-	X
85	MG	5	3683	-	X
85	MG	5	3693	-	X
85	MG	5	3695	-	X
85	MG	5	3697	-	X
85	MG	5	3700	-	X
85	MG	5	3706	-	X
85	MG	5	3707	-	X
85	MG	5	3710	-	X
85	MG	5	3717	-	X
85	MG	5	3721	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3726	-	X
85	MG	5	3727	-	X
85	MG	5	3730	-	X
85	MG	5	3731	-	X
85	MG	5	3732	-	X
85	MG	5	3734	-	X
85	MG	5	3737	-	X
85	MG	5	3738	-	X
85	MG	5	3743	-	X
85	MG	5	3746	-	X
85	MG	5	3748	-	X
85	MG	5	3751	-	X
85	MG	5	3755	-	X
85	MG	5	3756	-	X
85	MG	5	3757	-	X
85	MG	5	3763	-	X
85	MG	5	3764	-	X
85	MG	5	3766	-	X
85	MG	5	3770	-	X
85	MG	5	3772	-	X
85	MG	5	3776	-	X
85	MG	5	3780	-	X
85	MG	5	3783	-	X
85	MG	5	3785	-	X
85	MG	5	3786	-	X
85	MG	5	3790	-	X
85	MG	5	3793	-	X
85	MG	5	3796	-	X
85	MG	5	3802	-	X
85	MG	5	3803	-	X
85	MG	5	3807	-	X
85	MG	5	3813	-	X
85	MG	5	3815	-	X
85	MG	5	3821	-	X
85	MG	5	3823	-	X
85	MG	5	3825	-	X
85	MG	5	3827	-	X
85	MG	5	3828	-	X
85	MG	5	3832	-	X
85	MG	5	3833	-	X
85	MG	5	3841	-	X
85	MG	5	3844	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3846	-	X
85	MG	5	3847	-	X
85	MG	5	3848	-	X
85	MG	5	3853	-	X
85	MG	5	3855	-	X
85	MG	5	3856	-	X
85	MG	5	3858	-	X
85	MG	5	3864	-	X
85	MG	5	3867	-	X
85	MG	5	3868	-	X
85	MG	5	3869	-	X
85	MG	5	3871	-	X
85	MG	5	3872	-	X
85	MG	5	3874	-	X
85	MG	5	3875	-	X
85	MG	5	3877	-	X
85	MG	5	3880	-	X
85	MG	5	3881	-	X
85	MG	5	3882	-	X
85	MG	5	3884	-	X
85	MG	5	3887	-	X
85	MG	5	3892	-	X
85	MG	5	3894	-	X
85	MG	5	3896	-	X
85	MG	5	4253	-	X
85	MG	5	4254	-	X
85	MG	5	4255	-	X
85	MG	5	4257	-	X
85	MG	6	1901	-	X
85	MG	6	1903	-	X
85	MG	6	1904	-	X
85	MG	6	1906	-	X
85	MG	6	1907	-	X
85	MG	6	1908	-	X
85	MG	6	1909	-	X
85	MG	6	1910	-	X
85	MG	6	1911	-	X
85	MG	6	1912	-	X
85	MG	6	1913	-	X
85	MG	6	1914	-	X
85	MG	6	1916	-	X
85	MG	6	1917	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1918	-	X
85	MG	6	1919	-	X
85	MG	6	1920	-	X
85	MG	6	1921	-	X
85	MG	6	1922	-	X
85	MG	6	1923	-	X
85	MG	6	1925	-	X
85	MG	6	1926	-	X
85	MG	6	1927	-	X
85	MG	6	1928	-	X
85	MG	6	1929	-	X
85	MG	6	1931	-	X
85	MG	6	1933	-	X
85	MG	6	1934	-	X
85	MG	6	1935	-	X
85	MG	6	1936	-	X
85	MG	6	1937	-	X
85	MG	6	1939	-	X
85	MG	6	1940	-	X
85	MG	6	1942	-	X
85	MG	6	1943	-	X
85	MG	6	1944	-	X
85	MG	6	1945	-	X
85	MG	6	1946	-	X
85	MG	6	1947	-	X
85	MG	6	1948	-	X
85	MG	6	1949	-	X
85	MG	6	1950	-	X
85	MG	6	1951	-	X
85	MG	6	1952	-	X
85	MG	6	1954	-	X
85	MG	6	1955	-	X
85	MG	6	1956	-	X
85	MG	6	1957	-	X
85	MG	6	1958	-	X
85	MG	6	1959	-	X
85	MG	6	1960	-	X
85	MG	6	1961	-	X
85	MG	6	1963	-	X
85	MG	6	1964	-	X
85	MG	6	1965	-	X
85	MG	6	1966	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1968	-	X
85	MG	6	1971	-	X
85	MG	6	1975	-	X
85	MG	6	1977	-	X
85	MG	6	1980	-	X
85	MG	6	1983	-	X
85	MG	6	1985	-	X
85	MG	6	1987	-	X
85	MG	6	1991	-	X
85	MG	6	1997	-	X
85	MG	6	1998	-	X
85	MG	6	2000	-	X
85	MG	6	2005	-	X
85	MG	6	2011	-	X
85	MG	6	2012	-	X
85	MG	6	2013	-	X
85	MG	6	2015	-	X
85	MG	6	2018	-	X
85	MG	6	2019	-	X
85	MG	6	2020	-	X
85	MG	6	2021	-	X
85	MG	6	2027	-	X
85	MG	6	2028	-	X
85	MG	6	2029	-	X
85	MG	6	2030	-	X
85	MG	6	2035	-	X
85	MG	6	2038	-	X
85	MG	6	2039	-	X
85	MG	6	2040	-	X
85	MG	6	2042	-	X
85	MG	6	2043	-	X
85	MG	6	2046	-	X
85	MG	7	201	-	X
85	MG	7	202	-	X
85	MG	7	203	-	X
85	MG	7	204	-	X
85	MG	7	205	-	X
85	MG	7	206	-	X
85	MG	7	207	-	X
85	MG	7	209	-	X
85	MG	7	213	-	X
85	MG	7	215	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	8	201	-	X
85	MG	8	203	-	X
85	MG	8	206	-	X
85	MG	8	207	-	X
85	MG	8	213	-	X
85	MG	M3	202	-	X
85	MG	M7	201	-	X
85	MG	N3	201	-	X
85	MG	SM	301	-	X
85	MG	c7	201	-	X
85	MG	c8	201	-	X
85	MG	d3	201	-	X
85	MG	l3	401	-	X
85	MG	l5	301	-	X
85	MG	l7	301	-	X
85	MG	m1	201	-	X
85	MG	m4	201	-	X
85	MG	n3	201	-	X
85	MG	n8	203	-	X
85	MG	n8	204	-	X
85	MG	n9	3802	-	X
85	MG	o1	201	-	X
85	MG	o3	202	-	X
85	MG	o4	202	-	X
85	MG	s1	301	-	X
86	OHX	1	3868	-	X
86	OHX	1	3872	-	X
86	OHX	1	3874	-	X
86	OHX	1	3891	-	X
86	OHX	1	3915	-	X
86	OHX	1	3924	-	X
86	OHX	1	3982	-	X
86	OHX	1	4017	-	X
86	OHX	1	4023	-	X
86	OHX	1	4031	-	X
86	OHX	1	4049	-	X
86	OHX	1	4050	-	X
86	OHX	1	4061	-	X
86	OHX	1	4065	-	X
86	OHX	1	4066	-	X
86	OHX	1	4067	-	X
86	OHX	1	4071	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4073	-	X
86	OHX	1	4076	-	X
86	OHX	1	4081	-	X
86	OHX	1	4085	-	X
86	OHX	1	4086	-	X
86	OHX	1	4098	-	X
86	OHX	1	4102	-	X
86	OHX	1	4111	-	X
86	OHX	1	4113	-	X
86	OHX	1	4114	-	X
86	OHX	1	4116	-	X
86	OHX	1	4118	-	X
86	OHX	1	4122	-	X
86	OHX	1	4123	-	X
86	OHX	1	4124	-	X
86	OHX	1	4125	-	X
86	OHX	1	4128	-	X
86	OHX	1	4129	-	X
86	OHX	1	4130	-	X
86	OHX	1	4135	-	X
86	OHX	1	4136	-	X
86	OHX	1	4138	-	X
86	OHX	1	4140	-	X
86	OHX	1	4141	-	X
86	OHX	1	4142	-	X
86	OHX	1	4144	-	X
86	OHX	1	4145	-	X
86	OHX	1	4146	-	X
86	OHX	1	4148	-	X
86	OHX	1	4149	-	X
86	OHX	1	4150	-	X
86	OHX	1	4155	-	X
86	OHX	1	4156	-	X
86	OHX	1	4157	-	X
86	OHX	1	4160	-	X
86	OHX	1	4161	-	X
86	OHX	1	4162	-	X
86	OHX	1	4165	-	X
86	OHX	1	4166	-	X
86	OHX	1	4167	-	X
86	OHX	1	4169	-	X
86	OHX	1	4170	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4171	-	X
86	OHX	1	4172	-	X
86	OHX	1	4173	-	X
86	OHX	1	4174	-	X
86	OHX	1	4176	-	X
86	OHX	1	4177	-	X
86	OHX	1	4178	-	X
86	OHX	1	4179	-	X
86	OHX	1	4180	-	X
86	OHX	1	4183	-	X
86	OHX	1	4184	-	X
86	OHX	1	4185	-	X
86	OHX	1	4187	-	X
86	OHX	1	4188	-	X
86	OHX	1	4189	-	X
86	OHX	1	4191	-	X
86	OHX	1	4192	-	X
86	OHX	1	4193	-	X
86	OHX	1	4195	-	X
86	OHX	1	4197	-	X
86	OHX	1	4199	-	X
86	OHX	1	4201	-	X
86	OHX	1	4202	-	X
86	OHX	1	4203	-	X
86	OHX	1	4204	-	X
86	OHX	1	4205	-	X
86	OHX	1	4206	-	X
86	OHX	1	4208	-	X
86	OHX	1	4209	-	X
86	OHX	1	4210	-	X
86	OHX	1	4211	-	X
86	OHX	1	4212	-	X
86	OHX	1	4214	-	X
86	OHX	1	4215	-	X
86	OHX	2	2026	-	X
86	OHX	2	2031	-	X
86	OHX	2	2075	-	X
86	OHX	2	2080	-	X
86	OHX	2	2099	-	X
86	OHX	2	2103	-	X
86	OHX	2	2117	-	X
86	OHX	2	2119	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	2	2123	-	X
86	OHX	2	2126	-	X
86	OHX	2	2134	-	X
86	OHX	2	2136	-	X
86	OHX	2	2137	-	X
86	OHX	2	2138	-	X
86	OHX	2	2144	-	X
86	OHX	2	2146	-	X
86	OHX	2	2147	-	X
86	OHX	2	2149	-	X
86	OHX	2	2154	-	X
86	OHX	2	2155	-	X
86	OHX	2	2156	-	X
86	OHX	2	2158	-	X
86	OHX	2	2160	-	X
86	OHX	2	2161	-	X
86	OHX	2	2163	-	X
86	OHX	2	2164	-	X
86	OHX	2	2165	-	X
86	OHX	2	2167	-	X
86	OHX	2	2170	-	X
86	OHX	2	2172	-	X
86	OHX	2	2173	-	X
86	OHX	2	2174	-	X
86	OHX	2	2176	-	X
86	OHX	2	2177	-	X
86	OHX	2	2179	-	X
86	OHX	2	2180	-	X
86	OHX	3	223	-	X
86	OHX	3	225	-	X
86	OHX	4	227	-	X
86	OHX	4	232	-	X
86	OHX	4	233	-	X
86	OHX	4	235	-	X
86	OHX	4	236	-	X
86	OHX	5	3899	-	X
86	OHX	5	3900	-	X
86	OHX	5	3903	-	X
86	OHX	5	3909	-	X
86	OHX	5	3912	-	X
86	OHX	5	3913	-	X
86	OHX	5	3951	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4027	-	X
86	OHX	5	4039	-	X
86	OHX	5	4044	-	X
86	OHX	5	4089	-	X
86	OHX	5	4092	-	X
86	OHX	5	4099	-	X
86	OHX	5	4105	-	X
86	OHX	5	4108	-	X
86	OHX	5	4110	-	X
86	OHX	5	4112	-	X
86	OHX	5	4114	-	X
86	OHX	5	4125	-	X
86	OHX	5	4126	-	X
86	OHX	5	4127	-	X
86	OHX	5	4132	-	X
86	OHX	5	4134	-	X
86	OHX	5	4136	-	X
86	OHX	5	4137	-	X
86	OHX	5	4139	-	X
86	OHX	5	4140	-	X
86	OHX	5	4141	-	X
86	OHX	5	4142	-	X
86	OHX	5	4144	-	X
86	OHX	5	4145	-	X
86	OHX	5	4146	-	X
86	OHX	5	4147	-	X
86	OHX	5	4148	-	X
86	OHX	5	4149	-	X
86	OHX	5	4150	-	X
86	OHX	5	4151	-	X
86	OHX	5	4152	-	X
86	OHX	5	4154	-	X
86	OHX	5	4156	-	X
86	OHX	5	4157	-	X
86	OHX	5	4158	-	X
86	OHX	5	4159	-	X
86	OHX	5	4160	-	X
86	OHX	5	4161	-	X
86	OHX	5	4163	-	X
86	OHX	5	4164	-	X
86	OHX	5	4170	-	X
86	OHX	5	4171	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4172	-	X
86	OHX	5	4173	-	X
86	OHX	5	4175	-	X
86	OHX	5	4176	-	X
86	OHX	5	4177	-	X
86	OHX	5	4179	-	X
86	OHX	5	4181	-	X
86	OHX	5	4182	-	X
86	OHX	5	4183	-	X
86	OHX	5	4184	-	X
86	OHX	5	4185	-	X
86	OHX	5	4188	-	X
86	OHX	5	4189	-	X
86	OHX	5	4190	-	X
86	OHX	5	4191	-	X
86	OHX	5	4193	-	X
86	OHX	5	4194	-	X
86	OHX	5	4195	-	X
86	OHX	5	4199	-	X
86	OHX	5	4200	-	X
86	OHX	5	4201	-	X
86	OHX	5	4202	-	X
86	OHX	5	4203	-	X
86	OHX	5	4208	-	X
86	OHX	5	4210	-	X
86	OHX	5	4211	-	X
86	OHX	5	4212	-	X
86	OHX	5	4214	-	X
86	OHX	5	4216	-	X
86	OHX	5	4217	-	X
86	OHX	5	4218	-	X
86	OHX	5	4219	-	X
86	OHX	5	4220	-	X
86	OHX	5	4221	-	X
86	OHX	5	4225	-	X
86	OHX	5	4227	-	X
86	OHX	5	4228	-	X
86	OHX	5	4229	-	X
86	OHX	5	4230	-	X
86	OHX	5	4233	-	X
86	OHX	5	4234	-	X
86	OHX	5	4235	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4236	-	X
86	OHX	5	4238	-	X
86	OHX	5	4239	-	X
86	OHX	5	4244	-	X
86	OHX	5	4245	-	X
86	OHX	5	4246	-	X
86	OHX	5	4247	-	X
86	OHX	5	4248	-	X
86	OHX	6	2048	-	X
86	OHX	6	2053	-	X
86	OHX	6	2055	-	X
86	OHX	6	2126	-	X
86	OHX	6	2127	-	X
86	OHX	6	2144	-	X
86	OHX	6	2147	-	X
86	OHX	6	2157	-	X
86	OHX	6	2160	-	X
86	OHX	6	2161	-	X
86	OHX	6	2162	-	X
86	OHX	6	2163	-	X
86	OHX	6	2165	-	X
86	OHX	6	2168	-	X
86	OHX	6	2169	-	X
86	OHX	6	2171	-	X
86	OHX	6	2174	-	X
86	OHX	6	2176	-	X
86	OHX	6	2177	-	X
86	OHX	6	2178	-	X
86	OHX	6	2180	-	X
86	OHX	6	2181	-	X
86	OHX	6	2183	-	X
86	OHX	6	2184	-	X
86	OHX	6	2186	-	X
86	OHX	6	2187	-	X
86	OHX	6	2188	-	X
86	OHX	6	2189	-	X
86	OHX	6	2190	-	X
86	OHX	6	2191	-	X
86	OHX	6	2194	-	X
86	OHX	6	2195	-	X
86	OHX	6	2196	-	X
86	OHX	6	2197	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	6	2198	-	X
86	OHX	6	2199	-	X
86	OHX	6	2200	-	X
86	OHX	6	2203	-	X
86	OHX	6	2204	-	X
86	OHX	7	225	-	X
86	OHX	7	227	-	X
86	OHX	8	219	-	X
86	OHX	8	224	-	X
86	OHX	8	225	-	X
86	OHX	8	227	-	X
86	OHX	8	228	-	X
86	OHX	8	229	-	X
86	OHX	M7	207	-	X
86	OHX	M9	202	-	X
86	OHX	O9	101	-	X
86	OHX	l4	403	-	X
86	OHX	m7	206	-	X
86	OHX	s9	201	-	X
87	ZN	d7	101	-	X
88	3H3	1	4216	-	X

## 2 Entry composition

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

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 rRNA.

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		0	0	0
			1481	951	265	265				
9	s7	186	Total	C	N	O		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 *Saccharomyces cerevisiae* chromosome XII cosmid 9634.

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 Yeast 5S rRNA gene.

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 *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97.

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	l2	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	l3	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	l4	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	l5	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	l6	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	l7	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	l8	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	l9	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		0	0	0
			612	391	115	106				
74	o8	77	Total	C	N	O		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...*

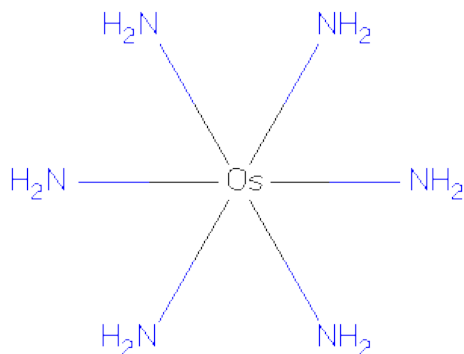
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N3	3	Total 3	Mg 3	0	0
85	N8	2	Total 2	Mg 2	0	0
85	4	21	Total 21	Mg 21	0	0
85	L2	1	Total 1	Mg 1	0	0
85	l5	3	Total 3	Mg 3	0	0
85	C3	1	Total 1	Mg 1	0	0
85	M7	6	Total 6	Mg 6	0	0
85	m4	1	Total 1	Mg 1	0	0
85	L6	1	Total 1	Mg 1	0	0
85	s1	1	Total 1	Mg 1	0	0
85	m6	1	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		

*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		

*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	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	S8	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		
86	C8	1	Total	N	Os	0	0
			7	6	1		
86	D9	1	Total	N	Os	0	0
			7	6	1		
86	SR	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		
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		
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		
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		
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	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 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L4	1	Total 7	N 6	Os 1	0	0
86	L6	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M6	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	N9	1	Total 7	N 6	Os 1	0	0
86	O2	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0

*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		
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		
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		
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...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	c8	1	Total	N	Os	0	0
			7	6	1		
86	d4	1	Total	N	Os	0	0
			7	6	1		
86	d9	1	Total	N	Os	0	0
			7	6	1		
86	sR	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		
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		
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		
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	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	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	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	19	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		

*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		

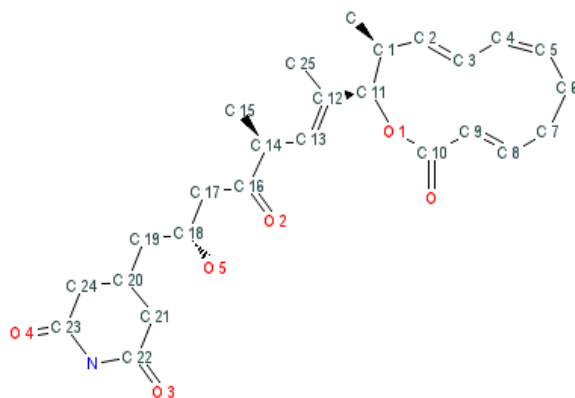
*Continued on next page...*



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: C<sub>26</sub>H<sub>35</sub>NO<sub>6</sub>).

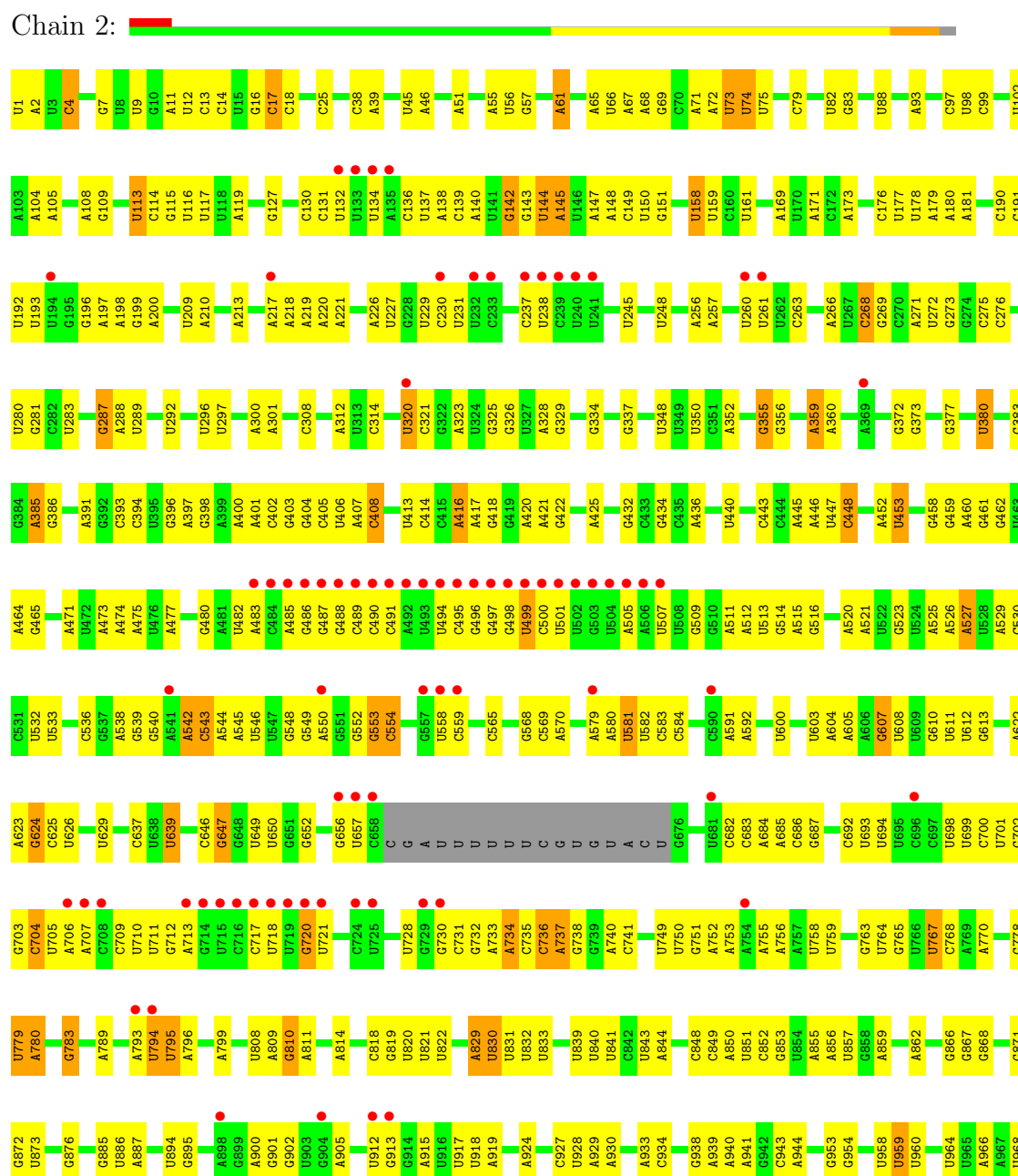


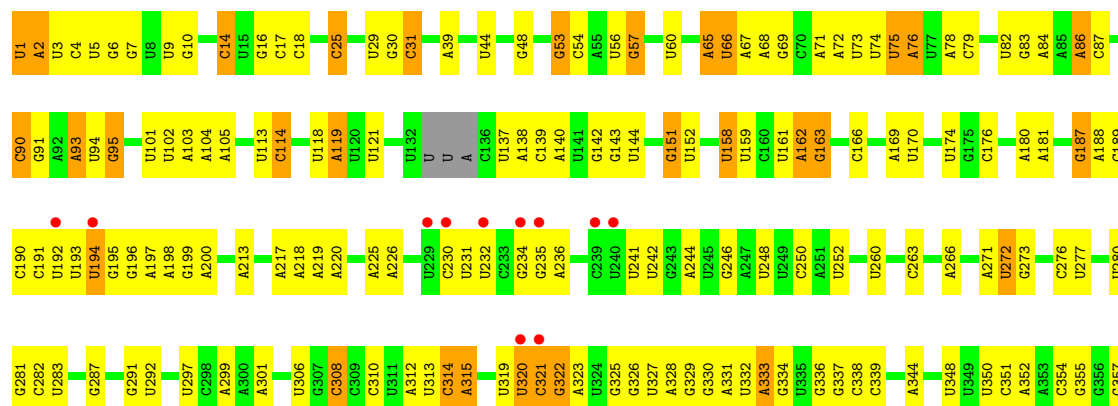
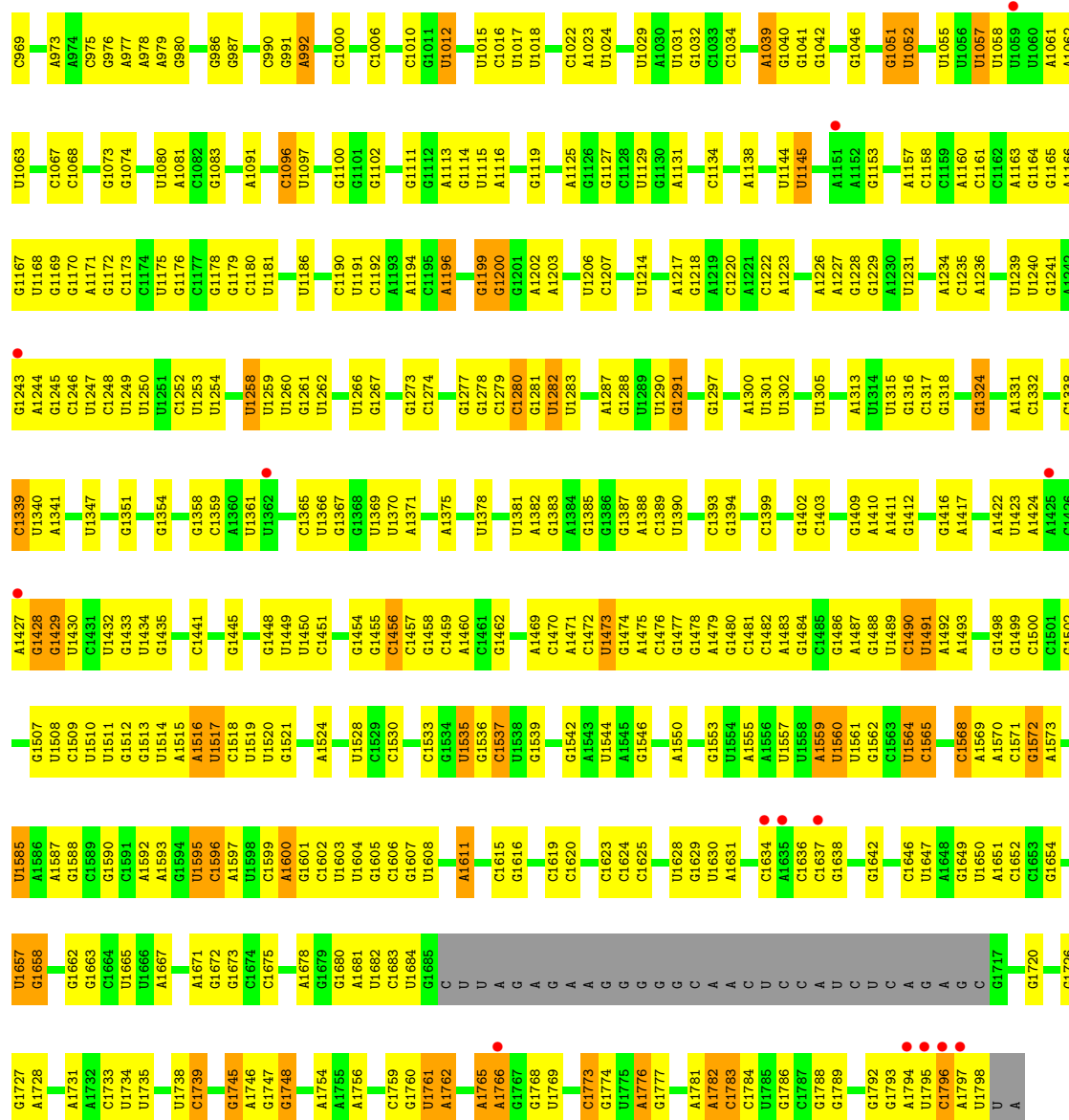
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			33	26	1	6		
88	5	1	Total	C	N	O	0	0
			33	26	1	6		

### 3 Residue-property plots

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

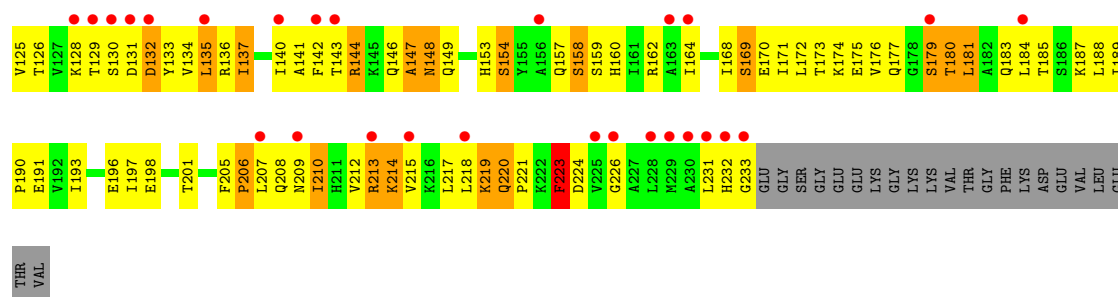
#### • Molecule 1: 18S rRNA





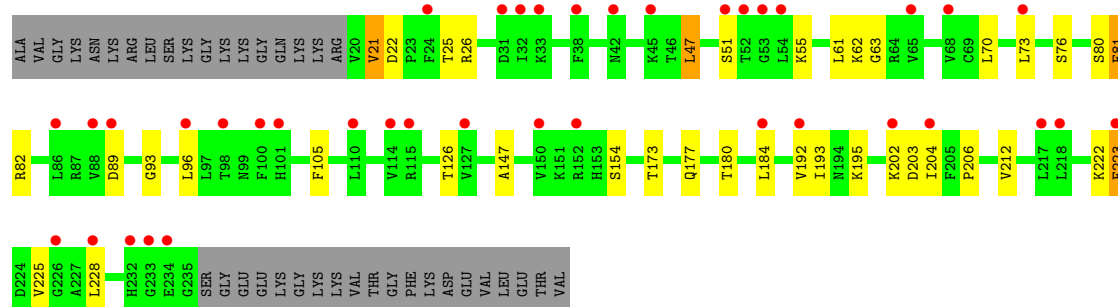
U1579	G1502	A1417	G1318	C1216	A1133	G1048	U965	U857	G765	U675	G597	A521	A437	U358
G1584	A1503	G1418	A1321	A1217	C1134	U1049	A956	G858	U766	G676	U600	G523	C443	A359
G1504	A1505	A1426	G1330	A1219	A1138	G1063	U968	A862	U767	A678	A601	G523	C443	A360
A1587	U1508	A1425	A1331	A1227	U1144	U1068	A973	A863	A770	U679	U603	A529	C449	G362
G1588	C1332	A1427	C1332	G1228	U1145	U1059	A978	U864	G775	U680	A604	U532	U453	A369
C1589	U1510	G1428	G1333	G1229	U1146	U1064	A979	G871	G778	C682	G607	U533	U454	A370
G1590	U1511	U1430	U1335	A1230	C1148	G1064	G980	G872	U782	C683	U609	C536	U455	U374
C1591	G1512	C1431	A1336	G1234	G1149	A1065	G986	U873	U783	U695	U610	C537	U456	U375
A1592	G1513	U1432	U1340	C1235	G1150	C1068	G987	C874	U788	C696	G613	A538	C376	G377
U1595	U1514	G1433	U1341	A1236	A1151	A1069	G988	G875	A788	C697	G614	C539	C459	G378
C1596	A1515	U1434	A1341	G1237	A1152	C1070	G989	G876	U793	C698	G615	G540	A470	A378
A1597	A1516	G1435	A1344	A1238	G1153	U1071	U989	U879	U794	U699	A615	A541	A471	U379
U1598	U1517	A1436	A1345	U1239	G1154	C1072	G990	G879	U795	C700	A623	C543	A474	U380
C1599	C1518	U1437	A1345	U1240	A1157	G1073	G991	G880	U800	G701	G624	A544	U476	C381
A1600	U1521	C1441	U1350	G1241	A1158	U1074	G992	U884	U801	U702	G625	A545	U477	C382
G1601	A1524	U1442	G1351	A1242	A1160	C1078	A993	G995	G801	G703	U629	U546	A478	A387
G1605	A1525	A1444	G1354	G1243	C1161	C1083	G994	G902	A804	C704	A630	U547	U481	G388
U1608	A1529	A1445	A1357	G1245	C1162	U1080	A995	G903	A805	U705	U633	U548	U482	G389
A1611	C1529	G1448	A1358	U1246	A1163	A1081	U996	G904	A806	A706	U634	A550	A483	G390
G1614	G1534	U1449	C1359	C1248	A1166	C1082	U1000	U901	U813	A713	A635	C554	C484	C393
A1615	U1535	G1455	A1360	U1249	G1167	U1083	A1001	G902	A814	G715	A636	C557	A485	C394
G1616	G1536	A1456	U1361	U1250	C1171	A1084	G1002	U903	G815	U716	U638	U558	C487	A397
C1617	C1537	C1457	U1362	U1251	A1171	G1085	A1003	G904	G816	C717	U639	U563	C488	G398
U1619	U1538	G1458	G1364	U1253	U1175	A1088	C1006	A915	A817	C718	U639	U564	C489	A399
C1620	G1539	C1459	G1365	U1254	G1176	A1091	C1010	U916	C818	U719	C646	G563	C490	A400
U1621	U1540	A1460	U1366	G1255	C1177	A1092	G1011	U917	G819	U720	C647	C565	C491	A401
G1622	G1541	C1461	U1370	U1257	G1178	U1095	G1014	U918	U820	G721	C648	C566	A492	C402
U1628	G1542	C1462	A1371	U1258	G1179	U1096	U1015	U919	U821	U722	U657	A567	U493	G403
G1629	A1543	G1464	C1379	U1259	C1180	U1097	C1016	U921	U822	G723	C652	G568	U494	G404
U1630	U1544	C1465	A1382	G1263	A1183	U1098	U1017	G922	G823	U724	C653	C569	C495	C405
A1631	C1549	U1471	A1382	G1264	C1192	U1099	U1018	A923	G824	U727	C654	A570	C496	U406
C1634	U1552	U1472	G1385	G1268	A1193	G1100	C1022	A926	U825	U728	C655	G571	C497	U407
A1635	G1553	U1473	G1385	U1269	A1194	G1101	U1026	C931	U826	G729	C656	C572	U498	C408
C1637	U1558	G1477	A1388	C1274	C1196	U1103	A1027	C934	U829	G730	C658	G577	C500	A410
G1638	A1559	A1478	C1389	C1279	C1197	G1107	A1028	C934	U830	U733	C659	A579	U501	A416
C1639	U1560	A1479	U1392	C1280	G1198	G1108	U1029	A944	U831	A734	C660	C583	U502	A417
U1645	G1562	C1481	C1393	G1281	G1199	U1109	A1030	U945	U832	G737	U662	C584	U503	G418
G1645	U1563	C1482	G1394	U1282	G1200	G1201	U1031	U946	U833	U738	U663	A585	A505	A421
U1649	U1564	A1487	G1395	U1283	G1201	G1119	G1032	U947	G837	C747	U664	G586	U507	G422
U1650	C1565	U1488	U1396	U1293	A1202	U1120	C1033	U951	G838	U751	U665	C587	U508	A425
A1651	U1566	G1489	U1397	U1294	A1203	C1121	G1034	A951	U843	G751	U666	U588	A511	G429
G1654	C1568	C1490	U1398	G1299	C1207	G1122	A1035	C956	U844	A752	U667	C589	A512	C430
A1655	U1569	U1491	A1400	C1309	A1208	C1123	A1036	G957	G846	G669	C590	A591	U513	G431
U1656	A1401	A1492	A1401	U1312	C1209	A1125	A1039	U958	A847	A754	G670	A592	G514	C431
U1657	G1402	A1493	G1402	A1312	C1210	G1126	G1040	U959	C848	A755	U670	U593	A515	G432
A1658	A1573	C1494	G1408	U1317	A1211	G1129	G1041	U960	C849	A756	G	A594	G516	C433
A1659	G1574	G1498	G1409	C1317	G1212	U1129	U1045	U964	A856	A757	U	G595	U517	G434
A1660					G1213	G1130							A518	





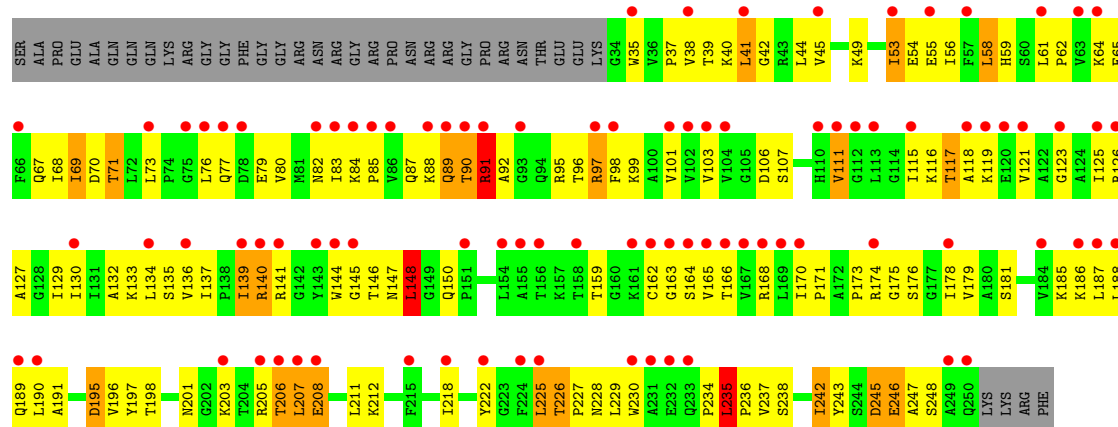
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



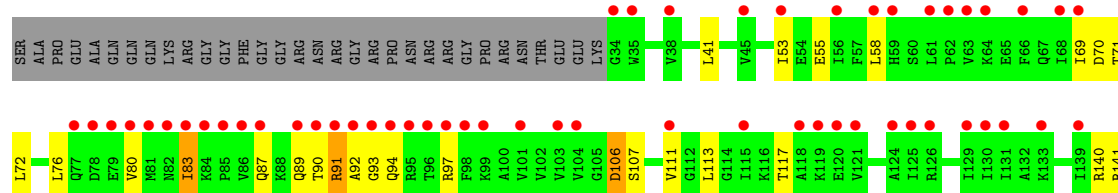
• Molecule 4: 40S ribosomal protein S2

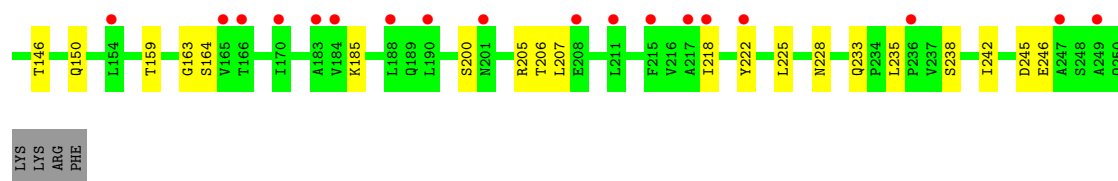
Chain S2:



• Molecule 4: 40S ribosomal protein S2

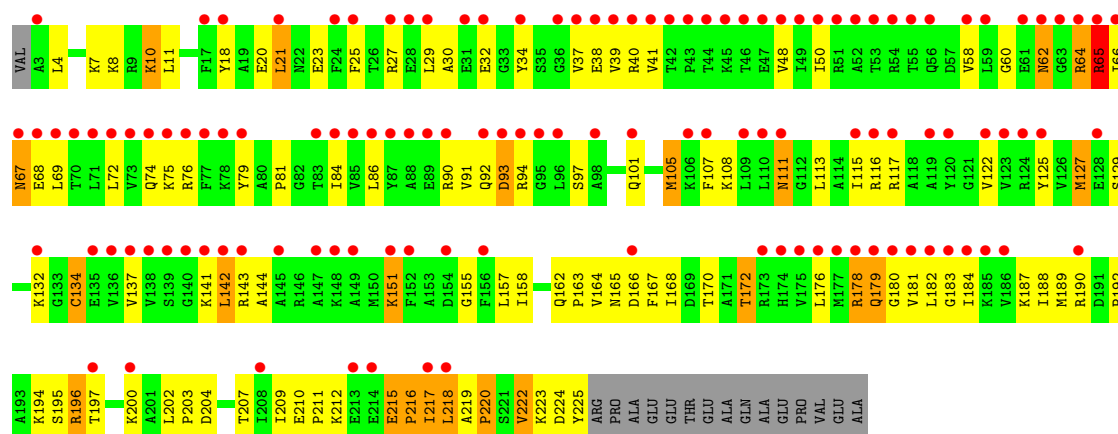
Chain s2:





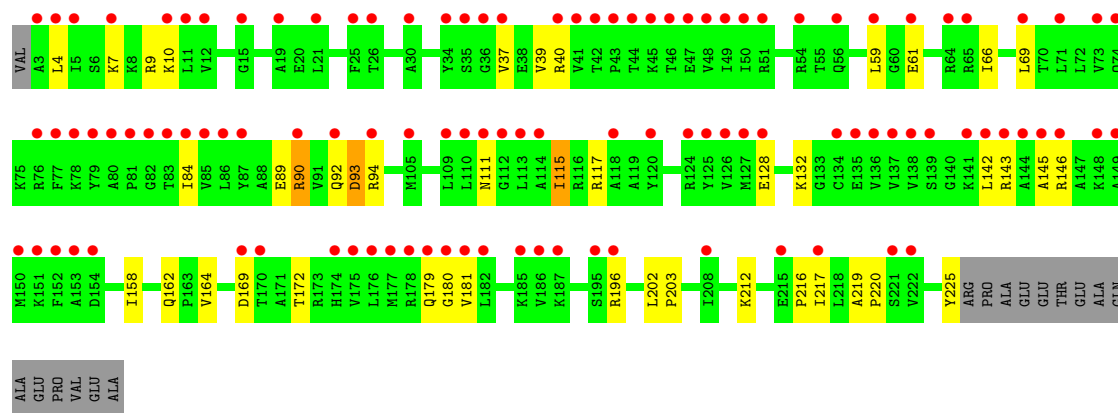
• Molecule 5: 40S ribosomal protein S3

Chain S3:



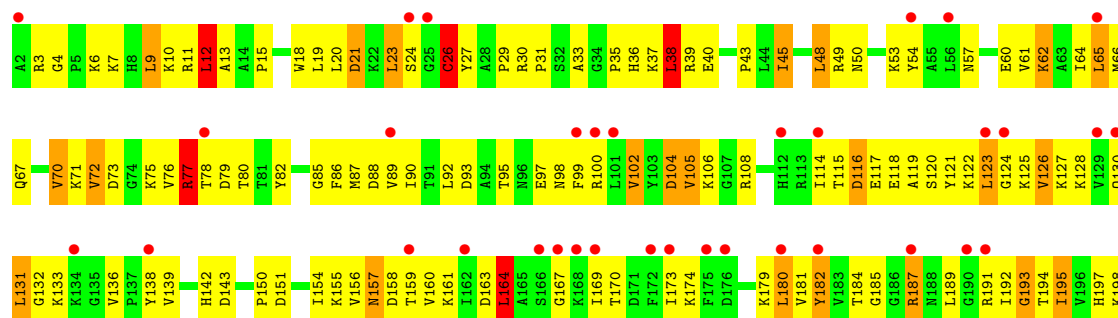
• Molecule 5: 40S ribosomal protein S3

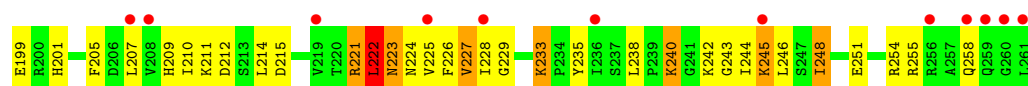
Chain s3:



• Molecule 6: 40S ribosomal protein S4-A

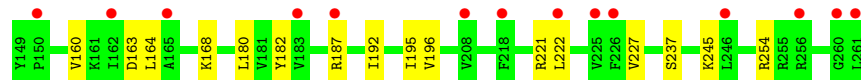
Chain S4:





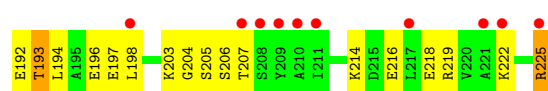
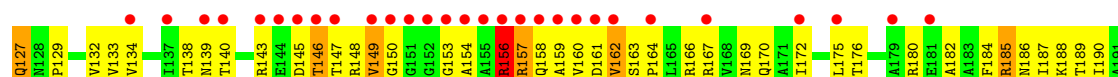
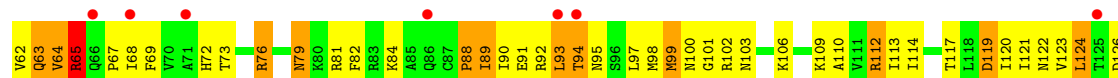
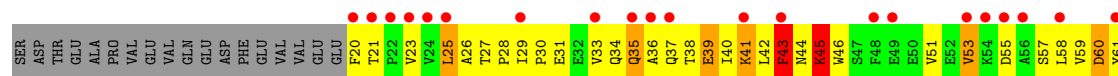
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



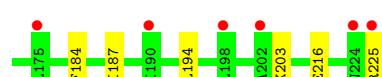
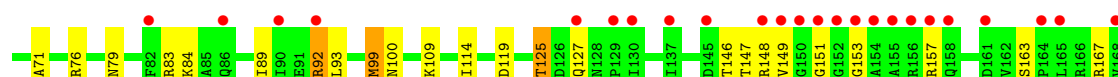
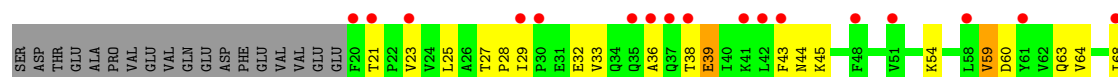
• Molecule 7: 40S ribosomal protein S5

Chain S5:



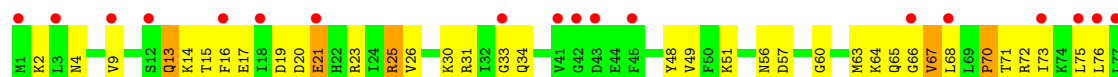
• Molecule 7: 40S ribosomal protein S5

Chain s5:

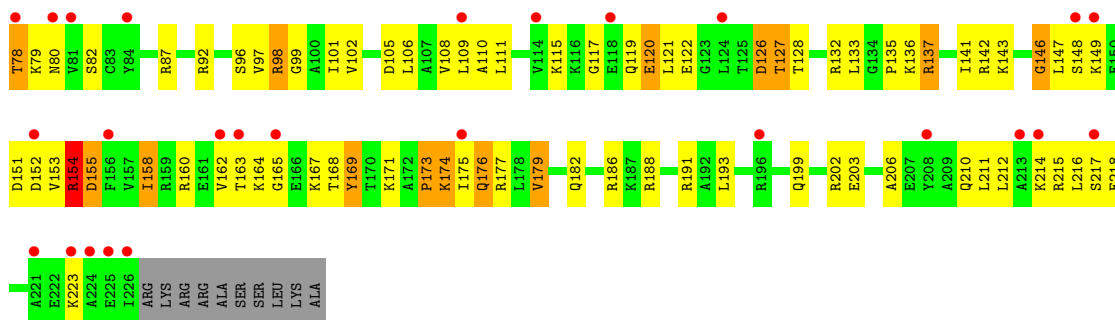


• Molecule 8: 40S ribosomal protein S6-A

Chain S6:

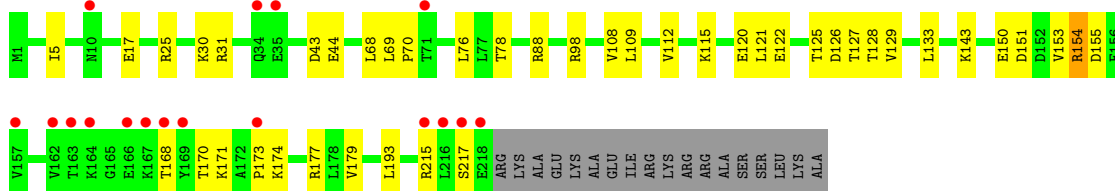






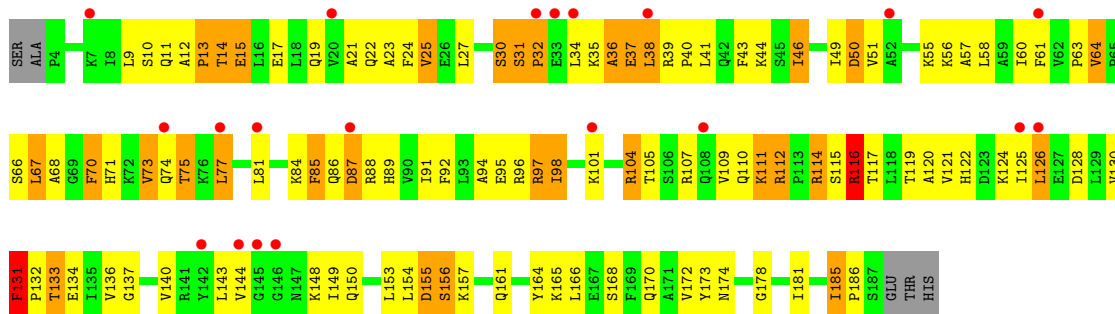
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



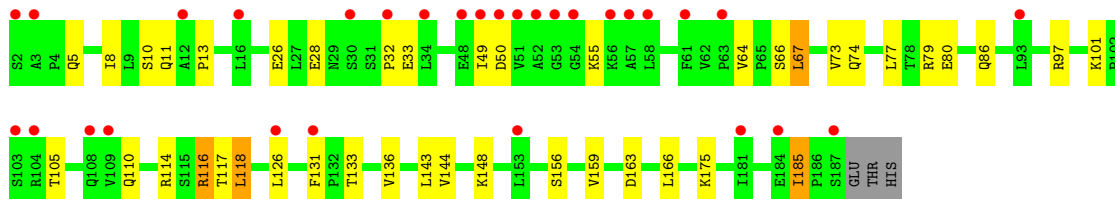
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



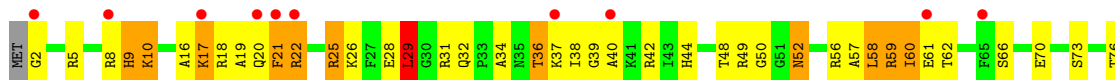
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:

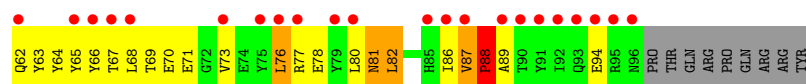


• Molecule 10: 40S ribosomal protein S8-A

Chain S8:

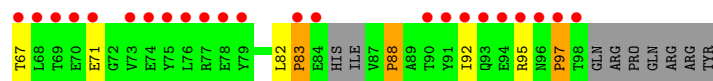
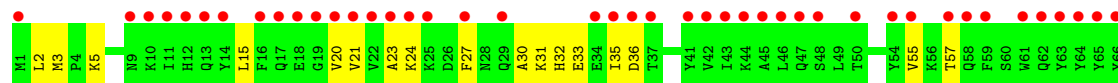






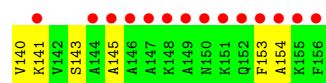
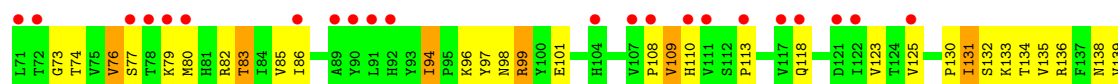
• Molecule 12: 40S ribosomal protein S10-A

Chain c0:



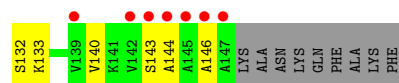
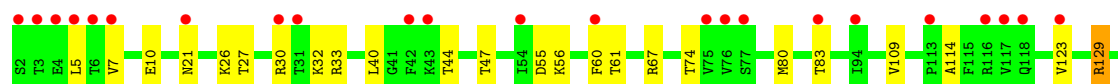
• Molecule 13: 40S ribosomal protein S11-A

Chain C1:



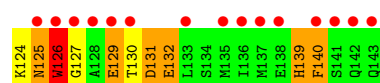
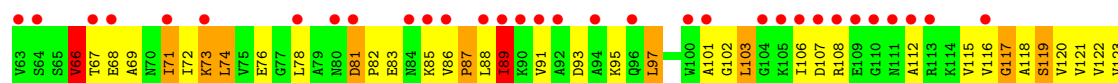
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



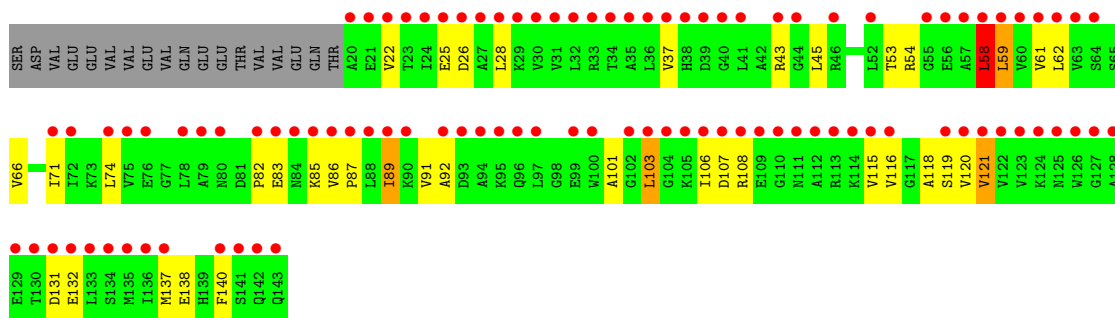
• Molecule 14: 40S ribosomal protein S12

Chain C2:



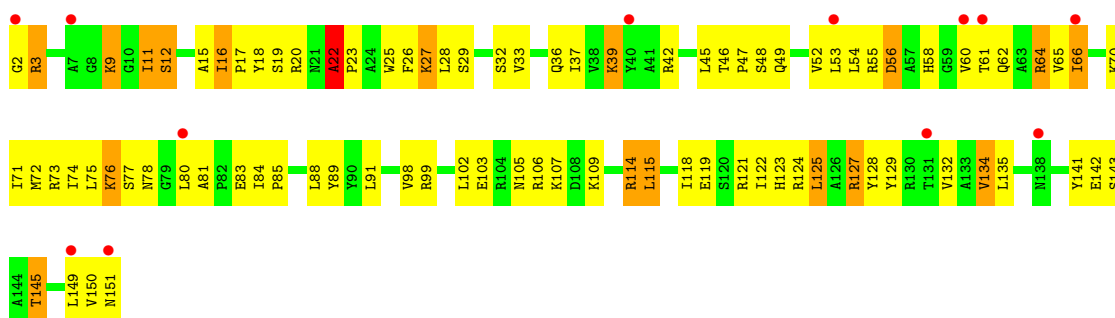
• Molecule 14: 40S ribosomal protein S12

Chain c2:



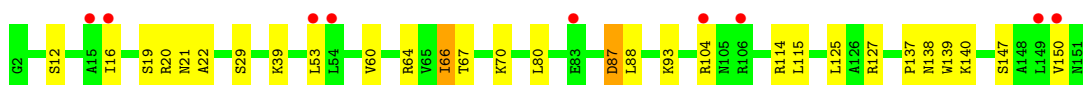
- Molecule 15: 40S ribosomal protein S13

Chain C3:



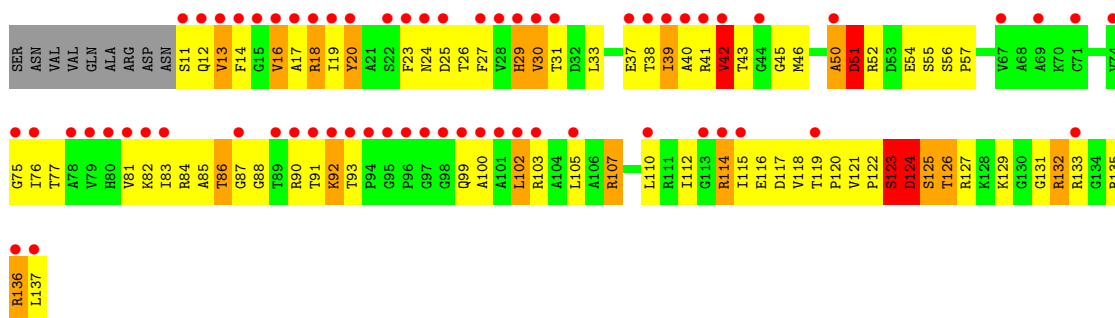
- Molecule 15: 40S ribosomal protein S13

Chain c3:



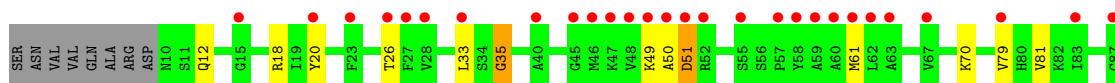
- Molecule 16: 40S ribosomal protein S14-A

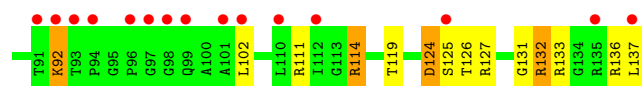
Chain C4:



- Molecule 16: 40S ribosomal protein S14-A

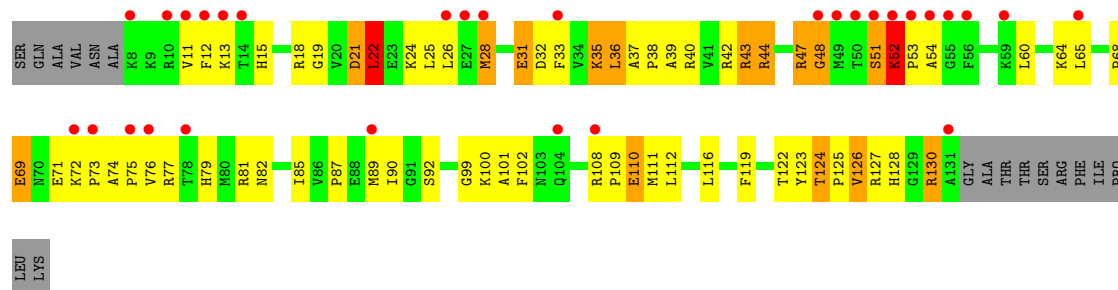
Chain c4:





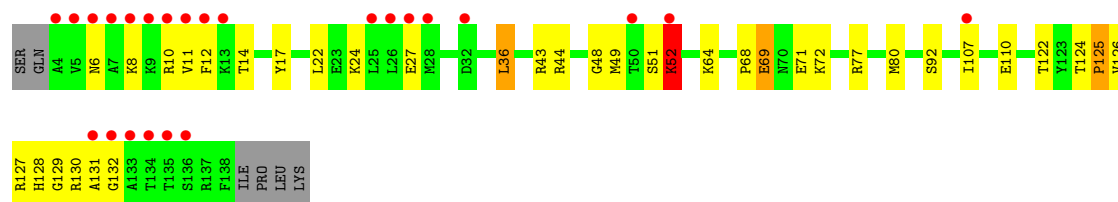
- Molecule 17: 40S ribosomal protein S15

Chain C5:



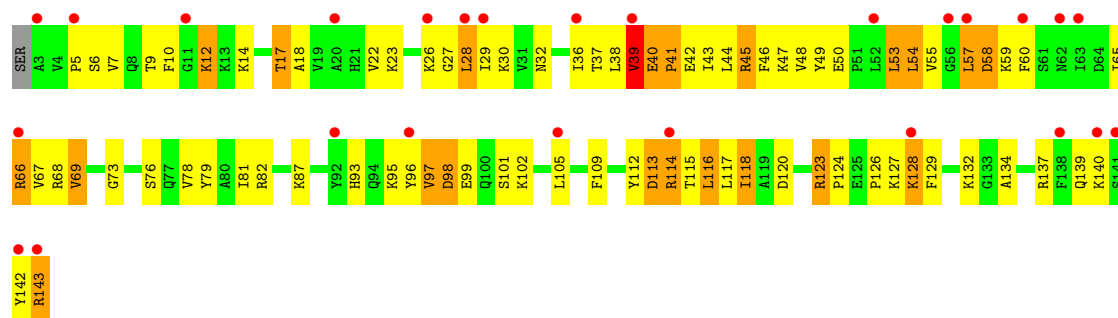
- Molecule 17: 40S ribosomal protein S15

Chain c5:



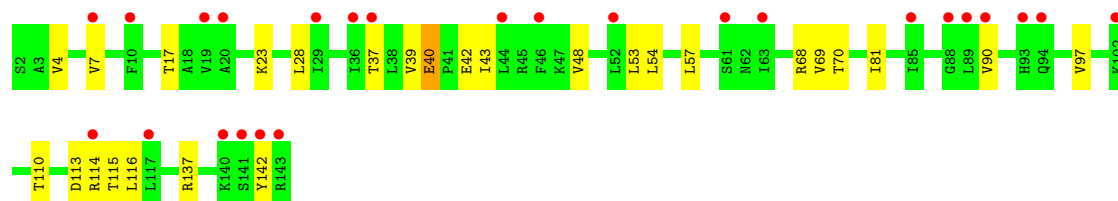
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



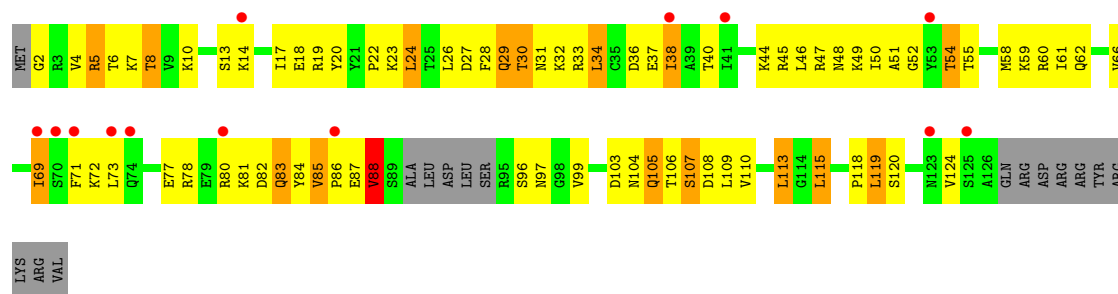
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:



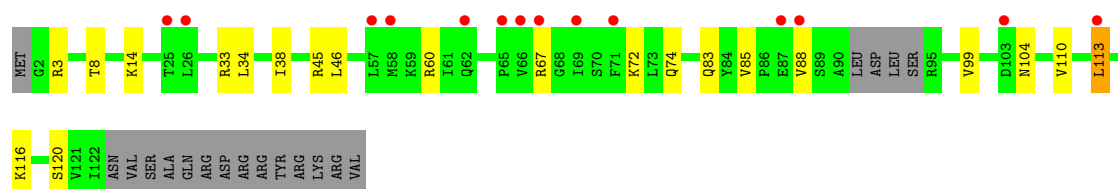
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 



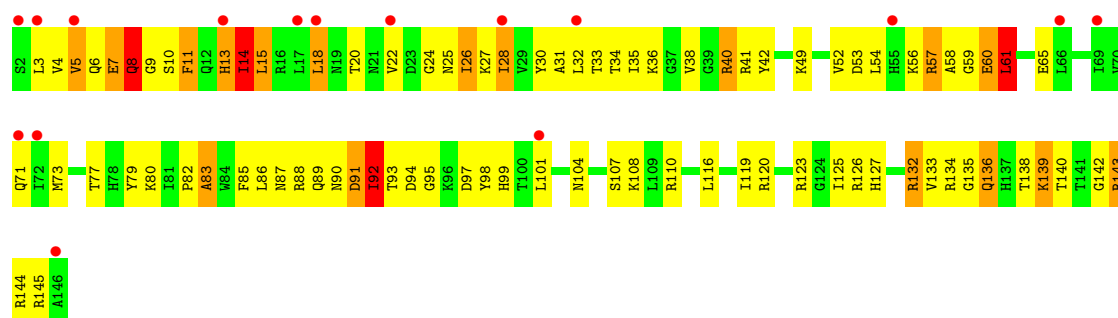
- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 



- Molecule 20: 40S ribosomal protein S18-A

Chain C8: 



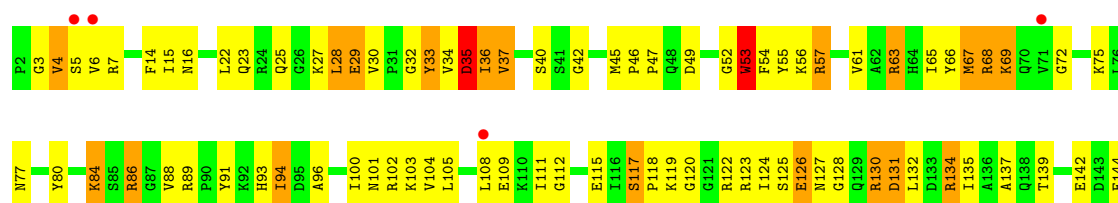
- Molecule 20: 40S ribosomal protein S18-A

Chain c8: 



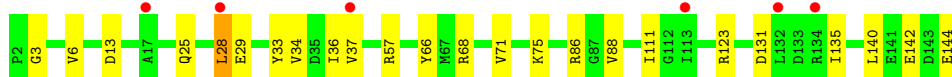
- Molecule 21: 40S ribosomal protein S19-A

Chain C9: 



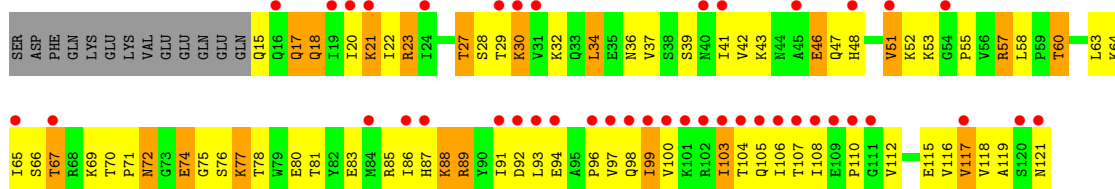
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



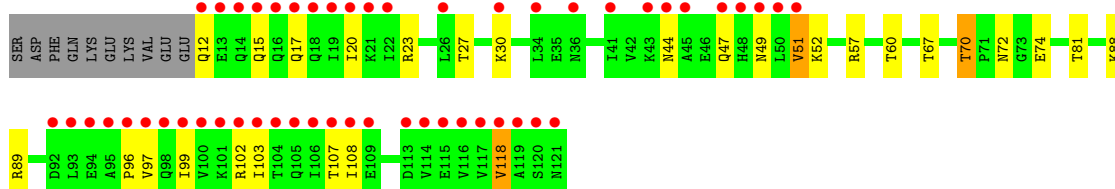
- Molecule 22: 40S ribosomal protein S20

Chain D0:



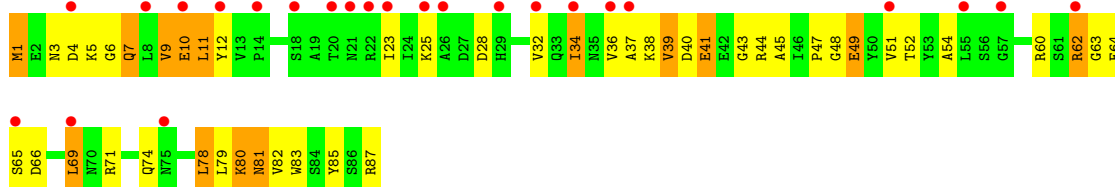
- Molecule 22: 40S ribosomal protein S20

Chain d0:



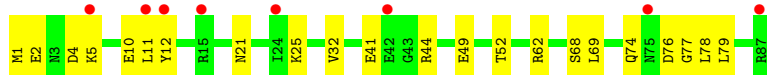
- Molecule 23: 40S ribosomal protein S21-A

Chain D1:



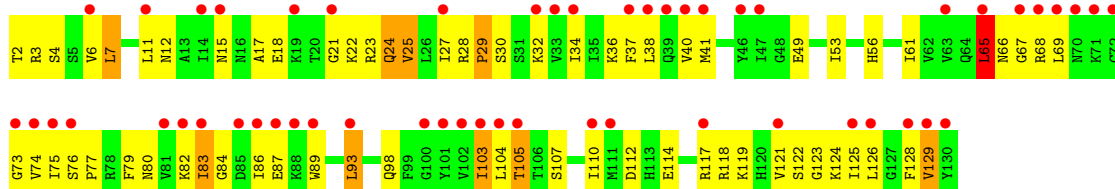
- Molecule 23: 40S ribosomal protein S21-A

Chain d1:



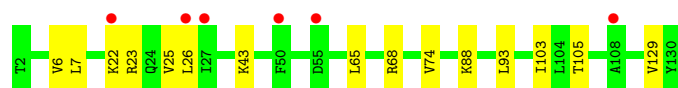
- Molecule 24: 40S ribosomal protein S22-A

Chain D2:



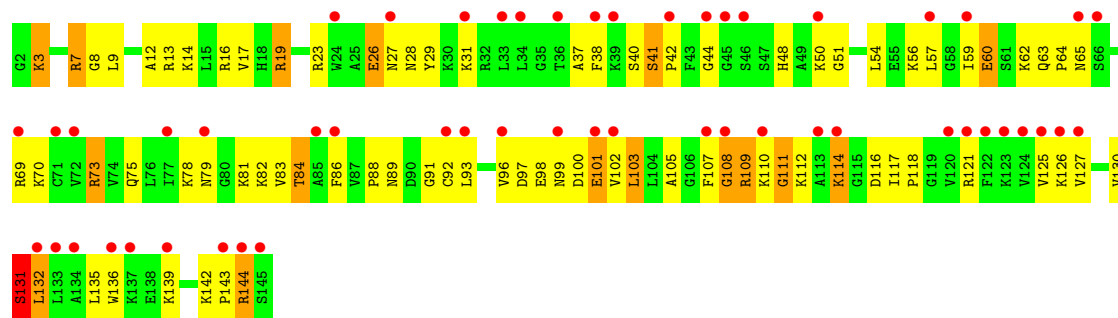
- Molecule 24: 40S ribosomal protein S22-A

Chain d2: 



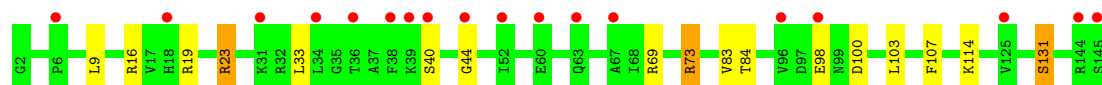
- Molecule 25: 40S ribosomal protein S23-A

Chain D3: 



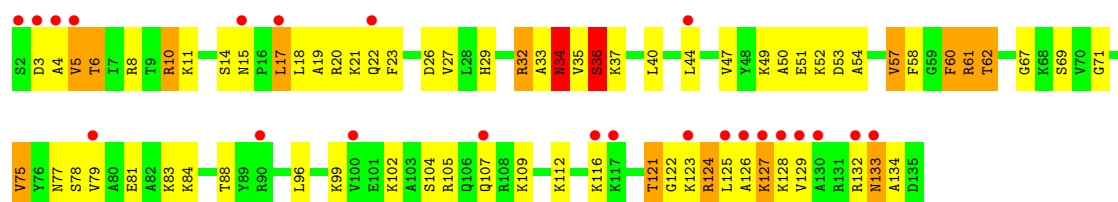
- Molecule 25: 40S ribosomal protein S23-A

Chain d3: 



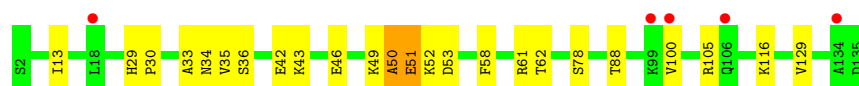
- Molecule 26: 40S ribosomal protein S24-A

Chain D4: 



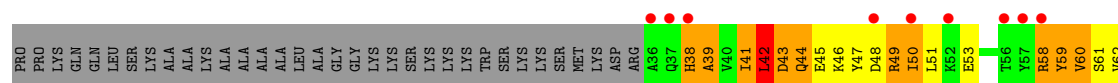
- Molecule 26: 40S ribosomal protein S24-A

Chain d4: 

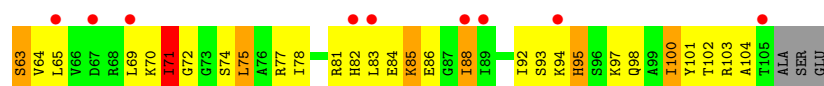


- Molecule 27: 40S ribosomal protein S25-A

Chain D5: 

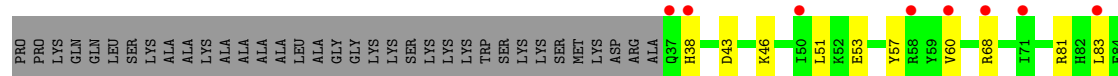






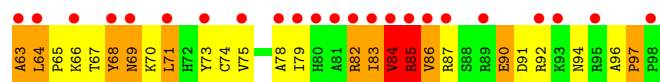
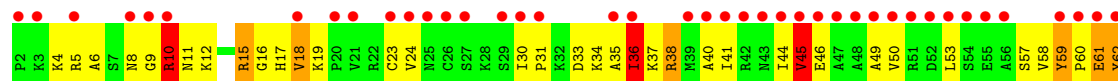
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:



- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



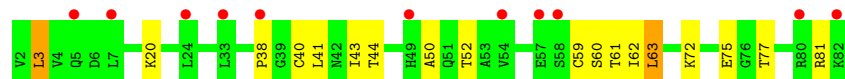
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



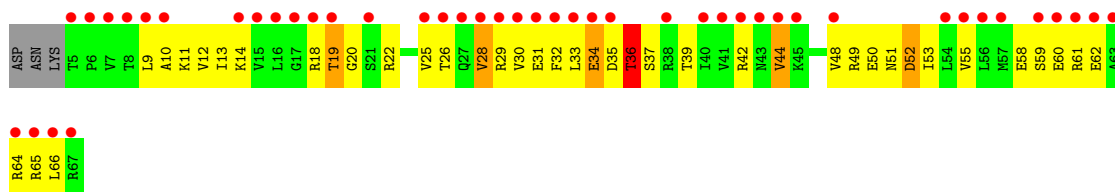
- Molecule 29: 40S ribosomal protein S27-A

Chain d7:



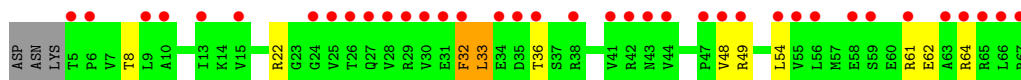
- Molecule 30: 40S ribosomal protein S28-A

Chain D8:



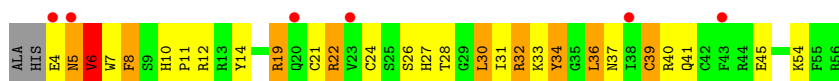
- Molecule 30: 40S ribosomal protein S28-A

Chain d8:



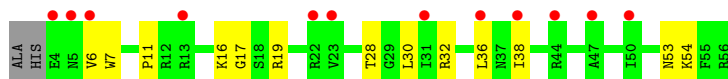
- Molecule 31: 40S ribosomal protein S29-A

Chain D9:



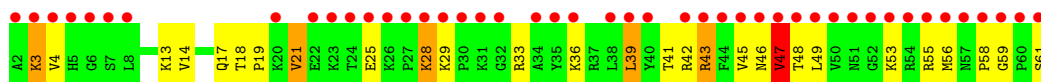
- Molecule 31: 40S ribosomal protein S29-A

Chain d9:



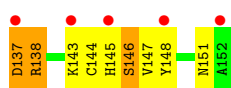
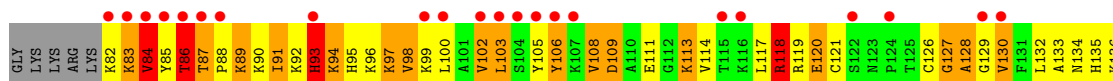
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:



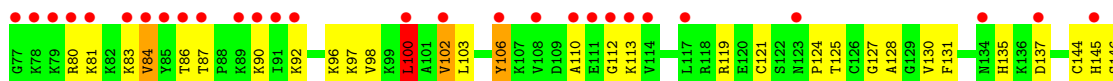
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:

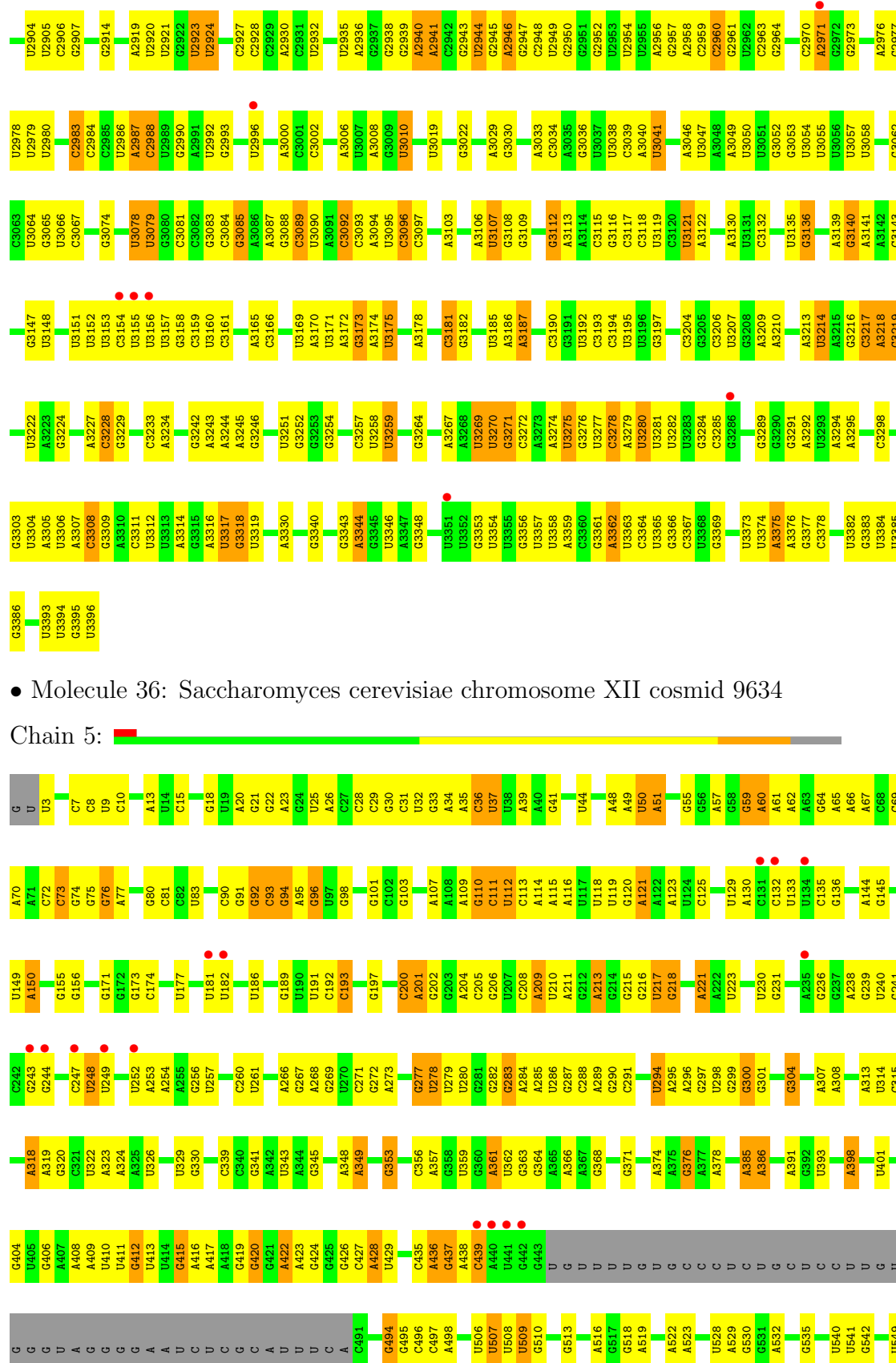






C1708	A1605	G1528	A1454	G1319	U1241	A1158	U1096	G999	A925	G857	A780	U689	G625
C1709	U1606	G1528	U1455	C1320	G1242	A1159	G1097	C1000	A926	A858	A781	A690	U626
G1713	C1608	G1536	A1456	G1321	G1243	G1160	U1100		C927	A859	G782	A691	U627
A1714	C1609			U1322	A1244	G1161	A1103	U1004	A929	G860	A783	A692	A628
A1715	G1610	U1540	C1459	U1323	G1245	U1162	G1104	G1005	U930	C861	A784	A693	U629
U1716	G1611	G1541	A1461	U1325	U1246	A1163	A1106	U1006	C931	U862	A785	C694	U631
U1717	A1612			A1326	U1247	G1164	G1104	A1007	U932	C863	A786	C695	G632
G1718	A1613	A1546	A1467	C1327	A1252	A1165	A1106	U1008	U933	G864	G787	A696	G633
G1719	C1614	G1547	A1468	U1328	C1255	U1167	G1107	A1009	G934	A867	C788	A697	C634
U1720	C1615	C1548	A1469	C1329	G1256	U1168	U1108	G1010	U935	G868	A789	C702	C635
U1721	U1616			A1330	G1256	A1169	U1109	U1010	A936	G869	A790	C636	C636
U1722				U1331	A1260	A1170	U1110	U1014	G937	G870	A791	U707	C637
A1723	A1621	G1551	G1473	U1334	G1261	G1171	U1111	U1015	C938	C871	G792	U708	C638
U1724	U1622	A1474	A1474	U1335	G1262	C1175	A1112	C1016		U871	C793	G708	G639
C1725	U1629	A1475	A1475	U1336	A1263	G1176	U1114	G1017	U942	U872	U794	A709	U640
U1730	U1630	G1553	G1476	U1337	G1263	G1177	U1114	G795	U943	C873	A710	A710	C641
A1741	C1631	U1554	A1477	A1338	G1264	G1178	G1116	G1024	C944	U874	U796	A711	U642
U1742		U1555	C1478	C1339	G1268	A1179	G1117	A1025	C945	G875	U797	G712	U643
G1743	U1636	U1556	U1479	C1340	U1269	A1180	C1118	U1028	G947	G878	A801	G714	G644
G1744	A1637	G1560	A1481	G1341	A1270	A1181	C1119	G1029	C948		C802	A715	A646
A1752	C1638	G1561	A1482	C1342	A1271	U1181	A1120	A1030	C949	A882	C803	A716	A647
G1753	U1639	C1562	G1483	G1345	C1272	A1184	U1121	U1035	U954	A883	C804	G717	C648
		U1563	U1484				U1122	G1036	U955	U884	G805	G718	A649
U1645	U1646	U1564	G1485	G1346	U1276	C1189	U1123	A1036	U956	U885	A806	U719	C650
C1759	U1653	A1566	G1486	U1348	C1277		U1124		U957	C886	A807	A720	G651
A1760	U1654	U1567	G1487	G1349	A1278	C1192	U1125	C1043	U958	A887	C808	G721	G652
C1761	G1655	U1568	A1488	U1350	C1279	A1193	G1126	U1048	C959	U888	G809	A736	
U1762	A1656	U1569	A1489	U1351	G1280	G1194	C1127	A1049	U960	U889	A810	G737	
G1763	G1656	U1570	G1492	A1352	G1281	A1195	U1128	U1060	C961	C890	U811	G728	C655
U1764	C1657	A1571	G1493	U1353	G1282	C1196	A1129	U1061	C962	G894	U814	C730	A656
U1765	G1658	U1572	U1494	C1424	C1283	A1200	A1130	U1051	A962	A895	G815		A657
G1766	U1659	G1573	U1495	U1355	G1284	C1201	C1131	A1054	G963	A896	A816	A735	G658
C1767	C1660	C1574	A1496	G1357	G1285	A1202	A1133	U1065	G971	U897	A817	A736	A660
U1768	G1661	U1575	C1497	U1427	A1286	A1202	G1134	U1060	U966	U898	C818	G737	G661
G1769		G1576	A1498	G1362	A1287		A1135	A1061	A967	U899	U819		G662
		U1577	G1499	U1363	U1293	G1207	A1136	A1062	G968	G900		G742	G663
G1778	C1665	U1578	C1500	C1364	A1294		C1137	G1063	C969		C824	C743	A664
C1779	G1668	C1579	G1501	G1365	G1295	U1211	U1138	A1064	A970	U903	U825		A665
U1780	C1669	A1580	U1504	C1366	C1296	A1212	G1139	A1065	G971	A904	G826	U748	
U1785	C1670	C1581	A1504	U1367	C1297	G1221	G1140	G1066	A972	U905	U829	C749	A671
G1786	C1671	U1582	C1505	A1368	A1301	G1222	C1141	C1069	A973	A906		G750	A672
A1787	U1672	G1586	A1506	A1369	A1302		G1142	U1070	G974	G907	A830		G673
C1788	G1673	A1587	G1507	G1370	A1303	C1227	U1144	U1071	C975	G908	G831	G760	G674
G1789	U1674	A1588	A1509	C1371	U1304	C1228	G1145	A1068	A976	G909	G832	U764	C675
U1790	A1683	G1590	G1510	U1372	U1305	G1229	U1146	U1074	G978	C911	U834	U764	A676
C1791				G1374	G1306	G1230	G1147	A1075	U979	G912	G835	U766	G678
G1792	U1686	G1591	G1513		G1307	A1231	G1148	U1078	A980	A913	A836	U767	U679
C1793	U1687	A1592	G1514	G1379	A1308	C1232	G1149	U1078	U981	A837		C768	G680
G1794	U1688	G1593	G1517	G1380	U1309	G1233	U1150	A1079	C982	G916	G838	G769	U681
U1795	U1689	C1596	A1521	A1381	G1310	U1234	U1151	A1080	A983	A917	C839	G770	U682
A1796		U1597	G1520	G1382	U1235	U1235	G1152	U1081		C840	C840	A771	U683
U1797	U1695	G1598	G1521	G1383	G1313	G1237	A1154	U1082	U988	A920	A841	U772	G684
A1798		U1599	U1522	U1387	C1314	G1237		G1083		A921		G773	G685
A1799	U1703	G1604	U1523	G1388	U1315	C1238	C1155	A1084	G993	U922	A846	U776	G686
A1804			A1524	G1389	C1316	C1239	G1157	U1095	U995	C923	A847	U777	G688

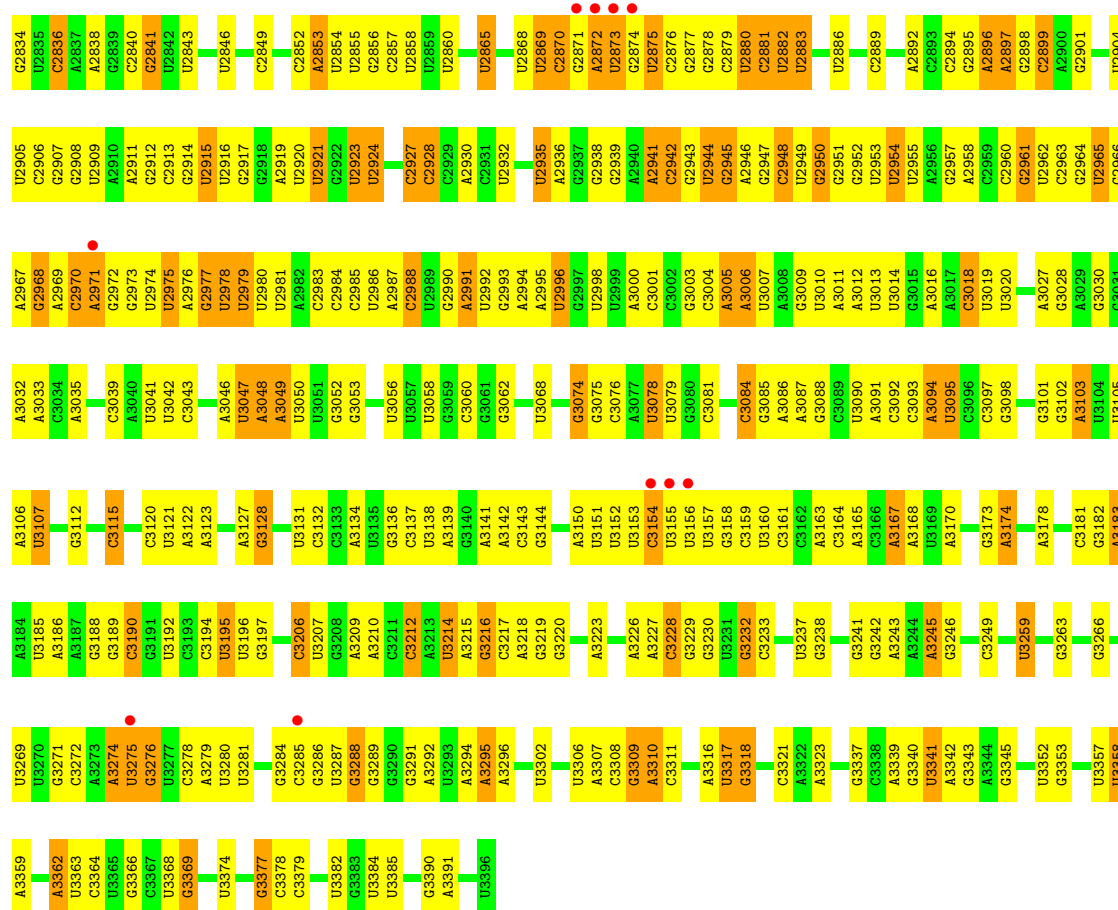
G2834	G2754	G2663	G2598	G2522	A	G2393	A2317	C2227	A2145	C	G	U	A1881	G1805
U2835	G2755	G2664	U2599	G2523	A	G2394	U2318		G2146	G	U	G	A1886	A1906
G2836	G2756		G2600	A2523	U	G2395	U2319	A2233	A2147	C	A	G	U1887	G1807
	A2757	G2677	G2601	A2601	A	G2396	A2320		U2148	U	G	G	U1888	G1808
U2842	A2758	G2678	G2602	G2528	A	G2397		G2236	A2149	U	G	C	G1889	G1811
U2843		G2679	G2603	G2603	U	A2398	G2323	C2237		C	C	C	U1890	G1812
A2845	G2761	G2680	U2604	A2529	G	G2399			G2155	G	C	C	A1891	A1913
U2846	U2766	G2682	G2606	U2532	U	G2400	U2327	U2241	G2156	U	G	C	U1892	A1914
A2847	U2767	U2683	G2533	G2534	G	A2401	G2328	A2242	G2157	A	G	U	A1893	A1814
G2848	U2768	G2684	G2608	G2607	G	A2402	C2329	A2243	A2158	C	C	U	G1894	U1815
U2849	U2769	G2685	A2609	A2535	G	G2403		A2244	A2159	A	A	G	A1897	A1816
G2850	G2770	A2686	G2610	U2537	C	A2404	C2333		G2160	A	A	C	G1897	U1817
A2851	U2771		U2611	G2538	U	G2405	U2334		G2161	U	C	U	G1898	U1818
C2852	G2772	A2695	U2612	C2539	U	G2406		G2251	U2162	A	U	C	G1899	U1819
U2853		A2696	G2613	U2540	C	G2407	C2338			A	U	C		U1820
A2854	U2775	A2697	G2614	U2541	G	U2408	U2340	A2255	G2165	G2094	C	A	U1902	U1821
U2855	G2776	G2698	G2615		G	G2409	U2341	A2256	G2169	G2095	C	G	U1903	C1822
	G2777	G2699	G2616	U2544	C	U2410	U2342	C2257	U2170	A2096	U	G	C1904	
U2859	G2778	G2700	U2617	C2545	G	G2411	C2343	C2258	G2171	U2097	G	C	G1905	U1831
U2860	A2779	U2701	G2618	G2546	C	A2413				C2098	C	A	G1906	C1832
U2861	U2780	A2702	G2619	A2547	C	G2414		U2259	U2175	A2099	C	C	A1907	
U2862	G2786	A2703	G2620	C2548	C	U2415	U2347	G2261	U2176	A2100	C	C	U1908	G1838
G2863	G2787		G2621	G2549	G	G2416		A2262	G2177	C2101	U	C	A1909	A1839
A2864		C2707	U2550	U2550	U	U2417	G2355	C2263	A2178		U	G	U1910	U1840
U2865	A2790		G2623	U2551	G	G2418	A2357		G2180	A2104	G	G	A1911	A1841
U2866		C2711	G2624		A	A2419	A2358	A2275		G2105	U	U	U1912	
G2794	U2795	U2712	A2624	A2554	A	G2420	C2359		G2181	A2106	C	G	A1913	G1843
U2796	G2796	U2713	G2626		A	U2421	C2360	C2278	A2183	A2107	C	G	G1914	C1844
G2797	G2797	A2714	C2627	U2558	U	G2422	A2361	A2279	U2184	C2108	A	G	U1915	
C2798	U2798	U2715	U2559	C2560	C	U2423	C2362	A2280	G2185		G	C	G1916	G1845
G2801	G2801	G2716	U2631	C2561	A	A2424	A2363	A2281	U2186		A	C	U1917	G1846
U2802	A2801	U2717	G2632	A2562	C	G2425	G2364	U2282	G2187	U2112	C	G	A1918	A1847
		G2718	U2633	G2563	U	U2426	C2365	G2283	G2188	G2114	C	G	G1919	G1848
		U2719	U2634	C2564	C	U2427	C2366	C2284		G2115	G	U	U1924	C1849
			U2635	U2565	U	U2428	A2367	C2285	U2191		C	U	U1925	
		U2723	A2636	G2566	A		A2368	U2286	C2192	C2118	C	G	G1926	G1852
G2805	G2805	U2724	U2637	C2567	C	U2433	G2369		U2193	A2119	C	G	U1927	U1853
G2806		U2725	G2567	C2568	A	U2434	G2370	A2291	G2194	A2120	U	C		G1854
U2808	C2808	C2726	C2638	C2569	U	G2435	G2371		C2195	G2121	G	U	U1931	U1855
U2809	A2808	A2727	G2639	C2568	U	G2437	A2372	A2295	G2196	G2122	G	G	A1932	G1856
G2810	G2810	G2728	A2640	U2571	U		A2373	A2296	G2197	G2123	C	C	G1857	G1857
A2811	U2729	U2641	G2572	C2572	A	G2440	C2374	U2297	A2198	G2124	U	U	A1858	A1859
G2812	G2730	A2642	U2643	G2573	U2501	U2441	G2375	A2298	G2201	A2125	G	G	U1937	
A2813	U2731	G2645	G2646	G2574	U2502	G2442	G2376	A2299	U2205		U	G	G1940	G1863
	G2732		G2647	G2575	G2503	A2443	G2377	G2300	G2206	G2131	U	G	C1941	G1866
G2816	A2733		A2649	U2578	U2504	G2444	C2378	U2301	G2207	A2131	C	U	G1947	
A2817	U2734		U2650	C2582	U2505	A2445	U2379	G2302	U2208	G2132	U	G	G1948	C1869
U2818	A2735		G2651	C2583	U2506		U2380	G2303	A2209	G2133	C	G	C1870	U1870
A2819	U2736	A2736	U2652	G2584	C2507	A	G2381	G2304	U2209	G2134	U	G	G1949	U1871
C2820	G2737		G2653	G2585	U2508	G	G2382	G2305	G2210		U	C	U1950	
G2821	A2740		C2654	G2586	U2510	G	A2384	G2306		U2137	C	U	G1951	
	C2741		U2655	G2587	U2512	C	G2385	C2308	A2214	A2138	A	U	C1951	A1874
U2827			U2656	G2589	U2513	U		C2309	A2215	A2139	G	C	G1952	G1875
G2828	A2746		A2657	U2592	U2514	G	U2388	U2310		U2140	A	C	G1953	U1876
U2829	A2747		G2593	A2515	U2515	U	C2389		A2223	A2142	C	C	G1954	U1877
A2890	A2748		G2594	A2516	U2516	G	A2390	A2313	A2224	A2143	C	C	U1955	U1878
U2891			G2595	A2517	U2517	U	G2391	U2314	U2225	A2144	A	C	A1956	G1879
A2892	U2752		U2596	G2518	C	A	G2392		U2226	C2145	U	C		U1880
C2893	A2892		U2597	G2519	A				U2227		U	C		U1881
G2894	A2893		G2598	G2520					U2228		U	C		



A1638	A1639	A1643	G1646	G1650	A1654	G1655	A1656	A1657	G1658	C1659	G1660	G1662	C1665	A1676	G1677	G1678	A1679	U1686	U1687	U1688	U1689	C1693	A1696	G1713	A1714	U1715	U1716	U1717	G1718	G1719	U1724	C1725	G1728	A1729	G1730	G1734	U1746	A1749	A1750	G1751															
U1555	C1556	A1557	A1558	G1559	G1560	C1562	C1563	A1564	G1565	A1566	U1567	U1568	U1569	U1570	G1571	A1572	G1573	C1574	A1575	C1578	C1579	A1580	G1581	C1582	G1586	A1587	A1588	A1589	G1590	G1591	U1592	U1595	C1596	C1597	U1601	A1602	A1603	G1604	A1605	U1606	U1607	A1613	C1614	C1615	U1629	U1630	C1631	A1632	C1633	G1634	U1635				
A1465	A1466	A1467	A1468	C1469	U1470	U1471	A1475	G1480	A1481	A1482	G1483	U1484	G1485	G1486	G1487	G1488	A1489	A1490	A1491	G1492	G1493	U1494	U1495	C1496	G1500	U1501	C1505	A1506	G1507	G1513	G1514	G1517	G1520	G1525	U1526	G1536	A1537	G1538	G1541	G1544	A1545	A1546	G1547	C1551	G1552	U1553	U1554								
C1391	G1392	A1393	A1394	C1395	C1396	C1397	U1398	A1399	C1402	G1403	G1404	U1405	A1406	U1407	G1408	G1409	U1410	U1411	G1412	G1413	G1414	U1415	G1416	G1417	A1418	A1419	C1420	G1421	C1426	U1427	U1428	G1429	U1430	G1431	C1432	A1433	G1434	A1435	U1436	C1437	U1438	U1439	U1445	A1446	G1447	U1448	A1449	G1450	C1451	A1452	A1456	C1461	U1464		
G1319	C1320	U1321	A1322	G1323	C1327	C1328	U1329	A1330	U1331	A1332	G1333	U1334	C1335	U1336	A1337	C1338	U1339	G1340	U1341	G1344	G1345	U1348	G1349	A1350	U1351	U1352	U1353	G1354	A1355	U1356	G1362	A1363	C1364	G1365	A1366	G1367	U1368	A1369	G1370	G1371	G1372	A1373	G1374	G1375	C1376	G1379	G1380	A1381	G1382	G1387	U1388	G1389	A1390		
G1236	G1237	C1238	U1239	G1242	G1243	A1244	A1245	G1246	G1249	G1250	A1251	A1252	C1254	G1255	G1256	G1257	U1258	A1259	A1260	G1261	G1262	A1263	G1264	U1276	G1284	A1290	A1291	C1292	G1295	C1296	C1297	U1298	U1299	G1300	A1301	A1302	A1303	A1304	U1305	G1306	G1307	A1308	U1309	G1310	G1311	C1312	G1313	C1314	U1315	G1316	A1317	A1318			
A1165	G1166	U1167	A1168	A1169	A1170	G1171	G1172	U1173	G1174	C1175	G1176	G1177	G1178	A1179	A1180	U1181	A1182	C1183	G1186	U1187	U1188	C1189	C1192	A1193	C1196	A1197	C1198	C1199	A1200	A1201	A1202	A1203	U1208	G1209	U1210	U1211	G1212	G1213	U1214	U1215	C1219	U1220	A1221	G1222	A1223	G1226	C1227	A1231	C1232	G1233	G1234	U1235			
U1096	G1097	A1098	A1099	U1100	U1101	A1102	A1103	G1104	C1107	U1108	U1109	U1110	U1111	A1112	G1113	U1114	G1115	G1116	G1117	C1118	C1119	A1120	U1121	U1122	U1123	U1124	U1128	A1129	A1130	G1131	C1132	U1133	G1134	C1141	G1142	U1143	U1144	G1145	C1146	U1147	G1148	G1149	U1151	G1152	A1153	A1154	G1157	U1158	A1159	C1160	G1161	U1162	A1163	G1164	
U1014	U1015	C1016	U1017	G1018	G1019	C1023	G1024	A1025	A1026	A1027	U1028	G1029	A1030	C1031	G1032	U1033	A1036	U1042	C1043	A1044	C1045	A1046	A1047	A1048	A1050	A1054	A1057	U1062	G1063	A1064	A1065	G1066	U1070	U1071	G1072	U1073	C1076	U1077	U1078	A1079	A1080	U1081	U1082	G1083	A1087	A1093	U1094	U1095							
C948	C949	G950	A951	A952	G953	U954	U955	U956	C957	C958	C959	U960	C961	A962	G963	U966	A967	G968	C969	A970	G971	G972	A973	G974	U979	A980	U981	U986	U987	U988	A989	U990	G991	A992	G993	G994	U995	A996	A997	A998	G999	C1000	U1001	A1002	A1003	U1004	G1005	A1006	G1010	A1011	U1012	G1013			
A882	A883	G887	A888	U889	C890	G891	U892	C893	G894	A895	U899	G900	C901	G902	U903	A904	U905	A906	G907	G908	G909	G910	C911	G912	A913	A914	A915	G916	A917	A920	U921	U922	C923	G924	A925	A926	C927	C928	A929	U930	C931	U932	A933	G934	U935	C936	G937	C938	G941	U942	U943	C944	U946	G947	
A810	U811	G812	G813	U814	G815	A816	A817	G818	U819	A820	U821	G822	C823	G824	U825	G826	A830	A837	G838	U839	G840	U841	G842	U843	A844	A847	A848	G849	U850	C851	U852	G853	G856	G857	U860	C861	U862	C863	G864	A869	U870	A871	G872	C873	U874	A875	A876	C877	U878	A806	A807				
C637	U640	G641	U642	U643	G644	A645	A646	A647	C648	A649	G652	A653	G654	C655	G656	A657	G658	A659	C661	U662	C663	U666	U667	C670	U671	G676	U677	U678	U679	G680	U682	U683	G684	U685	A691	A692	A693	U698	A699	C700	U623	G624	G701	C702	U627	A628	U629	A630	U631	A715	G632	C633	G634	U635	C636
A550	A551	G556	C641	G567	G568	A569	A570	G575	C577	A578	G579	C580	G583	G584	A585	C586	U594	G595	C596	G597	A598	C599	G600	A603	G604	A608	U609	G610	A611	U612	C618	A619	U620	A621	A622	U623	G624	G625	U626	U627	A628	U629	A630	U631	A715	G632	C633	G634	U635	C636					



A2758	A2766	A2767	A2768	A2769	A2770	A2771	A2772	A2773	A2777	A2787	A2790	A2791	A2792	A2793	A2794	A2795	A2796	A2797	A2798	A2799	A2800	A2803	A2804	A2805	A2808	A2809	A2810	A2813	A2814	A2815	A2816	A2817	A2818	A2819	A2820	A2821	A2822	A2823	A2824	A2825	A2826	A2827	A2828	A2829	A2830	A2831	A2832																																																																																																																																																																																																																																																																																																																																																																							
G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2919	G2920	G2921	G2922	G2923	G2924	G2925	G2926	G2927	G2928	G2929	G2930	G2931	G2932	G2933	G2934	G2935	G2936	G2937	G2938	G2939	G2940	G2941	G2942	G2943	G2944	G2945	G2946	G2947	G2948	G2949	G2950	G2951	G2952	G2953	G2954	G2955	G2956	G2957	G2958	G2959	G2960	G2961	G2962	G2963	G2964	G2965	G2966	G2967	G2968	G2969	G2970	G2971	G2972	G2973	G2974	G2975	G2976	G2977	G2978	G2979	G2980	G2981	G2982	G2983	G2984	G2985	G2986	G2987	G2988	G2989	G2990	G2991	G2992	G2993	G2994	G2995	G2996	G2997	G2998	G2999	G3000	G3001	G3002	G3003	G3004	G3005	G3006	G3007	G3008	G3009	G3010	G3011	G3012	G3013	G3014	G3015	G3016	G3017	G3018	G3019	G3020	G3021	G3022	G3023	G3024	G3025	G3026	G3027	G3028	G3029	G3030	G3031	G3032	G3033	G3034	G3035	G3036	G3037	G3038	G3039	G3040	G3041	G3042	G3043	G3044	G3045	G3046	G3047	G3048	G3049	G3050	G3051	G3052	G3053	G3054	G3055	G3056	G3057	G3058	G3059	G3060	G3061	G3062	G3063	G3064	G3065	G3066	G3067	G3068	G3069	G3070	G3071	G3072	G3073	G3074	G3075	G3076	G3077	G3078	G3079	G3080	G3081	G3082	G3083	G3084	G3085	G3086	G3087	G3088	G3089	G3090	G3091	G3092	G3093	G3094	G3095	G3096	G3097	G3098	G3099	G3100	G3101	G3102	G3103	G3104	G3105	G3106	G3107	G3108	G3109	G3110	G3111	G3112	G3113	G3114	G3115	G3116	G3117	G3118	G3119	G3120	G3121	G3122	G3123	G3124	G3125	G3126	G3127	G3128	G3129	G3130	G3131	G3132	G3133	G3134	G3135	G3136	G3137	G3138	G3139	G3140	G3141	G3142	G3143	G3144	G3145	G3146	G3147	G3148	G3149	G3150	G3151	G3152	G3153	G3154	G3155	G3156	G3157	G3158	G3159	G3160	G3161	G3162	G3163	G3164	G3165	G3166	G3167	G3168	G3169	G3170	G3171	G3172	G3173	G3174	G3175	G3176	G3177	G3178	G3179	G3180	G3181	G3182	G3183	G3184	G3185	G3186	G3187	G3188	G3189	G3190	G3191	G3192	G3193	G3194	G3195	G3196	G3197	G3198	G3199	G3200	G3201	G3202	G3203	G3204	G3205	G3206	G3207	G3208	G3209	G3210	G3211	G



• Molecule 37: Yeast 5S rRNA gene

Chain 3:



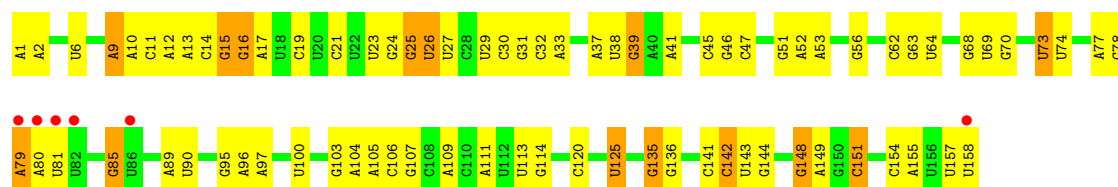
• Molecule 37: Yeast 5S rRNA gene

Chain 7:



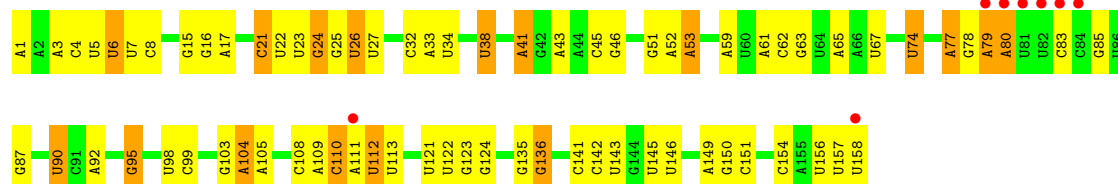
• Molecule 38: Saccharomyces cerevisiae genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 4:



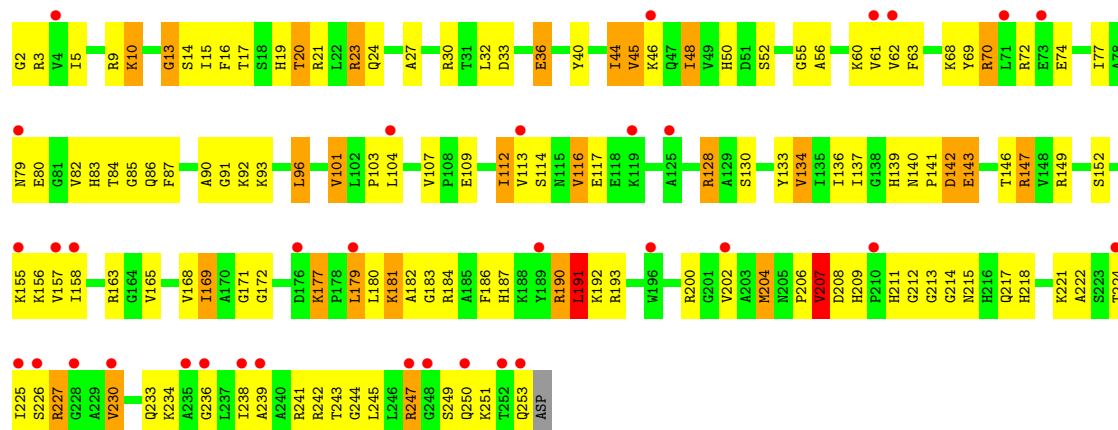
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 8:



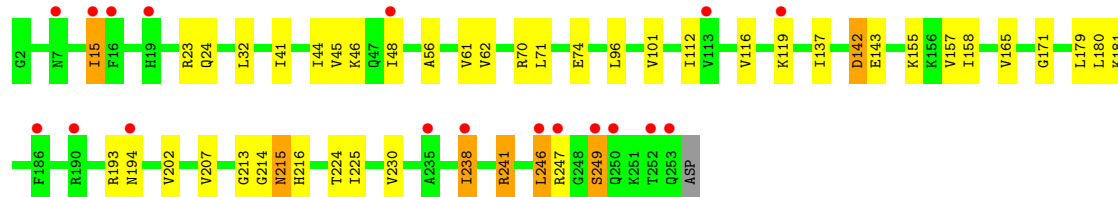
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



- Molecule 39: 60S ribosomal protein L2-A

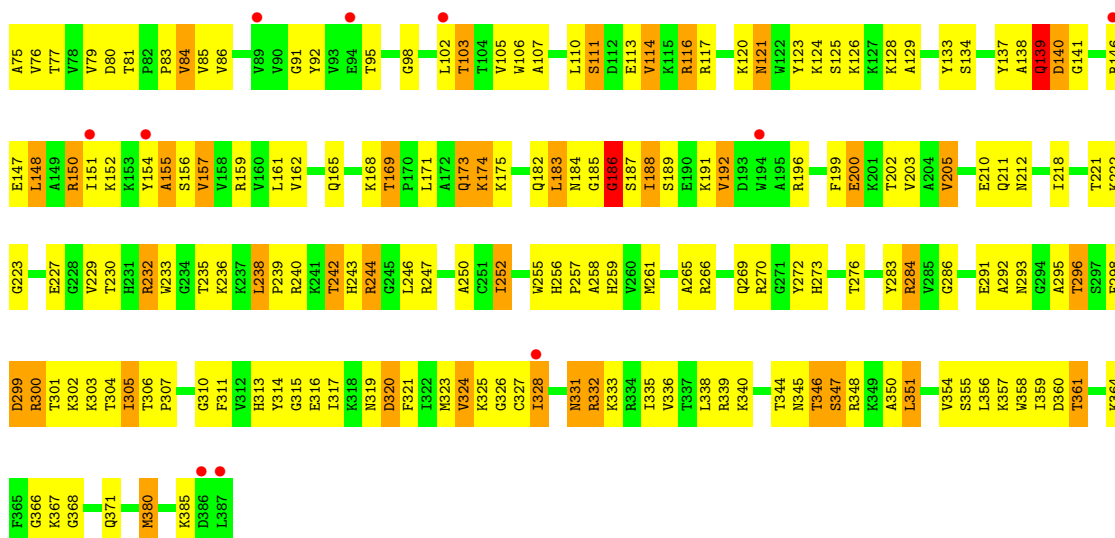
Chain L2:



- Molecule 40: 60S ribosomal protein L3

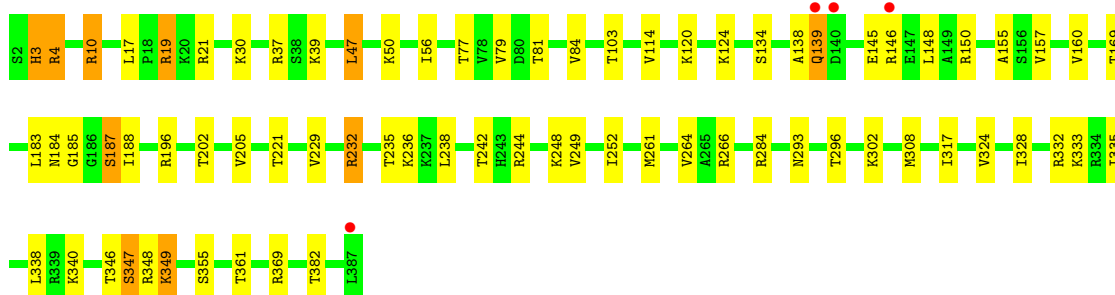
Chain L3:





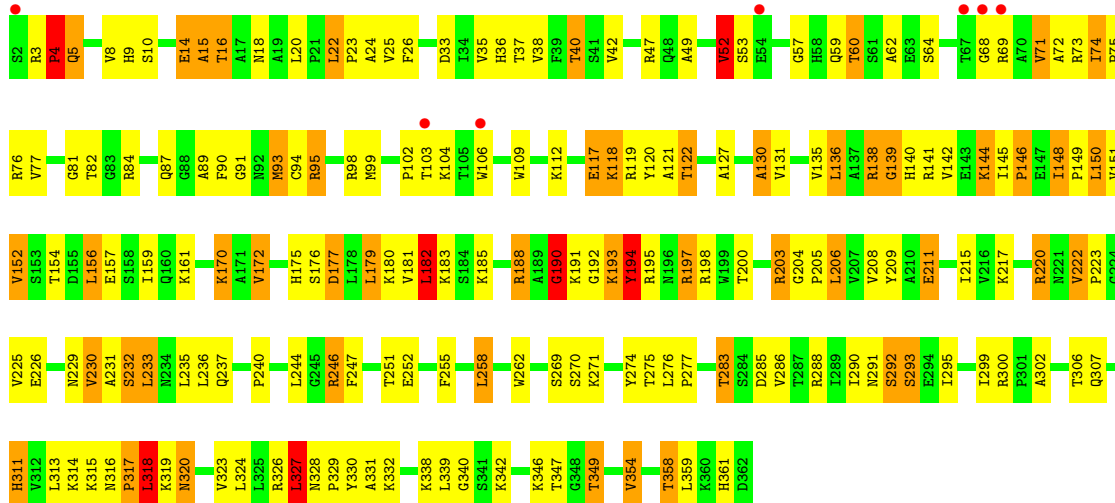
• Molecule 40: 60S ribosomal protein L3

Chain 13:



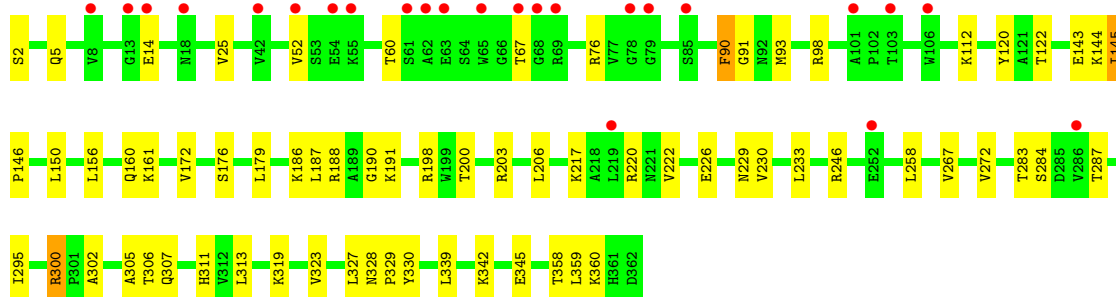
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



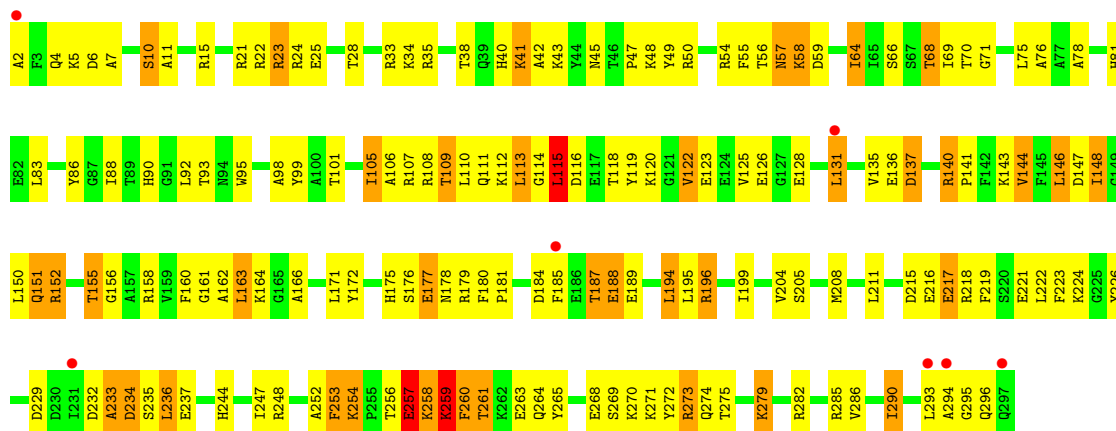
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



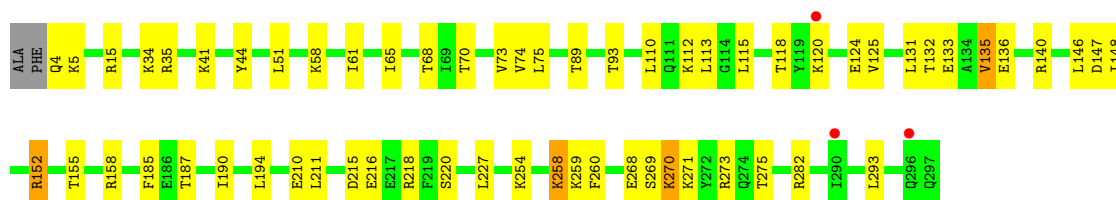
• Molecule 42: 60S ribosomal protein L5

Chain L5:



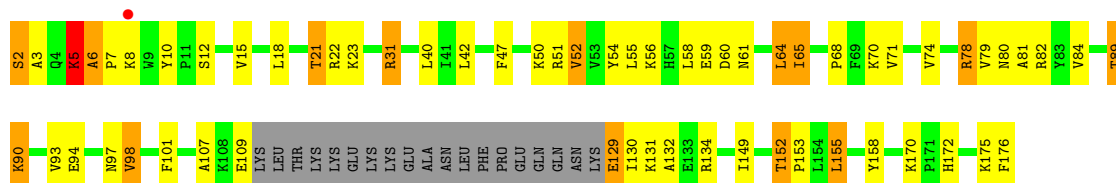
• Molecule 42: 60S ribosomal protein L5

Chain l5:



• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



• Molecule 43: 60S ribosomal protein L6-A

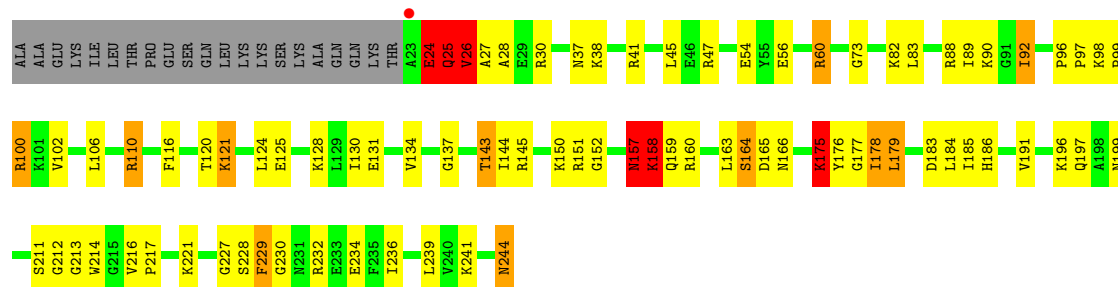
Chain l6:





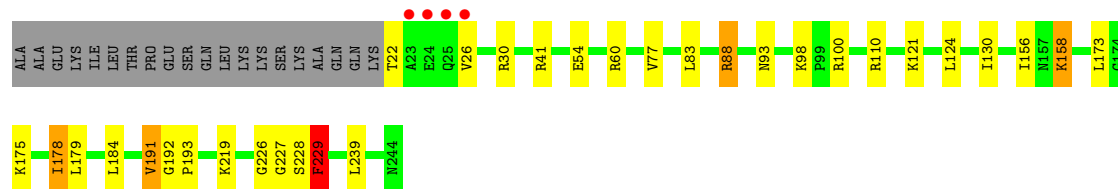
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



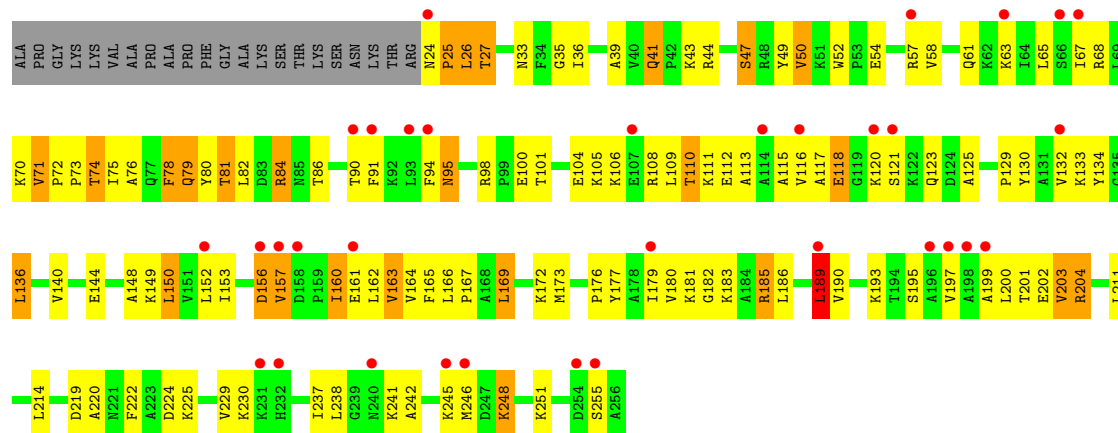
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



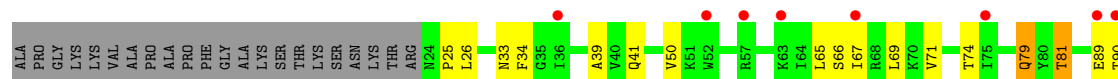
• Molecule 45: 60S ribosomal protein L8-A

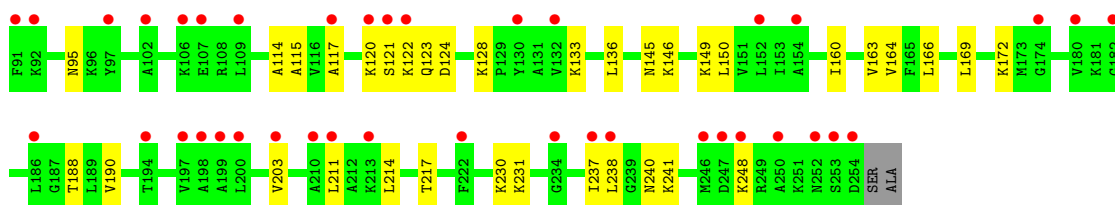
Chain L8:



• Molecule 45: 60S ribosomal protein L8-A

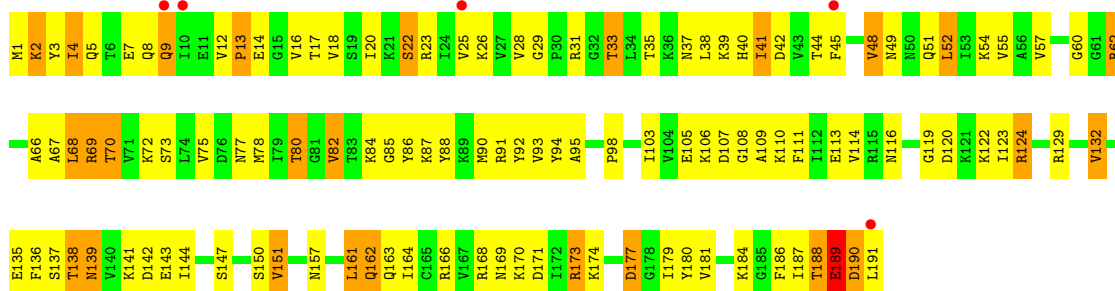
Chain L8:





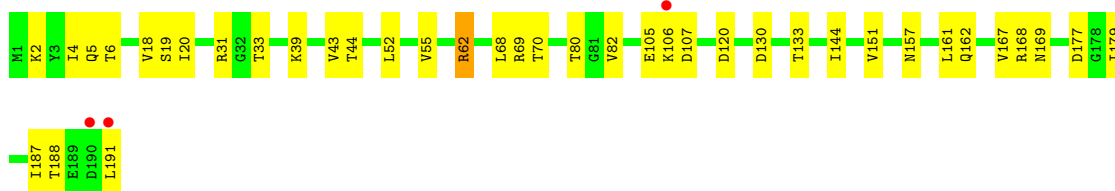
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



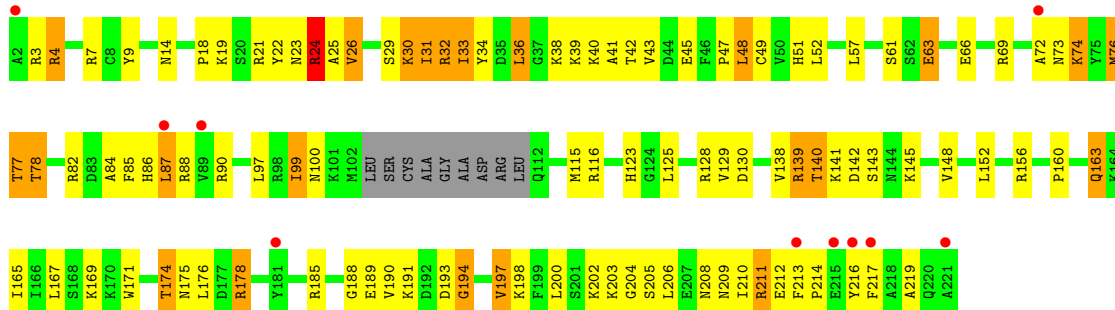
• Molecule 46: 60S ribosomal protein L9-A

Chain I9:



• Molecule 47: 60S ribosomal protein L10

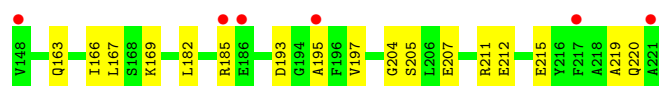
Chain M0:



• Molecule 47: 60S ribosomal protein L10

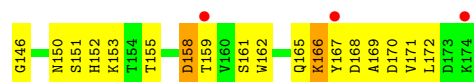
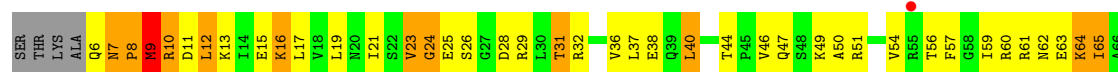
Chain m0:





• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



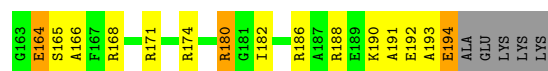
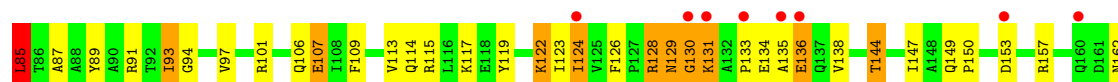
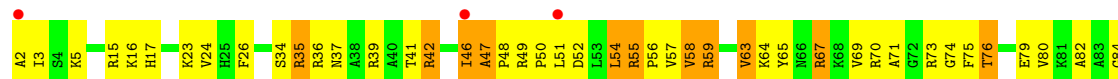
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



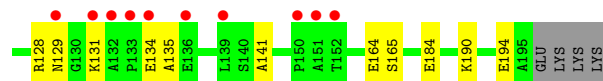
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



• Molecule 50: 60S ribosomal protein L14-A

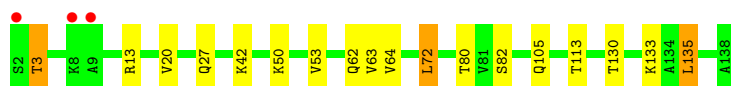
Chain M4:





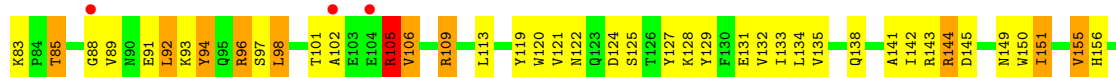
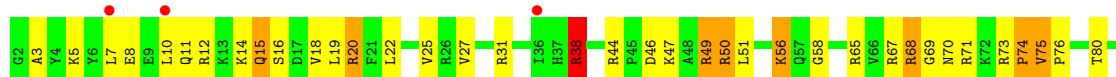
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



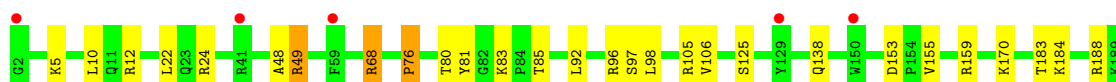
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



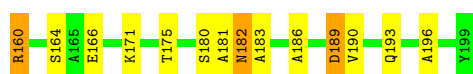
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



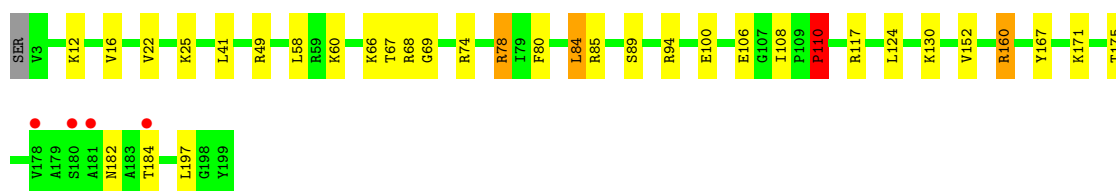
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



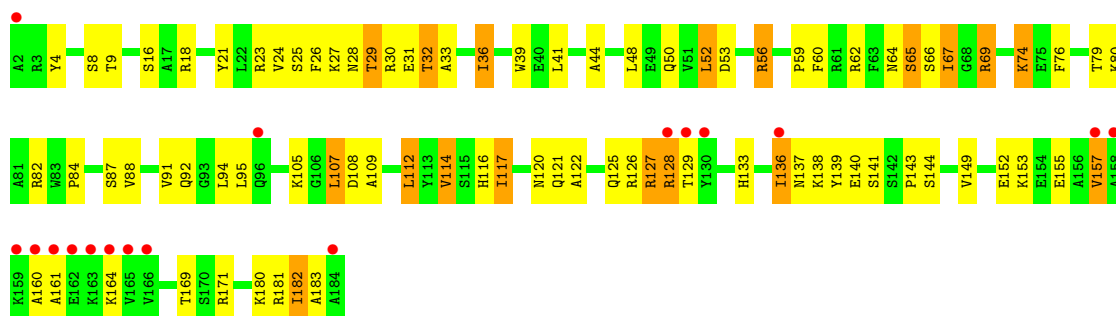
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



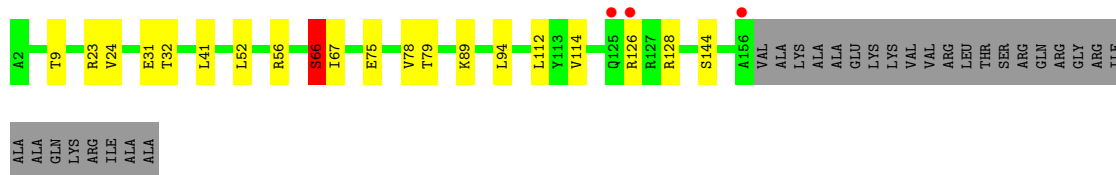
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:



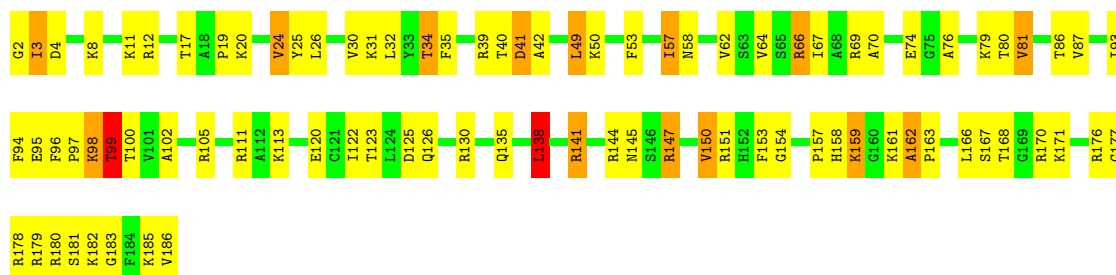
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:



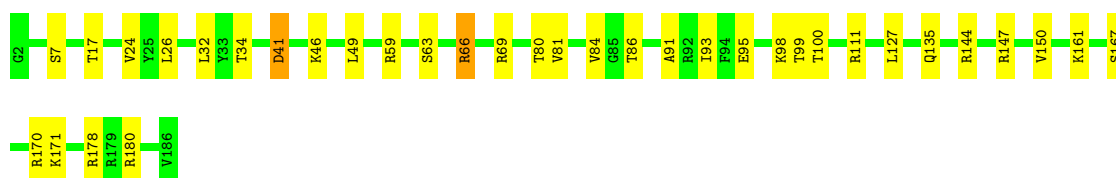
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



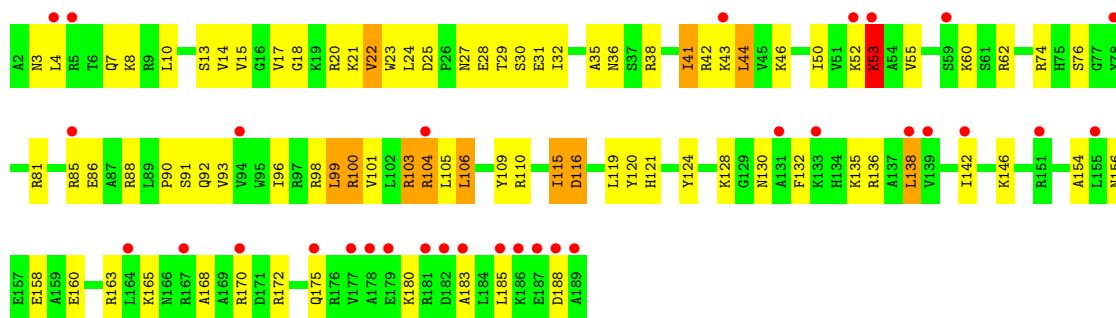
- Molecule 54: 60S ribosomal protein L18-A

Chain m8:



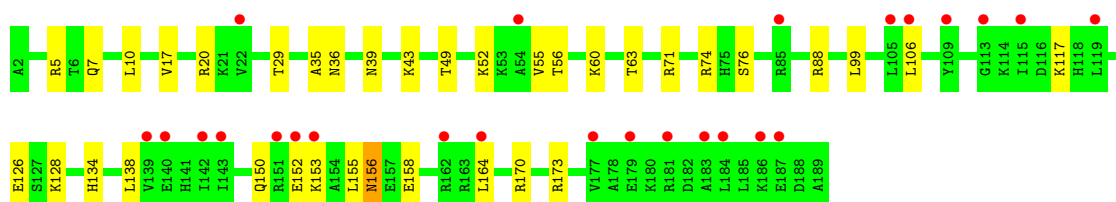
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



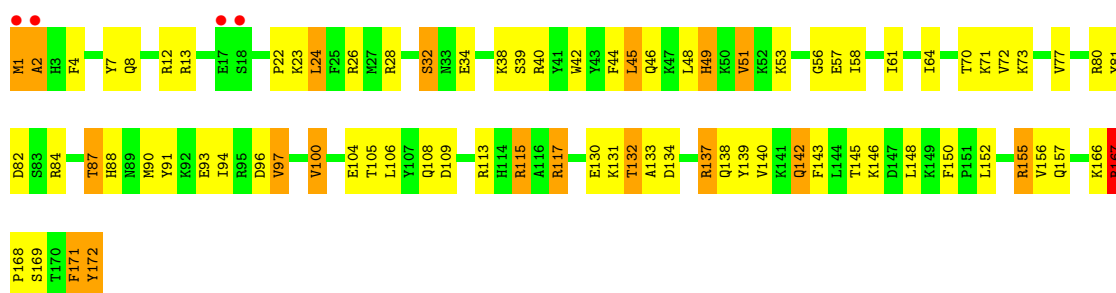
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:



- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



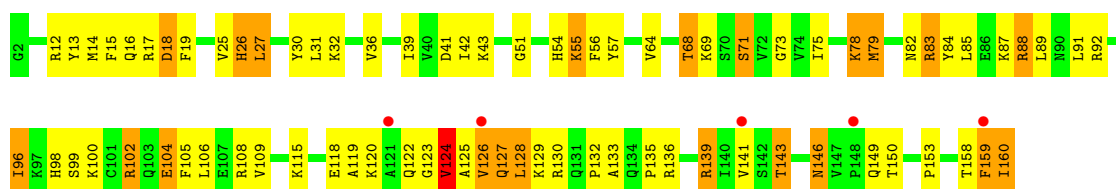
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



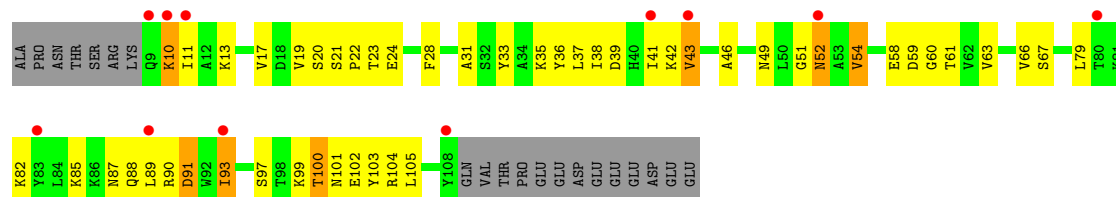
- Molecule 57: 60S ribosomal protein L21-A

Chain n1: 



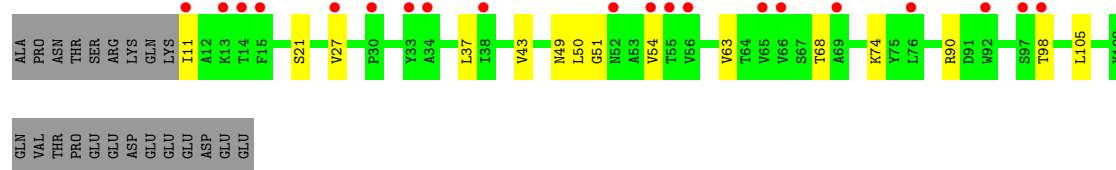
- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 



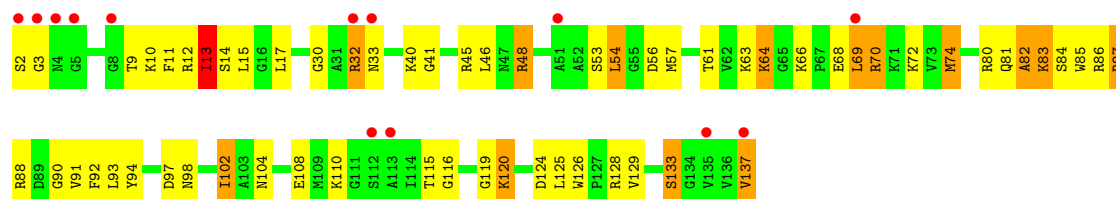
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 



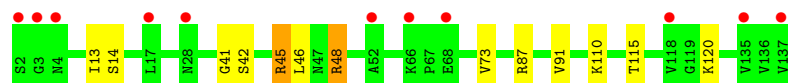
- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 



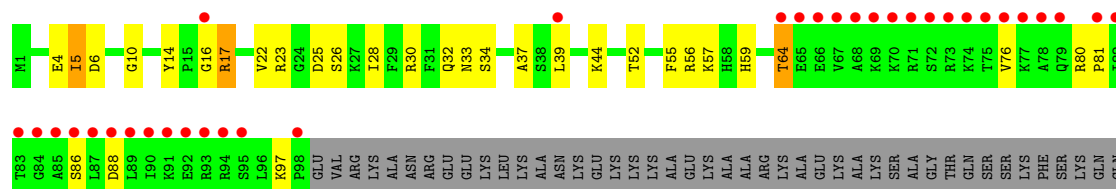
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 



- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 



ALA  
LYS  
GLY  
ALA  
PHE  
GLN  
LYS  
VAL  
ALA  
ALA  
THR  
SER  
ARG

- Molecule 60: 60S ribosomal protein L24-A

Chain n4:

M1 K2 I5 S26 L39 R43 L54 T63 T64 E65 E66 V67 A68 K69 R71 S72 R73 K74 T75 V76 K77 T83 L87 L96 E99 V100 K127 G132 S135 SER LYS PHE LYS GLN GLN ALA LYS GLY ALA PHE GLN LYS VAL ALA

THR  
SER  
ARG

- Molecule 61: 60S ribosomal protein L25

Chain N5:

ALA PRO SER ALA LYS THR ALA ALA LYS LYS VAL VAL LYS THR GLY ASN LYS K22 A23 L24 K25 V26 R27 K36 T37 L38 K39 L40 A41 P44 K45 Y46 A47 S48 K49 A50 V51 R56 L57 D58 S59 Y60 K61 V62 I63 T67 T68 T71 A72 M73 V76

E77 D78 G79 N80 I81 L82 V83 F84 Q85 V86 N91 K92 Y83 Q94 K100 E101 L102 Y103 E104 V105 D106 L108 K109 V110 L113 V114 R115 P116 N117 G118 T119 K120 K121 A122 Y123 V124 R125 L126 T127 Y130 D131 A132 L133 D134 I135 A136 N137 R138 I139 G140 Y141 I142

- Molecule 61: 60S ribosomal protein L25

Chain n5:

ALA PRO SER ALA LYS THR ALA ALA LYS LYS VAL VAL LYS THR ASN GLY LYS A23 L24 K25 V26 R27 F32 R33 L34 T37 L38 K39 L40 P44 K45 Y46 A47 P52 R56 L57 D58 S59 Y60 K61 V62 I63 E64 Q65 T71 F84 Q85 V86 S87

M88 T96 K96 K97 E101 Y102 E104 V105 D106 L108 K109 L113 V114 R115 P116 N117 G118 T119 V124 R125 L126 L133 D134 I135 A136 N137 I142

- Molecule 62: 60S ribosomal protein L26-A

Chain N6:

A2 K3 Q4 S5 L6 D7 V8 R12 R13 R16 S24 S25 Q26 K37 F38 L39 Q42 Y43 G44 I45 K46 A47 I50 R51 R52 D53 E55 V56 V58 V59 R60 K64 E67 T70 Y74 R75 L76 K77 F78 A79 V80 Q81 V82 D83 K84 V85 E88

N91 G92 A93 S94 T97 N98 S102 K103 L104 V105 K108 L109 H110 L111 D112 R115 I119 Q120 R121 K122 L125 L126 E127

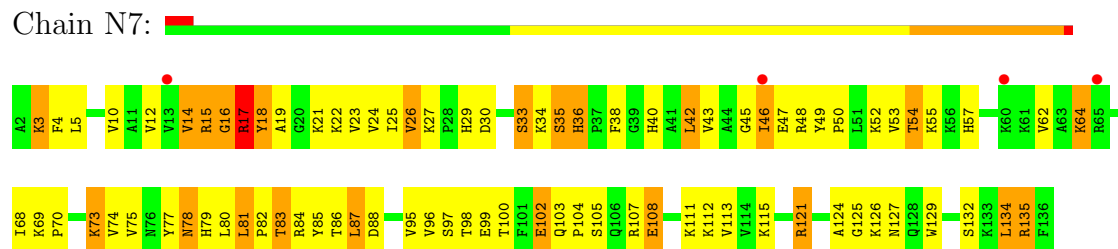
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:

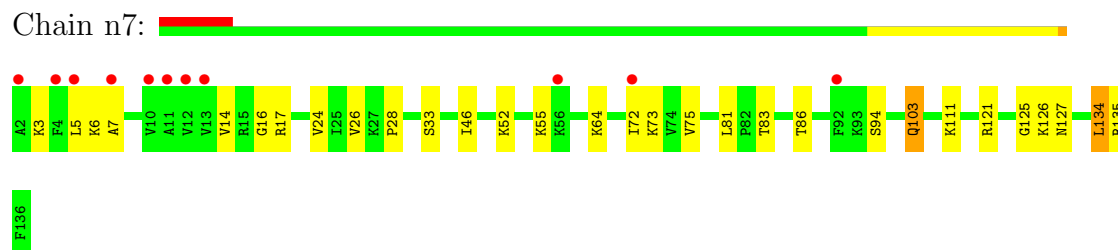
A2 S9 S10 D11 R12 R13 A18 L35 S36 K37 E38 L39 R40 Y43 G44 I45 I50 R51 R52 D53 E55 V56 L57 S62 Q66 K69 I70 S71 S72 Y73 Y74 L75 L76 V80 D83 K84 K87 E88 K89 V90 N91 G92 A93 S94 I97 N98

L104 V105 I106 T107 K108 L109 H110 L111 D112 K113 R115 S116 A117 L118 I119 Q120 R121 K125 L126 E127

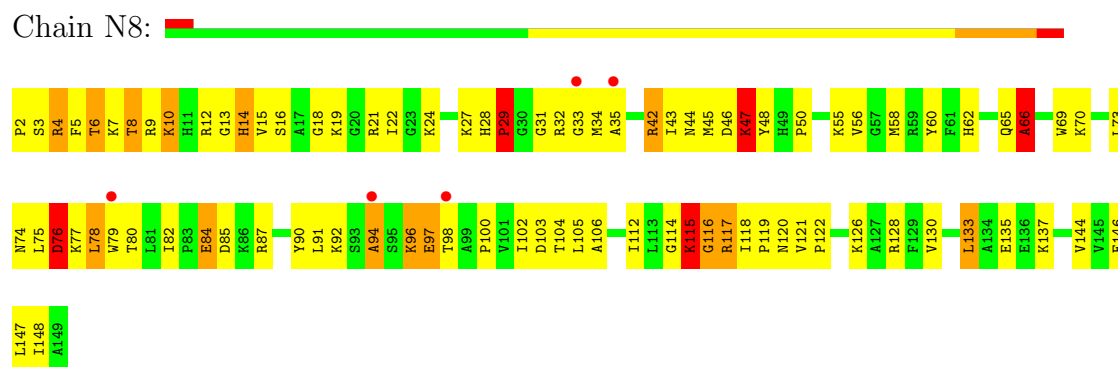
- Molecule 63: 60S ribosomal protein L27-A



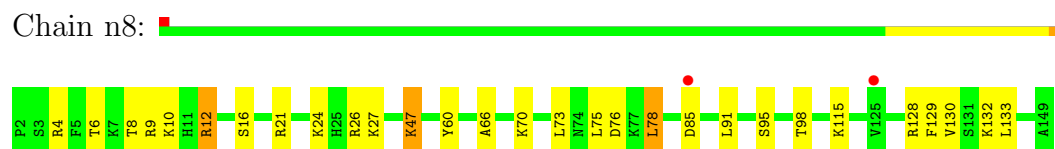
- Molecule 63: 60S ribosomal protein L27-A



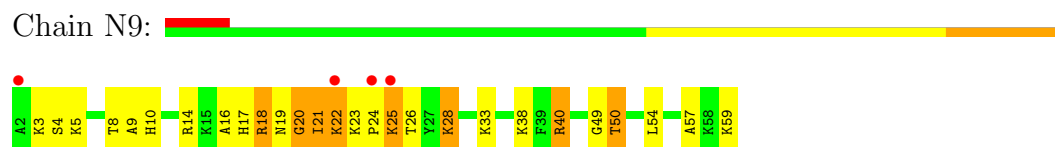
- Molecule 64: 60S ribosomal protein L28



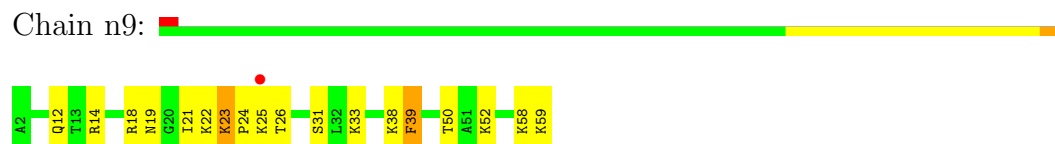
- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L29

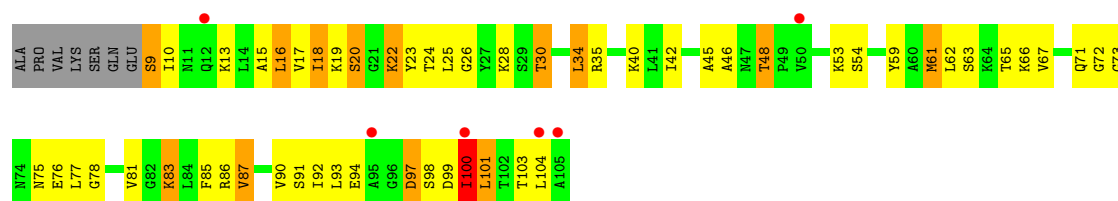


- Molecule 65: 60S ribosomal protein L29



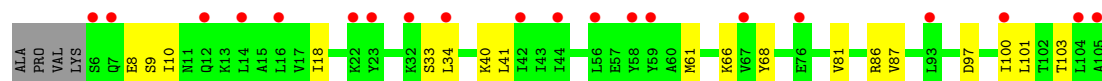
- Molecule 66: 60S ribosomal protein L30

Chain O0:



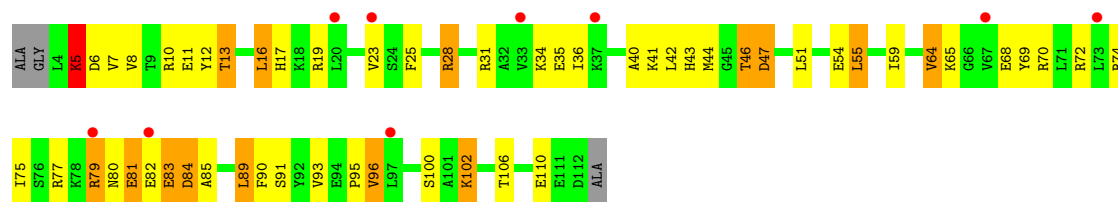
- Molecule 66: 60S ribosomal protein L30

Chain o0:



- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



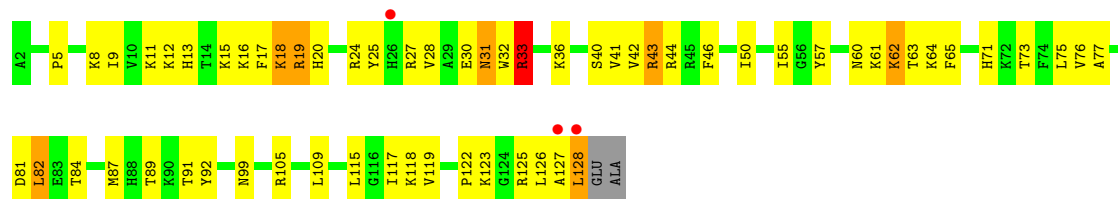
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



- Molecule 68: 60S ribosomal protein L32

Chain O2:



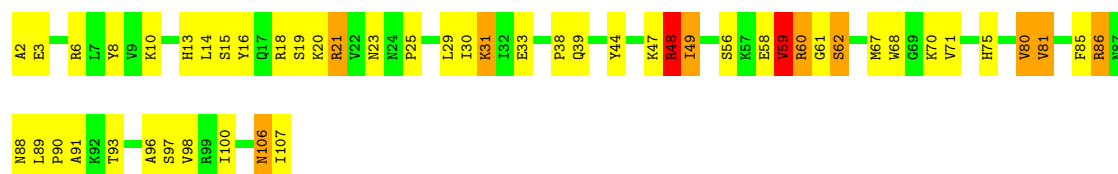
- Molecule 68: 60S ribosomal protein L32

Chain o2:



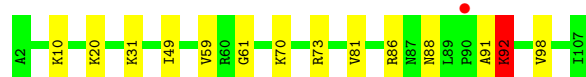
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



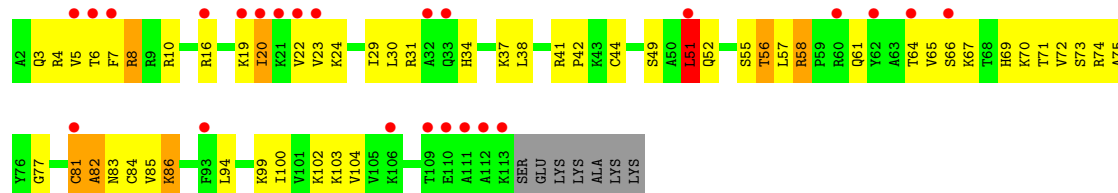
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



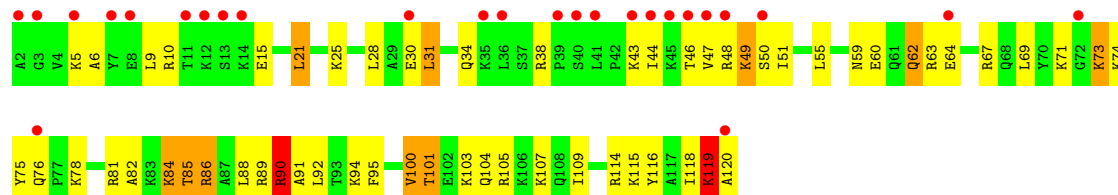
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



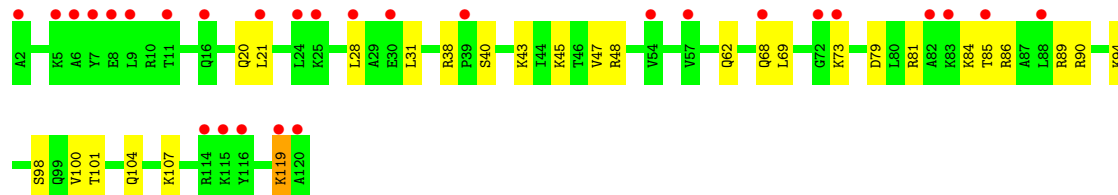
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



- Molecule 71: 60S ribosomal protein L35-A

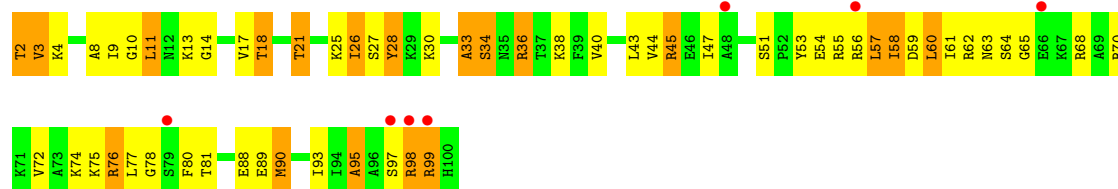
Chain o5:





- Molecule 72: 60S ribosomal protein L36-A

Chain O6: 



- Molecule 72: 60S ribosomal protein L36-A

Chain o6: 



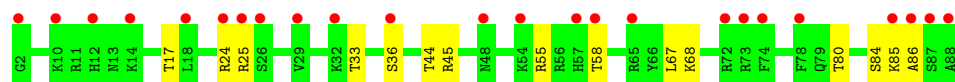
- Molecule 73: 60S ribosomal protein L37-A

Chain O7: 



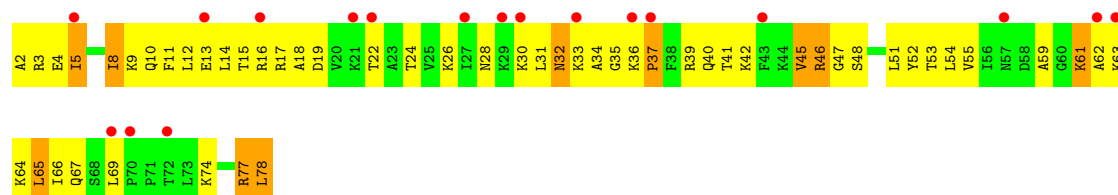
- Molecule 73: 60S ribosomal protein L37-A

Chain o7: 



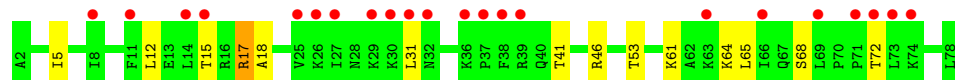
- Molecule 74: 60S ribosomal protein L38

Chain O8: 



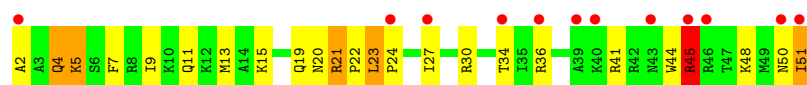
- Molecule 74: 60S ribosomal protein L38

Chain o8: 



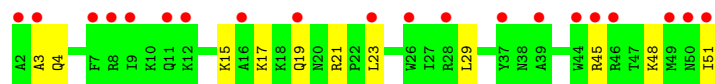
- Molecule 75: 60S ribosomal protein L39

Chain O9: 



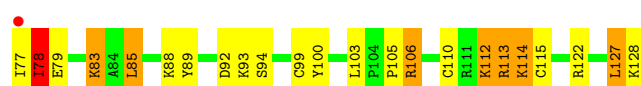
- Molecule 75: 60S ribosomal protein L39

Chain o9: 



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 



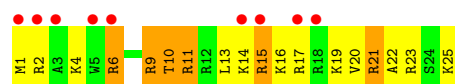
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 



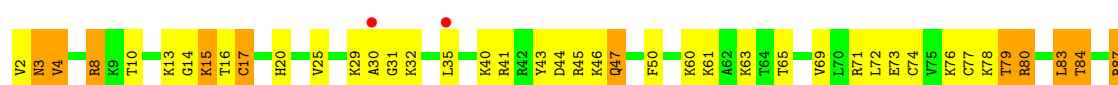
- Molecule 77: 60S ribosomal protein L41-A

Chain q1: 



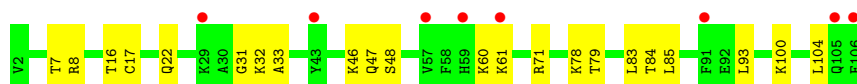
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 



- Molecule 78: 60S ribosomal protein L42-A

Chain q2: 



- Molecule 79: 60S ribosomal protein L43-A

Chain Q3: 



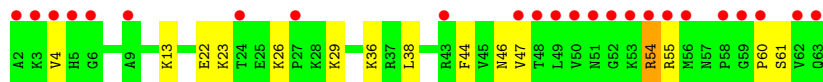
- Molecule 79: 60S ribosomal protein L43-A

Chain q3: 

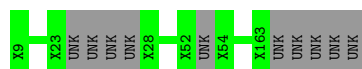


- Molecule 80: 40S ribosomal protein S30-A

Chain e0:

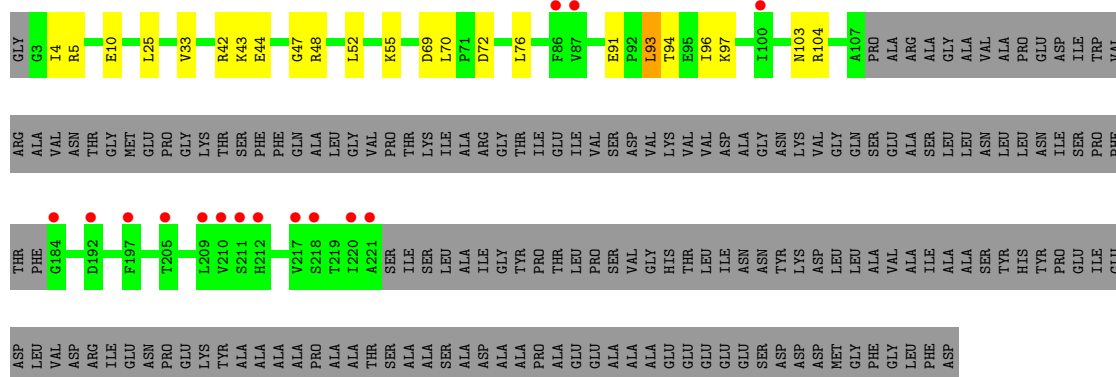


- Molecule 81: Unknown protein m2

Chain m2: 

- Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 



- Molecule 83: Unknown protein p1

Chain p1: 

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein p2

Chain p2: 

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	436.64Å 287.69Å 304.39Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	300.66 – 2.80 300.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (300.66-2.80) 99.5 (300.66-2.80)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.208 , 0.246 0.253 , 0.287	Depositor DCC
$R_{free}$ test set	26295 reflections (1.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 1805319 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	411226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	l5	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	l3	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	l2	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	l4	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	l3	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	l5	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	l3	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	l5	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 Close contacts

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

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	748	0
1	6	38238	0	19241	711	0
2	S0	1577	0	1567	139	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	145	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	111	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	93	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	146	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	130	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	106	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	106	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	98	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	116	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	58	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	59	0
13	c1	1168	0	1231	0	0
14	C2	890	0	887	64	0
14	c2	890	0	887	0	0
15	C3	1192	0	1255	76	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	91	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	74	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	90	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	68	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	89	0
20	c8	1192	0	1222	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C9	1112	0	1124	84	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	80	0
22	d0	882	0	939	0	0
23	D1	684	0	672	54	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	65	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	72	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	70	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	52	0
27	d5	558	0	598	0	0
28	D6	769	0	814	84	0
28	d6	769	0	814	0	0
29	D7	610	0	631	49	0
29	d7	610	0	631	0	0
30	D8	497	0	535	34	0
30	d8	497	0	535	0	0
31	D9	442	0	428	33	0
31	d9	442	0	428	0	0
32	E0	475	0	525	25	0
33	E1	566	0	602	63	0
33	e1	608	0	657	0	0
34	SR	2441	0	2395	133	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	67	0
35	sM	680	0	607	0	0
36	1	67355	0	33840	1037	0
36	5	67376	0	33857	1042	0
37	3	2579	0	1304	39	0
37	7	2579	0	1304	39	0
38	4	3353	0	1695	51	0
38	8	3353	0	1695	58	0
39	L2	1914	0	1981	137	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	218	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	173	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	169	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	61	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	74	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	114	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	106	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	107	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	84	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	94	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	54	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	118	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	83	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	81	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	87	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	77	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	71	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	72	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	29	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	62	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	18	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	65	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	51	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	94	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	28	0
65	n9	462	0	491	0	0
66	O0	743	0	797	52	0
66	o0	767	0	816	0	0
67	O1	876	0	912	40	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	48	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	45	0
69	o3	850	0	880	0	0
70	O4	880	0	945	53	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	61	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	55	0
72	o6	770	0	846	0	0
73	O7	681	0	683	55	0
73	o7	681	0	683	0	0
74	O8	612	0	682	46	0
74	o8	608	0	671	0	0
75	O9	436	0	475	31	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	26	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	25	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	51	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	44	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	175	0	0
82	p0	1077	0	1041	0	0
83	p1	235	0	51	0	0
84	p2	230	0	50	0	0
85	1	475	0	0	0	0
85	2	126	0	0	0	0
85	3	14	0	0	0	0
85	4	21	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	5	504	0	0	0	0
85	6	147	0	0	0	0
85	7	15	0	0	0	0
85	8	13	0	0	0	0
85	C3	1	0	0	0	0
85	L2	1	0	0	0	0
85	L3	2	0	0	0	0
85	L4	3	0	0	0	0
85	L5	1	0	0	0	0
85	L6	1	0	0	0	0
85	L7	2	0	0	0	0
85	L8	1	0	0	0	0
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	4	0	0	0	0
85	M5	2	0	0	0	0
85	M6	1	0	0	0	0
85	M7	6	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N8	2	0	0	0	0
85	O3	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	1	0	0	0	0
85	Q2	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	2	0	0	0	0
85	d2	1	0	0	0	0
85	d3	1	0	0	0	0
85	d6	1	0	0	0	0
85	l2	2	0	0	0	0
85	l3	1	0	0	0	0
85	l4	1	0	0	0	0
85	l5	3	0	0	0	0
85	l7	1	0	0	0	0
85	m1	2	0	0	0	0
85	m4	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	m5	1	0	0	0	0
85	m6	1	0	0	0	0
85	m7	5	0	0	0	0
85	n0	2	0	0	0	0
85	n3	2	0	0	0	0
85	n6	2	0	0	0	0
85	n8	4	0	0	0	0
85	n9	2	0	0	0	0
85	o1	1	0	0	0	0
85	o3	2	0	0	0	0
85	o4	2	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	1	0	0	0	0
85	s1	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2436	0	0	247	0
86	2	1106	0	0	132	0
86	3	84	0	0	5	0
86	4	105	0	0	5	0
86	5	2471	0	0	233	0
86	6	1106	0	0	97	0
86	7	84	0	0	12	0
86	8	112	0	0	21	0
86	C1	7	0	0	7	0
86	C3	7	0	0	1	0
86	C5	7	0	0	4	0
86	C8	7	0	0	1	0
86	D9	7	0	0	1	0
86	L3	14	0	0	1	0
86	L4	7	0	0	2	0
86	L6	7	0	0	0	0
86	M0	7	0	0	0	0
86	M5	14	0	0	2	0
86	M6	7	0	0	1	0
86	M7	14	0	0	1	0
86	M9	7	0	0	1	0
86	N9	7	0	0	1	0
86	O2	7	0	0	0	0
86	O3	7	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	O7	14	0	0	6	0
86	O9	7	0	0	4	0
86	Q2	7	0	0	2	0
86	S8	7	0	0	1	0
86	SR	7	0	0	0	0
86	c1	7	0	0	0	0
86	c3	7	0	0	0	0
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	21	0	0	0	0
86	l4	14	0	0	0	0
86	l5	21	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	m8	7	0	0	0	0
86	n3	7	0	0	0	0
86	n9	7	0	0	0	0
86	o2	7	0	0	0	0
86	o3	7	0	0	0	0
86	o4	7	0	0	0	0
86	o7	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	3	0
87	Q3	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	0	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	33	0	0	0	0
88	5	33	0	0	1	0
All	All	411226	0	297271	8412	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (8412) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
52:M6:66:LYS:NZ	52:M6:66:LYS:CE	1.48	1.54
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.09	1.40
78:Q2:17:CYS:CB	87:Q2:501:ZN:ZN	1.31	1.09
40:L3:296:THR:HG22	40:L3:298:PHE:H	1.82	1.07
36:5:2403:G:N2	36:5:2404:A:N7	2.03	1.03
36:1:979:U:H1'	36:1:980:A:C8	1.94	1.03
70:O4:74:ARG:NH2	36:5:1639:C:OP2	200.94	1.01
4:S2:140:ARG:NH1	23:D1:1:MET:SD	2.34	1.00
64:N8:21:ARG:NH2	36:5:640:U:OP1	182.19	0.99
47:M0:174:THR:HG23	47:M0:176:LEU:H	1.25	0.98
36:5:3274:A:H3'	36:5:3275:U:H5''	1.44	0.98
50:M4:113:THR:HG22	50:M4:116:GLU:H	1.48	0.97
10:S8:76:THR:HG22	10:S8:108:PRO:HG2	1.47	0.97
69:O3:48:ARG:HH11	69:O3:48:ARG:HG2	1.28	0.97
1:6:1011:G:OP2	86:6:2121:OHX:N3	1.97	0.96
51:M5:188:ARG:NH2	36:5:31:C:OP2	122.26	0.96
6:S4:49:ARG:NH1	1:6:448:C:OP2	379.39	0.95
1:2:1585:U:H3	1:2:1611:A:H2	1.10	0.95
36:1:640:U:OP1	64:N8:21:ARG:NH2	2.00	0.95
49:M3:46:ILE:HG22	49:M3:49:ARG:HB2	2.77	0.95
36:1:3346:U:H3	36:1:3359:A:H61	1.09	0.94
50:M4:128:ARG:NH2	36:5:3214:U:OP2	281.04	0.94
1:2:1339:C:O2'	1:2:1341:A:N7	1.99	0.94
47:M0:63:GLU:HB2	36:5:2853:A:H5'	297.32	0.94
1:2:1588:G:H1	1:2:1608:U:H3	1.16	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:31:C:OP2	51:M5:188:ARG:NH2	2.00	0.93
36:1:2403:G:N2	36:1:2404:A:N7	2.15	0.93
25:D3:64:PRO:O	86:6:2159:OHX:N2	360.90	0.93
36:1:3343:G:H21	36:1:3362:A:H2	1.09	0.92
78:Q2:17:CYS:SG	78:Q2:77:CYS:HB3	2.65	0.92
44:L7:217:PRO:O	86:5:4002:OHX:N3	259.50	0.92
36:5:3343:G:H21	36:5:3362:A:H2	1.10	0.92
36:5:2273:G:O6	86:5:4196:OHX:N5	2.04	0.90
36:1:1481:A:O2'	36:1:1858:A:N3	2.05	0.90
20:C8:41:ARG:NH2	21:C9:36:ILE:O	3.09	0.90
1:6:383:G:N7	86:6:2149:OHX:N5	2.18	0.90
16:C4:50:ALA:O	16:C4:52:ARG:N	2.24	0.90
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.79	0.90
50:M4:55:ARG:NH2	50:M4:76:ALA:O	2.18	0.90
52:M6:160:ARG:NH2	36:5:3182:G:OP1	280.20	0.90
25:D3:23:ARG:HG3	25:D3:23:ARG:HH11	1.80	0.90
1:6:1385:G:N7	86:6:2122:OHX:N6	2.20	0.90
36:1:837:A:OP2	79:Q3:4:ARG:NH1	2.05	0.90
1:6:1588:G:H1	1:6:1608:U:H3	1.20	0.90
86:5:3904:OHX:N6	38:8:16:G:O6	2.05	0.90
23:D1:74:GLN:NE2	23:D1:81:ASN:O	2.05	0.89
65:N9:24:PRO:HG2	65:N9:26:THR:HG22	8.01	0.89
36:5:2836:C:H5	36:5:2852:C:H42	1.17	0.89
41:L4:193:LYS:NZ	38:8:21:C:OP1	108.82	0.89
41:L4:99:MET:HE3	41:L4:103:THR:H	3.08	0.89
47:M0:175:ASN:OD1	47:M0:176:LEU:N	5.29	0.89
36:1:2208:A:N1	86:1:4047:OHX:N2	2.20	0.89
40:L3:139:GLN:O	40:L3:141:GLY:N	2.06	0.89
1:2:79:C:H1'	8:S6:174:LYS:HD3	1.55	0.89
19:C7:8:THR:HG21	1:6:1330:G:H21	420.57	0.89
36:1:687:U:OP2	49:M3:36:ARG:NH2	2.05	0.89
8:S6:163:THR:HG22	8:S6:168:THR:HG22	1.53	0.88
54:M8:170:ARG:NH1	64:N8:56:VAL:O	2.07	0.88
43:L6:78:ARG:NH1	36:5:3272:C:OP2	247.40	0.88
48:M1:94:ARG:O	48:M1:96:PHE:N	2.11	0.88
36:1:1233:G:H1	36:1:1255:C:H42	1.20	0.88
21:C9:57:ARG:HH11	21:C9:57:ARG:HG3	1.95	0.88
36:5:1875:G:H2'	36:5:1876:U:H5''	1.54	0.87
36:1:3344:A:H2	36:1:3361:G:H21	1.20	0.87
36:1:1222:G:HO2'	36:1:1285:G:H1	1.17	0.87
36:5:3153:U:H4'	36:5:3154:C:H5'	1.57	0.87
78:Q2:17:CYS:SG	87:Q2:501:ZN:ZN	1.62	0.87

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:1639:C:OP2	70:O4:74:ARG:NH2	2.07	0.87
41:L4:317:PRO:O	41:L4:319:LYS:N	2.07	0.87
1:6:1696:G:O2'	1:6:1698:G:N7	2.06	0.86
17:C5:43:ARG:NH2	1:6:1552:U:OP2	404.30	0.86
36:1:3214:U:H2'	50:M4:121:MET:HE1	1.57	0.86
39:L2:209:HIS:HD2	39:L2:211:HIS:H	1.22	0.86
86:1:3962:OHX:N4	44:L7:217:PRO:HA	1.91	0.86
36:1:3166:C:H42	36:1:3284:G:H1	1.21	0.86
36:1:2836:C:H5	36:1:2852:C:H42	1.23	0.86
40:L3:291:GLU:OE1	40:L3:302:LYS:NZ	3.74	0.86
1:2:68:A:OP1	8:S6:160:ARG:NH2	2.08	0.86
11:S9:93:LEU:HA	11:S9:96:VAL:HG13	1.57	0.86
15:C3:114:ARG:HH11	15:C3:114:ARG:HG2	1.86	0.86
36:1:3272:C:OP2	43:L6:78:ARG:NH1	2.08	0.86
36:5:1654:A:H2'	36:5:1655:G:H5''	1.57	0.86
3:S1:181:LEU:O	3:S1:185:THR:N	2.09	0.86
50:M4:132:LYS:HD3	36:5:3230:G:H4'	287.50	0.86
36:1:3182:G:OP1	52:M6:160:ARG:NH2	2.08	0.86
36:5:1078:U:O4	86:5:3999:OHX:N5	2.09	0.86
16:C4:85:ALA:H	16:C4:119:THR:HG22	1.37	0.86
47:M0:77:THR:HG22	47:M0:82:ARG:HA	2.64	0.86
36:1:2960:C:OP1	86:1:4005:OHX:N4	2.09	0.86
47:M0:3:ARG:NH2	36:5:2854:U:OP2	290.87	0.86
1:2:1010:C:OP2	86:2:2132:OHX:N6	2.09	0.86
19:C7:47:ARG:NH1	19:C7:48:ASN:OD1	2.09	0.85
1:2:740:A:H2'	1:2:741:C:H5''	1.57	0.85
36:5:272:G:OP2	86:5:4074:OHX:N6	2.09	0.85
1:2:9:U:O4	86:2:2156:OHX:N6	2.09	0.85
74:O8:46:ARG:NH2	36:5:1613:A:OP2	131.65	0.85
6:S4:9:LEU:HB2	6:S4:30:ARG:HB2	2.35	0.85
10:S8:162:ALA:HA	36:1:3353:G:H5'	1.58	0.85
2:S0:179:ARG:HD3	2:S0:183:ARG:HH11	1.41	0.85
38:4:70:G:O6	86:O7:103:OHX:N4	2.10	0.85
17:C5:126:VAL:HG13	17:C5:127:ARG:H	1.40	0.85
53:M7:69:ARG:HG2	53:M7:79:THR:HG23	4.85	0.85
71:O5:101:THR:HG22	71:O5:104:GLN:H	1.42	0.84
41:L4:16:THR:HG22	41:L4:18:ASN:H	1.51	0.84
36:1:2123:G:N7	86:1:4201:OHX:N2	2.26	0.84
10:S8:62:THR:HA	10:S8:76:THR:O	2.37	0.84
26:D4:8:ARG:NH1	26:D4:26:ASP:OD1	2.11	0.84
65:N9:50:THR:HG22	36:5:1073:U:H1'	206.13	0.84
1:2:895:G:H1	1:2:917:U:H3	1.23	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:142:G:H22	1:2:173:A:H2	1.25	0.84
10:S8:34:ALA:HB2	10:S8:56:ARG:HD3	2.57	0.83
36:5:2311:G:OP2	86:5:4196:OHX:N1	2.11	0.83
3:S1:201:THR:HG21	3:S1:207:LEU:HD22	1.58	0.83
13:C1:132:SER:O	13:C1:134:THR:N	3.40	0.83
37:3:49:G:N7	42:L5:58:LYS:HG3	1.92	0.83
2:S0:83:GLN:HG2	2:S0:99:ALA:HB1	1.60	0.83
1:6:1010:C:OP2	86:6:2171:OHX:N3	2.12	0.83
55:M9:27:ASN:O	86:M9:202:OHX:N6	2.11	0.83
77:Q1:9:ARG:HG3	77:Q1:9:ARG:HH11	1.84	0.83
78:Q2:73:GLU:OE1	78:Q2:80:ARG:NH2	2.10	0.83
53:M7:109:ALA:HA	53:M7:112:LEU:HD22	1.59	0.83
64:N8:6:THR:HG23	64:N8:8:THR:HG23	1.61	0.83
63:N7:135:ARG:HG2	63:N7:135:ARG:HH21	1.44	0.83
1:2:732:G:O6	86:2:2130:OHX:N5	2.10	0.83
36:1:2940:A:N7	40:L3:2:SER:N	2.27	0.82
41:L4:300:ARG:O	54:M8:39:ARG:NH1	2.18	0.82
1:2:1385:G:N7	86:2:2133:OHX:N3	2.25	0.82
11:S9:126:ARG:NH1	1:6:475:A:OP2	424.34	0.82
10:S8:36:THR:HG21	10:S8:173:PRO:HB2	1.61	0.82
1:2:992:A:H2	1:2:1012:U:H3	1.25	0.82
1:6:1726:G:N7	86:6:2147:OHX:N5	2.28	0.82
40:L3:347:SER:HB3	40:L3:350:ALA:H	1.65	0.82
18:C6:40:GLU:HA	18:C6:42:GLU:H	1.43	0.82
36:1:3214:U:OP2	50:M4:128:ARG:NH2	2.11	0.82
1:6:1041:G:OP1	86:6:2175:OHX:N4	2.13	0.82
44:L7:134:VAL:O	44:L7:229:PHE:HA	2.63	0.82
1:2:140:A:N6	1:2:281:G:OP1	2.12	0.82
1:6:755:A:O2'	1:6:756:A:O4'	1.98	0.82
36:5:658:G:OP1	86:5:4092:OHX:N5	2.12	0.82
40:L3:37:ARG:HG2	40:L3:187:SER:H	4.34	0.82
36:1:2794:G:N7	86:1:3938:OHX:N2	2.27	0.82
1:6:471:A:OP2	86:6:2103:OHX:N5	2.13	0.82
36:5:368:G:OP1	86:5:3924:OHX:N4	2.13	0.82
42:L5:40:HIS:HD2	42:L5:42:ALA:H	1.28	0.81
28:D6:79:ILE:HA	28:D6:84:VAL:HB	1.62	0.81
36:1:1814:A:H4'	36:1:1815:U:H5'	1.62	0.81
46:L9:22:SER:OG	46:L9:23:ARG:N	2.11	0.81
39:L2:193:ARG:NH1	36:5:2174:G:OP2	191.00	0.81
8:S6:87:ARG:NH2	1:6:161:U:OP2	315.22	0.81
1:2:237:C:H5''	1:2:238:U:H5'	1.61	0.81
3:S1:70:LEU:HB3	3:S1:79:HIS:HB3	5.33	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
41:L4:329:PRO:O	41:L4:331:ALA:N	3.33	0.81
36:1:2895:G:H2'	36:1:2896:A:H5''	1.62	0.81
22:D0:53:LYS:HB2	22:D0:92:ASP:HB2	2.50	0.81
1:6:990:C:OP2	86:6:2121:OHX:N2	2.12	0.81
21:C9:68:ARG:NH1	1:6:1521:G:O6	414.90	0.81
1:2:475:A:OP2	11:S9:126:ARG:NH1	2.13	0.81
34:SR:184:ASN:HD22	34:SR:185:GLN:H	5.40	0.81
32:E0:59:GLY:O	32:E0:61:SER:N	3.24	0.81
3:S1:70:LEU:HA	3:S1:73:LEU:HB3	1.63	0.81
53:M7:62:ARG:O	86:M7:207:OHX:N1	2.14	0.81
27:D5:38:HIS:HA	27:D5:70:LYS:HD3	7.74	0.81
36:1:1213:G:H4'	56:N0:90:MET:HG2	1.63	0.81
42:L5:120:LYS:O	42:L5:248:ARG:NH2	2.50	0.81
63:N7:88:ASP:O	63:N7:121:ARG:NH2	2.51	0.81
18:C6:82:ARG:HH22	18:C6:114:ARG:HB2	1.45	0.81
47:M0:76:MET:HE1	47:M0:148:VAL:HA	3.39	0.80
63:N7:46:ILE:HD13	63:N7:68:ILE:HG23	1.63	0.80
10:S8:103:GLN:HB3	10:S8:164:ARG:HG2	1.63	0.80
36:5:2255:A:H5'	36:5:2261:G:H22	1.46	0.80
41:L4:145:ILE:HD11	41:L4:148:ILE:HG13	1.62	0.80
36:1:1898:G:OP2	86:1:3935:OHX:N4	2.15	0.80
3:S1:62:LYS:O	3:S1:64:ARG:N	2.33	0.80
36:5:2233:A:OP2	86:5:3962:OHX:N5	2.14	0.80
1:2:991:G:OP2	86:2:2132:OHX:N1	2.15	0.80
56:N0:23:LYS:O	57:N1:146:ASN:ND2	2.10	0.80
44:L7:88:ARG:HD2	44:L7:90:LYS:O	1.89	0.80
22:D0:74:GLU:HG2	1:6:1429:G:H1'	378.46	0.80
36:1:770:G:N7	86:1:4099:OHX:N6	2.30	0.80
1:6:755:A:H2'	1:6:756:A:C8	2.16	0.80
42:L5:233:ALA:O	42:L5:235:SER:N	2.14	0.80
41:L4:338:LYS:O	41:L4:340:GLY:N	2.19	0.80
1:6:647:G:N2	1:6:687:G:H22	1.79	0.80
1:2:1202:A:OP1	86:2:2111:OHX:N1	2.15	0.80
73:O7:87:SER:O	86:O7:103:OHX:N3	2.14	0.80
2:S0:9:LEU:HD11	2:S0:14:ALA:HB2	2.36	0.80
36:1:2767:U:O2'	78:Q2:30:ALA:O	1.99	0.80
52:M6:110:PRO:O	52:M6:112:TYR:N	3.34	0.80
8:S6:153:VAL:O	8:S6:155:ASP:N	2.41	0.80
26:D4:29:HIS:HB3	26:D4:32:ARG:HB2	4.78	0.80
61:N5:115:ARG:HH11	61:N5:115:ARG:HG3	1.45	0.80
16:C4:38:THR:HG21	1:6:895:G:H21	264.62	0.80
72:O6:28:TYR:O	86:5:4187:OHX:N2	104.66	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:755:A:H2'	1:6:756:A:H8	1.45	0.80
7:S5:92:ARG:HH11	7:S5:92:ARG:HG2	2.43	0.80
25:D3:102:VAL:HG12	25:D3:127:VAL:HG12	1.64	0.80
46:L9:20:ILE:HD13	46:L9:25:VAL:HG22	2.81	0.80
44:L7:217:PRO:HA	86:5:4002:OHX:N5	263.33	0.79
46:L9:105:GLU:HA	46:L9:109:ALA:HB3	1.65	0.79
13:C1:99:ARG:NH1	25:D3:7:ARG:O	2.15	0.79
36:5:2620:G:O6	86:5:4241:OHX:N4	2.15	0.79
36:1:317:A:OP2	72:O6:30:LYS:NZ	2.15	0.79
1:6:1097:U:H4'	1:6:1098:U:H5'	1.63	0.79
1:2:1521:G:O6	21:C9:68:ARG:NH1	2.16	0.79
62:N6:45:ILE:HD11	62:N6:122:LYS:HB2	1.75	0.79
49:M3:3:ILE:HG21	64:N8:45:MET:HE3	5.40	0.79
6:S4:100:ARG:HG2	6:S4:102:VAL:HG12	2.06	0.79
4:S2:82:ASN:HD22	4:S2:207:LEU:HD13	1.47	0.79
1:2:1429:G:H1'	22:D0:74:GLU:HG2	1.62	0.79
47:M0:193:ASP:OD2	47:M0:194:GLY:N	2.16	0.79
2:S0:62:ARG:HG3	2:S0:62:ARG:HH11	2.27	0.79
2:S0:41:ARG:HH11	2:S0:45:VAL:HG21	2.02	0.79
53:M7:122:ALA:HB3	53:M7:143:PRO:HB2	1.89	0.79
36:1:830:A:OP1	86:1:4014:OHX:N4	2.16	0.79
63:N7:15:ARG:NH2	70:O4:83:ASN:OD1	2.15	0.79
1:2:1291:G:H5'	4:S2:119:LYS:HE2	1.63	0.79
36:1:329:U:OP2	86:1:4046:OHX:N4	2.16	0.78
71:O5:78:LYS:HA	71:O5:81:ARG:HD3	1.68	0.78
1:2:701:U:H3	1:2:737:A:H61	1.30	0.78
1:2:1203:A:OP2	86:2:2111:OHX:N5	2.16	0.78
1:2:471:A:OP2	86:2:2077:OHX:N4	2.17	0.78
7:S5:57:SER:O	7:S5:59:VAL:N	2.16	0.78
1:6:453:U:O4	86:6:2062:OHX:N4	2.16	0.78
36:1:2356:A:H61	36:1:2983:C:H5	1.28	0.78
1:6:1765:A:OP1	86:6:2126:OHX:N2	2.17	0.78
42:L5:4:GLN:NE2	42:L5:4:GLN:O	6.95	0.78
70:O4:41:ARG:HA	70:O4:56:THR:HG22	3.26	0.78
2:S0:41:ARG:HE	2:S0:45:VAL:HB	1.48	0.78
5:S3:7:LYS:NZ	22:D0:115:GLU:OE2	2.17	0.78
42:L5:270:LYS:HB3	37:7:1:G:O2'	322.66	0.78
38:4:62:C:O2	86:4:227:OHX:N5	2.17	0.78
36:5:2398:A:H5'	36:5:2398:A:H8	1.49	0.78
29:D7:29:ARG:HG3	29:D7:29:ARG:HH11	1.48	0.78
1:6:1695:G:H21	1:6:1706:C:H41	1.28	0.78
1:2:1681:A:H2'	1:2:1682:U:H5'	1.66	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:S2:69:ILE:HD11	4:S2:133:LYS:HG2	1.65	0.78
36:1:1740:U:H1'	36:1:1741:A:H2	1.49	0.78
36:1:819:U:OP1	73:O7:10:LYS:NZ	2.14	0.78
1:6:1280:C:H2'	1:6:1281:G:H8	1.49	0.78
53:M7:25:SER:O	53:M7:29:THR:HG23	1.84	0.78
4:S2:147:ASN:HB3	23:D1:4:ASP:HA	1.64	0.78
40:L3:171:LEU:O	86:L3:403:OHX:N6	2.17	0.78
34:SR:170:ILE:HG21	34:SR:211:ILE:HD11	1.64	0.78
36:5:2971:A:H3'	36:5:2971:A:N3	1.99	0.78
47:M0:76:MET:HE2	47:M0:148:VAL:HG22	1.65	0.77
1:2:702:G:O6	1:2:736:C:N4	2.14	0.77
51:M5:68:ARG:HG2	51:M5:68:ARG:HH11	1.49	0.77
64:N8:4:ARG:NH2	36:5:1427:U:OP2	135.33	0.77
36:5:1565:G:N1	36:5:1574:C:N3	2.32	0.77
36:1:776:U:H5	36:1:2719:U:O2	1.67	0.77
57:N1:51:GLY:HA3	57:N1:92:ARG:HG3	2.05	0.77
1:2:320:U:H3'	1:2:321:C:H5''	1.65	0.77
6:S4:79:ASP:HB3	6:S4:82:TYR:HB2	1.72	0.77
1:6:301:A:OP2	86:6:2093:OHX:N1	2.18	0.77
8:S6:67:VAL:HG21	8:S6:99:GLY:HA2	1.66	0.77
5:S3:7:LYS:HE2	22:D0:27:THR:HG21	1.65	0.77
46:L9:8:GLN:HG2	46:L9:68:LEU:HD13	1.64	0.77
73:O7:72:ARG:NH1	38:8:95:G:OP2	52.67	0.77
36:1:300:G:O6	86:1:4153:OHX:N1	2.17	0.77
11:S9:133:HIS:NE2	1:6:513:U:OP1	447.41	0.77
44:L7:163:LEU:O	44:L7:165:ASP:N	2.17	0.77
1:6:1665:U:O4	86:6:2124:OHX:N6	2.17	0.77
39:L2:147:ARG:HH22	39:L2:155:LYS:HG3	4.95	0.77
46:L9:166:ARG:HH21	46:L9:168:ARG:HH12	12.19	0.77
54:M8:158:HIS:H	54:M8:186:VAL:HG12	1.53	0.77
49:M3:166:ALA:HB1	64:N8:147:LEU:HD21	2.00	0.77
25:D3:91:GLY:O	25:D3:93:LEU:N	2.17	0.77
36:5:2818:U:H6	36:5:2818:U:H5'	1.48	0.77
54:M8:66:ARG:NH2	36:5:744:A:OP1	167.52	0.77
11:S9:3:ARG:HG2	11:S9:3:ARG:HH21	4.62	0.77
1:2:348:U:O4	86:2:2128:OHX:N5	2.17	0.77
7:S5:216:GLU:OE2	7:S5:219:ARG:NH2	2.16	0.77
36:1:1110:U:H2'	36:1:1111:U:C6	2.20	0.77
5:S3:108:LYS:HG2	5:S3:113:LEU:HD12	1.67	0.77
34:SR:161:LYS:O	34:SR:161:LYS:HG2	1.83	0.77
36:1:356:C:OP2	86:O9:101:OHX:N1	2.17	0.77
47:M0:24:ARG:HG3	47:M0:24:ARG:HH11	1.49	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
40:L3:296:THR:HG22	40:L3:298:PHE:N	2.19	0.77
1:2:127:G:N7	8:S6:202:ARG:NH2	2.32	0.77
68:O2:91:THR:HG22	68:O2:92:TYR:CD2	2.20	0.77
21:C9:105:LEU:HD13	21:C9:122:ARG:HD3	2.04	0.77
28:D6:37:LYS:O	28:D6:38:ARG:NH1	2.16	0.77
42:L5:270:LYS:HG3	42:L5:273:ARG:HB3	4.89	0.77
86:2:2032:OHX:N4	86:2:2147:OHX:N2	2.33	0.77
66:O0:63:SER:HG	66:O0:65:THR:HG1	1.28	0.77
36:1:662:U:OP1	64:N8:8:THR:HG21	1.85	0.76
33:E1:97:LYS:NZ	1:6:1253:U:O4	440.67	0.76
55:M9:62:ARG:NH2	36:5:3068:U:OP2	172.57	0.76
36:5:2975:U:OP1	86:5:4089:OHX:N3	2.17	0.76
48:M1:23:VAL:O	48:M1:25:GLU:N	2.17	0.76
51:M5:31:ARG:NH1	51:M5:124:ASP:OD1	2.49	0.76
56:N0:91:TYR:O	56:N0:137:ARG:NH1	2.19	0.76
22:D0:27:THR:HB	22:D0:88:LYS:HG2	2.18	0.76
69:O3:48:ARG:NH1	69:O3:48:ARG:HG2	1.99	0.76
36:1:1940:G:H21	36:1:3362:A:H8	1.33	0.76
3:S1:77:GLU:OE1	16:C4:114:ARG:NH2	2.18	0.76
40:L3:7:GLU:HG2	36:5:2915:U:C5	258.11	0.76
1:2:1459:C:OP1	20:C8:126:ARG:NH2	2.18	0.76
6:S4:139:VAL:HG13	6:S4:150:PRO:HG3	1.67	0.76
10:S8:36:THR:HB	10:S8:57:ALA:O	1.86	0.76
77:Q1:4:LYS:NZ	1:6:1774:G:N7	301.48	0.76
36:1:1196:C:O2	86:3:218:OHX:N2	2.17	0.76
73:O7:25:ARG:HB3	73:O7:25:ARG:HH11	3.63	0.76
1:6:542:A:C8	1:6:543:C:H2'	2.21	0.76
64:N8:82:ILE:HD11	64:N8:102:ILE:HG12	2.85	0.76
49:M3:113:VAL:HG12	49:M3:117:LYS:HD2	3.63	0.76
64:N8:77:LYS:O	64:N8:79:TRP:N	2.44	0.76
1:2:1479:A:OP1	21:C9:57:ARG:NH1	2.19	0.76
1:6:151:G:H1	1:6:163:G:H1	1.33	0.76
25:D3:125:VAL:HG12	25:D3:126:LYS:HG3	2.51	0.76
41:L4:152:VAL:HG23	41:L4:172:VAL:HG21	1.67	0.76
27:D5:41:ILE:HG23	27:D5:42:LEU:H	1.51	0.76
5:S3:7:LYS:HE3	22:D0:27:THR:HG21	3.10	0.76
1:2:1542:G:N2	1:2:1569:A:OP2	2.18	0.76
1:2:104:A:OP2	1:2:308:C:N4	2.18	0.76
19:C7:27:ASP:O	19:C7:31:ASN:ND2	3.77	0.76
11:S9:59:LEU:HD22	11:S9:69:ARG:HA	2.11	0.76
16:C4:13:VAL:HG13	16:C4:77:THR:H	1.50	0.76
36:1:3375:A:O2'	36:1:3378:C:OP2	2.03	0.76

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:C9:102:ARG:NH2	1:6:1502:G:N7	406.15	0.76
36:1:670:C:OP1	54:M8:147:ARG:NH2	2.16	0.76
63:N7:33:SER:OG	63:N7:35:SER:O	4.92	0.75
41:L4:232:SER:OG	41:L4:233:LEU:N	2.15	0.75
86:2:2032:OHX:N4	86:2:2147:OHX:N1	2.34	0.75
41:L4:197:ARG:NH1	36:5:1381:A:OP1	109.33	0.75
66:O0:101:LEU:HD22	66:O0:101:LEU:H	3.56	0.75
36:5:3276:G:OP2	36:5:3276:G:H2'	1.86	0.75
1:2:1508:U:O4	86:2:2032:OHX:N5	2.19	0.75
39:L2:96:LEU:HD22	79:Q3:83:ILE:HG23	1.67	0.75
47:M0:84:ALA:O	47:M0:140:THR:HG22	1.95	0.75
24:D2:27:ILE:HG12	24:D2:61:ILE:HB	1.66	0.75
36:5:776:U:H5	36:5:2719:U:O2	1.68	0.75
20:C8:30:TYR:HE2	20:C8:40:ARG:HH11	1.30	0.75
1:2:579:A:H2	5:S3:143:ARG:HG3	1.51	0.75
13:C1:4:GLU:HG2	13:C1:5:LEU:HG	1.66	0.75
72:O6:2:THR:OG1	72:O6:3:VAL:N	2.20	0.75
7:S5:94:THR:HG22	7:S5:114:ILE:HG13	2.12	0.75
71:O5:85:THR:HG22	71:O5:88:LEU:H	1.50	0.75
40:L3:139:GLN:HB2	40:L3:141:GLY:H	3.65	0.75
1:2:1720:G:O6	86:2:2083:OHX:N5	2.20	0.75
11:S9:64:GLU:OE1	11:S9:69:ARG:NH2	5.41	0.75
64:N8:94:ALA:HB1	64:N8:121:VAL:HA	1.69	0.75
35:SM:23:LYS:HD2	35:SM:23:LYS:H	1.51	0.75
36:1:2771:U:O2'	36:1:2772:C:O4'	2.04	0.75
2:S0:70:PRO:HB2	2:S0:94:GLY:HA3	1.79	0.75
58:N2:51:GLY:O	58:N2:52:ASN:ND2	2.17	0.75
36:1:2392:C:O2'	40:L3:266:ARG:NH2	2.18	0.75
41:L4:60:THR:HG21	41:L4:77:VAL:HG22	1.68	0.75
1:2:820:U:H2'	1:2:821:U:H4'	1.67	0.75
1:2:1572:G:H1'	7:S5:185:ARG:HH12	1.52	0.75
1:2:770:A:OP2	86:2:2139:OHX:N6	2.20	0.75
41:L4:291:ASN:O	41:L4:293:SER:N	2.20	0.75
37:3:60:G:OP2	86:3:226:OHX:N3	2.20	0.74
36:5:1541:G:OP2	86:5:4093:OHX:N4	2.20	0.74
9:S7:11:GLN:HG3	9:S7:13:PRO:HD2	1.68	0.74
1:2:1370:U:O4	86:2:2121:OHX:N1	2.19	0.74
1:6:65:A:H2	1:6:84:A:H62	1.36	0.74
36:5:2236:G:OP1	86:5:4247:OHX:N3	2.20	0.74
43:L6:31:ARG:HH11	69:O3:107:ILE:HG22	5.09	0.74
8:S6:33:GLY:HA2	8:S6:51:LYS:HE2	1.66	0.74
72:O6:54:GLU:HG2	72:O6:90:MET:HE1	2.94	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:C3:142:GLU:HB2	15:C3:145:THR:HG23	1.69	0.74
51:M5:38:ARG:HH11	51:M5:38:ARG:HG3	1.53	0.74
36:1:2513:U:H2'	36:1:2592:G:H1	1.53	0.74
25:D3:69:ARG:NH1	25:D3:116:ASP:OD1	2.19	0.74
1:6:1681:A:H2	1:6:1720:G:H21	1.33	0.74
41:L4:226:GLU:OE1	41:L4:237:GLN:NE2	2.47	0.74
18:C6:95:LYS:HE3	18:C6:96:TYR:CZ	2.70	0.74
36:1:3118:C:H4'	76:Q0:106:ARG:HH22	1.52	0.74
65:N9:26:THR:OG1	36:5:1065:A:N1	215.64	0.74
1:6:1150:G:O6	86:6:2115:OHX:N5	2.20	0.74
71:O5:10:ARG:NH1	71:O5:60:GLU:OE1	2.21	0.74
36:1:2532:U:O4	36:1:2547:A:N6	2.19	0.74
46:L9:62:ARG:NH2	36:5:3115:C:OP1	330.93	0.74
36:1:408:A:OP1	86:1:4060:OHX:N3	2.21	0.74
37:3:44:C:OP2	48:M1:137:ARG:NH2	2.20	0.74
3:S1:144:ARG:NH2	3:S1:207:LEU:O	3.46	0.74
86:2:2032:OHX:N3	86:2:2147:OHX:N5	2.36	0.74
58:N2:42:LYS:HG2	58:N2:46:ALA:HA	3.66	0.74
71:O5:90:ARG:NH1	36:5:20:A:OP2	86.44	0.74
86:1:3962:OHX:N3	44:L7:217:PRO:O	2.21	0.74
20:C8:134:ARG:O	20:C8:136:GLN:N	3.50	0.74
55:M9:105:LEU:HD13	55:M9:135:LYS:HD2	1.70	0.73
1:6:1595:U:H3	1:6:1600:A:H2	1.35	0.73
75:O9:23:LEU:HD22	75:O9:24:PRO:HD2	1.98	0.73
51:M5:190:THR:O	51:M5:194:GLN:HG2	1.88	0.73
36:5:2234:G:O6	86:5:3962:OHX:N1	2.21	0.73
66:O0:18:ILE:HG22	66:O0:19:LYS:HD3	5.27	0.73
29:D7:28:PRO:HB3	1:6:959:U:H5''	352.31	0.73
16:C4:87:GLY:HA3	16:C4:120:PRO:HG2	2.19	0.73
4:S2:174:ARG:O	11:S9:53:ARG:NH2	2.21	0.73
36:1:2255:A:H5'	36:1:2261:G:H22	1.53	0.73
1:2:1597:A:OP2	31:D9:32:ARG:NH2	2.20	0.73
44:L7:216:VAL:HG11	44:L7:227:GLY:HA3	4.65	0.73
36:1:1240:A:H61	36:1:1244:A:H5''	1.53	0.73
36:1:924:G:OP1	86:1:4146:OHX:N5	2.21	0.73
21:C9:57:ARG:NH1	1:6:1479:A:OP1	392.66	0.73
10:S8:197:THR:HA	10:S8:200:LYS:HB2	1.71	0.73
35:SM:79:SER:HA	35:SM:82:THR:HG23	1.71	0.73
53:M7:138:LYS:HG3	53:M7:140:GLU:HG3	2.03	0.73
10:S8:89:GLU:OE1	10:S8:92:ARG:NH2	2.19	0.73
36:1:3155:U:H3'	36:1:3156:U:H4'	1.71	0.73
1:2:169:A:H5''	8:S6:176:GLN:HG2	1.69	0.73

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
39:L2:224:THR:HG21	36:5:2201:G:H21	222.61	0.73
74:O8:66:ILE:HA	74:O8:69:LEU:HD23	1.69	0.73
36:5:3280:U:O2'	36:5:3281:U:H5''	1.89	0.73
42:L5:56:THR:O	42:L5:58:LYS:N	2.19	0.73
36:1:18:G:OP1	71:O5:81:ARG:NH2	2.19	0.73
1:2:1562:G:OP1	21:C9:89:ARG:NH2	2.21	0.73
13:C1:94:ILE:HG12	25:D3:16:ARG:HD2	4.65	0.73
1:2:1520:U:OP2	21:C9:75:LYS:NZ	2.20	0.73
46:L9:171:ASP:OD1	46:L9:173:ARG:HD3	1.93	0.73
18:C6:50:GLU:OE2	18:C6:82:ARG:NH2	2.53	0.73
1:6:1151:A:O2'	1:6:1766:A:N7	2.21	0.73
1:6:1637:C:OP2	86:6:2115:OHX:N4	2.22	0.73
26:D4:14:SER:OG	1:6:783:G:OP2	417.67	0.73
33:E1:108:VAL:HB	33:E1:114:VAL:HG22	1.70	0.73
40:L3:173:GLN:O	40:L3:175:LYS:N	2.22	0.73
36:1:1724:U:H1'	36:1:1725:C:C6	2.24	0.73
49:M3:50:PRO:O	49:M3:52:ASP:N	3.33	0.73
3:S1:137:ILE:HD11	3:S1:172:LEU:HD22	1.69	0.73
36:1:3122:A:N1	46:L9:70:THR:HG21	2.04	0.73
34:SR:89:LEU:HB2	34:SR:103:PHE:HB2	1.70	0.73
36:5:2248:C:OP2	86:5:3978:OHX:N6	2.22	0.72
39:L2:209:HIS:CD2	39:L2:211:HIS:H	2.06	0.72
1:6:140:A:N6	1:6:281:G:OP1	2.21	0.72
54:M8:154:GLY:O	54:M8:159:LYS:HE2	1.89	0.72
19:C7:14:LYS:NZ	19:C7:18:GLU:OE2	2.22	0.72
59:N3:48:ARG:HH11	59:N3:48:ARG:HG3	1.86	0.72
45:L8:182:GLY:HA3	45:L8:185:ARG:HB2	1.70	0.72
25:D3:27:ASN:OD1	25:D3:31:LYS:NZ	2.21	0.72
1:2:1181:U:O4	86:2:2119:OHX:N6	2.23	0.72
46:L9:28:VAL:HG22	46:L9:33:THR:HB	2.08	0.72
36:5:2398:A:C8	36:5:2398:A:H5'	2.24	0.72
36:1:1878:G:OP1	86:1:3931:OHX:N4	2.23	0.72
4:S2:65:GLU:HB2	4:S2:68:ILE:HD12	1.71	0.72
36:1:1355:A:H5''	36:1:1356:U:H5	1.54	0.72
18:C6:40:GLU:HA	18:C6:42:GLU:N	2.03	0.72
1:2:7:G:O6	4:S2:205:ARG:NH2	2.23	0.72
36:1:283:G:OP1	78:Q2:45:ARG:NH2	2.22	0.72
86:2:2032:OHX:N6	86:2:2147:OHX:N5	2.36	0.72
51:M5:183:THR:OG1	51:M5:183:THR:O	2.69	0.72
1:2:452:A:OP2	86:2:2039:OHX:N5	2.22	0.72
36:1:1230:G:H1	36:1:1279:C:H42	1.35	0.72
28:D6:58:VAL:HG22	28:D6:59:TYR:H	2.28	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:439:C:H3'	36:1:440:A:C8	2.23	0.72
21:C9:49:ASP:HB3	21:C9:53:TRP:HB3	1.71	0.72
42:L5:40:HIS:HB3	42:L5:43:LYS:HG3	1.72	0.72
52:M6:110:PRO:O	52:M6:113:ASP:N	5.38	0.72
40:L3:218:ILE:HG12	40:L3:276:THR:HG23	3.25	0.72
2:S0:50:VAL:HG23	19:C7:109:LEU:HD21	3.33	0.72
41:L4:300:ARG:HG2	41:L4:300:ARG:HH11	3.12	0.72
1:6:542:A:H2'	1:6:542:A:OP1	1.90	0.72
62:N6:3:LYS:HD2	62:N6:8:VAL:HG23	2.70	0.72
48:M1:82:ARG:NH1	48:M1:112:LEU:O	3.09	0.72
27:D5:46:LYS:HG2	27:D5:70:LYS:HE3	1.72	0.72
1:2:868:G:H1	1:2:960:U:H3	1.37	0.72
24:D2:82:LYS:O	24:D2:84:GLY:N	2.20	0.72
4:S2:206:THR:HG21	1:6:14:C:OP2	376.80	0.72
47:M0:38:LYS:HG2	47:M0:41:ALA:HB2	1.90	0.72
41:L4:60:THR:HG23	36:5:364:G:OP1	128.93	0.72
86:5:3942:OHX:N2	86:5:4232:OHX:N6	2.38	0.72
36:5:2258:U:OP2	86:5:3948:OHX:N4	2.22	0.72
5:S3:141:LYS:HE3	5:S3:179:GLN:HG3	1.71	0.72
12:C0:29:GLN:NE2	12:C0:31:LYS:O	4.72	0.72
40:L3:120:LYS:NZ	36:5:3001:C:OP1	205.30	0.72
36:1:3353:G:O2'	36:1:3356:G:OP2	2.07	0.72
1:2:687:G:H5'	24:D2:119:LYS:HG2	1.71	0.72
36:5:2568:C:N4	36:5:2574:G:O6	2.23	0.72
36:5:1840:U:OP2	86:5:4039:OHX:N4	2.23	0.72
49:M3:46:ILE:HG23	49:M3:49:ARG:HB2	1.72	0.71
27:D5:65:LEU:HB3	27:D5:71:ILE:HD12	1.71	0.71
70:O4:57:LEU:HB3	70:O4:61:GLN:HB2	2.44	0.71
63:N7:26:VAL:HG21	63:N7:96:VAL:HB	1.71	0.71
2:S0:52:LYS:HD2	23:D1:82:VAL:HA	1.71	0.71
1:2:1207:C:H42	1:2:1456:C:H5	1.37	0.71
1:6:1171:A:H2'	1:6:1172:G:C8	2.25	0.71
51:M5:96:ARG:HG2	51:M5:96:ARG:HH11	1.55	0.71
1:6:1:U:O2'	1:6:370:A:H5'	1.90	0.71
70:O4:102:LYS:HB3	70:O4:103:LYS:HE3	3.67	0.71
36:1:2236:G:OP1	86:1:4122:OHX:N6	2.23	0.71
40:L3:293:ASN:HB2	40:L3:304:THR:HA	2.08	0.71
4:S2:245:ASP:N	4:S2:245:ASP:OD1	2.21	0.71
34:SR:164:ASP:O	34:SR:166:SER:N	2.67	0.71
1:6:1595:U:N3	1:6:1600:A:H2	1.87	0.71
1:2:1034:C:HO2'	24:D2:2:THR:N	1.87	0.71
15:C3:65:VAL:HG23	15:C3:66:ILE:HG23	6.06	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
55:M9:76:SER:O	55:M9:81:ARG:NH1	2.23	0.71
3:S1:157:GLN:O	3:S1:159:SER:N	2.24	0.71
5:S3:27:ARG:HD2	12:C0:60:SER:HB2	1.72	0.71
36:1:980:A:OP2	36:1:980:A:H8	1.74	0.71
8:S6:31:ARG:HH11	8:S6:34:GLN:HE22	2.67	0.71
1:2:829:A:O2'	1:2:830:U:OP2	2.09	0.71
36:1:637:C:H2'	36:1:638:C:C6	2.26	0.71
22:D0:48:HIS:O	22:D0:48:HIS:ND1	2.24	0.71
1:2:1228:G:H1	14:C2:67:THR:HB	1.54	0.71
36:5:2840:C:OP1	86:5:4136:OHX:N3	2.24	0.71
40:L3:296:THR:HG22	40:L3:299:ASP:H	1.55	0.71
16:C4:117:ASP:OD1	16:C4:119:THR:HG23	1.91	0.71
25:D3:130:VAL:O	25:D3:131:SER:HB3	2.02	0.71
36:1:2098:C:H2'	36:1:2099:A:H8	1.56	0.71
4:S2:225:LEU:HD13	24:D2:68:ARG:HA	2.25	0.71
21:C9:52:GLY:O	21:C9:54:PHE:N	2.23	0.71
78:Q2:71:ARG:HG3	78:Q2:71:ARG:HH11	2.10	0.71
1:2:1585:U:N3	1:2:1611:A:H2	1.86	0.71
40:L3:116:ARG:HG2	40:L3:175:LYS:HA	1.72	0.71
1:2:1046:G:OP1	3:S1:157:GLN:NE2	2.23	0.71
62:N6:52:ARG:O	62:N6:54:ASP:N	2.23	0.71
51:M5:172:ARG:HB3	51:M5:174:ILE:HD13	3.17	0.71
42:L5:34:LYS:O	42:L5:38:THR:HG23	1.89	0.71
36:1:3243:A:H4'	40:L3:95:THR:HG22	1.73	0.71
3:S1:48:VAL:HG13	3:S1:61:LEU:HD21	1.73	0.71
19:C7:51:ALA:O	19:C7:55:THR:HG23	5.09	0.71
36:1:2112:U:H4'	36:1:2113:A:H5'	1.73	0.71
49:M3:74:GLY:O	49:M3:101:ARG:NH1	2.24	0.71
36:1:2397:A:OP1	36:1:2398:A:H4'	1.91	0.71
41:L4:302:ALA:HB2	54:M8:39:ARG:CZ	2.76	0.71
18:C6:39:VAL:HG12	18:C6:41:PRO:HD2	5.40	0.71
14:C2:28:LEU:HD11	14:C2:89:ILE:HG21	3.85	0.71
1:2:887:A:H1'	16:C4:122:PRO:HB3	1.73	0.71
1:6:1370:U:H4'	1:6:1371:A:H4'	1.73	0.71
41:L4:181:VAL:O	41:L4:182:LEU:HB2	1.91	0.71
18:C6:82:ARG:HH22	18:C6:114:ARG:HG3	4.06	0.70
4:S2:168:ARG:NE	1:6:1098:U:OP2	384.74	0.70
1:2:218:A:O2'	1:2:219:A:OP1	2.08	0.70
1:2:1657:U:H4'	1:2:1658:G:O5'	1.89	0.70
7:S5:222:LYS:HA	7:S5:225:ARG:HH11	4.17	0.70
36:1:1238:C:N4	36:1:1245:A:OP2	2.20	0.70
6:S4:158:ASP:OD2	6:S4:174:LYS:NZ	2.23	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
62:N6:112:ASP:HB3	62:N6:115:ARG:HB2	4.06	0.70
1:2:656:G:O2'	1:2:657:U:O4'	2.08	0.70
36:1:2734:A:OP1	86:1:4010:OHX:N3	2.24	0.70
17:C5:44:ARG:NH2	17:C5:82:ASN:O	2.86	0.70
36:1:1952:G:H3'	36:1:1953:G:H5''	1.73	0.70
36:1:595:G:N1	36:1:609:G:H5''	2.06	0.70
73:O7:59:THR:HG22	38:8:41:A:O2'	92.25	0.70
24:D2:2:THR:N	1:6:1034:C:HO2'	339.16	0.70
16:C4:86:THR:HB	16:C4:91:THR:HG22	2.26	0.70
36:1:3312:U:H5''	40:L3:25:ILE:HD12	1.73	0.70
4:S2:90:THR:O	4:S2:92:ALA:N	2.55	0.70
9:S7:50:ASP:N	9:S7:50:ASP:OD1	2.23	0.70
36:1:299:G:N7	86:1:4084:OHX:N2	2.39	0.70
21:C9:37:VAL:HG11	21:C9:100:ILE:HD11	2.57	0.70
86:5:3942:OHX:N2	86:5:4232:OHX:N4	2.38	0.70
76:Q0:114:LYS:NZ	36:5:3107:U:OP1	300.81	0.70
48:M1:49:LYS:HB3	48:M1:62:ASN:HA	1.73	0.70
33:E1:127:GLY:O	33:E1:129:GLY:N	2.24	0.70
63:N7:70:PRO:HG3	63:N7:115:LYS:HB2	1.73	0.70
41:L4:59:GLN:OE1	73:O7:55:ARG:NH2	2.45	0.70
30:D8:36:THR:OG1	30:D8:37:SER:N	2.25	0.70
19:C7:82:ASP:O	19:C7:83:GLN:NE2	2.21	0.70
10:S8:57:ALA:HB2	10:S8:177:GLY:HA2	2.01	0.70
56:N0:137:ARG:HG2	56:N0:139:TYR:CE1	2.37	0.70
17:C5:39:ALA:HA	17:C5:42:ARG:HH21	1.55	0.70
68:O2:81:ASP:O	68:O2:84:THR:HG23	1.90	0.70
41:L4:36:HIS:O	41:L4:40:THR:HG23	2.00	0.70
1:6:193:U:C2	1:6:195:G:H1'	2.26	0.70
1:6:1670:G:N7	86:6:2190:OHX:N4	2.38	0.70
1:6:1492:A:O2'	1:6:1493:A:H8	1.75	0.70
59:N3:87:ARG:HH22	59:N3:137:VAL:CG2	2.05	0.70
47:M0:174:THR:OG1	47:M0:175:ASN:O	6.66	0.70
1:2:1796:C:H5	28:D6:6:ALA:H	1.39	0.70
78:Q2:45:ARG:NH2	36:5:283:G:OP1	147.81	0.70
36:1:3298:C:OP1	53:M7:74:LYS:NZ	2.23	0.70
1:2:833:U:OP2	86:2:2142:OHX:N4	2.25	0.70
1:6:176:C:OP1	86:6:2096:OHX:N6	2.25	0.70
1:6:25:C:OP2	1:6:25:C:H4'	1.90	0.70
36:5:2123:G:N7	86:5:4099:OHX:N1	2.39	0.70
1:2:1428:G:H8	1:2:1428:G:H5'	1.56	0.70
1:6:1542:G:N2	1:6:1569:A:OP2	2.25	0.70
36:1:980:A:H2'	36:1:981:U:N1	2.06	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:S8:50:GLY:HA2	1:6:397:A:O3'	315.54	0.70
17:C5:111:MET:HG2	20:C8:119:ILE:HG13	4.36	0.70
36:5:770:G:N7	86:5:4096:OHX:N6	2.39	0.70
40:L3:239:PRO:O	40:L3:242:THR:HG23	1.92	0.70
86:2:2090:OHX:N6	77:Q1:25:LYS:O	2.24	0.70
10:S8:138:ASN:HA	10:S8:141:ARG:HD3	4.56	0.70
36:1:1790:G:O6	86:1:4171:OHX:N4	2.25	0.70
1:6:1202:A:OP1	86:6:2130:OHX:N2	2.24	0.70
54:M8:30:VAL:O	54:M8:34:THR:HG23	1.91	0.70
36:5:979:U:H1'	36:5:980:A:C4	2.26	0.70
2:S0:71:GLU:O	2:S0:96:THR:HG22	1.91	0.70
64:N8:104:THR:HG21	64:N8:112:ILE:HD11	2.21	0.70
5:S3:225:TYR:OH	34:SR:191:ASP:OD2	3.67	0.70
6:S4:19:LEU:HD11	6:S4:108:ARG:HD2	1.90	0.70
36:1:2107:A:H2	36:1:3344:A:H8	1.39	0.70
45:L8:78:PHE:O	45:L8:79:GLN:HB3	2.63	0.70
9:S7:38:LEU:HD23	9:S7:41:LEU:HD12	1.73	0.70
1:6:67:A:O2'	1:6:69:G:OP1	2.06	0.69
36:1:2736:A:O2'	57:N1:68:THR:HG21	1.92	0.69
14:C2:61:VAL:HG13	14:C2:121:VAL:HG23	3.21	0.69
14:C2:66:VAL:HG11	14:C2:71:ILE:HD12	1.74	0.69
10:S8:8:ARG:HH21	10:S8:22:ARG:HH11	8.63	0.69
1:2:1199:G:O6	22:D0:67:THR:HG23	1.92	0.69
36:1:2818:U:H6	36:1:2818:U:H5'	1.56	0.69
36:1:2585:G:N7	45:L8:47:SER:OG	2.25	0.69
46:L9:48:VAL:HG11	46:L9:52:LEU:HD13	1.74	0.69
2:S0:49:ASN:HB3	2:S0:52:LYS:HG3	1.74	0.69
86:2:2032:OHX:N3	86:2:2147:OHX:N1	2.40	0.69
1:2:1460:A:OP2	35:SM:68:ARG:HD3	1.91	0.69
36:1:3047:U:O2'	40:L3:53:MET:HE1	1.91	0.69
35:SM:65:THR:OG1	35:SM:66:ALA:N	3.81	0.69
42:L5:270:LYS:HG3	42:L5:273:ARG:CB	5.67	0.69
1:2:513:U:H2'	1:2:514:G:C8	2.27	0.69
1:2:885:G:OP1	3:S1:136:ARG:NH1	2.25	0.69
36:1:2120:A:OP2	86:1:4012:OHX:N2	2.25	0.69
36:1:1495:U:H5	36:1:1835:A:N1	1.91	0.69
1:2:1537:C:N3	86:2:2155:OHX:N3	2.39	0.69
41:L4:269:SER:O	41:L4:271:LYS:N	2.22	0.69
7:S5:123:VAL:O	27:D5:58:ARG:NH1	2.24	0.69
28:D6:87:ARG:NH1	1:6:1796:C:OP1	345.75	0.69
36:1:364:G:OP1	41:L4:60:THR:HG23	1.92	0.69
9:S7:13:PRO:HB3	9:S7:14:THR:HB	1.73	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:C7:105:GLN:HA	19:C7:108:ASP:HB2	2.09	0.69
36:5:2101:C:O2'	36:5:2102:U:OP1	2.10	0.69
17:C5:69:GLU:OE1	86:C5:201:OHX:N4	2.25	0.69
38:4:106:C:O2'	86:4:232:OHX:N4	2.25	0.69
42:L5:294:ALA:HB1	47:M0:217:PHE:HB3	1.73	0.69
45:L8:160:ILE:HD12	45:L8:164:VAL:HG13	5.48	0.69
72:O6:76:ARG:HA	72:O6:76:ARG:HE	1.57	0.69
41:L4:354:VAL:O	41:L4:358:THR:HG23	1.92	0.69
20:C8:30:TYR:O	20:C8:33:THR:OG1	2.28	0.69
36:5:2836:C:H5	36:5:2852:C:N4	1.90	0.69
39:L2:204:MET:HE2	39:L2:209:HIS:HB2	2.31	0.69
3:S1:169:SER:O	3:S1:173:THR:HG23	2.35	0.69
53:M7:29:THR:HG22	53:M7:87:SER:OG	1.92	0.69
36:5:2970:C:H4'	36:5:2971:A:N1	2.07	0.69
68:O2:91:THR:HG22	68:O2:92:TYR:HD2	1.56	0.69
51:M5:183:THR:HG22	51:M5:187:ARG:HB2	4.47	0.69
36:1:3107:U:OP1	76:Q0:114:LYS:NZ	2.25	0.69
75:O9:19:GLN:NE2	38:8:53:A:OP1	90.43	0.69
1:2:134:U:OP1	1:2:136:C:N4	2.25	0.69
37:3:62:U:O3'	42:L5:285:ARG:NH1	2.25	0.69
1:2:176:C:OP1	86:2:2074:OHX:N3	2.25	0.69
71:O5:76:GLN:O	71:O5:81:ARG:NH1	2.69	0.69
31:D9:33:LYS:HE2	31:D9:34:TYR:CZ	3.32	0.69
56:N0:155:ARG:HD3	56:N0:172:TYR:CG	2.31	0.69
1:2:1592:A:H2'	1:2:1593:A:H8	1.58	0.69
4:S2:139:ILE:HD11	4:S2:191:ALA:HB1	2.11	0.69
36:1:1409:G:N7	86:1:4070:OHX:N3	2.41	0.69
36:5:1772:U:H5''	36:5:1773:C:H5'	1.74	0.69
46:L9:17:THR:HG21	50:M4:3:THR:HB	1.73	0.69
36:5:1875:G:C2'	36:5:1876:U:H5''	2.23	0.69
1:2:732:G:O2'	1:2:733:A:O4'	2.10	0.69
13:C1:33:ARG:NH2	13:C1:51:GLY:O	3.51	0.69
47:M0:3:ARG:NH1	47:M0:63:GLU:HG3	2.07	0.69
47:M0:38:LYS:NZ	47:M0:45:GLU:OE2	3.50	0.69
73:O7:21:ARG:NH2	73:O7:41:ALA:O	2.29	0.69
1:2:759:U:OP1	86:2:2161:OHX:N1	2.26	0.69
1:2:1533:C:H4'	1:2:1539:G:N1	2.08	0.69
10:S8:172:ARG:NH1	1:6:330:G:OP2	280.81	0.69
36:5:3295:A:H2'	36:5:3296:A:C8	2.27	0.69
36:1:1493:G:O6	75:O9:2:ALA:HA	1.93	0.69
62:N6:60:ARG:NH1	36:5:200:C:OP1	86.48	0.69
18:C6:32:ASN:O	18:C6:66:ARG:NH1	2.25	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:2307:G:O2'	36:1:2310:U:OP2	2.10	0.69
63:N7:135:ARG:HB3	63:N7:135:ARG:HH21	2.96	0.69
34:SR:184:ASN:HD22	34:SR:185:GLN:N	5.47	0.69
36:5:2211:U:O4	86:5:3962:OHX:N4	2.26	0.69
55:M9:105:LEU:HD23	55:M9:138:LEU:HD13	1.75	0.69
19:C7:34:LEU:O	19:C7:38:ILE:HG22	1.93	0.69
57:N1:39:ILE:HD12	57:N1:102:ARG:HG2	1.74	0.69
41:L4:47:ARG:NH1	41:L4:109:TRP:O	2.25	0.69
4:S2:116:LYS:HG2	4:S2:127:ALA:HB3	1.74	0.69
36:1:3358:U:H2'	36:1:3359:A:O4'	1.93	0.69
24:D2:76:SER:OG	24:D2:77:PRO:HD3	1.93	0.69
34:SR:52:GLN:HG2	34:SR:53:LYS:H	2.12	0.69
1:6:915:A:OP1	86:6:2071:OHX:N6	2.26	0.69
36:5:1804:A:H2'	36:5:1805:C:C6	2.28	0.69
11:S9:110:GLN:HE22	11:S9:126:ARG:HG2	1.58	0.68
8:S6:67:VAL:HG23	8:S6:68:LEU:O	2.27	0.68
18:C6:49:TYR:HB3	18:C6:53:LEU:HD21	1.86	0.68
36:1:824:C:H5''	39:L2:21:ARG:HD3	1.76	0.68
1:2:1726:G:N7	86:2:2099:OHX:N4	2.41	0.68
38:4:136:G:OP1	61:N5:48:SER:OG	2.11	0.68
42:L5:95:TRP:CH2	42:L5:181:PRO:HD3	4.52	0.68
15:C3:132:VAL:HG23	15:C3:134:VAL:HG13	1.74	0.68
39:L2:114:SER:HB2	39:L2:169:ILE:HD12	1.75	0.68
11:S9:109:LEU:HB2	11:S9:146:PHE:HB3	1.75	0.68
15:C3:25:TRP:HA	15:C3:27:LYS:HE2	6.64	0.68
1:6:578:U:H4'	1:6:579:A:H5'	1.75	0.68
1:2:61:A:H8	1:2:269:G:HO2'	1.39	0.68
45:L8:94:PHE:HB3	45:L8:189:LEU:HD11	2.86	0.68
1:6:1769:U:OP2	86:6:2144:OHX:N2	2.26	0.68
1:2:150:U:OP1	26:D4:123:LYS:NZ	2.24	0.68
86:1:3876:OHX:N5	38:4:2:A:OP2	2.26	0.68
36:1:3087:A:OP1	86:1:4184:OHX:N5	2.26	0.68
47:M0:87:LEU:HD23	47:M0:138:VAL:HG22	3.45	0.68
1:6:320:U:H2'	1:6:321:C:C2	2.28	0.68
66:O0:9:SER:OG	66:O0:10:ILE:N	2.39	0.68
7:S5:92:ARG:NH2	7:S5:169:ASN:OD1	2.26	0.68
48:M1:143:ARG:NH2	37:7:5:G:OP1	292.32	0.68
19:C7:5:ARG:NH1	1:6:1402:G:OP2	410.05	0.68
36:1:1320:C:O2	56:N0:115:ARG:NH2	2.25	0.68
36:5:1387:G:OP1	86:5:4198:OHX:N3	2.27	0.68
36:1:978:G:O2'	36:1:979:U:O2	2.11	0.68
36:1:2854:U:OP2	47:M0:3:ARG:NH2	2.27	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
86:1:4084:OHX:N1	72:O6:28:TYR:O	2.26	0.68
42:L5:269:SER:OG	37:7:1:G:N3	316.20	0.68
53:M7:29:THR:HA	53:M7:32:THR:HG23	1.75	0.68
53:M7:125:GLN:HB2	53:M7:141:SER:HB2	2.13	0.68
3:S1:34:ALA:HB3	3:S1:41:ARG:HA	1.76	0.68
57:N1:127:GLN:HG3	36:5:1095:U:H3	262.38	0.68
1:2:377:G:O6	86:2:2079:OHX:N5	2.25	0.68
33:E1:144:CYS:HB3	33:E1:147:VAL:HG13	1.81	0.68
19:C7:103:ASP:O	19:C7:104:ASN:ND2	6.32	0.68
1:6:822:U:H2'	1:6:823:G:H5''	1.76	0.68
30:D8:22:ARG:HD2	1:6:1619:C:C2	344.18	0.68
2:S0:24:LEU:O	2:S0:163:ASN:ND2	2.27	0.68
31:D9:19:ARG:NH2	1:6:1597:A:OP1	408.12	0.68
9:S7:114:ARG:O	9:S7:117:THR:HB	2.88	0.68
48:M1:51:ARG:NH2	36:5:2682:C:OP2	303.14	0.68
18:C6:58:ASP:O	18:C6:60:PHE:N	2.25	0.68
36:1:2548:C:OP2	39:L2:93:LYS:NZ	2.25	0.68
3:S1:70:LEU:O	3:S1:74:GLN:N	2.26	0.68
8:S6:102:VAL:HG13	8:S6:106:LEU:HD12	1.75	0.68
36:1:2924:U:O4	86:1:4021:OHX:N1	2.26	0.68
47:M0:36:LEU:HD21	47:M0:69:ARG:HH11	1.58	0.68
64:N8:3:SER:O	64:N8:6:THR:HB	2.33	0.68
20:C8:123:ARG:HG3	20:C8:133:VAL:HG21	1.76	0.68
64:N8:28:HIS:CD2	64:N8:32:ARG:HG2	2.59	0.68
76:Q0:92:ASP:O	76:Q0:105:PRO:HG3	1.94	0.68
18:C6:143:ARG:HH12	35:SM:84:LYS:HZ3	1.40	0.68
1:2:1595:U:H3	1:2:1600:A:H2	1.42	0.68
58:N2:103:TYR:OH	36:5:1677:G:OP2	147.45	0.68
57:N1:139:ARG:HG2	57:N1:139:ARG:HH21	4.38	0.68
61:N5:51:VAL:HG21	71:O5:62:GLN:HB3	2.15	0.68
1:2:68:A:H5'	8:S6:160:ARG:HH12	1.59	0.68
59:N3:87:ARG:HH22	59:N3:137:VAL:HG21	1.59	0.68
36:1:541:U:O4	86:1:4196:OHX:N2	2.27	0.68
44:L7:110:ARG:NH2	36:5:1364:C:OP1	223.32	0.68
36:1:368:G:OP1	86:1:3887:OHX:N1	2.27	0.68
36:5:1110:U:H2'	36:5:1111:U:C6	2.29	0.68
38:4:97:A:OP1	71:O5:67:ARG:NH2	2.26	0.68
54:M8:153:PHE:O	54:M8:161:LYS:HG2	4.21	0.68
86:5:3978:OHX:N2	86:5:4196:OHX:N1	2.41	0.68
1:6:513:U:H2'	1:6:514:G:C8	2.29	0.68
66:O0:13:LYS:NZ	66:O0:99:ASP:OD2	2.26	0.68
9:S7:50:ASP:HB3	9:S7:56:LYS:HG2	1.76	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
34:SR:7:LEU:HG	34:SR:315:VAL:HG22	2.63	0.68
1:2:151:G:O6	26:D4:124:ARG:NH2	2.25	0.68
58:N2:19:VAL:O	58:N2:23:THR:OG1	2.18	0.68
45:L8:33:ASN:O	45:L8:35:GLY:N	3.28	0.68
86:6:2121:OHX:N6	86:6:2171:OHX:N3	2.42	0.67
1:6:895:G:H1	1:6:917:U:H3	1.41	0.67
1:2:514:G:H1	1:2:543:C:H5	1.42	0.67
2:S0:74:VAL:HG22	2:S0:96:THR:HG23	1.76	0.67
36:5:600:G:N2	36:5:603:A:OP2	2.28	0.67
36:5:1806:A:OP2	86:5:4024:OHX:N5	2.27	0.67
36:5:1688:U:H2'	36:5:1689:U:C6	2.29	0.67
52:M6:110:PRO:O	52:M6:111:PRO:C	3.67	0.67
33:E1:119:ARG:NH2	33:E1:120:GLU:O	8.76	0.67
36:5:2877:G:OP1	86:5:4054:OHX:N4	2.28	0.67
36:1:1078:U:O4	86:1:3970:OHX:N2	2.28	0.67
36:1:1794:G:H4'	39:L2:191:LEU:HD13	1.74	0.67
20:C8:120:ARG:NH2	35:SM:58:GLU:OE1	2.26	0.67
1:6:1533:C:H4'	1:6:1539:G:N1	2.08	0.67
36:5:155:G:H5''	36:5:156:G:C8	2.29	0.67
1:2:66:U:H5	8:S6:173:PRO:HG3	1.59	0.67
7:S5:36:ALA:HB1	7:S5:42:LEU:HD12	5.01	0.67
46:L9:9:GLN:HG2	46:L9:52:LEU:HD21	1.75	0.67
5:S3:211:PRO:HG2	19:C7:19:ARG:HB2	1.75	0.67
12:C0:32:HIS:CD2	12:C0:33:GLU:H	4.35	0.67
49:M3:122:LYS:NZ	71:O5:119:LYS:O	2.26	0.67
36:5:118:U:O2	36:5:121:A:H5'	1.93	0.67
70:O4:7:PHE:CD1	70:O4:20:ILE:HD12	4.92	0.67
22:D0:71:PRO:O	22:D0:72:ASN:ND2	6.08	0.67
20:C8:134:ARG:O	20:C8:136:GLN:NE2	5.28	0.67
1:2:197:A:H61	10:S8:138:ASN:ND2	1.92	0.67
36:1:103:G:OP1	49:M3:70:ARG:NH2	2.26	0.67
36:1:3316:A:O2'	36:1:3317:U:OP2	2.08	0.67
47:M0:14:ASN:O	47:M0:128:ARG:NH2	2.28	0.67
1:2:1680:G:O6	86:2:2110:OHX:N5	2.27	0.67
63:N7:38:PHE:O	63:N7:40:HIS:ND1	2.23	0.67
13:C1:101:GLU:OE2	25:D3:16:ARG:NH2	2.58	0.67
1:6:1492:A:HO2'	1:6:1493:A:H8	1.42	0.67
9:S7:67:LEU:HG	9:S7:94:ALA:HB2	2.20	0.67
17:C5:65:LEU:O	86:C5:201:OHX:N2	5.04	0.67
5:S3:164:VAL:HG13	5:S3:168:ILE:HD11	1.76	0.67
86:7:218:OHX:N3	86:7:226:OHX:N6	2.43	0.67
43:L6:149:ILE:HG23	43:L6:155:LEU:HD13	2.41	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:M5:15:GLN:HB3	72:O6:51:SER:HB2	1.76	0.67
86:1:3943:OHX:N5	86:1:4200:OHX:N6	2.42	0.67
54:M8:64:VAL:HG22	54:M8:96:PHE:CE2	2.29	0.67
29:D7:56:CYS:SG	29:D7:57:GLU:N	2.85	0.67
64:N8:96:LYS:O	64:N8:98:THR:N	2.27	0.67
78:Q2:77:CYS:SG	78:Q2:79:THR:HG23	2.35	0.67
86:6:2121:OHX:N6	86:6:2171:OHX:N5	2.43	0.67
36:5:343:U:OP2	86:5:3924:OHX:N3	2.28	0.67
65:N9:14:ARG:HH22	65:N9:18:ARG:HH11	1.42	0.67
45:L8:81:THR:OG1	45:L8:82:LEU:N	2.97	0.67
1:2:523:G:OP2	26:D4:37:LYS:NZ	2.20	0.67
45:L8:241:LYS:HB2	36:5:2586:G:N7	185.23	0.67
76:Q0:77:ILE:HG22	76:Q0:78:ILE:H	1.59	0.67
36:5:1466:G:O6	86:5:3912:OHX:N5	2.28	0.67
22:D0:106:ILE:HG23	22:D0:107:THR:HG23	1.77	0.67
11:S9:171:ARG:NH1	11:S9:174:ARG:HD3	3.58	0.67
1:6:1590:G:OP2	86:6:2157:OHX:N6	2.27	0.67
1:2:702:G:HO2'	1:2:703:G:H8	1.43	0.67
1:6:647:G:H22	1:6:687:G:H22	1.41	0.67
75:O9:50:ASN:OD1	86:O9:101:OHX:N6	2.28	0.67
49:M3:56:PRO:HG3	49:M3:74:GLY:O	2.22	0.67
42:L5:296:GLN:HG2	47:M0:214:PRO:HB3	9.38	0.67
36:1:223:U:O4	86:1:4198:OHX:N5	2.27	0.67
38:4:52:A:H62	75:O9:27:ILE:HD13	1.59	0.67
61:N5:38:LEU:HD11	61:N5:40:LEU:HD13	1.77	0.67
57:N1:42:ILE:HG12	57:N1:96:ILE:HD11	2.00	0.67
8:S6:71:THR:HG22	8:S6:72:ARG:H	4.39	0.67
9:S7:50:ASP:HA	9:S7:56:LYS:HA	1.77	0.67
4:S2:163:GLY:O	4:S2:164:SER:HB3	4.25	0.67
26:D4:47:VAL:O	26:D4:49:LYS:NZ	2.21	0.67
57:N1:129:LYS:HB2	36:5:1098:A:O5'	253.36	0.67
1:2:915:A:OP1	86:2:2095:OHX:N3	2.27	0.67
42:L5:105:ILE:O	42:L5:109:THR:HG23	2.02	0.67
5:S3:125:TYR:O	5:S3:129:SER:OG	3.03	0.67
5:S3:222:VAL:HG11	34:SR:229:LYS:HA	2.41	0.67
36:5:92:G:H5'	36:5:93:C:H5''	1.76	0.67
26:D4:20:ARG:HE	26:D4:22:GLN:HE21	4.96	0.67
42:L5:265:TYR:O	42:L5:269:SER:HB3	4.26	0.67
38:4:95:G:OP2	73:O7:72:ARG:NH1	2.27	0.67
1:2:1745:G:O6	86:2:2087:OHX:N6	2.28	0.67
4:S2:178:ILE:O	4:S2:185:LYS:NZ	2.21	0.67
25:D3:79:ASN:HB3	25:D3:81:LYS:H	1.58	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:1752:A:OP2	86:1:4051:OHX:N3	2.28	0.67
1:6:1762:A:H1'	1:6:1783:C:H5'	1.77	0.67
1:6:729:G:O2'	1:6:730:G:O5'	2.12	0.67
40:L3:41:VAL:HA	40:L3:185:GLY:CA	2.41	0.66
8:S6:136:LYS:NZ	1:6:66:U:OP1	336.23	0.66
31:D9:19:ARG:HD2	31:D9:32:ARG:HD2	1.76	0.66
42:L5:294:ALA:O	42:L5:296:GLN:N	2.23	0.66
51:M5:150:TRP:CH2	51:M5:151:ILE:HG12	2.29	0.66
1:2:178:U:C4	8:S6:191:ARG:HD3	2.30	0.66
1:6:868:G:H1	1:6:960:U:H3	1.42	0.66
47:M0:171:TRP:O	47:M0:174:THR:HB	1.95	0.66
1:2:1202:A:N6	1:2:1457:C:H5''	2.11	0.66
22:D0:58:LEU:HD13	22:D0:88:LYS:HE3	2.31	0.66
2:S0:31:VAL:HG12	2:S0:33:GLN:H	1.60	0.66
20:C8:13:HIS:HA	20:C8:24:GLY:HA3	2.47	0.66
44:L7:151:ARG:NH1	44:L7:244:ASN:O	2.75	0.66
29:D7:37:CYS:O	29:D7:39:GLY:N	2.50	0.66
36:5:398:A:O2'	36:5:1416:C:OP1	2.11	0.66
39:L2:204:MET:CE	39:L2:209:HIS:HB2	2.54	0.66
1:6:1280:C:H2'	1:6:1281:G:C8	2.31	0.66
36:5:15:C:H6	36:5:15:C:H5'	1.59	0.66
20:C8:28:ILE:HD11	20:C8:56:LYS:HB2	7.10	0.66
43:L6:50:LYS:HG2	43:L6:74:VAL:HG21	2.02	0.66
36:1:1636:U:H5''	63:N7:73:LYS:NZ	2.10	0.66
2:S0:185:ARG:HB2	23:D1:45:ALA:HB3	1.76	0.66
24:D2:25:VAL:HG22	24:D2:65:LEU:HD21	4.47	0.66
35:SM:34:LYS:NZ	36:1:2707:C:OP1	2.28	0.66
41:L4:170:LYS:HG2	41:L4:175:HIS:HB2	2.81	0.66
38:8:79:A:H3'	38:8:80:A:C8	2.30	0.66
38:8:79:A:H2'	38:8:80:A:O4'	1.94	0.66
4:S2:101:VAL:HG22	4:S2:115:ILE:HG12	1.76	0.66
1:6:482:U:H3	1:6:505:A:H61	1.42	0.66
1:6:484:C:H42	1:6:503:G:H1	1.41	0.66
49:M3:89:TYR:CE1	49:M3:93:ILE:HD11	4.58	0.66
56:N0:23:LYS:O	56:N0:24:LEU:HB2	1.95	0.66
1:6:647:G:H22	1:6:687:G:N2	1.93	0.66
1:2:1254:U:OP2	14:C2:46:ARG:NH1	2.27	0.66
51:M5:65:ARG:HG2	51:M5:127:TYR:CD1	2.57	0.66
20:C8:145:ARG:HB2	35:SM:68:ARG:NH2	2.11	0.66
39:L2:48:ILE:HD13	79:Q3:65:ALA:HB2	2.50	0.66
40:L3:139:GLN:CB	40:L3:141:GLY:H	4.06	0.66
36:1:2563:G:H5''	45:L8:27:THR:HG23	1.76	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:3074:G:OP1	86:1:4042:OHX:N1	2.28	0.66
16:C4:81:VAL:H	16:C4:115:ILE:HG22	1.61	0.66
29:D7:29:ARG:NH1	29:D7:29:ARG:HG3	2.10	0.66
86:2:2032:OHX:N6	86:2:2147:OHX:N2	2.43	0.66
41:L4:140:HIS:NE2	41:L4:246:ARG:HG2	3.03	0.66
59:N3:86:ARG:HG3	59:N3:92:PHE:CE2	2.47	0.66
4:S2:144:TRP:CE2	4:S2:173:PRO:HG3	2.31	0.66
1:2:301:A:OP2	86:2:2065:OHX:N2	2.28	0.66
56:N0:2:ALA:HB3	56:N0:32:SER:HB3	1.78	0.66
64:N8:115:LYS:HG3	36:5:715:A:H8	148.59	0.66
5:S3:32:GLU:OE1	5:S3:65:ARG:NH2	2.28	0.66
16:C4:107:ARG:HH21	16:C4:107:ARG:HB2	2.02	0.66
2:S0:79:ARG:NH1	2:S0:164:ASN:O	2.60	0.66
18:C6:112:TYR:OH	18:C6:114:ARG:NH1	2.28	0.66
11:S9:129:ILE:HG12	11:S9:134:ILE:HD12	1.78	0.66
36:5:1249:G:H2'	36:5:1250:G:H8	1.61	0.66
42:L5:148:ILE:HG23	42:L5:151:GLN:HB3	2.58	0.66
28:D6:23:CYS:HB2	28:D6:74:CYS:HB3	1.78	0.66
36:1:2227:C:OP1	78:Q2:32:LYS:NZ	2.28	0.66
45:L8:54:GLU:HG2	45:L8:57:ARG:HH21	1.61	0.66
40:L3:296:THR:CG2	40:L3:298:PHE:H	2.40	0.66
75:O9:5:LYS:HD3	75:O9:13:MET:HE1	2.44	0.66
1:2:1490:C:H4'	1:2:1491:U:OP1	1.94	0.66
79:Q3:8:VAL:HB	79:Q3:11:THR:HG22	1.77	0.66
6:S4:66:MET:HE1	6:S4:78:THR:HG23	3.55	0.66
8:S6:63:MET:HE2	8:S6:106:LEU:HD13	1.77	0.66
1:2:1760:G:H2'	1:2:1761:U:H5'	1.78	0.66
36:1:3376:A:OP2	86:1:3911:OHX:N5	2.29	0.66
34:SR:25:THR:OG1	34:SR:26:SER:N	3.54	0.66
36:1:1235:U:H4'	36:1:1236:G:H5'	1.77	0.66
45:L8:144:GLU:OE1	72:O6:36:ARG:NH2	2.41	0.66
49:M3:64:LYS:HE3	64:N8:69:TRP:CD1	2.31	0.66
46:L9:13:PRO:HD2	46:L9:16:VAL:HG22	1.78	0.66
36:1:2107:A:H2	36:1:3344:A:C8	2.14	0.65
51:M5:49:ARG:NH2	36:5:115:A:OP1	101.61	0.65
47:M0:86:HIS:HB3	47:M0:139:ARG:HG2	1.89	0.65
74:O8:5:ILE:HG22	74:O8:54:LEU:HB2	1.78	0.65
40:L3:102:LEU:HD23	40:L3:102:LEU:H	1.60	0.65
1:2:565:C:O2	86:2:2040:OHX:N5	2.29	0.65
36:1:1010:G:N2	47:M0:193:ASP:OD2	2.29	0.65
86:1:3943:OHX:N5	86:1:4200:OHX:N2	2.43	0.65
9:S7:66:SER:O	9:S7:68:ALA:N	3.54	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
44:L7:178:ILE:HA	44:L7:183:ASP:HB3	2.08	0.65
1:6:833:U:O4	86:6:2101:OHX:N2	2.30	0.65
36:1:3242:G:H21	36:1:3245:A:H5''	1.60	0.65
1:2:66:U:C5	8:S6:173:PRO:HG3	2.30	0.65
36:1:2836:C:H5	36:1:2852:C:N4	1.94	0.65
36:1:1213:G:OP1	56:N0:137:ARG:HD3	1.95	0.65
1:2:1796:C:C2	28:D6:5:ARG:HG2	2.31	0.65
49:M3:174:ARG:HB2	72:O6:9:ILE:HD12	1.78	0.65
59:N3:2:SER:HA	59:N3:56:ASP:OD1	5.33	0.65
36:1:1422:G:H21	43:L6:5:LYS:NZ	1.94	0.65
47:M0:74:LYS:O	47:M0:78:THR:HG23	1.96	0.65
36:5:3377:G:O6	86:5:4088:OHX:N2	2.28	0.65
36:5:299:G:N7	86:5:4187:OHX:N1	2.45	0.65
1:2:1795:U:O2	28:D6:10:ARG:HD2	1.97	0.65
5:S3:179:GLN:OE1	5:S3:180:GLY:N	6.44	0.65
19:C7:50:ILE:O	19:C7:54:THR:HG23	2.02	0.65
36:5:2444:C:H42	36:5:2503:G:H1	1.43	0.65
36:5:2996:U:OP1	36:5:2996:U:H4'	1.94	0.65
36:1:1103:A:H1'	36:1:1104:G:OP1	1.96	0.65
43:L6:31:ARG:NH1	69:O3:107:ILE:HG22	5.82	0.65
69:O3:86:ARG:NH2	36:5:497:C:O3'	214.80	0.65
39:L2:9:ARG:NH1	36:5:912:G:OP2	180.45	0.65
36:1:2680:A:C2	48:M1:24:GLY:HA3	2.31	0.65
30:D8:26:THR:HB	30:D8:44:VAL:HG22	1.77	0.65
36:1:73:C:O2	49:M3:59:ARG:HD3	1.97	0.65
36:5:2718:U:O4	86:5:4230:OHX:N6	2.29	0.65
36:5:2211:U:H5	36:5:2234:G:O6	1.79	0.65
8:S6:57:ASP:HA	8:S6:106:LEU:HA	1.78	0.65
1:2:1471:A:OP1	7:S5:185:ARG:NH1	2.30	0.65
2:S0:142:PRO:HB3	23:D1:34:ILE:HD13	2.35	0.65
33:E1:146:SER:HB3	1:6:1235:C:H5'	434.42	0.65
58:N2:19:VAL:HG12	58:N2:105:LEU:HD22	2.44	0.65
1:2:420:A:OP1	8:S6:96:SER:OG	2.11	0.65
36:5:2407:C:H2'	36:5:2408:U:H6	1.62	0.65
36:5:1764:U:H3'	36:5:1765:U:H5''	1.78	0.65
1:2:734:A:H5''	1:2:735:C:OP1	1.96	0.65
42:L5:166:ALA:HB1	42:L5:171:LEU:HD12	1.79	0.65
66:O0:13:LYS:HB3	66:O0:100:ILE:HG23	1.76	0.65
13:C1:5:LEU:O	13:C1:7:VAL:N	2.26	0.65
1:2:818:C:N4	1:2:819:G:O6	2.29	0.65
72:O6:58:ILE:HG22	72:O6:90:MET:HG3	2.37	0.65
45:L8:33:ASN:O	45:L8:33:ASN:ND2	4.29	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:S7:86:GLN:HG3	9:S7:87:ASP:H	1.62	0.65
36:1:3010:U:OP2	86:1:4203:OHX:N5	2.30	0.65
39:L2:45:VAL:HG22	39:L2:84:THR:HA	1.79	0.65
86:5:4020:OHX:N6	86:5:4215:OHX:N2	2.44	0.65
10:S8:76:THR:HG21	10:S8:105:ASP:O	5.55	0.65
3:S1:58:SER:HA	3:S1:62:LYS:HD3	1.78	0.65
36:1:2310:U:OP1	86:1:4142:OHX:N2	2.29	0.65
36:1:3276:G:N7	53:M7:171:ARG:NH1	2.44	0.65
15:C3:91:LEU:HD12	15:C3:125:LEU:HD12	2.80	0.65
66:O0:22:LYS:HD3	66:O0:94:GLU:HG3	3.46	0.65
46:L9:75:VAL:HA	46:L9:78:MET:HE2	1.78	0.65
50:M4:37:GLU:HG3	50:M4:38:ILE:H	1.60	0.65
36:5:1329:U:H4'	36:5:1330:A:OP1	1.96	0.65
36:5:3274:A:H3'	36:5:3275:U:C5'	2.24	0.65
10:S8:76:THR:HG23	10:S8:108:PRO:HG2	2.89	0.65
1:2:1760:G:C2'	1:2:1761:U:H5'	2.27	0.65
40:L3:25:ILE:H	40:L3:25:ILE:HD13	1.62	0.65
49:M3:64:LYS:HG3	64:N8:69:TRP:CG	2.32	0.65
3:S1:129:THR:HA	3:S1:177:GLN:HA	1.78	0.65
41:L4:91:GLY:HA3	41:L4:93:MET:HE1	1.77	0.65
86:5:3973:OHX:N3	86:5:4241:OHX:N5	2.45	0.65
36:5:2398:A:OP1	36:5:2873:U:H4'	1.96	0.65
1:2:568:G:N7	25:D3:69:ARG:NH2	2.45	0.65
31:D9:33:LYS:O	31:D9:36:LEU:HD23	1.97	0.65
36:5:1236:G:N2	36:5:1244:A:OP1	2.28	0.65
10:S8:52:ASN:OD1	86:6:2136:OHX:N3	310.82	0.65
12:C0:12:HIS:NE2	12:C0:49:LEU:HD21	2.11	0.65
4:S2:234:PRO:O	4:S2:235:LEU:HB2	1.97	0.65
36:1:837:A:OP1	79:Q3:5:THR:OG1	2.14	0.64
16:C4:11:SER:OG	16:C4:12:GLN:N	4.23	0.64
43:L6:31:ARG:NH2	43:L6:81:ALA:O	2.29	0.64
52:M6:65:ASN:OD1	52:M6:67:THR:HB	1.99	0.64
34:SR:154:VAL:HG12	34:SR:171:SER:HB3	1.78	0.64
36:5:540:U:H3	36:5:551:A:H61	1.45	0.64
36:1:709:A:OP1	54:M8:179:ARG:NH2	2.24	0.64
86:6:2121:OHX:N2	86:6:2171:OHX:N1	2.45	0.64
42:L5:106:ALA:O	42:L5:110:LEU:HD22	3.69	0.64
1:2:1502:G:O6	21:C9:102:ARG:NH2	2.30	0.64
7:S5:62:VAL:HG13	7:S5:89:ILE:HG12	1.86	0.64
4:S2:45:VAL:HG21	4:S2:68:ILE:HG23	2.72	0.64
15:C3:26:PHE:HE2	15:C3:66:ILE:HD13	1.61	0.64
36:1:118:U:O2	36:1:121:A:H5'	1.96	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:1239:U:O4	86:6:2097:OHX:N1	2.31	0.64
52:M6:12:LYS:O	56:N0:167:ARG:NH2	2.34	0.64
2:S0:140:ASN:ND2	4:S2:62:PRO:HD3	4.00	0.64
36:1:1352:A:H4'	36:1:1353:U:OP1	1.98	0.64
5:S3:178:ARG:H	5:S3:178:ARG:HE	1.45	0.64
36:5:690:A:H4'	36:5:691:A:OP1	1.97	0.64
86:6:2121:OHX:N4	86:6:2171:OHX:N3	2.45	0.64
1:2:142:G:N2	1:2:173:A:H2	1.95	0.64
63:N7:88:ASP:HB3	63:N7:121:ARG:HH22	1.62	0.64
36:1:1596:C:H2'	36:1:1597:C:C6	2.31	0.64
5:S3:163:PRO:HA	5:S3:166:ASP:HB2	1.78	0.64
3:S1:110:LEU:HD11	3:S1:213:ARG:HD2	1.79	0.64
69:O3:59:VAL:HG23	69:O3:60:ARG:H	1.97	0.64
1:2:159:U:O2'	8:S6:87:ARG:NH1	2.31	0.64
18:C6:95:LYS:O	34:SR:59:ARG:NH2	2.59	0.64
59:N3:2:SER:O	59:N3:57:MET:N	5.22	0.64
59:N3:11:PHE:CG	59:N3:88:ARG:HD2	2.44	0.64
36:1:2242:A:H5'	39:L2:243:THR:HG23	1.79	0.64
40:L3:284:ARG:NH2	40:L3:295:ALA:O	2.23	0.64
47:M0:156:ARG:HG2	47:M0:163:GLN:HG2	2.07	0.64
36:1:718:G:C2	36:1:721:G:H1'	2.33	0.64
36:1:563:U:OP1	56:N0:71:LYS:NZ	2.25	0.64
37:3:49:G:C5	42:L5:58:LYS:HG3	2.32	0.64
36:1:2767:U:OP2	86:1:4136:OHX:N2	2.31	0.64
36:1:2897:A:H2'	36:1:2899:C:H5'	1.80	0.64
51:M5:172:ARG:HH11	36:5:30:G:P	107.91	0.64
53:M7:59:PRO:HG3	53:M7:76:PHE:CD1	2.33	0.64
1:2:73:U:H1'	1:2:74:U:H5'	1.80	0.64
36:5:1643:A:H4'	36:5:1822:C:H5'	1.79	0.64
1:2:1367:G:N7	86:2:2109:OHX:N6	2.46	0.64
34:SR:144:LEU:HD21	34:SR:186:PHE:HB3	4.55	0.64
36:5:132:C:H2'	36:5:133:U:H5''	1.79	0.64
18:C6:38:LEU:O	18:C6:40:GLU:N	2.30	0.64
1:6:151:G:N2	1:6:163:G:N2	2.45	0.64
1:2:190:C:N4	1:2:196:G:O6	2.31	0.64
36:5:980:A:H2'	36:5:981:U:C2	2.33	0.64
69:O3:86:ARG:NH1	36:5:498:A:H5'	216.48	0.64
1:6:1058:U:H4'	1:6:1059:U:OP1	1.97	0.64
47:M0:99:ILE:HG13	47:M0:123:HIS:HB2	5.03	0.64
2:S0:56:LYS:NZ	23:D1:66:ASP:OD1	2.31	0.64
1:2:740:A:C2'	1:2:741:C:H5''	2.28	0.64
36:1:1613:A:OP2	74:O8:46:ARG:NH2	2.30	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:702:G:O2'	1:2:703:G:H8	1.80	0.64
8:S6:87:ARG:NH1	1:6:159:U:O2'	321.09	0.64
1:2:1683:C:O2'	1:2:1684:U:O5'	2.13	0.64
54:M8:158:HIS:H	54:M8:186:VAL:CG1	2.11	0.64
19:C7:104:ASN:O	19:C7:106:THR:N	3.61	0.64
52:M6:182:ASN:OD1	52:M6:186:ALA:HB2	4.86	0.64
36:5:1952:G:H1	36:5:2094:C:H42	1.46	0.64
36:5:528:U:H2'	36:5:529:A:C8	2.32	0.64
33:E1:135:HIS:HB2	33:E1:138:ARG:HB3	1.80	0.64
46:L9:86:TYR:CE2	46:L9:151:VAL:HG22	2.42	0.64
86:6:2121:OHX:N2	86:6:2171:OHX:N5	2.45	0.64
36:1:595:G:H1	36:1:609:G:H5''	1.63	0.64
86:7:218:OHX:N3	86:7:226:OHX:N5	2.45	0.64
36:1:12:A:OP1	86:1:4205:OHX:N6	2.31	0.64
44:L7:26:VAL:HG23	44:L7:27:ALA:H	1.63	0.64
5:S3:94:ARG:NH2	35:SM:134:ASP:OD1	2.23	0.64
71:O5:81:ARG:NH2	36:5:18:G:OP1	77.54	0.64
66:O0:15:ALA:O	66:O0:18:ILE:HG22	1.98	0.64
52:M6:62:THR:H	52:M6:69:GLY:HA3	2.10	0.64
59:N3:13:ILE:HG22	59:N3:85:TRP:CD1	2.33	0.64
26:D4:3:ASP:O	26:D4:5:VAL:N	2.30	0.64
39:L2:172:GLY:HA3	79:Q3:68:ALA:H	4.08	0.64
36:1:2573:G:O6	86:1:4002:OHX:N3	2.30	0.64
34:SR:38:ARG:HG2	34:SR:67:ILE:HG23	2.03	0.64
47:M0:76:MET:CE	47:M0:148:VAL:HA	2.66	0.64
36:1:917:A:OP2	86:1:4146:OHX:N2	2.31	0.64
36:1:13:A:OP2	86:1:4205:OHX:N5	2.30	0.64
36:5:3128:G:OP2	86:5:4157:OHX:N3	2.31	0.64
36:1:1507:G:N7	53:M7:129:THR:HG22	2.12	0.64
9:S7:130:VAL:HG11	9:S7:154:LEU:HD21	2.89	0.64
78:Q2:41:ARG:NH1	36:5:284:A:OP2	157.46	0.64
62:N6:91:ASN:O	62:N6:93:ALA:N	2.88	0.64
1:2:260:U:H3'	1:2:261:U:H5''	1.78	0.64
36:1:2278:C:OP1	77:Q1:23:ARG:NH1	2.31	0.64
45:L8:156:ASP:OD2	45:L8:156:ASP:N	2.30	0.64
21:C9:42:GLY:HA2	21:C9:84:LYS:HB2	1.80	0.64
2:S0:63:ILE:HG12	23:D1:36:VAL:HG22	1.80	0.64
28:D6:84:VAL:O	28:D6:86:VAL:N	2.31	0.63
3:S1:51:SER:HA	3:S1:57:ALA:H	1.61	0.63
28:D6:5:ARG:NH2	1:6:1793:G:O2'	335.25	0.63
9:S7:131:PHE:O	9:S7:133:THR:N	2.31	0.63
86:7:218:OHX:N1	86:7:226:OHX:N5	2.47	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
34:SR:33:LEU:HB3	34:SR:45:TRP:HB2	1.79	0.63
30:D8:10:ALA:HB1	30:D8:30:VAL:HB	2.03	0.63
36:1:2554:A:N7	79:Q3:62:LYS:NZ	2.45	0.63
36:1:2209:U:O2'	36:1:2210:G:OP1	2.14	0.63
1:6:656:G:N2	1:6:675:U:O2	2.31	0.63
1:6:1564:U:H2'	1:6:1565:C:C6	2.34	0.63
7:S5:43:PHE:CZ	7:S5:90:ILE:HG21	2.33	0.63
21:C9:139:THR:O	21:C9:142:GLU:HG3	4.88	0.63
18:C6:126:PRO:O	18:C6:128:LYS:NZ	2.26	0.63
44:L7:96:PRO:O	44:L7:99:PRO:HD2	2.30	0.63
11:S9:163:PRO:O	11:S9:165:GLY:N	2.31	0.63
72:O6:57:LEU:O	72:O6:61:ILE:HG12	3.98	0.63
7:S5:225:ARG:NH2	30:D8:58:GLU:HB2	5.52	0.63
10:S8:10:LYS:NZ	1:6:339:C:OP2	284.18	0.63
9:S7:117:THR:HG22	9:S7:120:ALA:H	2.37	0.63
2:S0:56:LYS:HE3	2:S0:158:VAL:HG23	4.01	0.63
36:5:1308:A:C8	36:5:1308:A:OP2	2.52	0.63
36:5:990:U:O4	86:5:4182:OHX:N6	2.31	0.63
63:N7:95:VAL:HG21	63:N7:113:VAL:HG11	1.78	0.63
36:5:1878:G:O2'	36:5:1879:A:OP1	2.16	0.63
36:5:1881:A:OP2	86:5:4030:OHX:N6	2.31	0.63
54:M8:170:ARG:O	54:M8:171:LYS:HB2	3.43	0.63
36:1:410:U:O4	86:1:4060:OHX:N5	2.30	0.63
15:C3:26:PHE:CE2	15:C3:28:LEU:HB2	2.75	0.63
18:C6:32:ASN:N	18:C6:67:VAL:O	2.25	0.63
86:5:4020:OHX:N3	86:5:4215:OHX:N1	2.47	0.63
34:SR:19:TRP:HB2	34:SR:38:ARG:HG3	2.60	0.63
8:S6:199:GLN:O	8:S6:203:GLU:HG3	3.33	0.63
36:5:1345:G:N7	86:5:4066:OHX:N5	2.45	0.63
3:S1:111:ARG:HB3	28:D6:68:TYR:CD2	2.33	0.63
67:O1:19:ARG:HD3	67:O1:35:GLU:HG3	1.80	0.63
1:2:45:U:O2'	1:2:46:A:H2'	1.99	0.63
46:L9:84:LYS:HE2	46:L9:191:LEU:HD13	1.79	0.63
36:1:979:U:C2	36:1:980:A:C4	2.87	0.63
1:6:151:G:H22	1:6:163:G:N2	1.96	0.63
36:5:304:G:N3	36:5:304:G:H5'	2.12	0.63
46:L9:48:VAL:HG13	46:L9:52:LEU:HB3	1.81	0.63
61:N5:48:SER:OG	38:8:136:G:OP1	83.91	0.63
2:S0:150:ASP:OD1	2:S0:165:ARG:NH2	2.25	0.63
7:S5:140:THR:HA	7:S5:214:LYS:HD2	2.81	0.63
36:1:272:G:OP2	86:1:4034:OHX:N3	2.31	0.63
1:6:1160:A:H2'	1:6:1161:C:C6	2.33	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
42:L5:187:THR:O	42:L5:189:GLU:N	2.31	0.63
22:D0:20:ILE:HD13	22:D0:22:ILE:HD13	1.80	0.63
1:6:546:U:H2'	1:6:547:U:C6	2.34	0.63
1:6:987:G:O6	86:6:2120:OHX:N4	2.32	0.63
39:L2:224:THR:HG23	36:5:2202:C:O4'	219.23	0.63
36:5:3047:U:O2'	36:5:3048:A:H5'	1.98	0.63
9:S7:44:LYS:NZ	9:S7:95:GLU:HG2	2.13	0.63
36:1:3169:U:H2'	36:1:3170:A:O4'	1.99	0.63
57:N1:32:LYS:HE3	57:N1:98:HIS:HD2	7.89	0.63
34:SR:136:ILE:H	34:SR:136:ILE:HD13	1.64	0.63
36:1:2403:G:N2	36:1:2404:A:H62	1.97	0.63
3:S1:157:GLN:H	3:S1:160:HIS:HB2	1.64	0.63
1:6:194:U:O2	1:6:195:G:O2'	2.15	0.63
38:4:135:G:OP2	61:N5:56:ARG:NH2	2.31	0.63
1:2:1600:A:H4'	1:2:1601:G:OP1	1.98	0.63
36:1:883:A:H5'	53:M7:133:HIS:HA	1.80	0.63
1:6:1579:U:OP1	86:6:2182:OHX:N4	2.32	0.63
36:5:1655:G:H5'	36:5:1655:G:H8	1.62	0.63
16:C4:85:ALA:H	16:C4:119:THR:CG2	2.12	0.63
8:S6:98:ARG:NH2	8:S6:101:ILE:O	2.32	0.63
20:C8:145:ARG:HD3	35:SM:68:ARG:NE	3.70	0.63
1:2:1114:G:O6	86:2:2075:OHX:N5	2.32	0.63
36:5:739:G:O6	86:5:3966:OHX:N6	2.31	0.63
50:M4:19:ARG:HA	50:M4:69:THR:HG22	2.41	0.63
2:S0:11:PRO:O	2:S0:15:GLN:HG3	2.17	0.63
40:L3:247:ARG:NH2	36:5:2341:A:OP2	219.19	0.63
36:1:1243:G:N2	36:1:1244:A:N7	2.47	0.63
36:1:1724:U:H4'	36:1:1725:C:OP1	1.99	0.63
2:S0:163:ASN:O	2:S0:165:ARG:N	2.59	0.63
57:N1:17:ARG:O	57:N1:18:ASP:HB2	1.98	0.63
1:2:794:U:O2'	1:2:795:U:O2	2.10	0.63
36:1:1176:C:OP1	52:M6:25:LYS:HE3	1.99	0.63
36:1:3259:U:H6	36:1:3259:U:H5'	1.64	0.63
40:L3:92:TYR:O	40:L3:155:ALA:HA	1.98	0.63
40:L3:41:VAL:CA	40:L3:185:GLY:HA3	2.46	0.62
36:1:1286:A:N3	36:1:1287:A:H1'	2.14	0.62
7:S5:90:ILE:O	7:S5:94:THR:HG23	2.36	0.62
51:M5:38:ARG:NH2	38:8:143:U:OP1	108.95	0.62
42:L5:64:ILE:HG13	42:L5:109:THR:HG21	4.65	0.62
68:O2:123:LYS:HA	68:O2:126:LEU:HD12	2.14	0.62
42:L5:155:THR:HG22	42:L5:179:ARG:NH1	2.14	0.62
36:5:1817:G:OP1	86:5:4178:OHX:N1	2.31	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:5:2676:A:H4'	36:5:2677:G:O5'	1.99	0.62
63:N7:83:THR:HG23	63:N7:85:TYR:H	1.63	0.62
31:D9:21:CYS:HB2	31:D9:39:CYS:HB3	2.01	0.62
86:2:2091:OHX:N3	86:2:2132:OHX:N6	2.47	0.62
25:D3:126:LYS:HA	25:D3:131:SER:HA	1.81	0.62
36:1:1308:A:C8	36:1:1308:A:OP2	2.52	0.62
46:L9:129:ARG:O	46:L9:132:VAL:HG13	2.21	0.62
1:6:1690:G:H1	1:6:1711:C:H42	1.47	0.62
48:M1:108:GLU:HG2	48:M1:122:ILE:HG21	1.81	0.62
36:5:59:G:H2'	38:8:33:A:O2'	1.99	0.62
70:O4:16:ARG:HH11	70:O4:16:ARG:HG3	4.36	0.62
1:6:486:G:O6	1:6:488:G:N2	2.32	0.62
11:S9:157:ASP:OD1	11:S9:158:PHE:N	3.99	0.62
36:1:1014:U:H2'	36:1:1015:U:H5''	1.79	0.62
86:2:2040:OHX:N1	25:D3:64:PRO:O	2.32	0.62
20:C8:35:ILE:HB	20:C8:38:VAL:HG22	2.24	0.62
50:M4:48:GLY:HA3	50:M4:53:VAL:HG13	1.92	0.62
25:D3:23:ARG:NH2	1:6:375:U:OP1	343.86	0.62
77:Q1:1:MET:HB2	1:6:1783:C:OP2	309.96	0.62
22:D0:18:GLN:O	22:D0:96:PRO:HB3	3.88	0.62
3:S1:109:LYS:HG3	3:S1:113:MET:HE3	1.80	0.62
67:O1:36:ILE:HD12	67:O1:59:ILE:HD11	1.81	0.62
2:S0:124:THR:HG22	2:S0:174:TRP:HE1	1.64	0.62
66:O0:24:THR:HG22	66:O0:91:SER:HB3	1.80	0.62
10:S8:76:THR:HG22	10:S8:105:ASP:HB3	2.87	0.62
47:M0:73:ASN:O	47:M0:77:THR:HG23	1.98	0.62
47:M0:86:HIS:HB3	47:M0:139:ARG:CG	2.43	0.62
36:5:438:A:C8	36:5:439:C:H5	2.17	0.62
48:M1:59:ILE:HG21	48:M1:65:ILE:HD11	1.80	0.62
86:5:4020:OHX:N5	86:5:4215:OHX:N2	2.47	0.62
1:6:86:A:OP2	86:6:2188:OHX:N1	2.33	0.62
6:S4:31:PRO:HG2	6:S4:38:LEU:HD13	1.80	0.62
1:2:434:G:N7	86:2:2049:OHX:N4	2.46	0.62
1:2:649:U:O2'	1:2:650:U:O5'	2.17	0.62
36:1:1846:C:OP1	36:1:1849:C:N4	2.31	0.62
79:Q3:4:ARG:NH2	36:5:838:G:O6	236.75	0.62
53:M7:84:PRO:HB2	53:M7:87:SER:HB2	1.81	0.62
36:5:2818:U:C6	36:5:2818:U:H5'	2.33	0.62
1:2:1595:U:N3	1:2:1600:A:H2	1.97	0.62
12:C0:15:LEU:HD22	12:C0:46:LEU:HD11	1.81	0.62
5:S3:170:THR:HG22	5:S3:187:LYS:HG2	1.80	0.62
34:SR:64:HIS:ND1	34:SR:86:ASP:OD2	2.31	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
42:L5:261:THR:H	42:L5:264:GLN:NE2	3.21	0.62
44:L7:176:TYR:CZ	44:L7:197:GLN:HG2	2.34	0.62
12:C0:58:GLN:HB3	12:C0:65:TYR:HB2	2.38	0.62
36:1:2663:G:H5'	42:L5:152:ARG:HD3	1.81	0.62
36:5:1093:A:H4'	36:5:1093:A:OP1	1.98	0.62
10:S8:188:GLU:OE2	13:C1:15:LYS:NZ	2.29	0.62
41:L4:9:HIS:CE1	41:L4:146:PRO:HB2	2.35	0.62
3:S1:126:THR:HG22	3:S1:136:ARG:HE	1.94	0.62
10:S8:8:ARG:HD3	10:S8:21:PHE:HB3	1.80	0.62
1:6:837:G:O6	86:6:2101:OHX:N1	2.31	0.62
36:5:2128:C:OP1	86:5:4090:OHX:N3	2.33	0.62
66:O0:26:GLY:O	66:O0:30:THR:HG23	2.01	0.62
1:2:533:U:H4'	26:D4:33:ALA:HB2	1.81	0.62
36:1:2534:G:H2'	36:1:2535:A:H8	1.65	0.62
5:S3:195:SER:O	5:S3:197:THR:N	2.29	0.62
5:S3:40:ARG:HG2	22:D0:110:PRO:HB3	1.81	0.62
4:S2:103:VAL:HG12	4:S2:190:LEU:HD12	1.81	0.62
52:M6:10:ASP:OD2	52:M6:37:ARG:NH2	2.74	0.62
45:L8:163:VAL:O	45:L8:166:LEU:HB2	2.43	0.62
69:O3:56:SER:OG	36:5:3170:A:OP2	204.27	0.62
17:C5:12:PHE:CZ	48:M1:85:LYS:HE2	8.29	0.62
70:O4:42:PRO:HB2	70:O4:51:LEU:HD12	5.50	0.62
21:C9:45:MET:HE3	21:C9:46:PRO:HD2	2.01	0.62
86:2:2162:OHX:N4	8:S6:155:ASP:OD1	2.33	0.62
2:S0:41:ARG:NH1	2:S0:45:VAL:HG21	2.76	0.62
38:4:107:G:OP2	86:4:232:OHX:N2	2.33	0.62
1:2:25:C:H4'	1:2:25:C:OP2	2.00	0.62
36:1:2717:U:OP1	86:1:3987:OHX:N6	2.33	0.62
50:M4:60:LEU:HD13	56:N0:152:LEU:HD11	1.81	0.62
36:5:1481:A:O4'	36:5:1481:A:OP1	2.18	0.62
36:1:2108:C:H1'	36:1:3344:A:C8	2.35	0.62
25:D3:69:ARG:NH2	1:6:568:G:N7	366.04	0.62
41:L4:139:GLY:O	41:L4:180:LYS:HE2	5.18	0.62
36:5:1765:U:H4'	36:5:1765:U:OP1	1.99	0.62
5:S3:178:ARG:NE	5:S3:178:ARG:H	1.98	0.62
1:2:434:G:H5'	25:D3:78:LYS:HB3	1.82	0.62
1:2:1382:A:H5''	22:D0:60:THR:HG22	1.82	0.62
34:SR:295:SER:HB2	34:SR:300:THR:HB	1.81	0.62
33:E1:82:LYS:O	33:E1:84:VAL:N	4.96	0.62
5:S3:105:MET:HG2	5:S3:122:VAL:HG21	1.80	0.62
1:2:730:G:O6	86:2:2157:OHX:N4	2.33	0.62
10:S8:163:GLY:HA3	36:1:3354:U:H1'	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:C5:119:PHE:HE1	20:C8:119:ILE:HG23	2.41	0.62
54:M8:34:THR:HG22	54:M8:49:LEU:HD21	1.82	0.62
86:7:218:OHX:N4	86:7:226:OHX:N2	2.47	0.62
11:S9:29:LYS:O	11:S9:33:GLU:HG2	4.33	0.62
52:M6:16:VAL:CG2	52:M6:43:ILE:HG12	2.53	0.62
41:L4:20:LEU:HD11	41:L4:252:GLU:HG3	1.84	0.62
1:2:591:A:H2'	1:2:592:A:C8	2.35	0.62
36:1:3393:U:H2'	36:1:3394:U:C6	2.34	0.62
68:O2:16:LYS:O	68:O2:17:PHE:HB2	4.66	0.62
3:S1:212:VAL:O	3:S1:214:LYS:N	2.32	0.62
27:D5:82:HIS:O	27:D5:85:LYS:N	3.31	0.62
36:1:1541:G:OP2	86:1:4023:OHX:N5	2.33	0.62
50:M4:124:ARG:NH2	36:5:3212:C:OP2	290.06	0.62
23:D1:9:VAL:HG22	23:D1:10:GLU:H	2.24	0.62
1:6:823:G:H2'	1:6:824:G:O4'	1.98	0.62
48:M1:50:ALA:HB2	48:M1:65:ILE:HD12	1.82	0.62
1:6:1239:U:O2	1:6:1246:C:N4	2.33	0.62
36:1:2572:C:O2'	36:1:2573:G:O4'	2.18	0.62
13:C1:80:MET:HB3	13:C1:83:THR:HG23	1.81	0.62
10:S8:18:ARG:NH1	1:6:105:A:OP1	305.69	0.62
39:L2:3:ARG:HD3	36:5:911:C:H42	179.04	0.62
75:O9:44:TRP:CZ3	75:O9:45:ARG:HG3	2.35	0.62
78:Q2:99:GLN:OE1	78:Q2:102:GLN:NE2	2.25	0.62
36:1:735:A:H2'	36:1:736:A:C8	2.34	0.62
67:O1:79:ARG:HA	67:O1:89:LEU:HD12	1.81	0.62
5:S3:48:VAL:HB	5:S3:86:LEU:HD12	1.81	0.62
3:S1:154:SER:OG	3:S1:154:SER:O	2.23	0.62
36:5:1025:A:H3'	36:5:1026:A:H4'	1.82	0.62
36:5:924:G:OP1	86:5:4212:OHX:N4	2.33	0.62
1:2:359:A:C2	25:D3:38:PHE:HB3	2.34	0.62
1:6:1776:A:H2'	1:6:1777:G:C8	2.35	0.62
61:N5:56:ARG:NH2	38:8:135:G:OP2	82.71	0.61
2:S0:185:ARG:HG3	23:D1:47:PRO:HD3	1.81	0.61
1:6:833:U:O4	86:6:2101:OHX:N5	2.33	0.61
36:1:562:C:H2'	36:1:563:U:C6	2.35	0.61
36:5:1024:G:N7	36:5:1027:A:N6	2.47	0.61
51:M5:46:ASP:OD1	51:M5:50:ARG:NH2	2.37	0.61
34:SR:22:SER:OG	34:SR:70:ASP:HA	3.01	0.61
78:Q2:63:LYS:NZ	36:5:2761:G:N7	212.21	0.61
36:1:2867:C:H5'	36:1:2867:C:H6	1.65	0.61
16:C4:25:ASP:OD1	16:C4:26:THR:N	2.69	0.61
1:6:476:U:OP1	1:6:477:A:O2'	2.17	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
52:M6:61:ALA:HB1	52:M6:66:LYS:HG3	2.25	0.61
47:M0:66:GLU:CD	47:M0:69:ARG:HH21	2.03	0.61
73:O7:88:ALA:O	86:O7:103:OHX:N4	2.33	0.61
20:C8:36:LYS:NZ	1:6:1568:C:OP1	335.64	0.61
1:2:1234:A:H4'	33:E1:146:SER:HB3	1.82	0.61
36:1:807:A:H61	36:1:934:G:H22	1.48	0.61
13:C1:59:PRO:HG2	13:C1:60:PHE:CE2	2.35	0.61
20:C8:94:ASP:OD1	20:C8:98:TYR:OH	2.15	0.61
1:6:770:A:OP2	86:6:2138:OHX:N3	2.33	0.61
41:L4:98:ARG:HD2	41:L4:99:MET:O	2.02	0.61
1:2:706:A:N1	1:2:734:A:N6	2.49	0.61
46:L9:171:ASP:OD2	46:L9:173:ARG:NH1	2.33	0.61
73:O7:55:ARG:HD3	36:5:353:G:N7	108.79	0.61
1:6:213:A:OP2	86:6:2150:OHX:N1	2.32	0.61
86:7:218:OHX:N4	86:7:226:OHX:N6	2.49	0.61
2:S0:185:ARG:H	23:D1:45:ALA:H	2.17	0.61
45:L8:101:THR:HG23	45:L8:104:GLU:H	1.65	0.61
1:2:1650:U:H2'	1:2:1651:A:C8	2.35	0.61
36:1:2697:A:H2'	36:1:2698:G:C8	2.36	0.61
86:1:4007:OHX:N6	86:1:4175:OHX:N1	2.48	0.61
33:E1:90:LYS:HB2	33:E1:93:HIS:CE1	11.06	0.61
7:S5:133:VAL:HG22	7:S5:198:LEU:HD13	1.97	0.61
36:1:1808:G:O6	86:1:3986:OHX:N3	2.34	0.61
1:2:1450:U:OP2	86:2:2063:OHX:N5	2.33	0.61
43:L6:40:LEU:HD11	43:L6:54:TYR:HB2	2.37	0.61
49:M3:80:VAL:HG12	49:M3:85:LEU:O	2.12	0.61
1:6:104:A:OP2	1:6:308:C:N4	2.31	0.61
56:N0:108:GLN:NE2	36:5:1322:U:O2	293.45	0.61
1:2:741:C:O2	9:S7:107:ARG:NH1	2.25	0.61
1:2:780:A:C8	26:D4:8:ARG:HB3	2.35	0.61
27:D5:43:ASP:O	27:D5:45:GLU:N	2.33	0.61
1:2:1592:A:H2'	1:2:1593:A:C8	2.34	0.61
86:7:218:OHX:N1	86:7:226:OHX:N2	2.49	0.61
40:L3:211:GLN:NE2	40:L3:283:TYR:O	2.33	0.61
1:2:1665:U:O4	86:2:2137:OHX:N4	2.32	0.61
62:N6:120:GLN:OE1	62:N6:126:LEU:HA	8.00	0.61
55:M9:86:GLU:OE2	55:M9:91:SER:N	2.30	0.61
1:6:820:U:O2'	1:6:821:U:H5''	2.00	0.61
44:L7:121:LYS:HB2	57:N1:133:ALA:HB3	1.81	0.61
52:M6:108:ILE:HG12	52:M6:108:ILE:O	4.82	0.61
48:M1:15:GLU:HB3	48:M1:130:VAL:HG22	1.82	0.61
1:2:569:C:H41	25:D3:69:ARG:HH12	1.48	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:C2:88:LEU:H	14:C2:140:PHE:HE1	1.75	0.61
19:C7:20:TYR:CE1	19:C7:38:ILE:HD11	2.36	0.61
20:C8:53:ASP:HB3	20:C8:56:LYS:HG3	1.81	0.61
86:5:4020:OHX:N6	86:5:4215:OHX:N4	2.47	0.61
36:5:3103:A:OP2	86:5:4157:OHX:N4	2.34	0.61
1:2:57:G:OP1	26:D4:112:LYS:NZ	2.30	0.61
1:6:1427:A:O2'	1:6:1428:G:OP1	2.17	0.61
11:S9:17:ARG:O	11:S9:23:ARG:NH2	2.33	0.61
47:M0:21:ARG:NH2	47:M0:22:TYR:OH	2.33	0.61
1:2:1280:C:H2'	1:2:1281:G:H8	1.66	0.61
3:S1:171:ILE:HD12	3:S1:197:ILE:HD13	1.80	0.61
71:O5:101:THR:HG22	71:O5:104:GLN:HB2	2.64	0.61
61:N5:67:ILE:HD12	61:N5:121:LYS:HG3	1.82	0.61
38:4:52:A:N6	75:O9:27:ILE:HD13	2.15	0.61
36:5:438:A:H2'	36:5:494:G:H21	1.64	0.61
48:M1:54:VAL:HG13	48:M1:59:ILE:HD11	5.16	0.61
36:5:2407:C:H2'	36:5:2408:U:C6	2.34	0.61
9:S7:49:ILE:O	9:S7:57:ALA:N	2.28	0.61
1:2:1564:U:H2'	1:2:1565:C:C6	2.35	0.61
36:1:1472:U:H5'	55:M9:4:LEU:HB2	1.82	0.61
7:S5:158:GLN:HG2	30:D8:66:LEU:HD11	2.40	0.61
79:Q3:73:THR:HG22	79:Q3:76:ALA:H	1.90	0.61
1:2:143:G:N7	8:S6:177:ARG:NH2	2.48	0.61
62:N6:2:ALA:N	36:5:213:A:H5''	80.94	0.61
36:5:1152:G:N2	36:5:1200:A:H61	1.97	0.61
53:M7:155:GLU:OE2	53:M7:155:GLU:N	4.81	0.61
71:O5:95:PHE:CG	36:5:136:G:H5'	61.72	0.61
55:M9:8:LYS:HD2	55:M9:22:VAL:HG23	1.81	0.61
36:5:2403:G:H22	36:5:2404:A:H62	1.49	0.61
10:S8:39:GLY:HA2	10:S8:61:GLU:HB3	1.82	0.61
40:L3:346:THR:O	40:L3:348:ARG:N	2.90	0.61
34:SR:170:ILE:HG13	34:SR:202:LEU:HD21	3.98	0.61
39:L2:56:ALA:HB2	39:L2:130:SER:HB3	2.78	0.61
1:6:986:G:OP2	86:6:2120:OHX:N2	2.33	0.61
36:5:1818:U:H2'	36:5:1819:U:H6	1.64	0.61
48:M1:90:GLN:HG2	48:M1:170:ASP:HB2	1.83	0.61
1:2:843:U:H2'	1:2:844:A:H8	1.65	0.61
13:C1:6:THR:O	13:C1:8:GLN:N	2.32	0.61
36:5:1355:A:H1'	36:5:1356:U:OP2	1.99	0.61
1:6:1524:A:H2'	1:6:1525:A:C8	2.36	0.61
45:L8:225:LYS:O	45:L8:229:VAL:HG23	2.00	0.61
1:2:1073:G:H2'	1:2:1074:G:H5''	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:717:C:H42	1:2:720:G:H22	1.48	0.61
36:5:1638:A:H5''	36:5:1639:C:OP2	2.00	0.61
24:D2:30:SER:HA	24:D2:34:ILE:HD12	1.82	0.61
1:2:1207:C:N4	1:2:1456:C:H5	1.99	0.61
40:L3:53:MET:HE1	40:L3:327:CYS:HB3	2.48	0.61
40:L3:103:THR:HG21	40:L3:147:GLU:OE2	2.07	0.61
16:C4:30:VAL:HG22	16:C4:39:ILE:HG13	1.83	0.61
3:S1:71:ALA:HB3	16:C4:114:ARG:HH12	2.01	0.61
3:S1:206:PRO:O	3:S1:207:LEU:HB2	1.98	0.61
42:L5:268:GLU:O	42:L5:270:LYS:N	3.34	0.61
54:M8:177:GLY:O	54:M8:186:VAL:N	2.39	0.61
20:C8:143:ARG:NH2	1:6:1462:G:N7	339.43	0.61
51:M5:168:GLY:O	51:M5:172:ARG:HB2	2.59	0.61
1:6:191:C:O2'	1:6:192:U:O5'	2.19	0.61
74:O8:45:VAL:HG23	74:O8:52:TYR:HB2	1.81	0.61
36:1:2341:A:OP2	40:L3:247:ARG:NH2	2.34	0.61
34:SR:300:THR:HG23	34:SR:314:GLN:HG3	1.82	0.61
41:L4:5:GLN:HA	41:L4:20:LEU:O	2.01	0.61
1:6:819:G:O2'	1:6:821:U:OP2	2.19	0.61
1:6:417:A:H4'	1:6:418:G:O5'	2.01	0.61
35:SM:48:ARG:HB3	35:SM:50:ASN:H	4.95	0.61
2:S0:84:ARG:HH21	2:S0:201:LEU:HD12	4.03	0.61
41:L4:295:ILE:O	41:L4:299:ILE:HG12	2.19	0.61
57:N1:91:LEU:HD12	57:N1:96:ILE:HD11	1.83	0.61
40:L3:70:ARG:HH22	59:N3:120:LYS:HE3	1.66	0.61
54:M8:161:LYS:O	54:M8:162:ALA:HB3	2.01	0.61
5:S3:75:LYS:HB3	12:C0:22:VAL:HG22	2.64	0.61
70:O4:7:PHE:HD1	70:O4:20:ILE:HD12	4.09	0.61
36:1:3317:U:H4'	36:1:3318:G:O5'	2.01	0.61
42:L5:76:ALA:HB3	42:L5:109:THR:HG22	2.30	0.61
36:1:1334:U:O2'	44:L7:151:ARG:NH2	2.31	0.61
40:L3:247:ARG:HD3	36:5:1888:U:OP1	210.46	0.61
63:N7:23:VAL:HG12	63:N7:45:GLY:HA3	1.95	0.61
6:S4:151:ASP:OD1	8:S6:215:ARG:NH1	3.24	0.61
15:C3:84:ILE:HG22	15:C3:135:LEU:HD21	1.83	0.61
27:D5:59:TYR:HD2	27:D5:60:VAL:N	1.99	0.61
1:2:1239:U:O4	86:2:2048:OHX:N2	2.34	0.61
21:C9:4:VAL:HG11	21:C9:137:ALA:HB2	1.83	0.61
40:L3:299:ASP:OD1	40:L3:301:THR:HG23	2.12	0.60
28:D6:24:VAL:HG21	28:D6:71:LEU:HD12	1.83	0.60
53:M7:32:THR:HG21	53:M7:87:SER:HB3	1.82	0.60
24:D2:27:ILE:HD11	24:D2:61:ILE:HD12	1.82	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S0:121:VAL:HG23	2:S0:141:ILE:HG21	1.81	0.60
36:5:1815:U:O2'	36:5:1816:A:OP2	2.16	0.60
73:O7:5:THR:HA	73:O7:8:PHE:CD2	2.36	0.60
36:1:2535:A:H61	36:1:2544:U:H3	1.48	0.60
36:1:1806:A:OP2	86:1:3986:OHX:N4	2.34	0.60
28:D6:11:ASN:O	28:D6:11:ASN:ND2	3.17	0.60
1:2:839:U:H2'	1:2:840:U:H5'	1.83	0.60
53:M7:67:ILE:HD12	53:M7:82:ARG:CZ	2.30	0.60
36:1:276:U:O2	51:M5:93:LYS:NZ	2.32	0.60
44:L7:102:VAL:HG12	44:L7:130:ILE:HD12	4.16	0.60
36:1:1854:C:OP2	86:1:4037:OHX:N5	2.33	0.60
32:E0:18:THR:HG21	1:6:584:C:H1'	389.95	0.60
40:L3:47:LEU:HG	40:L3:335:ILE:HD11	2.45	0.60
36:1:3078:U:H4'	36:1:3079:U:O5'	1.96	0.60
36:5:1064:A:N6	36:5:1096:U:H3	1.99	0.60
64:N8:6:THR:HG22	64:N8:9:ARG:HG2	1.84	0.60
6:S4:77:ARG:HD2	6:S4:82:TYR:CE1	5.32	0.60
19:C7:28:PHE:HA	19:C7:55:THR:HG21	3.22	0.60
1:2:499:U:O2'	1:2:500:C:H5"	2.01	0.60
26:D4:36:SER:O	26:D4:40:LEU:HG	2.01	0.60
12:C0:50:THR:HG22	12:C0:55:VAL:HG22	1.83	0.60
47:M0:156:ARG:HD3	47:M0:163:GLN:O	2.39	0.60
6:S4:251:GLU:O	6:S4:255:ARG:HG2	3.98	0.60
34:SR:238:ASP:N	34:SR:238:ASP:OD1	2.33	0.60
38:4:79:A:H2'	38:4:80:A:H1'	1.82	0.60
35:SM:64:LYS:O	35:SM:66:ALA:N	3.15	0.60
56:N0:13:ARG:HH11	56:N0:13:ARG:HG3	4.20	0.60
25:D3:127:VAL:O	25:D3:130:VAL:HG22	2.01	0.60
1:2:1290:U:H2'	1:2:1291:G:C8	2.36	0.60
1:6:1695:G:H21	1:6:1706:C:N4	1.99	0.60
55:M9:101:VAL:HG13	55:M9:104:ARG:NH1	2.15	0.60
36:1:1924:U:OP1	77:Q1:25:LYS:NZ	2.34	0.60
1:2:1460:A:O2'	35:SM:72:ARG:NH2	2.34	0.60
36:5:3049:A:H8	36:5:3049:A:H5'	1.66	0.60
36:5:510:G:O6	86:5:4023:OHX:N2	2.34	0.60
36:1:2278:C:OP1	86:1:3961:OHX:N3	2.35	0.60
86:1:4007:OHX:N3	86:1:4175:OHX:N3	2.50	0.60
1:2:116:U:H2'	1:2:117:U:C6	2.37	0.60
26:D4:83:LYS:HE2	26:D4:96:LEU:HB3	1.84	0.60
67:O1:54:GLU:OE2	67:O1:54:GLU:N	2.29	0.60
36:1:2683:U:H2'	36:1:2684:C:C6	2.36	0.60
49:M3:180:ARG:HD3	72:O6:11:LEU:HD21	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
86:1:3962:OHX:N6	44:L7:217:PRO:O	2.34	0.60
1:2:1428:G:H5'	1:2:1428:G:C8	2.35	0.60
56:N0:155:ARG:NH2	56:N0:171:PHE:O	2.35	0.60
36:1:3050:U:OP2	86:1:4184:OHX:N4	2.35	0.60
37:3:4:U:H2'	37:3:5:G:C8	2.36	0.60
24:D2:114:GLU:HG2	24:D2:118:ARG:HH21	4.66	0.60
53:M7:33:ALA:HB1	53:M7:117:ILE:HG12	1.84	0.60
36:5:1717:U:H2'	36:5:1718:G:C8	2.37	0.60
36:1:3066:U:O4	86:1:4138:OHX:N5	2.34	0.60
54:M8:170:ARG:O	54:M8:171:LYS:HB3	2.00	0.60
34:SR:211:ILE:HG22	34:SR:223:TRP:HD1	1.66	0.60
46:L9:70:THR:HG21	36:5:3122:A:N1	324.75	0.60
1:6:874:C:H2'	1:6:875:G:C8	2.37	0.60
7:S5:163:SER:HB2	30:D8:48:VAL:HG23	1.83	0.60
33:E1:135:HIS:ND1	1:6:1250:U:O2	433.23	0.60
2:S0:188:LEU:HD12	2:S0:189:VAL:HG12	1.83	0.60
69:O3:75:HIS:HB3	69:O3:80:VAL:HG12	1.83	0.60
1:6:1508:U:O4	86:6:2055:OHX:N4	2.34	0.60
36:5:1716:U:H6	36:5:1716:U:H5'	1.67	0.60
41:L4:33:ASP:O	41:L4:37:THR:HG23	2.00	0.60
21:C9:32:GLY:H	21:C9:34:VAL:HG12	1.67	0.60
36:1:3218:A:H5''	36:1:3219:G:C5	2.37	0.60
36:5:1103:A:H3'	36:5:1104:G:H5'	1.83	0.60
4:S2:226:THR:OG1	4:S2:228:ASN:OD1	2.19	0.60
1:2:1338:C:H1'	1:2:1410:A:C4	2.37	0.60
1:2:1769:U:OP2	86:2:2146:OHX:N1	2.34	0.60
44:L7:47:ARG:NH1	44:L7:183:ASP:OD2	2.35	0.60
86:5:4001:OHX:N4	86:5:4090:OHX:N2	2.49	0.60
5:S3:40:ARG:HG3	22:D0:110:PRO:HB3	3.09	0.60
39:L2:230:VAL:O	39:L2:233:GLN:HB2	2.16	0.60
36:1:1764:U:H5''	55:M9:43:LYS:HE2	1.84	0.60
34:SR:216:LYS:HA	34:SR:239:GLU:HG3	1.99	0.60
86:8:215:OHX:N2	86:8:223:OHX:N1	2.48	0.60
45:L8:133:LYS:HB2	45:L8:199:ALA:O	3.56	0.60
1:2:1067:C:H2'	1:2:1068:C:H6	1.65	0.60
36:1:2736:A:OP1	57:N1:92:ARG:NH1	2.34	0.60
36:1:1278:A:O2'	36:1:1279:C:O5'	2.19	0.60
36:5:2569:A:H4'	36:5:2570:U:H5'	1.84	0.60
11:S9:145:SER:OG	1:6:474:A:OP1	419.57	0.60
26:D4:60:PHE:O	1:6:523:G:H5'	413.89	0.60
56:N0:166:LYS:O	56:N0:167:ARG:HB2	2.01	0.60
36:1:1176:C:H2'	36:1:1177:G:N2	2.17	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:M5:119:TYR:OH	51:M5:131:GLU:OE1	2.82	0.60
36:1:1609:C:H5''	61:N5:125:ARG:HH11	1.67	0.60
1:6:1081:A:H1'	1:6:1082:C:H5	1.67	0.60
36:5:2514:U:OP1	36:5:2514:U:H6	1.85	0.60
62:N6:37:LYS:H	62:N6:37:LYS:HE2	1.71	0.60
48:M1:155:THR:O	48:M1:159:THR:HG23	5.28	0.60
39:L2:202:VAL:HG13	39:L2:217:GLN:HB3	1.83	0.60
41:L4:16:THR:HG22	41:L4:18:ASN:N	2.32	0.60
42:L5:107:ARG:HH22	42:L5:120:LYS:HA	1.66	0.60
1:6:1766:A:H5''	86:6:2126:OHX:N3	2.16	0.60
51:M5:68:ARG:HA	51:M5:98:LEU:HD21	2.80	0.60
1:2:1542:G:N2	1:2:1568:C:H1'	2.16	0.60
55:M9:88:ARG:NH1	36:5:2103:U:OP1	213.74	0.60
36:5:1804:A:H2'	36:5:1805:C:H6	1.65	0.60
25:D3:51:GLY:O	25:D3:101:GLU:HA	2.62	0.60
44:L7:228:SER:HA	44:L7:232:ARG:HH21	2.52	0.60
1:6:716:C:H42	1:6:722:G:H1	1.50	0.60
63:N7:87:LEU:HB2	63:N7:127:ASN:ND2	2.15	0.60
36:1:1615:C:OP1	86:1:4182:OHX:N3	2.35	0.60
36:1:1599:G:OP1	86:1:4088:OHX:N5	2.35	0.60
36:1:381:U:O4	86:1:4065:OHX:N4	2.34	0.60
1:6:1672:G:H2'	1:6:1673:G:C8	2.37	0.60
17:C5:18:ARG:NH1	20:C8:90:ASN:O	2.34	0.60
77:Q1:9:ARG:NH1	77:Q1:9:ARG:HG3	2.41	0.60
42:L5:120:LYS:HD3	42:L5:123:GLU:OE1	3.19	0.60
4:S2:70:ASP:OD1	4:S2:133:LYS:NZ	3.40	0.60
8:S6:57:ASP:OD1	8:S6:72:ARG:NH1	2.35	0.60
1:2:514:G:N1	1:2:543:C:H5	2.00	0.60
20:C8:140:THR:HA	20:C8:143:ARG:NH1	2.31	0.60
6:S4:126:VAL:HG13	6:S4:158:ASP:O	2.18	0.60
10:S8:8:ARG:NH2	10:S8:19:ALA:O	2.34	0.60
75:O9:2:ALA:N	36:5:1493:G:O6	121.77	0.60
19:C7:4:VAL:HG22	1:6:1402:G:H5'	401.11	0.60
3:S1:103:MET:HB3	3:S1:215:VAL:HG12	2.35	0.60
1:2:4:C:O2'	11:S9:17:ARG:NH1	2.35	0.60
1:2:1280:C:H2'	1:2:1281:G:C8	2.36	0.60
49:M3:37:ASN:O	49:M3:41:THR:HG23	5.27	0.60
39:L2:112:ILE:HD11	39:L2:168:VAL:HG12	6.91	0.60
64:N8:116:GLY:HA2	64:N8:137:LYS:NZ	2.17	0.60
36:5:955:U:H2'	36:5:956:U:C6	2.37	0.60
36:5:223:U:O4	86:5:4242:OHX:N4	2.34	0.60
1:6:489:C:O2'	1:6:490:C:O4'	2.19	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:1934:G:N7	86:1:3888:OHX:N2	2.50	0.60
55:M9:23:TRP:CZ3	55:M9:25:ASP:HB2	2.37	0.60
50:M4:121:MET:HG3	36:5:3214:U:C4	282.61	0.60
40:L3:169:THR:HG21	40:L3:171:LEU:HD12	1.84	0.60
36:1:776:U:C5	36:1:2719:U:O2	2.53	0.60
40:L3:53:MET:HE1	40:L3:327:CYS:CB	3.07	0.60
76:Q0:78:ILE:HD11	76:Q0:83:LYS:HA	7.41	0.60
1:6:697:C:OP2	86:6:2074:OHX:N5	2.35	0.60
51:M5:125:SER:HB3	36:5:2433:U:H1'	161.32	0.60
1:2:851:U:H2'	1:2:852:C:C6	2.37	0.60
26:D4:62:THR:HA	26:D4:69:SER:HA	1.84	0.60
36:1:3113:A:OP1	46:L9:73:SER:OG	2.19	0.60
63:N7:21:LYS:HG2	63:N7:46:ILE:O	2.03	0.59
36:1:2818:U:C6	36:1:2818:U:H5'	2.37	0.59
20:C8:145:ARG:HD3	35:SM:68:ARG:CZ	2.81	0.59
48:M1:24:GLY:HA2	48:M1:65:ILE:HG23	3.77	0.59
52:M6:68:ARG:NH1	36:5:2988:C:P	216.69	0.59
53:M7:129:THR:HG23	53:M7:139:TYR:HB2	1.84	0.59
45:L8:163:VAL:HG22	45:L8:166:LEU:HD12	1.84	0.59
53:M7:64:ASN:O	53:M7:67:ILE:HG12	2.38	0.59
1:2:1477:G:H2'	1:2:1478:G:C8	2.37	0.59
36:1:3103:A:OP2	86:1:4170:OHX:N1	2.35	0.59
23:D1:71:ARG:HG3	23:D1:83:TRP:CH2	2.37	0.59
36:5:385:A:H2'	36:5:386:A:C8	2.37	0.59
40:L3:81:THR:O	40:L3:81:THR:HG22	2.02	0.59
49:M3:133:PRO:O	49:M3:135:ALA:N	3.51	0.59
36:1:2799:A:H1'	64:N8:42:ARG:NH2	2.16	0.59
1:6:1688:U:H2'	1:6:1689:A:C8	2.37	0.59
42:L5:10:SER:HB2	37:7:67:G:H5'	312.97	0.59
49:M3:42:ARG:O	49:M3:46:ILE:HG12	3.16	0.59
41:L4:145:ILE:O	86:L4:404:OHX:N5	2.35	0.59
1:6:152:U:C2	1:6:163:G:N2	2.70	0.59
4:S2:56:ILE:HG23	4:S2:61:LEU:HB2	1.84	0.59
52:M6:42:ASN:OD1	52:M6:125:ARG:HD3	2.02	0.59
48:M1:101:ASN:HB3	48:M1:130:VAL:HA	2.38	0.59
34:SR:255:ALA:HB2	34:SR:292:LEU:HD22	1.85	0.59
36:1:2518:C:OP1	86:1:4209:OHX:N5	2.35	0.59
10:S8:116:HIS:O	10:S8:146:ARG:NH1	2.35	0.59
1:2:1358:G:H2'	1:2:1359:C:C6	2.38	0.59
72:O6:63:ASN:O	72:O6:65:GLY:N	4.71	0.59
36:5:2528:G:N7	86:5:4206:OHX:N3	2.50	0.59
36:5:2717:U:OP1	86:5:4068:OHX:N3	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
70:O4:44:CYS:SG	70:O4:81:CYS:HB3	2.42	0.59
47:M0:72:ALA:O	47:M0:76:MET:HG2	4.42	0.59
6:S4:73:ASP:OD2	6:S4:122:LYS:NZ	2.24	0.59
55:M9:106:LEU:HD13	55:M9:138:LEU:HD11	2.47	0.59
1:6:500:C:O2'	1:6:501:U:O4'	2.21	0.59
22:D0:28:SER:HB3	22:D0:34:LEU:HD12	4.25	0.59
17:C5:100:LYS:HD3	1:6:1183:A:C4	366.26	0.59
6:S4:121:TYR:HA	6:S4:163:ASP:O	2.19	0.59
1:6:1697:G:H8	1:6:1705:C:N3	2.00	0.59
73:O7:2:GLY:N	36:5:2138:A:HO2'	174.09	0.59
40:L3:4:ARG:HG3	40:L3:4:ARG:HH11	3.37	0.59
39:L2:27:ALA:O	39:L2:128:ARG:NH2	2.60	0.59
74:O8:8:ILE:HD12	74:O8:8:ILE:H	1.67	0.59
37:3:17:A:OP1	42:L5:2:ALA:N	2.34	0.59
1:6:75:U:O2'	1:6:76:A:O4'	2.20	0.59
36:1:2223:A:OP2	36:1:2223:A:H8	1.84	0.59
36:1:2107:A:C2	36:1:3344:A:H8	2.19	0.59
17:C5:126:VAL:O	17:C5:127:ARG:HB2	2.29	0.59
46:L9:57:VAL:HG23	46:L9:68:LEU:HG	2.03	0.59
1:2:1657:U:O4	86:2:2090:OHX:N4	2.36	0.59
40:L3:77:THR:HG23	40:L3:326:GLY:O	2.02	0.59
17:C5:68:PRO:O	86:C5:201:OHX:N1	6.49	0.59
43:L6:50:LYS:HG2	43:L6:74:VAL:CG2	2.58	0.59
12:C0:46:LEU:O	12:C0:50:THR:HG23	2.02	0.59
69:O3:18:ARG:HD3	36:5:1178:G:H5'	238.29	0.59
1:2:843:U:H2'	1:2:844:A:C8	2.38	0.59
36:5:330:G:OP2	86:5:4049:OHX:N1	2.35	0.59
1:2:482:U:H2'	1:2:483:A:H8	1.66	0.59
20:C8:26:ILE:HD11	20:C8:31:ALA:HA	3.47	0.59
1:2:530:C:O2	26:D4:61:ARG:NH2	2.36	0.59
36:1:1383:G:O3'	41:L4:138:ARG:NH2	2.36	0.59
1:2:539:G:OP2	1:2:539:G:H8	1.86	0.59
18:C6:47:LYS:NZ	18:C6:114:ARG:HD3	4.53	0.59
19:C7:27:ASP:OD2	19:C7:30:THR:HG22	2.01	0.59
21:C9:52:GLY:HA2	21:C9:55:TYR:CD2	2.37	0.59
47:M0:210:ILE:HA	47:M0:217:PHE:HE2	1.68	0.59
41:L4:354:VAL:HG11	57:N1:143:THR:HG21	1.83	0.59
86:1:3943:OHX:N1	86:1:4200:OHX:N4	2.50	0.59
86:5:4020:OHX:N5	86:5:4215:OHX:N1	2.49	0.59
36:5:1235:U:H4'	36:5:1236:G:H5'	1.83	0.59
14:C2:81:ASP:O	14:C2:83:GLU:N	2.66	0.59
36:5:2977:G:OP1	86:5:4151:OHX:N4	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:876:G:H1'	1:2:944:A:O4'	2.02	0.59
63:N7:14:VAL:HG13	70:O4:86:LYS:HG2	1.83	0.59
38:8:43:A:OP1	86:8:224:OHX:N3	2.35	0.59
41:L4:191:LYS:HG3	41:L4:194:TYR:CZ	3.86	0.59
26:D4:122:GLY:HA2	26:D4:125:LEU:HB3	3.26	0.59
1:6:918:U:H2'	1:6:919:A:H8	1.68	0.59
41:L4:68:GLY:O	36:5:2401:A:H1'	173.13	0.59
1:6:1207:C:H42	1:6:1456:C:H5	1.50	0.59
56:N0:82:ASP:OD1	56:N0:87:THR:HB	2.02	0.59
27:D5:47:TYR:CZ	27:D5:51:LEU:HD11	3.07	0.59
1:2:1429:G:C1'	22:D0:74:GLU:HG2	2.31	0.59
21:C9:30:VAL:HG12	21:C9:54:PHE:CD2	2.37	0.59
10:S8:138:ASN:OD1	10:S8:138:ASN:N	2.36	0.59
10:S8:8:ARG:CZ	10:S8:22:ARG:HE	7.27	0.59
36:1:3242:G:N2	36:1:3245:A:H5''	2.18	0.59
36:5:1877:U:H5''	36:5:1878:G:H5'	1.83	0.59
26:D4:122:GLY:O	26:D4:126:ALA:N	3.23	0.59
36:5:2810:C:OP1	86:5:4079:OHX:N3	2.36	0.59
36:5:1586:G:OP1	86:5:3991:OHX:N3	2.36	0.59
52:M6:78:ARG:HG2	52:M6:78:ARG:HH11	1.68	0.59
86:1:3976:OHX:N3	86:1:4159:OHX:N1	2.51	0.59
1:2:280:U:O2'	1:2:281:G:OP2	2.17	0.59
46:L9:166:ARG:HH21	46:L9:168:ARG:NH1	11.99	0.59
7:S5:43:PHE:HZ	7:S5:90:ILE:HG21	1.66	0.59
21:C9:52:GLY:HA2	21:C9:55:TYR:HD2	1.68	0.59
1:2:1657:U:C4	86:2:2090:OHX:N2	2.70	0.59
73:O7:21:ARG:HD2	73:O7:37:CYS:SG	2.52	0.59
75:O9:9:ILE:HG22	75:O9:13:MET:HE2	1.85	0.59
1:2:1619:C:H1'	30:D8:22:ARG:HH21	1.67	0.59
36:1:2443:A:N6	36:1:2504:U:O4	2.35	0.59
36:1:1043:C:O3'	47:M0:90:ARG:NH1	2.35	0.59
36:5:2284:C:O2	86:5:4177:OHX:N1	2.36	0.59
3:S1:85:LYS:HB3	3:S1:101:HIS:HB3	1.84	0.59
2:S0:26:ALA:HB3	2:S0:149:LEU:HB2	1.84	0.59
70:O4:74:ARG:HG2	70:O4:75:ALA:N	2.18	0.59
51:M5:96:ARG:NH1	51:M5:96:ARG:HG2	2.17	0.59
49:M3:42:ARG:O	49:M3:46:ILE:HB	2.03	0.59
86:5:3978:OHX:N6	86:5:4196:OHX:N3	2.50	0.59
8:S6:162:VAL:HG21	8:S6:171:LYS:HD3	4.57	0.59
41:L4:316:ASN:OD1	41:L4:318:LEU:HB2	2.03	0.59
86:2:2091:OHX:N5	86:2:2132:OHX:N6	2.51	0.59
75:O9:48:LYS:O	86:O9:101:OHX:N2	2.35	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:M5:38:ARG:HH11	51:M5:38:ARG:CG	2.15	0.59
15:C3:27:LYS:HE2	15:C3:27:LYS:H	1.66	0.59
30:D8:12:VAL:HG22	30:D8:28:VAL:HG11	1.84	0.59
68:O2:122:PRO:O	68:O2:123:LYS:HB2	4.63	0.59
24:D2:86:ILE:HG13	24:D2:87:GLU:N	2.17	0.59
1:6:800:U:H2'	1:6:801:G:H8	1.66	0.59
42:L5:279:LYS:HD3	42:L5:282:ARG:NH2	5.02	0.59
64:N8:13:GLY:O	68:O2:36:LYS:HE2	2.21	0.59
57:N1:135:PRO:O	57:N1:136:ARG:HB2	4.60	0.59
60:N4:4:GLU:HG2	60:N4:30:ARG:CD	2.33	0.59
36:1:1481:A:O2'	36:1:1858:A:C2	2.49	0.59
4:S2:99:LYS:HG3	4:S2:117:THR:HG22	3.17	0.59
44:L7:244:ASN:HD22	44:L7:244:ASN:C	2.06	0.59
2:S0:56:LYS:HD2	2:S0:158:VAL:HG23	1.83	0.59
36:5:3317:U:H4'	36:5:3318:G:O5'	2.03	0.59
60:N4:23:ARG:NH2	60:N4:25:ASP:OD1	3.22	0.59
36:5:3078:U:O2'	86:5:4193:OHX:N1	2.36	0.59
36:5:1506:A:H1'	36:5:1848:G:O6	2.03	0.59
16:C4:29:HIS:HB2	16:C4:41:ARG:HA	1.85	0.59
36:1:2295:A:OP1	59:N3:63:LYS:NZ	2.36	0.59
32:E0:46:ASN:HD21	32:E0:48:THR:HG23	3.87	0.59
8:S6:70:PRO:O	8:S6:98:ARG:NH1	2.36	0.59
33:E1:96:LYS:O	33:E1:97:LYS:HB3	2.33	0.59
40:L3:25:ILE:HD13	40:L3:25:ILE:N	2.18	0.59
20:C8:125:ILE:HG12	35:SM:61:ILE:HG23	1.84	0.59
51:M5:49:ARG:NH1	36:5:149:U:OP2	101.23	0.59
34:SR:13:LEU:HB2	34:SR:310:ILE:HB	1.84	0.59
34:SR:20:VAL:HG11	34:SR:310:ILE:HG12	2.34	0.59
36:1:1845:G:H5'	36:1:1846:C:H5'	1.84	0.59
1:6:75:U:O2'	1:6:76:A:O5'	2.21	0.59
39:L2:187:HIS:ND1	39:L2:190:ARG:NH1	3.87	0.59
1:2:855:A:C2	1:2:857:U:H1'	2.37	0.59
38:8:83:C:H4'	38:8:85:G:N3	2.18	0.59
1:6:624:G:H2'	1:6:625:C:H6	1.67	0.59
36:1:2169:G:O6	86:M5:303:OHX:N4	2.35	0.59
4:S2:98:PHE:CZ	35:SM:116:GLU:HG3	2.38	0.59
13:C1:40:LEU:HD22	1:6:246:G:C2	327.26	0.59
39:L2:245:LEU:HD23	39:L2:247:ARG:HH11	1.68	0.59
14:C2:52:LEU:O	14:C2:85:LYS:NZ	2.35	0.59
21:C9:115:GLU:OE1	21:C9:123:ARG:NH1	5.47	0.59
36:5:1781:C:H2'	36:5:1782:U:C6	2.38	0.59
30:D8:52:ASP:OD1	30:D8:52:ASP:N	2.36	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:3115:C:OP1	46:L9:62:ARG:NH2	2.35	0.58
86:1:3943:OHX:N3	86:1:4200:OHX:N6	2.51	0.58
16:C4:107:ARG:NH2	16:C4:107:ARG:HB2	2.77	0.58
67:O1:70:ARG:HD2	67:O1:102:LYS:HE2	3.42	0.58
24:D2:89:TRP:O	24:D2:93:LEU:HB2	5.07	0.58
36:1:612:U:OP1	43:L6:21:THR:HB	2.03	0.58
1:6:826:U:O4	86:6:2066:OHX:N3	2.35	0.58
36:5:2875:U:H3	36:5:2952:G:H1	1.50	0.58
3:S1:82:ARG:NH2	3:S1:188:LEU:O	3.05	0.58
77:Q1:6:ARG:O	77:Q1:10:THR:HG23	2.02	0.58
7:S5:110:ALA:HA	7:S5:113:ILE:HD12	1.85	0.58
36:1:1565:G:N2	36:1:1574:C:O2	2.36	0.58
36:1:627:U:H2'	36:1:628:A:C8	2.38	0.58
19:C7:6:THR:OG1	19:C7:8:THR:HG23	4.73	0.58
3:S1:180:THR:HG23	3:S1:183:GLN:OE1	9.53	0.58
46:L9:106:LYS:H	46:L9:109:ALA:HB2	1.68	0.58
1:2:514:G:O2'	1:2:515:A:H5'	2.03	0.58
86:5:4020:OHX:N3	86:5:4215:OHX:N4	2.51	0.58
16:C4:29:HIS:ND1	16:C4:29:HIS:O	2.36	0.58
3:S1:81:PHE:HD2	3:S1:82:ARG:HG3	1.68	0.58
21:C9:61:VAL:O	21:C9:65:ILE:HG13	2.03	0.58
28:D6:17:HIS:ND1	28:D6:18:VAL:O	2.36	0.58
49:M3:24:VAL:HG21	49:M3:26:PHE:CE2	2.38	0.58
6:S4:194:THR:O	6:S4:195:ILE:HB	2.03	0.58
49:M3:16:LYS:O	49:M3:17:HIS:HB2	4.64	0.58
36:1:1427:U:OP2	64:N8:4:ARG:NH2	2.26	0.58
36:1:1355:A:H5''	36:1:1356:U:C5	2.37	0.58
40:L3:53:MET:HB2	36:5:3049:A:H5''	233.86	0.58
1:2:1006:C:O2	86:2:2146:OHX:N2	2.36	0.58
38:8:90:U:O2	86:8:219:OHX:N2	2.36	0.58
4:S2:170:ILE:HB	4:S2:197:TYR:HB2	1.87	0.58
74:O8:31:LEU:HA	74:O8:37:PRO:HA	1.84	0.58
12:C0:2:LEU:HD22	1:6:1258:U:H4'	434.13	0.58
4:S2:228:ASN:ND2	23:D1:1:MET:HB3	2.17	0.58
1:6:66:U:H4'	1:6:67:A:OP1	2.03	0.58
36:1:1233:G:N2	36:1:1255:C:N3	2.43	0.58
86:2:2091:OHX:N1	86:2:2132:OHX:N2	2.52	0.58
18:C6:47:LYS:HZ1	18:C6:114:ARG:HG2	1.68	0.58
1:6:151:G:N2	1:6:163:G:H22	2.01	0.58
36:1:2514:U:H5'	45:L8:68:ARG:HG3	1.86	0.58
41:L4:73:ARG:NH2	36:5:2814:G:OP1	172.84	0.58
36:1:1947:G:H1	36:1:2101:C:H42	1.49	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
40:L3:2:SER:O	40:L3:3:HIS:HB3	2.06	0.58
56:N0:12:ARG:HG3	56:N0:13:ARG:O	2.24	0.58
36:5:3278:C:O2'	36:5:3279:A:OP2	2.21	0.58
1:2:639:U:OP1	9:S7:117:THR:OG1	2.20	0.58
86:1:3943:OHX:N3	86:1:4200:OHX:N4	2.51	0.58
52:M6:16:VAL:HG21	52:M6:43:ILE:HG12	1.99	0.58
42:L5:279:LYS:HD3	42:L5:282:ARG:CZ	4.53	0.58
1:6:138:A:N6	1:6:266:A:H61	2.01	0.58
36:5:1614:C:H2'	36:5:1615:C:H6	1.68	0.58
6:S4:11:ARG:N	6:S4:26:CYS:O	2.97	0.58
36:5:783:A:OP2	86:5:4191:OHX:N6	2.37	0.58
1:2:1331:A:OP1	19:C7:45:ARG:NH2	2.37	0.58
36:5:1596:C:H2'	36:5:1597:C:C6	2.39	0.58
10:S8:5:ARG:HD3	10:S8:29:LEU:O	2.07	0.58
47:M0:3:ARG:HH22	36:5:2854:U:P	291.48	0.58
86:2:2091:OHX:N5	86:2:2132:OHX:N2	2.52	0.58
41:L4:141:ARG:NH1	41:L4:180:LYS:HD3	2.39	0.58
1:6:1669:U:OP2	86:6:2190:OHX:N3	2.36	0.58
10:S8:8:ARG:NH2	10:S8:22:ARG:HE	7.65	0.58
41:L4:269:SER:O	41:L4:269:SER:OG	2.19	0.58
70:O4:20:ILE:HD11	70:O4:34:HIS:CE1	2.39	0.58
67:O1:79:ARG:H	67:O1:79:ARG:NE	2.00	0.58
86:8:215:OHX:N6	86:8:223:OHX:N3	2.50	0.58
36:1:1554:U:HO2'	36:1:1582:C:H5	1.50	0.58
36:5:3035:A:OP2	86:5:4051:OHX:N5	2.36	0.58
36:5:1070:U:O4	86:5:4110:OHX:N6	2.36	0.58
1:6:1657:U:O2'	1:6:1658:G:OP2	2.10	0.58
36:1:2873:U:H5''	36:1:2873:U:O2	2.03	0.58
55:M9:17:VAL:HG21	55:M9:52:LYS:HE3	1.84	0.58
40:L3:303:LYS:HZ2	40:L3:361:THR:HB	2.36	0.58
53:M7:92:GLN:HA	53:M7:95:LEU:HB2	1.86	0.58
60:N4:6:ASP:HB3	60:N4:10:GLY:H	1.67	0.58
20:C8:135:GLY:H	1:6:1559:A:H5''	364.29	0.58
10:S8:152:ILE:O	10:S8:153:GLU:HB2	2.03	0.58
36:1:2105:G:C2'	36:1:2106:A:H5'	2.33	0.58
65:N9:23:LYS:HB3	65:N9:24:PRO:HD3	2.68	0.58
10:S8:56:ARG:HH22	1:6:332:U:P	287.64	0.58
1:6:158:U:O2'	1:6:159:U:H3'	2.03	0.58
28:D6:10:ARG:HB2	28:D6:34:LYS:HA	2.53	0.58
1:2:1459:C:OP2	20:C8:138:THR:OG1	2.20	0.58
36:1:353:G:N7	73:O7:55:ARG:HD3	2.18	0.58
19:C7:5:ARG:O	19:C7:10:LYS:HE2	2.04	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
45:L8:54:GLU:O	45:L8:58:VAL:HG23	2.12	0.58
2:S0:182:LEU:HB3	2:S0:188:LEU:HD23	1.85	0.58
86:8:215:OHX:N6	86:8:223:OHX:N4	2.52	0.58
36:1:1581:C:H2'	36:1:1582:C:H5''	1.86	0.58
1:6:407:A:H2'	1:6:408:C:C6	2.39	0.58
36:1:2828:G:OP1	47:M0:7:ARG:NH1	2.37	0.58
36:1:1322:U:OP1	56:N0:117:ARG:HD2	2.04	0.58
13:C1:96:LYS:NZ	1:6:374:U:OP1	348.01	0.58
26:D4:11:LYS:NZ	1:6:775:G:N7	414.04	0.58
13:C1:132:SER:O	13:C1:132:SER:OG	3.55	0.58
1:2:1291:G:H22	1:2:1324:G:N2	2.01	0.58
8:S6:64:LYS:O	8:S6:67:VAL:HG22	2.04	0.58
51:M5:184:LYS:H	51:M5:186:GLY:H	1.54	0.58
45:L8:161:GLU:HA	45:L8:164:VAL:HG22	1.90	0.58
79:Q3:56:THR:HB	79:Q3:63:THR:OG1	2.03	0.58
36:1:715:A:H8	64:N8:115:LYS:HG2	1.69	0.58
30:D8:44:VAL:HG11	30:D8:48:VAL:HG21	2.50	0.58
9:S7:49:ILE:HG13	9:S7:57:ALA:HB3	2.79	0.58
45:L8:113:ALA:O	45:L8:115:ALA:N	4.10	0.58
36:5:3053:G:OP2	86:5:4170:OHX:N3	2.37	0.58
7:S5:203:LYS:HE2	7:S5:203:LYS:HA	4.36	0.58
56:N0:96:ASP:OD1	56:N0:97:VAL:N	2.69	0.58
40:L3:76:VAL:HG12	40:L3:325:LYS:HA	1.83	0.58
36:1:1478:C:H2'	36:1:1479:U:H6	1.69	0.58
17:C5:15:HIS:HB3	17:C5:22:LEU:HD23	1.86	0.58
12:C0:51:SER:OG	1:6:1219:A:N3	432.72	0.58
1:2:866:G:OP1	15:C3:2:GLY:HA2	2.04	0.58
86:2:2091:OHX:N1	86:2:2132:OHX:N4	2.52	0.58
74:O8:64:LYS:HG3	74:O8:65:LEU:N	5.31	0.58
1:2:868:G:OP1	15:C3:121:ARG:NH1	2.36	0.58
40:L3:25:ILE:H	40:L3:25:ILE:CD1	2.17	0.58
43:L6:3:ALA:HB2	68:O2:77:ALA:HB2	1.98	0.58
1:6:190:C:N4	1:6:196:G:O6	2.37	0.58
13:C1:33:ARG:HH22	13:C1:51:GLY:C	4.01	0.58
86:1:4007:OHX:N3	86:1:4175:OHX:N5	2.51	0.58
64:N8:42:ARG:NH2	36:5:2799:A:H1'	193.62	0.58
56:N0:26:ARG:HH11	57:N1:150:THR:HG21	3.16	0.58
36:1:772:U:H2'	36:1:773:G:C8	2.39	0.58
17:C5:60:LEU:HD23	17:C5:76:VAL:HG21	3.44	0.58
1:2:1483:A:H2'	1:2:1484:G:C8	2.39	0.58
1:2:138:A:O2'	8:S6:149:LYS:NZ	2.37	0.58
70:O4:38:LEU:H	70:O4:38:LEU:HD12	2.83	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
68:O2:40:SER:O	68:O2:44:ARG:HG3	2.03	0.58
1:2:919:A:H5'	16:C4:18:ARG:HH12	1.68	0.58
47:M0:73:ASN:O	47:M0:77:THR:OG1	4.01	0.58
36:1:3308:C:N3	53:M7:69:ARG:NH1	2.51	0.58
1:6:647:G:H1	1:6:687:G:H1	1.52	0.58
40:L3:77:THR:CG2	40:L3:327:CYS:HA	2.56	0.58
42:L5:155:THR:HG22	42:L5:179:ARG:HH11	1.67	0.58
62:N6:43:TYR:CD1	62:N6:126:LEU:HA	2.39	0.58
41:L4:35:VAL:HG21	41:L4:244:LEU:HD21	1.85	0.58
1:2:1097:U:O4	4:S2:201:ASN:ND2	2.36	0.58
36:1:768:C:OP1	49:M3:186:ARG:NH2	2.37	0.58
1:6:1680:G:O6	86:6:2189:OHX:N1	2.37	0.58
9:S7:168:SER:O	9:S7:172:VAL:HG23	2.51	0.58
59:N3:3:GLY:HA2	59:N3:40:LYS:HB3	6.13	0.58
14:C2:36:LEU:HD21	14:C2:102:GLY:HA3	1.86	0.58
1:6:1000:C:N4	1:6:1003:A:OP2	2.37	0.58
39:L2:13:GLY:O	39:L2:17:THR:HG23	2.03	0.58
36:5:3275:U:H4'	36:5:3276:G:OP2	2.04	0.57
27:D5:44:GLN:NE2	27:D5:48:ASP:OD2	2.37	0.57
63:N7:46:ILE:HD11	63:N7:49:TYR:CD2	4.20	0.57
36:5:2397:A:OP1	36:5:2398:A:H5''	2.03	0.57
37:3:60:G:H2'	37:3:61:G:H8	1.68	0.57
10:S8:21:PHE:O	10:S8:22:ARG:HG2	2.04	0.57
36:5:1808:G:O6	86:5:4024:OHX:N3	2.36	0.57
57:N1:130:ARG:HD3	36:5:1098:A:OP2	255.43	0.57
36:5:1878:G:OP1	86:5:3957:OHX:N5	2.37	0.57
36:5:3242:G:H5'	36:5:3245:A:H8	1.69	0.57
32:E0:14:VAL:O	32:E0:18:THR:HG23	2.18	0.57
86:2:2037:OHX:N2	10:S8:17:LYS:O	2.37	0.57
1:2:1387:G:OP1	19:C7:32:LYS:NZ	2.34	0.57
2:S0:193:GLN:O	2:S0:195:TRP:N	2.37	0.57
36:1:1365:G:OP2	86:1:3971:OHX:N6	2.37	0.57
36:5:996:A:H2'	36:5:997:A:O4'	2.04	0.57
1:6:700:C:H2'	1:6:701:U:C6	2.39	0.57
15:C3:18:TYR:O	15:C3:19:SER:HB2	4.52	0.57
3:S1:176:VAL:HG12	3:S1:177:GLN:H	1.69	0.57
66:O0:99:ASP:O	66:O0:103:THR:HG23	2.04	0.57
43:L6:31:ARG:NH1	69:O3:107:ILE:O	2.34	0.57
49:M3:76:THR:HG22	49:M3:101:ARG:HB3	1.85	0.57
1:6:217:A:C8	1:6:218:A:C8	2.92	0.57
36:1:562:C:H2'	36:1:563:U:H6	1.67	0.57
19:C7:29:GLN:HG2	34:SR:67:ILE:HD11	2.55	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
86:1:4036:OHX:N6	86:1:4048:OHX:N3	2.52	0.57
4:S2:132:ALA:O	4:S2:135:SER:OG	3.08	0.57
58:N2:43:VAL:HG23	58:N2:49:ASN:HB3	2.69	0.57
22:D0:69:LYS:HE2	22:D0:80:GLU:HB2	1.86	0.57
36:1:385:A:H2'	36:1:386:A:C8	2.39	0.57
50:M4:55:ARG:HD3	56:N0:70:THR:OG1	2.37	0.57
1:2:780:A:H8	26:D4:8:ARG:HB3	1.68	0.57
42:L5:122:VAL:HG23	42:L5:123:GLU:N	3.15	0.57
62:N6:115:ARG:HG3	62:N6:115:ARG:HH11	2.61	0.57
7:S5:143:ARG:HD3	30:D8:55:VAL:HG11	1.87	0.57
1:2:542:A:H5''	1:2:544:A:C8	2.40	0.57
37:3:60:G:H2'	37:3:61:G:C8	2.38	0.57
36:5:917:A:OP2	86:5:4222:OHX:N3	2.38	0.57
14:C2:54:ARG:O	14:C2:56:GLU:N	2.32	0.57
36:5:173:G:HO2'	36:5:174:C:H6	1.52	0.57
13:C1:3:THR:HG1	13:C1:82:ARG:HE	1.49	0.57
1:2:312:A:C2	1:2:314:C:H2'	2.39	0.57
25:D3:73:ARG:HE	25:D3:84:THR:HG22	1.69	0.57
36:5:920:A:OP1	36:5:922:U:H5	1.87	0.57
45:L8:181:LYS:HD3	38:8:154:C:H5''	150.40	0.57
36:5:1015:U:O3'	36:5:1016:C:H2'	2.04	0.57
51:M5:85:THR:HG22	86:Q2:503:OHX:N1	2.19	0.57
1:6:469:C:H2'	1:6:470:A:H5''	1.86	0.57
27:D5:41:ILE:HG13	27:D5:42:LEU:HG	1.86	0.57
1:6:1720:G:O6	86:6:2094:OHX:N4	2.38	0.57
9:S7:131:PHE:HB3	9:S7:132:PRO:HD3	1.85	0.57
11:S9:143:ILE:HD13	1:6:767:U:C5	422.47	0.57
1:2:1248:C:H2'	1:2:1249:U:H6	1.69	0.57
36:5:1152:G:H22	36:5:1200:A:H61	1.50	0.57
86:8:215:OHX:N2	86:8:223:OHX:N4	2.52	0.57
86:1:3976:OHX:N6	86:1:4159:OHX:N4	2.52	0.57
14:C2:124:LYS:O	14:C2:126:TRP:N	2.37	0.57
1:2:862:A:N7	15:C3:64:ARG:NH2	2.49	0.57
1:2:1127:G:OP1	77:Q1:11:ARG:NH2	2.36	0.57
1:2:1629:G:H2'	1:2:1630:U:C6	2.40	0.57
41:L4:120:TYR:CE2	41:L4:277:PRO:HB3	2.39	0.57
1:2:326:G:OP1	13:C1:57:LYS:NZ	2.35	0.57
36:5:2896:A:H8	36:5:2896:A:H5''	1.70	0.57
43:L6:129:GLU:OE2	43:L6:130:ILE:N	2.37	0.57
72:O6:27:SER:O	72:O6:28:TYR:HB2	2.03	0.57
36:1:20:A:OP2	71:O5:90:ARG:NH1	2.38	0.57
48:M1:82:ARG:HB3	48:M1:112:LEU:HB2	3.91	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:M5:172:ARG:HD2	36:5:30:G:O5'	111.18	0.57
36:1:2818:U:C5'	36:1:2818:U:H6	2.17	0.57
27:D5:58:ARG:HB3	27:D5:103:ARG:HH11	6.29	0.57
3:S1:41:ARG:HH22	3:S1:232:HIS:HA	2.83	0.57
1:6:1762:A:C1'	1:6:1783:C:H5'	2.35	0.57
22:D0:22:ILE:HG22	22:D0:93:LEU:HB2	1.96	0.57
48:M1:15:GLU:HG2	48:M1:16:LYS:HD3	1.86	0.57
86:1:3976:OHX:N3	86:1:4159:OHX:N4	2.53	0.57
6:S4:95:THR:HG23	6:S4:97:GLU:HG2	7.00	0.57
45:L8:86:THR:O	45:L8:90:THR:OG1	2.85	0.57
24:D2:104:LEU:HB2	24:D2:125:ILE:HA	1.87	0.57
55:M9:85:ARG:NH2	36:5:1916:U:O3'	231.18	0.57
36:1:3160:U:H2'	36:1:3161:C:C6	2.38	0.57
71:O5:34:GLN:HB3	71:O5:38:ARG:HH22	3.68	0.57
78:Q2:17:CYS:SG	78:Q2:76:LYS:HB2	2.44	0.57
16:C4:82:LYS:HG3	16:C4:118:VAL:HG11	4.92	0.57
78:Q2:25:VAL:HG22	78:Q2:72:LEU:HD23	1.86	0.57
11:S9:110:GLN:NE2	11:S9:126:ARG:HG2	2.19	0.57
36:5:1573:G:C6	36:5:1574:C:H1'	2.39	0.57
1:6:542:A:H8	1:6:543:C:H5'	1.69	0.57
7:S5:43:PHE:N	7:S5:46:TRP:O	2.84	0.57
7:S5:89:ILE:HD12	7:S5:90:ILE:H	1.70	0.57
63:N7:53:VAL:HG21	63:N7:62:VAL:HG13	1.87	0.57
1:6:830:U:H2'	1:6:831:U:H5'	1.86	0.57
52:M6:68:ARG:NH1	36:5:2988:C:OP1	217.97	0.57
5:S3:167:PHE:CE1	5:S3:192:PRO:HB3	3.00	0.57
18:C6:22:VAL:HG22	18:C6:65:ILE:HG12	1.86	0.57
1:2:380:U:H5	11:S9:5:PRO:HA	1.69	0.57
46:L9:1:MET:O	46:L9:2:LYS:HB2	2.38	0.57
36:1:3092:C:O2'	36:1:3094:A:OP2	2.19	0.57
61:N5:82:LEU:HD12	61:N5:126:LEU:HD21	1.87	0.57
36:1:1819:U:O4	86:1:4044:OHX:N6	2.37	0.57
36:5:2580:A:O2'	86:5:4129:OHX:N1	2.36	0.57
36:5:3152:U:O2	86:5:4224:OHX:N5	2.38	0.57
1:2:1220:C:OP1	12:C0:48:SER:OG	2.21	0.57
5:S3:64:ARG:O	5:S3:67:ASN:N	2.36	0.57
34:SR:76:ASP:OD1	34:SR:76:ASP:N	2.26	0.57
44:L7:54:GLU:OE2	44:L7:186:HIS:NE2	2.34	0.57
40:L3:332:ARG:HH11	40:L3:332:ARG:HG2	1.69	0.57
73:O7:88:ALA:O	86:O7:103:OHX:N1	2.36	0.57
10:S8:44:HIS:O	10:S8:56:ARG:N	2.52	0.57
3:S1:144:ARG:HB3	3:S1:208:GLN:HB3	1.85	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:1410:A:H2'	1:2:1411:A:O4'	2.05	0.57
7:S5:61:TYR:HE2	7:S5:164:PRO:HG2	3.21	0.57
36:5:1572:U:HO2'	36:5:1573:G:H8	1.51	0.57
1:6:542:A:H8	1:6:543:C:H2'	1.67	0.57
40:L3:232:ARG:NH1	40:L3:269:GLN:O	2.36	0.57
1:6:218:A:H2'	1:6:219:A:H5''	1.87	0.57
36:1:561:C:H2'	36:1:562:C:H6	1.68	0.57
1:6:486:G:H22	1:6:501:U:H3	1.52	0.57
1:2:25:C:O2	86:2:2085:OHX:N1	2.38	0.57
36:5:3241:G:H2'	36:5:3245:A:H8	1.70	0.57
38:4:78:G:H2'	38:4:79:A:C8	2.39	0.57
20:C8:91:ASP:O	20:C8:92:ILE:HB	2.25	0.57
61:N5:80:ASN:HD21	61:N5:126:LEU:HB2	1.69	0.57
1:6:235:G:H2'	1:6:236:A:H8	1.70	0.57
1:2:199:G:HO2'	1:2:200:A:H8	1.53	0.57
36:5:1081:U:O2'	36:5:1082:U:O5'	2.22	0.57
36:1:1159:A:O2'	36:1:1160:C:H5''	2.05	0.57
22:D0:55:PRO:HA	22:D0:91:ILE:HG12	1.87	0.57
36:5:2787:G:OP2	86:5:4034:OHX:N6	2.37	0.57
39:L2:193:ARG:NH2	36:5:2181:C:OP1	198.08	0.57
28:D6:70:LYS:HE3	1:6:931:C:P	317.97	0.57
41:L4:182:LEU:HD11	41:L4:223:PRO:HG2	2.20	0.57
36:5:2942:C:O2	86:5:4108:OHX:N2	2.38	0.57
20:C8:27:LYS:HG3	20:C8:57:ARG:HH21	1.69	0.57
86:1:4036:OHX:N4	86:1:4048:OHX:N1	2.52	0.57
59:N3:84:SER:HA	59:N3:94:TYR:HB3	2.16	0.57
18:C6:18:ALA:HB2	18:C6:69:VAL:HG13	2.01	0.57
1:2:1214:U:OP1	1:2:1246:C:H1'	2.05	0.57
36:5:2440:G:O2'	36:5:2441:A:OP1	2.23	0.57
1:2:905:A:H5''	16:C4:52:ARG:HD3	1.87	0.57
1:2:1479:A:P	21:C9:57:ARG:HH12	2.28	0.57
41:L4:300:ARG:CG	41:L4:300:ARG:HH11	2.77	0.57
27:D5:39:ALA:O	27:D5:72:GLY:N	2.35	0.57
56:N0:13:ARG:NH1	56:N0:13:ARG:HG3	4.69	0.57
56:N0:12:ARG:HB3	56:N0:24:LEU:HD23	1.90	0.57
36:5:979:U:H1'	36:5:980:A:N3	2.20	0.57
86:2:2045:OHX:N1	86:2:2099:OHX:N3	2.53	0.57
79:Q3:50:GLY:O	79:Q3:54:ILE:HD13	5.02	0.57
36:5:1239:C:H42	36:5:1249:G:H1	1.51	0.57
46:L9:188:THR:O	46:L9:188:THR:OG1	2.22	0.57
2:S0:200:ASP:HB2	19:C7:85:VAL:HG22	1.87	0.57
18:C6:6:SER:HA	18:C6:23:LYS:HA	2.14	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
63:N7:4:PHE:CZ	66:O0:35:ARG:HA	2.40	0.57
36:5:2683:U:H2'	36:5:2684:C:C6	2.40	0.57
35:SM:101:ASP:O	35:SM:102:THR:HB	2.05	0.57
9:S7:170:GLN:HA	9:S7:181:ILE:HG22	1.87	0.57
52:M6:171:LYS:O	52:M6:175:THR:HG23	2.04	0.57
1:2:520:A:H2'	1:2:521:A:C8	2.39	0.57
36:1:3152:U:O2'	36:1:3153:U:H5'	2.04	0.57
1:2:1646:C:H2'	1:2:1647:U:C6	2.40	0.57
70:O4:52:GLN:HG2	36:5:1639:C:H5'	197.97	0.57
36:1:2403:G:H1'	36:1:2404:A:H5''	1.87	0.57
36:5:1940:G:H21	36:5:3362:A:H8	1.53	0.57
48:M1:92:ARG:HH21	48:M1:94:ARG:HD2	7.21	0.57
41:L4:8:VAL:O	41:L4:16:THR:HB	2.08	0.57
3:S1:61:LEU:O	3:S1:62:LYS:NZ	2.35	0.57
9:S7:15:GLU:O	9:S7:19:GLN:HG2	2.05	0.57
17:C5:108:ARG:HH21	20:C8:119:ILE:HD12	3.79	0.57
36:5:604:G:N7	86:5:4166:OHX:N2	2.52	0.57
36:1:2444:C:H3'	36:1:2445:A:H5''	1.87	0.57
21:C9:33:TYR:HD1	21:C9:34:VAL:H	2.25	0.57
40:L3:56:ILE:HD11	40:L3:359:ILE:HG12	1.91	0.57
39:L2:20:THR:HA	39:L2:23:ARG:HD3	1.87	0.57
36:5:541:U:H2'	36:5:542:G:C8	2.40	0.57
1:6:694:U:H3'	1:6:695:U:O2	2.05	0.57
36:5:1450:G:OP1	86:5:4227:OHX:N4	2.38	0.57
45:L8:95:ASN:OD1	45:L8:98:ARG:NH1	4.09	0.57
1:6:1620:C:H2'	1:6:1621:U:H6	1.70	0.57
59:N3:30:GLY:HA3	59:N3:66:LYS:HD2	1.86	0.57
54:M8:182:LYS:NZ	64:N8:55:LYS:O	2.52	0.57
21:C9:112:GLY:O	21:C9:125:SER:OG	3.05	0.57
36:5:1696:A:OP2	86:5:4183:OHX:N6	2.38	0.57
42:L5:83:LEU:HB3	42:L5:88:ILE:HB	1.87	0.57
44:L7:196:LYS:HE2	36:5:1100:U:OP2	246.10	0.57
36:1:750:G:P	65:N9:40:ARG:HH21	2.27	0.57
1:2:1339:C:O2'	1:2:1340:U:OP1	2.23	0.56
41:L4:144:LYS:HG2	41:L4:145:ILE:H	5.51	0.56
1:2:1796:C:OP2	28:D6:5:ARG:NH1	2.38	0.56
45:L8:26:LEU:HD13	63:N7:53:VAL:HG11	1.85	0.56
69:O3:60:ARG:NH2	69:O3:60:ARG:HB2	2.20	0.56
33:E1:135:HIS:ND1	33:E1:138:ARG:HD2	2.20	0.56
86:1:4088:OHX:N4	55:M9:14:VAL:O	2.38	0.56
22:D0:34:LEU:HD23	22:D0:112:VAL:HG13	1.86	0.56
26:D4:105:ARG:HB2	1:6:443:C:OP2	372.63	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:1679:G:O6	86:6:2189:OHX:N3	2.38	0.56
40:L3:10:ARG:NH1	40:L3:11:HIS:O	2.39	0.56
36:1:3148:U:O4	86:1:4113:OHX:N2	2.38	0.56
16:C4:51:ASP:OD1	1:6:902:G:N1	283.84	0.56
3:S1:119:THR:HB	3:S1:143:THR:HG23	1.87	0.56
74:O8:39:ARG:NH1	74:O8:63:LYS:HE2	9.96	0.56
86:5:4055:OHX:N5	86:5:4197:OHX:N6	2.53	0.56
36:1:1016:C:O2	36:1:1028:U:N3	2.38	0.56
6:S4:9:LEU:HD12	6:S4:30:ARG:HA	2.54	0.56
8:S6:173:PRO:HG3	1:6:66:U:C5	334.16	0.56
1:2:778:G:H22	26:D4:10:ARG:NH2	2.03	0.56
63:N7:135:ARG:NH2	36:5:2556:C:O2'	200.51	0.56
36:1:623:U:OP1	86:1:4135:OHX:N1	2.38	0.56
46:L9:166:ARG:NH2	46:L9:168:ARG:HH12	12.10	0.56
7:S5:91:GLU:HA	7:S5:94:THR:HG23	1.86	0.56
45:L8:78:PHE:O	45:L8:80:TYR:N	2.34	0.56
39:L2:171:GLY:O	79:Q3:68:ALA:HB2	2.27	0.56
42:L5:152:ARG:HH11	42:L5:152:ARG:HG3	2.05	0.56
8:S6:177:ARG:NH2	1:6:143:G:N7	311.92	0.56
2:S0:198:MET:SD	19:C7:85:VAL:HG11	2.45	0.56
53:M7:67:ILE:HD11	36:5:1447:G:H3'	165.11	0.56
1:2:458:G:OP2	26:D4:105:ARG:NH2	2.38	0.56
42:L5:226:TYR:HE1	42:L5:236:LEU:HD11	5.72	0.56
9:S7:119:THR:HG23	1:6:639:U:OP2	370.08	0.56
14:C2:30:VAL:HB	14:C2:132:GLU:HG3	1.87	0.56
30:D8:13:ILE:HB	30:D8:29:ARG:HG2	5.04	0.56
36:5:1810:A:H2'	36:5:1811:G:C8	2.40	0.56
36:5:201:A:OP2	86:5:3987:OHX:N1	2.39	0.56
30:D8:32:PHE:O	30:D8:34:GLU:N	4.42	0.56
68:O2:27:ARG:HB3	36:5:655:C:OP1	162.35	0.56
67:O1:46:THR:HG23	67:O1:47:ASP:N	3.23	0.56
1:2:12:U:H2'	1:2:13:C:C6	2.39	0.56
39:L2:15:ILE:HD12	36:5:822:G:H1'	176.54	0.56
36:5:3343:G:N2	36:5:3362:A:H2	1.91	0.56
25:D3:23:ARG:HB3	25:D3:29:TYR:CE1	2.61	0.56
36:5:1876:U:H6	36:5:1876:U:C5'	2.19	0.56
1:6:1698:G:N2	1:6:1699:G:N7	2.53	0.56
16:C4:85:ALA:N	16:C4:119:THR:HG22	2.16	0.56
1:2:704:C:OP2	1:2:704:C:H3'	2.05	0.56
36:5:662:U:H2'	36:5:663:C:C6	2.40	0.56
36:1:2943:G:OP2	40:L3:2:SER:HB2	2.05	0.56
8:S6:155:ASP:OD2	8:S6:155:ASP:N	2.68	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:M5:163:GLY:HA2	51:M5:168:GLY:HA3	2.22	0.56
77:Q1:22:ALA:HA	77:Q1:25:LYS:HG3	1.87	0.56
75:O9:9:ILE:O	75:O9:13:MET:HG3	2.05	0.56
15:C3:22:ALA:HB1	15:C3:23:PRO:HA	2.08	0.56
15:C3:27:LYS:H	15:C3:27:LYS:CE	2.18	0.56
36:5:3164:C:H1'	36:5:3165:A:H5'	1.86	0.56
36:1:1636:U:H5''	63:N7:73:LYS:HZ2	1.69	0.56
1:6:484:C:N4	1:6:503:G:H1	2.02	0.56
59:N3:81:GLN:NE2	59:N3:83:LYS:O	2.39	0.56
18:C6:99:GLU:HG2	34:SR:57:PRO:HB2	2.40	0.56
1:2:793:A:H5''	1:2:794:U:C5	2.40	0.56
13:C1:59:PRO:HB3	13:C1:66:ILE:HD11	1.86	0.56
86:1:4007:OHX:N5	86:1:4175:OHX:N5	2.53	0.56
36:5:182:U:H4'	36:5:182:U:OP1	2.04	0.56
36:1:2872:A:O2'	36:1:2873:U:H5'	2.05	0.56
1:2:355:G:OP2	86:2:2037:OHX:N4	2.38	0.56
36:1:3152:U:O2	86:1:4147:OHX:N4	2.38	0.56
78:Q2:43:TYR:CZ	78:Q2:47:GLN:NE2	2.74	0.56
15:C3:127:ARG:HH11	15:C3:127:ARG:HG2	1.69	0.56
6:S4:222:LEU:O	6:S4:224:ASN:N	2.38	0.56
51:M5:74:PRO:O	51:M5:75:VAL:HG22	2.05	0.56
36:1:2973:G:N7	86:1:4102:OHX:N2	2.54	0.56
36:1:3289:G:N7	86:1:4134:OHX:N4	2.54	0.56
34:SR:133:VAL:O	34:SR:141:LEU:N	2.62	0.56
1:6:1535:U:H4'	1:6:1535:U:OP1	2.05	0.56
34:SR:80:ALA:HB3	34:SR:92:TRP:HB2	2.47	0.56
1:6:1754:A:H4'	1:6:1755:A:O5'	2.06	0.56
36:1:261:U:H2'	36:1:262:U:C6	2.40	0.56
36:1:2155:G:O2'	39:L2:227:ARG:NH2	2.37	0.56
11:S9:148:VAL:HG11	11:S9:156:ILE:HD11	1.86	0.56
16:C4:84:ARG:HG3	16:C4:85:ALA:O	3.28	0.56
53:M7:62:ARG:NH1	36:5:412:G:OP1	159.74	0.56
6:S4:100:ARG:NH2	6:S4:122:LYS:HA	2.43	0.56
2:S0:62:ARG:HG3	2:S0:62:ARG:NH1	2.66	0.56
7:S5:42:LEU:HD21	7:S5:45:LYS:HD2	1.87	0.56
36:5:3279:A:H2'	36:5:3280:U:H5'	1.88	0.56
1:6:564:G:O6	86:6:2154:OHX:N5	2.39	0.56
36:1:1095:U:N3	57:N1:127:GLN:OE1	2.35	0.56
12:C0:14:TYR:CE1	12:C0:18:GLU:HG3	2.41	0.56
2:S0:148:ASP:OD1	2:S0:149:LEU:N	2.58	0.56
36:5:22:G:H1'	38:8:104:A:N3	2.20	0.56
39:L2:68:LYS:HG2	39:L2:70:ARG:HG2	3.44	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:437:G:H2'	36:1:438:A:C8	2.41	0.56
36:5:1659:U:H2'	36:5:1660:C:C6	2.40	0.56
36:5:1560:G:O2'	36:5:1561:G:OP1	2.23	0.56
1:2:527:A:OP2	86:2:2054:OHX:N4	2.38	0.56
36:5:1581:C:OP2	36:5:1581:C:H4'	2.03	0.56
6:S4:205:PHE:HB3	6:S4:221:ARG:HD2	1.88	0.56
36:1:658:G:OP1	86:1:4049:OHX:N4	2.38	0.56
45:L8:41:GLN:HG3	45:L8:44:ARG:HH12	1.71	0.56
40:L3:98:GLY:HA3	36:5:3005:A:H5'	249.50	0.56
70:O4:74:ARG:HG2	70:O4:75:ALA:H	1.71	0.56
20:C8:41:ARG:NE	21:C9:46:PRO:HD3	2.20	0.56
66:O0:16:LEU:HB3	66:O0:98:SER:HB2	1.87	0.56
4:S2:203:LYS:O	4:S2:206:THR:HG23	2.08	0.56
36:1:1064:A:H4'	36:1:1065:A:O5'	2.05	0.56
17:C5:22:LEU:HA	17:C5:25:LEU:HD12	2.81	0.56
3:S1:119:THR:HB	3:S1:143:THR:CG2	2.36	0.56
86:5:4055:OHX:N1	86:5:4197:OHX:N2	2.54	0.56
36:1:2510:U:O2'	36:1:2511:A:H5''	2.05	0.56
64:N8:35:ALA:HB2	36:5:39:A:H5''	167.79	0.56
36:5:1258:U:O2	36:5:1260:A:H8	1.88	0.56
1:6:336:G:H2'	1:6:338:C:H5	1.70	0.56
3:S1:40:ASN:ND2	3:S1:42:ASN:O	2.39	0.56
54:M8:166:LEU:O	54:M8:167:SER:HB2	4.53	0.56
45:L8:195:SER:O	45:L8:197:VAL:N	2.38	0.56
36:1:2406:C:H2'	36:1:2407:C:C6	2.40	0.56
48:M1:92:ARG:NH2	48:M1:94:ARG:HD2	6.58	0.56
77:Q1:9:ARG:CG	77:Q1:9:ARG:HH11	2.37	0.56
37:3:121:U:OP2	42:L5:265:TYR:OH	2.15	0.56
51:M5:68:ARG:HG3	36:5:291:C:OP1	145.31	0.56
7:S5:37:GLN:OE1	18:C6:53:LEU:HD22	2.07	0.56
7:S5:68:ILE:HD13	7:S5:69:PHE:H	5.21	0.56
36:1:2592:G:H4'	36:1:2594:C:C2	2.39	0.56
8:S6:179:VAL:HG21	1:6:140:A:H1'	328.42	0.56
36:5:2568:C:O2'	36:5:2569:A:O5'	2.16	0.56
45:L8:33:ASN:ND2	36:5:2549:G:N3	215.60	0.56
36:1:3318:G:H2'	36:1:3318:G:OP2	2.05	0.56
5:S3:60:GLY:HA3	5:S3:65:ARG:HB3	3.61	0.56
36:1:1507:G:C8	53:M7:129:THR:HG22	2.40	0.56
36:5:3241:G:H2'	36:5:3245:A:C8	2.40	0.56
1:2:1229:G:H1	14:C2:47:GLU:HG3	1.69	0.56
1:6:230:C:H42	1:6:235:G:H1	1.52	0.56
52:M6:127:LEU:HD11	56:N0:168:PRO:HG3	2.49	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
74:O8:42:LYS:HG2	74:O8:55:VAL:HG22	1.87	0.56
44:L7:157:ASN:O	44:L7:158:LYS:HB3	3.02	0.56
41:L4:192:GLY:HA2	41:L4:195:ARG:HG3	4.01	0.56
4:S2:53:ILE:HD11	4:S2:73:LEU:HD13	3.68	0.56
43:L6:175:LYS:O	50:M4:117:ARG:NH2	2.39	0.56
36:1:1804:A:H2'	36:1:1805:C:C6	2.41	0.56
67:O1:13:THR:HG22	67:O1:72:ARG:HD3	1.87	0.56
36:5:2998:U:O4	86:5:4140:OHX:N4	2.38	0.56
47:M0:30:LYS:HG3	47:M0:63:GLU:OE1	4.39	0.56
86:6:2060:OHX:N2	86:6:2147:OHX:N4	2.54	0.56
35:SM:83:LYS:HE2	1:6:1178:G:H4'	339.90	0.56
22:D0:67:THR:HG22	1:6:1199:G:O6	401.66	0.56
86:5:4011:OHX:N3	86:5:4198:OHX:N5	2.53	0.56
29:D7:2:VAL:O	29:D7:3:LEU:HB2	2.21	0.56
45:L8:24:ASN:HB3	45:L8:25:PRO:HD2	2.97	0.56
36:1:1564:U:H2'	36:1:1565:G:C8	2.40	0.56
10:S8:26:LYS:O	10:S8:26:LYS:HG3	2.06	0.56
22:D0:80:GLU:HG3	31:D9:54:LYS:HZ3	1.71	0.56
5:S3:74:GLN:HA	5:S3:79:TYR:HB2	2.53	0.56
17:C5:122:THR:HG22	17:C5:123:TYR:HD1	5.71	0.56
36:1:1524:A:OP1	61:N5:92:LYS:NZ	2.25	0.56
36:5:129:U:H2'	36:5:130:A:C8	2.40	0.56
41:L4:316:ASN:O	41:L4:319:LYS:O	2.53	0.56
46:L9:106:LYS:H	46:L9:109:ALA:CB	2.19	0.56
44:L7:150:LYS:HD3	44:L7:244:ASN:HD21	1.71	0.56
2:S0:168:HIS:O	2:S0:172:LEU:HB2	2.45	0.56
86:5:4055:OHX:N3	86:5:4197:OHX:N6	2.54	0.56
17:C5:122:THR:HG22	1:6:1558:U:H3	368.18	0.56
1:6:1631:A:OP2	86:6:2168:OHX:N3	2.38	0.56
36:1:2614:G:OP1	86:1:4179:OHX:N6	2.39	0.56
40:L3:36:ASP:OD1	40:L3:38:SER:OG	2.20	0.56
54:M8:67:ILE:HG23	54:M8:81:VAL:HG11	2.23	0.56
56:N0:48:LEU:O	56:N0:49:HIS:ND1	2.88	0.56
6:S4:185:GLY:N	6:S4:189:LEU:HD13	2.20	0.56
86:5:4094:OHX:N3	86:5:4234:OHX:N4	2.54	0.56
67:O1:10:ARG:HH12	67:O1:44:MET:HG3	5.35	0.56
22:D0:46:GLU:HB2	22:D0:52:LYS:NZ	2.20	0.56
48:M1:139:THR:HG22	48:M1:146:GLY:O	2.54	0.56
42:L5:254:LYS:O	42:L5:254:LYS:HG3	3.49	0.56
37:3:10:C:OP2	57:N1:26:HIS:HD2	1.88	0.56
36:1:3165:A:H2'	36:1:3166:C:C6	2.41	0.56
86:2:2091:OHX:N3	86:2:2132:OHX:N4	2.53	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:C5:127:ARG:CZ	35:SM:66:ALA:HB2	5.57	0.56
1:2:1798:U:C5	28:D6:38:ARG:NH2	2.74	0.56
33:E1:91:ILE:HG12	33:E1:92:LYS:HG2	6.40	0.56
33:E1:90:LYS:HD3	33:E1:93:HIS:HE1	11.58	0.56
34:SR:81:LEU:HG	34:SR:91:LEU:HD13	1.87	0.56
39:L2:70:ARG:CZ	39:L2:72:ARG:HE	5.01	0.56
65:N9:22:LYS:HA	36:5:983:A:OP1	216.26	0.56
86:1:4032:OHX:N2	86:1:4149:OHX:N5	2.53	0.56
15:C3:53:LEU:HD13	29:D7:52:THR:HG21	2.57	0.56
60:N4:32:GLN:OE1	60:N4:33:ASN:ND2	2.76	0.56
36:1:3008:A:OP2	52:M6:74:ARG:NH1	2.37	0.56
36:1:1874:A:OP2	55:M9:21:LYS:HE2	2.05	0.56
1:6:1588:G:OP1	86:6:2125:OHX:N2	2.39	0.56
39:L2:204:MET:HG2	36:5:914:A:C2	196.04	0.56
86:6:2060:OHX:N1	86:6:2147:OHX:N4	2.54	0.56
18:C6:109:PHE:CD2	18:C6:117:LEU:HD21	2.41	0.56
1:2:1202:A:H61	1:2:1457:C:H5''	1.70	0.56
2:S0:62:ARG:CG	2:S0:62:ARG:HH11	2.61	0.56
7:S5:61:TYR:OH	30:D8:52:ASP:OD1	3.36	0.56
28:D6:6:ALA:H	1:6:1796:C:H5	345.48	0.56
7:S5:94:THR:HG22	7:S5:114:ILE:CG1	2.78	0.56
26:D4:121:THR:HG22	26:D4:123:LYS:HB2	7.85	0.56
64:N8:65:GLN:O	64:N8:66:ALA:HB2	2.06	0.56
36:1:1103:A:N3	36:1:1103:A:H2'	2.20	0.56
21:C9:118:PRO:HD2	21:C9:123:ARG:NH2	2.21	0.56
1:2:918:U:O3'	16:C4:18:ARG:NH1	2.39	0.56
44:L7:158:LYS:HD2	44:L7:159:GLN:HA	4.99	0.56
14:C2:74:LEU:HD11	33:E1:106:TYR:HD1	1.70	0.56
1:2:1041:G:H2'	1:2:1042:G:C8	2.40	0.56
36:1:619:A:H5''	36:1:620:U:OP1	2.06	0.56
1:6:660:G:H2'	1:6:661:A:H4'	1.88	0.56
7:S5:187:ILE:H	7:S5:187:ILE:HD12	1.97	0.56
49:M3:73:ARG:NH1	36:5:110:G:OP2	75.76	0.56
36:5:410:U:O4	86:5:4102:OHX:N1	2.39	0.56
18:C6:115:THR:HG23	18:C6:118:ILE:O	5.04	0.55
26:D4:29:HIS:HB2	26:D4:67:GLY:HA2	5.46	0.55
8:S6:176:GLN:HG2	1:6:169:A:H5''	328.90	0.55
36:1:1119:C:OP2	86:1:3958:OHX:N1	2.39	0.55
8:S6:73:ILE:HD12	8:S6:75:LEU:HD21	2.40	0.55
54:M8:122:ILE:HD11	54:M8:130:ARG:NH1	3.45	0.55
36:1:2529:A:OP1	45:L8:248:LYS:NZ	2.39	0.55
40:L3:66:LYS:HE3	59:N3:124:ASP:OD2	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:S5:182:ALA:O	7:S5:186:ASN:ND2	2.39	0.55
1:2:271:A:H5'	1:2:272:U:OP2	2.06	0.55
1:6:1699:G:C2	1:6:1701:A:H5''	2.40	0.55
41:L4:232:SER:O	41:L4:233:LEU:HB2	2.05	0.55
86:2:2045:OHX:N1	86:2:2099:OHX:N5	2.54	0.55
42:L5:261:THR:HG23	42:L5:264:GLN:HE21	2.15	0.55
24:D2:89:TRP:O	24:D2:93:LEU:HD22	2.06	0.55
71:O5:34:GLN:HB3	71:O5:38:ARG:NH2	3.37	0.55
46:L9:120:ASP:OD1	46:L9:124:ARG:NH2	2.39	0.55
42:L5:274:GLN:OE1	37:7:60:G:N2	332.40	0.55
1:6:1091:A:H4'	1:6:1092:A:O5'	2.07	0.55
8:S6:49:VAL:HB	8:S6:115:LYS:HG2	4.49	0.55
1:6:1767:G:OP1	1:6:1770:U:H4'	2.06	0.55
36:1:2854:U:H5''	47:M0:160:PRO:HD3	1.88	0.55
10:S8:39:GLY:N	10:S8:60:ILE:O	2.33	0.55
36:1:1949:G:OP1	55:M9:104:ARG:NH1	2.39	0.55
36:1:2433:U:H1'	51:M5:125:SER:HB3	1.88	0.55
36:1:3159:C:H2'	36:1:3160:U:H6	1.70	0.55
36:1:2318:U:O4	86:1:4043:OHX:N2	2.40	0.55
1:2:407:A:H2'	1:2:408:C:C6	2.42	0.55
1:2:1783:C:H2'	1:2:1784:C:H6	1.71	0.55
10:S8:16:ALA:HB2	1:6:354:C:H5''	298.58	0.55
18:C6:73:GLY:H	18:C6:76:SER:HB2	1.71	0.55
36:1:544:C:H1'	36:1:548:G:H22	1.71	0.55
67:O1:80:ASN:HA	67:O1:90:PHE:CE2	5.87	0.55
15:C3:55:ARG:HD2	15:C3:56:ASP:OD1	4.87	0.55
86:1:4084:OHX:N2	86:1:4153:OHX:N1	2.54	0.55
86:5:3973:OHX:N4	86:5:4241:OHX:N2	2.54	0.55
14:C2:73:LYS:NZ	33:E1:108:VAL:HG13	2.22	0.55
35:SM:58:GLU:O	35:SM:62:ARG:HB2	2.78	0.55
76:Q0:77:ILE:O	76:Q0:78:ILE:HG23	5.06	0.55
1:2:260:U:H3'	1:2:261:U:C5'	2.37	0.55
1:2:1449:U:H2'	1:2:1450:U:C6	2.41	0.55
36:1:1581:C:C2	36:1:1582:C:H5'	2.41	0.55
4:S2:98:PHE:CE1	35:SM:116:GLU:HG3	2.42	0.55
36:1:792:G:H2'	36:1:793:C:C6	2.42	0.55
46:L9:90:MET:O	46:L9:91:ARG:HD2	2.80	0.55
36:5:830:A:O2'	36:5:1866:C:H2'	2.06	0.55
42:L5:55:PHE:CZ	42:L5:158:ARG:HB3	5.06	0.55
29:D7:62:ILE:HG13	29:D7:63:LEU:H	1.87	0.55
36:1:2860:U:H6	36:1:2860:U:H5'	1.71	0.55
36:1:742:G:N7	86:1:3979:OHX:N1	2.54	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
41:L4:161:LYS:NZ	36:5:209:A:OP1	74.92	0.55
68:O2:9:ILE:HG12	68:O2:63:THR:HB	1.88	0.55
46:L9:147:SER:HB2	46:L9:187:ILE:HD11	1.88	0.55
36:1:155:G:H5''	36:1:156:G:C8	2.41	0.55
28:D6:36:ILE:HG21	28:D6:78:ALA:HB2	1.89	0.55
1:6:514:G:HO2'	1:6:515:A:H8	1.54	0.55
71:O5:6:ALA:O	71:O5:10:ARG:HG3	2.52	0.55
19:C7:109:LEU:O	19:C7:113:LEU:HB2	4.07	0.55
1:2:885:G:H21	16:C4:123:SER:HB2	1.72	0.55
1:6:1542:G:N2	1:6:1568:C:H1'	2.22	0.55
64:N8:74:ASN:HB2	64:N8:76:ASP:HB2	1.87	0.55
1:6:656:G:H2'	1:6:657:U:C6	2.41	0.55
63:N7:10:VAL:HB	63:N7:83:THR:HG21	1.86	0.55
63:N7:83:THR:HG23	63:N7:85:TYR:N	2.21	0.55
27:D5:59:TYR:HE2	27:D5:61:SER:HB3	1.71	0.55
36:1:3153:U:O2	36:1:3158:G:N1	2.39	0.55
36:1:2946:A:H5''	36:1:2947:G:H5'	1.87	0.55
1:6:404:G:H2'	1:6:405:C:C6	2.42	0.55
54:M8:86:THR:HG22	54:M8:105:ARG:HB2	1.88	0.55
36:5:2509:U:H2'	36:5:2510:U:H5''	1.87	0.55
36:5:1149:G:N2	36:5:1198:C:N3	2.45	0.55
36:5:2140:U:O2'	36:5:2978:U:H5'	2.06	0.55
1:2:1244:A:O2'	1:2:1245:G:OP1	2.21	0.55
23:D1:41:GLU:N	23:D1:41:GLU:OE2	2.40	0.55
41:L4:209:TYR:OH	36:5:689:U:O4	86.91	0.55
36:5:945:C:H2'	36:5:946:U:C6	2.42	0.55
40:L3:188:ILE:HA	40:L3:191:LYS:HD2	1.89	0.55
46:L9:44:THR:HG22	36:5:3186:A:C2	327.40	0.55
21:C9:57:ARG:NH2	21:C9:80:TYR:HB3	2.21	0.55
13:C1:53:TYR:CD1	13:C1:113:PRO:HG2	2.42	0.55
33:E1:144:CYS:O	33:E1:146:SER:N	2.61	0.55
45:L8:33:ASN:HA	36:5:2549:G:N2	212.35	0.55
71:O5:119:LYS:HA	71:O5:119:LYS:HE2	1.88	0.55
11:S9:160:PRO:O	11:S9:167:ALA:HB2	2.06	0.55
71:O5:95:PHE:CD2	36:5:136:G:H5'	63.08	0.55
36:1:1819:U:O4	86:1:4044:OHX:N4	2.40	0.55
16:C4:54:GLU:OE1	1:6:901:G:N2	282.75	0.55
36:1:2883:U:H2'	36:1:2884:C:C6	2.41	0.55
43:L6:89:THR:HG21	50:M4:115:PHE:HB2	1.98	0.55
72:O6:43:LEU:HD13	72:O6:47:ILE:HD11	2.72	0.55
69:O3:90:PRO:O	69:O3:91:ALA:HB3	2.06	0.55
1:2:1175:U:H2'	1:2:1176:G:C8	2.42	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:S7:35:LYS:O	9:S7:37:GLU:N	2.32	0.55
36:1:1171:G:O6	86:1:3962:OHX:N2	2.40	0.55
20:C8:33:THR:HA	20:C8:38:VAL:HG23	2.27	0.55
36:1:624:G:OP2	86:1:4135:OHX:N3	2.39	0.55
21:C9:28:LEU:CD1	21:C9:29:GLU:H	2.20	0.55
1:2:61:A:H8	1:2:269:G:O2'	1.89	0.55
26:D4:60:PHE:H	26:D4:71:GLY:HA2	1.72	0.55
44:L7:151:ARG:HD2	44:L7:244:ASN:OD1	3.58	0.55
74:O8:3:ARG:NH2	36:5:1824:U:OP1	149.05	0.55
36:1:3259:U:H5'	36:1:3259:U:C6	2.42	0.55
20:C8:95:GLY:O	86:C8:201:OHX:N2	2.40	0.55
18:C6:7:VAL:HG12	18:C6:22:VAL:HB	6.08	0.55
9:S7:150:GLN:HB3	9:S7:181:ILE:HD12	1.88	0.55
43:L6:175:LYS:O	43:L6:176:PHE:HB2	4.47	0.55
40:L3:339:ARG:HG2	40:L3:340:LYS:O	2.15	0.55
46:L9:180:TYR:HB2	76:Q0:85:LEU:HD13	1.89	0.55
36:1:3195:U:O2'	36:1:3197:G:N2	2.40	0.55
1:2:1145:U:O2'	4:S2:89:GLN:O	2.19	0.55
36:1:1413:G:N7	86:1:4125:OHX:N4	2.55	0.55
36:1:171:G:H2'	36:1:172:G:O4'	2.06	0.55
37:3:85:G:O6	86:3:216:OHX:N4	2.40	0.55
2:S0:177:LEU:O	2:S0:181:VAL:HG13	2.07	0.55
1:6:9:U:O4	86:6:2146:OHX:N3	2.39	0.55
44:L7:120:THR:HB	57:N1:132:PRO:HB2	1.88	0.55
37:7:3:U:H2'	37:7:4:U:C6	2.42	0.55
1:2:1735:U:OP2	59:N3:32:ARG:NH1	2.40	0.55
38:4:69:U:OP2	86:O7:103:OHX:N3	2.40	0.55
86:6:2060:OHX:N1	86:6:2147:OHX:N3	2.54	0.55
63:N7:88:ASP:HB3	63:N7:121:ARG:NH2	2.20	0.55
28:D6:5:ARG:HG2	1:6:1796:C:C2	345.12	0.55
8:S6:98:ARG:HD2	8:S6:99:GLY:N	3.86	0.55
1:2:1370:U:H1'	1:2:1371:A:OP2	2.07	0.55
1:2:1518:C:OP1	86:2:2121:OHX:N5	2.40	0.55
4:S2:205:ARG:NH2	1:6:7:G:N7	369.73	0.55
1:2:191:C:O2'	1:2:192:U:O5'	2.25	0.55
1:6:1490:C:H4'	1:6:1491:U:OP1	2.05	0.55
1:6:25:C:O2	86:6:2108:OHX:N6	2.40	0.55
7:S5:119:ASP:O	7:S5:123:VAL:HG23	3.17	0.55
36:1:2310:U:OP1	86:1:4142:OHX:N4	2.40	0.55
45:L8:134:TYR:CG	45:L8:190:VAL:HG21	2.42	0.55
30:D8:11:LYS:HB2	30:D8:33:LEU:HD23	2.74	0.55
36:1:2718:U:OP1	78:Q2:13:LYS:NZ	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:3393:U:H2'	36:1:3394:U:H6	1.72	0.55
6:S4:151:ASP:HB3	6:S4:154:ILE:HG13	1.89	0.55
53:M7:31:GLU:HG3	53:M7:60:PHE:HA	3.24	0.55
40:L3:361:THR:HG22	40:L3:371:GLN:HB3	2.16	0.55
5:S3:144:ALA:HB1	35:SM:101:ASP:OD2	2.07	0.55
36:1:3246:G:O6	86:1:4111:OHX:N4	2.39	0.55
1:2:1535:U:O2'	1:2:1536:G:N3	2.38	0.55
41:L4:38:VAL:HG21	41:L4:121:ALA:HB2	2.37	0.55
36:1:2927:C:H2'	36:1:2928:C:C6	2.41	0.55
36:1:1717:U:H2'	36:1:1718:G:C8	2.42	0.55
36:1:2664:C:OP2	48:M1:142:LYS:NZ	2.39	0.55
26:D4:23:PHE:HE2	26:D4:75:VAL:HG12	1.71	0.55
70:O4:81:CYS:O	70:O4:83:ASN:N	3.36	0.55
21:C9:28:LEU:HD13	21:C9:29:GLU:H	1.71	0.55
1:2:1550:A:OP2	17:C5:42:ARG:NH2	2.40	0.55
36:5:1556:C:C5	36:5:2169:G:C4	2.95	0.55
79:Q3:73:THR:HG22	79:Q3:75:ALA:N	2.20	0.55
55:M9:46:LYS:HZ1	36:5:1766:G:H8	101.61	0.55
36:1:3159:C:H2'	36:1:3160:U:C6	2.42	0.55
86:5:4094:OHX:N5	86:5:4234:OHX:N6	2.55	0.55
34:SR:63:GLY:HA3	34:SR:90:ARG:NH1	3.01	0.55
36:5:1724:U:H1'	36:5:1725:C:C6	2.42	0.55
1:6:1166:A:H2'	1:6:1167:G:O4'	2.07	0.55
1:2:226:A:H2'	1:2:227:U:H5'	1.89	0.55
36:1:1919:G:N7	86:1:4017:OHX:N5	2.55	0.55
1:6:1639:C:OP1	86:6:2156:OHX:N5	2.40	0.55
50:M4:108:ARG:NH2	52:M6:196:ALA:O	2.39	0.55
36:1:1744:G:O6	86:1:4098:OHX:N2	2.40	0.55
49:M3:75:PHE:H	49:M3:97:VAL:HA	1.95	0.55
36:5:1657:C:N4	36:5:1798:A:OP2	2.36	0.55
8:S6:173:PRO:HG3	1:6:66:U:H5	333.73	0.55
17:C5:43:ARG:NH1	17:C5:47:ARG:HD3	4.12	0.55
36:5:1655:G:C5'	36:5:1655:G:H8	2.20	0.55
36:5:2397:A:H8	36:5:2941:A:N1	2.05	0.55
53:M7:28:ASN:O	53:M7:32:THR:HG22	2.07	0.55
6:S4:104:ASP:HB3	6:S4:106:LYS:H	1.72	0.55
63:N7:29:HIS:HB2	63:N7:40:HIS:O	2.82	0.55
26:D4:44:LEU:HA	26:D4:47:VAL:HG13	5.14	0.55
49:M3:93:ILE:HG22	49:M3:94:GLY:H	4.58	0.55
4:S2:176:SER:HB2	4:S2:195:ASP:HB3	2.22	0.55
22:D0:118:VAL:HG22	22:D0:119:ALA:H	1.72	0.55
33:E1:90:LYS:HD3	33:E1:93:HIS:CE1	11.00	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
53:M7:60:PHE:CE2	53:M7:82:ARG:HB2	2.42	0.55
55:M9:23:TRP:CH2	55:M9:25:ASP:HB2	2.43	0.55
86:1:4036:OHX:N4	86:1:4048:OHX:N3	2.54	0.55
36:1:2947:G:C2	40:L3:250:ALA:HB1	2.41	0.55
1:6:1213:G:O6	86:6:2073:OHX:N6	2.40	0.55
48:M1:28:ASP:HA	48:M1:31:THR:HG23	2.00	0.55
36:5:3227:A:H2'	36:5:3228:C:H5'	1.88	0.55
36:5:1192:C:N4	36:5:1301:A:O3'	2.39	0.55
1:2:1217:A:H8	1:2:1217:A:H5'	1.72	0.55
36:1:565:U:H2'	36:1:566:G:H8	1.72	0.55
16:C4:84:ARG:HB2	16:C4:118:VAL:HG23	1.89	0.54
1:6:196:G:O2'	1:6:197:A:OP2	2.25	0.54
9:S7:132:PRO:O	9:S7:133:THR:OG1	4.74	0.54
86:5:4011:OHX:N6	86:5:4198:OHX:N2	2.54	0.54
22:D0:103:ILE:HA	22:D0:106:ILE:HG22	2.56	0.54
12:C0:15:LEU:HD22	12:C0:68:LEU:HD22	4.96	0.54
36:5:528:U:H2'	36:5:529:A:H8	1.72	0.54
36:5:3242:G:H5'	36:5:3245:A:C8	2.41	0.54
49:M3:24:VAL:HG23	49:M3:24:VAL:O	2.07	0.54
9:S7:164:TYR:CE1	9:S7:165:LYS:HG3	3.51	0.54
69:O3:16:TYR:OH	69:O3:91:ALA:HB2	2.07	0.54
36:5:2364:G:H22	36:5:2396:G:H1'	1.71	0.54
66:O0:75:ASN:HA	66:O0:86:ARG:HB2	2.69	0.54
1:2:1620:C:OP2	86:2:2167:OHX:N6	2.40	0.54
36:1:3395:G:N2	36:1:3396:U:O4	2.33	0.54
1:6:1350:U:H2'	1:6:1351:G:C8	2.41	0.54
50:M4:21:VAL:HB	50:M4:63:VAL:HG13	1.88	0.54
1:6:1263:G:H2'	1:6:1264:G:O4'	2.07	0.54
63:N7:77:TYR:HA	63:N7:80:LEU:HD12	3.01	0.54
36:5:1661:G:H2'	36:5:1662:G:C8	2.42	0.54
36:1:1221:A:H3'	36:1:1222:G:H5''	1.87	0.54
1:2:1555:A:P	17:C5:47:ARG:HH21	2.30	0.54
3:S1:77:GLU:O	3:S1:79:HIS:N	2.37	0.54
20:C8:11:PHE:CD2	20:C8:59:GLY:HA3	2.42	0.54
18:C6:114:ARG:O	18:C6:115:THR:HB	3.94	0.54
46:L9:105:GLU:HG3	46:L9:109:ALA:H	1.73	0.54
42:L5:272:TYR:CZ	37:7:22:A:H1'	333.92	0.54
36:5:2971:A:H5''	36:5:2972:G:O5'	2.07	0.54
36:1:1240:A:H3'	36:1:1241:U:H5'	1.90	0.54
14:C2:119:SER:OG	14:C2:120:VAL:N	2.40	0.54
40:L3:53:MET:HG2	40:L3:77:THR:HG22	1.87	0.54
75:O9:5:LYS:HE3	75:O9:13:MET:HE1	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:D4:49:LYS:N	26:D4:49:LYS:HD3	2.66	0.54
36:5:437:G:H1	36:5:622:A:H61	1.55	0.54
36:5:438:A:H2'	36:5:494:G:N2	2.23	0.54
7:S5:161:ASP:OD2	30:D8:42:ARG:NH1	3.58	0.54
7:S5:158:GLN:HG2	30:D8:66:LEU:HD21	1.90	0.54
40:L3:150:ARG:HD2	36:5:3242:G:N7	251.88	0.54
86:8:215:OHX:N5	86:8:223:OHX:N3	2.54	0.54
14:C2:33:ARG:HA	14:C2:36:LEU:HD12	1.88	0.54
43:L6:176:PHE:H	50:M4:117:ARG:NH2	5.32	0.54
6:S4:185:GLY:HA2	6:S4:189:LEU:HD22	3.39	0.54
51:M5:12:ARG:HG3	36:5:268:A:C4	127.75	0.54
57:N1:122:GLN:O	57:N1:124:VAL:HG23	6.90	0.54
11:S9:88:GLU:O	11:S9:91:LYS:HD2	3.80	0.54
3:S1:87:ARG:NH2	3:S1:89:ASP:OD1	5.66	0.54
86:6:2060:OHX:N5	86:6:2147:OHX:N6	2.56	0.54
25:D3:103:LEU:HD12	25:D3:126:LYS:HD3	3.25	0.54
62:N6:51:ARG:HB3	62:N6:115:ARG:NH2	2.20	0.54
11:S9:3:ARG:HG2	11:S9:3:ARG:NH2	4.85	0.54
24:D2:30:SER:HB2	24:D2:61:ILE:HG13	1.89	0.54
1:2:959:U:C6	15:C3:17:PRO:HG2	2.43	0.54
1:2:789:A:O2'	6:S4:106:LYS:NZ	2.39	0.54
47:M0:210:ILE:HA	47:M0:217:PHE:CE2	2.42	0.54
61:N5:48:SER:OG	61:N5:49:LYS:N	3.14	0.54
12:C0:21:VAL:HG12	12:C0:66:TYR:HB2	4.32	0.54
59:N3:17:LEU:HD21	59:N3:98:ASN:CG	2.28	0.54
2:S0:84:ARG:HD3	2:S0:203:PHE:O	2.99	0.54
53:M7:36:ILE:HD11	53:M7:95:LEU:HD11	1.89	0.54
14:C2:42:ALA:HB2	14:C2:124:LYS:HD2	2.25	0.54
47:M0:43:VAL:HG21	47:M0:197:VAL:HB	2.29	0.54
1:6:1703:C:H2'	1:6:1704:U:H6	1.72	0.54
36:5:725:G:H3'	36:5:726:G:H5''	1.89	0.54
1:6:828:U:H2'	1:6:829:A:H5''	1.89	0.54
36:1:1229:G:H1	36:1:1280:C:H42	1.56	0.54
36:5:308:A:H5'	36:5:2223:A:O2'	2.06	0.54
1:6:1244:A:H3'	1:6:1244:A:N3	2.23	0.54
22:D0:23:ARG:HB3	22:D0:117:VAL:HG12	1.88	0.54
6:S4:130:GLN:HB3	6:S4:138:TYR:CZ	3.96	0.54
36:1:2402:A:C5	36:1:2871:G:C2	2.96	0.54
86:5:3978:OHX:N2	86:5:4196:OHX:N5	2.56	0.54
86:5:3978:OHX:N4	86:5:4196:OHX:N1	2.55	0.54
3:S1:131:ASP:HB3	3:S1:180:THR:CG2	2.38	0.54
3:S1:185:THR:O	3:S1:189:ILE:HG13	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:S1:71:ALA:HB3	16:C4:114:ARG:NH1	2.31	0.54
41:L4:15:ALA:O	41:L4:16:THR:OG1	2.21	0.54
1:2:894:U:H2'	1:2:895:G:C8	2.43	0.54
1:2:1796:C:H4'	1:2:1797:A:OP2	2.07	0.54
1:2:1034:C:OP1	15:C3:9:LYS:NZ	2.38	0.54
15:C3:36:GLN:OE1	15:C3:58:HIS:NE2	2.40	0.54
36:5:3047:U:C2'	36:5:3048:A:H5'	2.37	0.54
1:2:1235:C:O2	33:E1:138:ARG:NH2	2.41	0.54
36:5:1480:G:H4'	36:5:1481:A:OP1	2.07	0.54
62:N6:37:LYS:H	62:N6:37:LYS:CD	2.31	0.54
1:2:753:A:H5'	6:S4:221:ARG:HG3	1.89	0.54
86:1:4032:OHX:N6	86:1:4149:OHX:N5	2.55	0.54
29:D7:54:VAL:O	29:D7:63:LEU:HB2	2.12	0.54
16:C4:19:ILE:HB	16:C4:83:ILE:HD12	1.89	0.54
74:O8:26:LYS:NZ	74:O8:28:ASN:OD1	2.30	0.54
36:1:1310:G:O6	86:1:4031:OHX:N1	2.40	0.54
62:N6:82:VAL:O	62:N6:84:LYS:N	2.98	0.54
86:1:4056:OHX:N6	86:1:4163:OHX:N4	2.56	0.54
1:6:914:G:H8	1:6:914:G:OP2	1.90	0.54
75:O9:20:ASN:ND2	75:O9:20:ASN:O	2.41	0.54
36:5:2507:C:O2'	36:5:2508:U:OP1	2.24	0.54
42:L5:211:LEU:HB3	42:L5:219:PHE:HB2	2.18	0.54
42:L5:110:LEU:HA	42:L5:113:LEU:HB2	3.04	0.54
1:6:1:U:H5''	1:6:2:A:OP1	2.08	0.54
1:2:487:G:H3'	1:2:488:G:H5''	1.88	0.54
1:6:831:U:O2'	1:6:832:U:H5'	2.07	0.54
1:2:72:A:C2	1:2:73:U:N3	2.75	0.54
45:L8:101:THR:OG1	45:L8:104:GLU:HG3	5.62	0.54
1:6:235:G:H2'	1:6:236:A:C8	2.43	0.54
1:2:462:G:N7	86:2:2144:OHX:N1	2.54	0.54
40:L3:227:GLU:HG3	40:L3:270:ARG:HE	3.89	0.54
41:L4:179:LEU:HD22	41:L4:183:LYS:HG2	2.38	0.54
86:1:4059:OHX:N6	86:1:4166:OHX:N5	2.55	0.54
46:L9:93:VAL:O	46:L9:177:ASP:HA	2.29	0.54
78:Q2:17:CYS:HB2	87:Q2:501:ZN:ZN	1.26	0.54
1:2:701:U:H3	1:2:737:A:N6	2.01	0.54
8:S6:67:VAL:O	8:S6:68:LEU:HB2	2.13	0.54
75:O9:48:LYS:O	86:5:4207:OHX:N1	118.05	0.54
51:M5:38:ARG:HG3	51:M5:38:ARG:NH1	2.23	0.54
41:L4:139:GLY:O	41:L4:141:ARG:NH1	5.04	0.54
36:1:439:C:H3'	36:1:440:A:H8	1.73	0.54
36:1:1024:G:N7	86:1:4168:OHX:N6	2.55	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:3087:A:P	86:1:4184:OHX:N5	2.80	0.54
46:L9:77:ASN:HA	46:L9:80:THR:HG23	2.37	0.54
51:M5:93:LYS:HG3	36:5:289:A:C2	147.06	0.54
36:1:3064:U:O4	86:1:4138:OHX:N6	2.41	0.54
55:M9:17:VAL:CG2	55:M9:52:LYS:HE3	2.37	0.54
1:2:296:U:H2'	1:2:297:U:C6	2.41	0.54
41:L4:64:SER:HA	41:L4:75:PRO:HA	1.89	0.54
36:5:2659:G:H4'	36:5:2751:G:O2'	2.07	0.54
36:1:692:A:OP1	51:M5:201:ARG:NH2	2.40	0.54
34:SR:16:HIS:CE1	34:SR:43:ILE:HG12	2.42	0.54
36:1:2726:C:O2'	36:1:2727:A:H2'	2.08	0.54
36:1:242:C:HO2'	36:1:243:G:H8	1.54	0.54
1:6:1017:U:H2'	1:6:1018:U:C6	2.43	0.54
36:1:3033:A:H2'	36:1:3034:C:C6	2.43	0.54
1:6:363:G:OP1	86:6:2112:OHX:N1	2.39	0.54
79:Q3:91:GLU:OE2	79:Q3:91:GLU:N	2.39	0.54
68:O2:105:ARG:NH2	36:5:1412:G:OP1	147.10	0.54
8:S6:163:THR:HA	8:S6:168:THR:HG22	3.01	0.54
11:S9:85:VAL:HG12	11:S9:99:LEU:HD11	1.89	0.54
36:5:2211:U:OP2	86:5:4221:OHX:N1	2.41	0.54
7:S5:53:VAL:O	7:S5:55:ASP:N	3.05	0.54
48:M1:137:ARG:NH2	37:7:44:C:OP2	296.49	0.54
1:2:14:C:OP2	4:S2:206:THR:HG21	2.08	0.54
36:1:1064:A:H5''	36:1:1066:G:O4'	2.07	0.54
36:1:1103:A:H4'	36:1:1103:A:OP2	2.08	0.54
1:6:485:A:N6	1:6:486:G:N3	2.55	0.54
25:D3:97:ASP:O	25:D3:100:ASP:HB2	2.27	0.54
59:N3:66:LYS:HB3	59:N3:68:GLU:OE1	2.06	0.54
86:5:4055:OHX:N5	86:5:4197:OHX:N2	2.55	0.54
86:5:4094:OHX:N5	86:5:4234:OHX:N2	2.55	0.54
52:M6:58:LEU:HA	52:M6:72:HIS:CD2	2.91	0.54
15:C3:55:ARG:HD3	29:D7:47:PHE:CD1	2.92	0.54
40:L3:188:ILE:HD12	40:L3:189:SER:H	1.73	0.54
1:6:913:G:H3'	1:6:914:G:H5'	1.88	0.54
38:4:103:G:O6	86:4:223:OHX:N4	2.40	0.54
24:D2:37:PHE:CE2	24:D2:103:ILE:HD12	2.45	0.54
49:M3:128:ARG:NH2	71:O5:109:ILE:O	2.31	0.54
34:SR:93:ASP:HB3	34:SR:96:THR:HG22	1.89	0.54
45:L8:74:THR:HB	45:L8:230:LYS:NZ	2.22	0.54
36:5:2765:C:H2'	36:5:2766:U:H6	1.71	0.54
36:5:3358:U:H2'	36:5:3359:A:C8	2.43	0.54
36:5:2228:A:H5''	36:5:2228:A:H8	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
41:L4:299:ILE:HG23	54:M8:39:ARG:HB3	2.44	0.54
42:L5:260:PHE:CE2	37:7:121:U:H5'	321.25	0.54
35:SM:23:LYS:HE3	35:SM:24:GLU:H	6.95	0.54
36:5:2897:A:H2'	36:5:2899:C:C5'	2.38	0.54
15:C3:33:VAL:HG11	15:C3:66:ILE:HG12	1.88	0.54
41:L4:181:VAL:O	41:L4:182:LEU:CB	2.56	0.54
1:2:1786:G:OP1	16:C4:136:ARG:NH2	2.33	0.54
45:L8:100:GLU:OE2	45:L8:108:ARG:NH1	2.82	0.54
1:6:1081:A:O2'	1:6:1082:C:O5'	2.26	0.54
6:S4:184:THR:C	6:S4:189:LEU:HD13	2.91	0.54
36:1:3340:G:O6	86:1:4056:OHX:N4	2.41	0.54
1:2:1765:A:OP2	86:2:2093:OHX:N5	2.41	0.54
36:5:420:G:O5'	36:5:420:G:OP2	2.26	0.54
36:1:3295:A:OP2	40:L3:126:LYS:N	2.29	0.54
68:O2:11:LYS:O	68:O2:12:LYS:HB2	2.19	0.54
40:L3:111:SER:OG	40:L3:113:GLU:HB2	2.08	0.54
1:6:565:C:N3	86:6:2159:OHX:N4	2.56	0.54
1:2:158:U:O2'	1:2:159:U:H3'	2.08	0.54
1:6:152:U:O2	1:6:163:G:N2	2.41	0.54
38:4:38:U:C4	71:O5:89:ARG:HD2	2.43	0.54
1:2:819:G:O2'	1:2:821:U:OP2	2.13	0.54
46:L9:70:THR:HB	36:5:3112:G:O2'	329.52	0.54
14:C2:97:LEU:HD11	14:C2:121:VAL:HG22	3.43	0.54
11:S9:171:ARG:HH11	11:S9:174:ARG:HB3	4.67	0.54
11:S9:171:ARG:HE	11:S9:174:ARG:HB2	4.80	0.54
36:1:1422:G:H21	43:L6:5:LYS:HZ1	1.56	0.54
52:M6:67:THR:HG23	86:M6:202:OHX:N4	2.23	0.54
2:S0:187:ALA:O	2:S0:188:LEU:HD22	2.08	0.54
28:D6:17:HIS:CE1	28:D6:18:VAL:O	2.61	0.54
9:S7:126:LEU:HD11	9:S7:181:ILE:HG12	1.90	0.54
34:SR:93:ASP:HB2	34:SR:100:TYR:CE1	2.42	0.54
1:2:958:U:OP2	29:D7:20:LYS:HE3	2.08	0.54
1:2:404:G:H2'	1:2:405:C:C6	2.42	0.54
16:C4:132:ARG:HB3	1:6:1787:C:OP2	292.79	0.54
1:6:751:G:H2'	1:6:752:A:C8	2.43	0.54
18:C6:123:ARG:HG3	18:C6:124:PRO:HD2	1.89	0.54
36:5:3:U:H3	38:8:156:U:H3	1.54	0.54
36:5:3259:U:H5'	36:5:3259:U:C6	2.43	0.54
42:L5:217:GLU:HG2	42:L5:218:ARG:N	2.21	0.54
58:N2:36:TYR:OH	58:N2:82:LYS:HG2	2.08	0.54
36:5:2962:U:OP1	86:5:3978:OHX:N4	2.41	0.54
41:L4:295:ILE:HG23	41:L4:299:ILE:HD11	2.80	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:2895:G:C2'	36:1:2896:A:H5''	2.36	0.54
36:1:1899:G:N7	86:1:3935:OHX:N3	2.56	0.54
22:D0:58:LEU:HD12	22:D0:88:LYS:HB3	1.89	0.54
4:S2:67:GLN:HA	4:S2:70:ASP:HB2	2.27	0.54
21:C9:53:TRP:HH2	21:C9:100:ILE:HD12	2.11	0.54
59:N3:87:ARG:HH22	59:N3:137:VAL:HG22	1.84	0.54
36:1:1495:U:C5	36:1:1835:A:N1	2.74	0.54
22:D0:106:ILE:HG13	22:D0:107:THR:H	1.73	0.54
38:4:52:A:OP1	75:O9:21:ARG:NH2	2.28	0.54
36:1:561:C:H2'	36:1:562:C:C6	2.43	0.54
12:C0:1:MET:HG2	12:C0:2:LEU:H	1.73	0.54
45:L8:90:THR:HA	45:L8:214:LEU:HD21	1.90	0.54
1:2:1015:U:OP1	86:2:2046:OHX:N3	2.41	0.54
1:6:241:U:H2'	1:6:242:U:C6	2.43	0.54
6:S4:161:LYS:HB3	6:S4:170:THR:O	4.66	0.54
36:5:644:G:H2'	36:5:2372:A:N7	2.22	0.54
36:5:2317:A:OP2	86:5:4185:OHX:N6	2.40	0.54
7:S5:93:LEU:HD23	7:S5:172:ILE:HG23	2.97	0.54
36:5:2771:U:H2'	36:5:2772:C:C6	2.43	0.54
2:S0:28:ASN:OD1	2:S0:28:ASN:N	4.39	0.54
1:6:393:C:H2'	1:6:394:C:C6	2.43	0.54
40:L3:324:VAL:HG11	40:L3:328:ILE:HD13	1.90	0.54
45:L8:193:LYS:HB3	36:5:7:C:H5''	122.86	0.54
36:1:980:A:C8	36:1:980:A:OP2	2.57	0.53
17:C5:43:ARG:NH1	1:6:1553:G:N7	402.15	0.53
3:S1:175:GLU:HG2	3:S1:193:ILE:HD13	4.07	0.53
40:L3:345:ASN:OD1	40:L3:346:THR:N	2.62	0.53
28:D6:10:ARG:NE	1:6:1795:U:O2	329.10	0.53
8:S6:63:MET:HE2	8:S6:106:LEU:CD1	2.38	0.53
1:6:1458:G:H5''	1:6:1459:C:OP2	2.07	0.53
1:6:542:A:H1'	1:6:543:C:H5'	1.90	0.53
65:N9:14:ARG:NH2	65:N9:18:ARG:HH11	2.09	0.53
39:L2:48:ILE:HG12	79:Q3:63:THR:HG22	2.13	0.53
46:L9:75:VAL:HA	46:L9:78:MET:CE	2.52	0.53
52:M6:60:LYS:NZ	36:5:1307:G:H5''	251.51	0.53
1:6:74:U:H5''	1:6:75:U:OP2	2.07	0.53
2:S0:195:TRP:NE1	2:S0:197:ILE:HD13	3.33	0.53
1:6:737:A:H2'	1:6:738:G:C8	2.43	0.53
13:C1:3:THR:OG1	13:C1:82:ARG:NE	2.35	0.53
1:2:1629:G:H2'	1:2:1630:U:H6	1.74	0.53
26:D4:21:LYS:HB2	26:D4:75:VAL:HG13	1.90	0.53
41:L4:156:LEU:HD23	41:L4:159:ILE:HD12	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:3089:C:OP1	40:L3:222:LYS:NZ	2.39	0.53
36:5:2204:C:H4'	36:5:2205:U:OP1	2.08	0.53
1:2:1158:C:OP2	86:2:2174:OHX:N5	2.41	0.53
38:4:77:A:OP2	86:4:224:OHX:N2	2.41	0.53
36:1:655:C:H2'	36:1:656:A:C8	2.43	0.53
41:L4:136:LEU:HD23	41:L4:142:VAL:HG23	1.90	0.53
1:2:1253:U:H4'	33:E1:143:LYS:N	2.23	0.53
41:L4:139:GLY:O	41:L4:140:HIS:HB2	2.07	0.53
48:M1:162:TRP:CZ2	48:M1:166:LYS:HD2	2.44	0.53
12:C0:32:HIS:HD2	12:C0:35:ILE:HB	1.72	0.53
5:S3:60:GLY:O	5:S3:62:ASN:N	3.31	0.53
46:L9:86:TYR:CD1	46:L9:151:VAL:HG13	2.42	0.53
23:D1:36:VAL:HG11	23:D1:78:LEU:HD21	4.81	0.53
1:6:486:G:N2	1:6:487:G:N7	2.56	0.53
45:L8:153:ILE:HD13	45:L8:166:LEU:HB3	2.49	0.53
1:2:1450:U:H2'	1:2:1451:C:C6	2.44	0.53
36:5:3074:G:OP1	86:5:4118:OHX:N4	2.41	0.53
35:SM:48:ARG:HA	36:5:1019:G:OP1	334.53	0.53
48:M1:155:THR:OG1	48:M1:158:ASP:HB2	2.15	0.53
86:1:4032:OHX:N6	86:1:4149:OHX:N3	2.55	0.53
1:2:385:A:OP1	10:S8:25:ARG:NH1	2.38	0.53
36:5:2734:A:OP1	86:5:4046:OHX:N6	2.41	0.53
36:1:955:U:H2'	36:1:956:U:C6	2.44	0.53
42:L5:86:TYR:CE1	42:L5:247:ILE:HA	2.43	0.53
36:1:1313:G:OP1	52:M6:82:LYS:HE2	2.08	0.53
36:5:374:A:N3	36:5:376:G:H5''	2.23	0.53
40:L3:105:VAL:HG21	40:L3:148:LEU:HD13	1.89	0.53
53:M7:108:ASP:N	53:M7:152:GLU:OE2	2.96	0.53
24:D2:7:LEU:HD13	24:D2:74:VAL:HG23	2.15	0.53
55:M9:90:PRO:HG2	55:M9:93:VAL:HG23	2.66	0.53
40:L3:123:TYR:CZ	40:L3:124:LYS:HG3	2.44	0.53
42:L5:114:GLY:C	42:L5:116:ASP:H	2.10	0.53
1:6:539:G:OP2	1:6:539:G:H8	1.92	0.53
36:1:2157:G:O6	39:L2:152:SER:HB3	2.08	0.53
46:L9:3:TYR:HA	56:N0:142:GLN:OE1	2.08	0.53
63:N7:22:LYS:HE2	63:N7:129:TRP:CZ2	3.37	0.53
36:1:3:U:H2'	36:1:4:U:O4'	2.08	0.53
86:5:3973:OHX:N3	86:5:4241:OHX:N2	2.57	0.53
53:M7:87:SER:O	53:M7:91:VAL:HG23	3.36	0.53
1:2:513:U:OP1	11:S9:133:HIS:NE2	2.37	0.53
36:1:785:G:OP1	54:M8:66:ARG:NH1	2.40	0.53
40:L3:95:THR:HG22	36:5:3243:A:H4'	255.87	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
76:Q0:99:CYS:HB2	76:Q0:114:LYS:HD3	2.54	0.53
45:L8:50:VAL:HG22	45:L8:52:TRP:CE2	2.43	0.53
1:2:523:G:H5'	26:D4:60:PHE:O	2.09	0.53
19:C7:45:ARG:NH2	1:6:1331:A:OP1	413.42	0.53
36:1:1363:A:OP2	86:1:4048:OHX:N6	2.42	0.53
69:O3:49:ILE:HG23	69:O3:100:ILE:HG13	1.93	0.53
1:2:393:C:H2'	1:2:394:C:C6	2.44	0.53
36:5:253:A:HO2'	36:5:254:A:H8	1.55	0.53
34:SR:267:PRO:HG2	34:SR:269:TYR:HE1	1.72	0.53
51:M5:155:VAL:HG23	51:M5:156:HIS:ND1	2.24	0.53
36:1:829:U:H3	36:1:895:A:H62	1.55	0.53
18:C6:140:LYS:NZ	1:6:1192:C:O3'	364.09	0.53
14:C2:27:ALA:O	14:C2:31:VAL:HG23	2.08	0.53
36:1:719:U:H5''	36:1:719:U:H6	1.72	0.53
1:2:287:G:O2'	1:2:288:A:OP2	2.25	0.53
1:2:1191:U:O2'	18:C6:142:TYR:O	2.18	0.53
36:5:2403:G:N2	36:5:2404:A:H62	2.05	0.53
48:M1:95:ASN:HD22	48:M1:95:ASN:N	2.06	0.53
63:N7:46:ILE:HD11	63:N7:49:TYR:CG	3.79	0.53
3:S1:48:VAL:HG21	3:S1:61:LEU:HD22	5.07	0.53
7:S5:35:GLN:O	7:S5:37:GLN:N	2.76	0.53
49:M3:79:GLU:OE2	49:M3:101:ARG:NH2	3.00	0.53
17:C5:111:MET:HG2	20:C8:119:ILE:CG1	4.51	0.53
36:5:3049:A:C8	36:5:3049:A:H5'	2.42	0.53
45:L8:94:PHE:HB3	45:L8:189:LEU:HD13	1.90	0.53
74:O8:5:ILE:HD12	74:O8:52:TYR:HB3	2.88	0.53
12:C0:53:GLY:O	12:C0:55:VAL:N	2.40	0.53
36:5:1024:G:N2	36:5:1026:A:OP2	2.41	0.53
6:S4:199:GLU:OE1	6:S4:201:HIS:HE1	1.91	0.53
36:5:3155:U:OP1	86:5:4224:OHX:N2	2.41	0.53
86:1:4032:OHX:N2	86:1:4149:OHX:N1	2.56	0.53
52:M6:116:LYS:HG3	52:M6:117:ARG:N	2.24	0.53
45:L8:116:VAL:C	45:L8:118:GLU:H	2.37	0.53
79:Q3:49:ARG:HB2	79:Q3:55:TRP:CZ3	2.80	0.53
36:1:685:G:P	49:M3:35:ARG:NH1	2.81	0.53
36:1:871:U:H2'	36:1:872:U:C6	2.43	0.53
38:4:104:A:C8	38:4:105:A:C8	2.97	0.53
21:C9:3:GLY:HA3	1:6:1364:G:N2	431.36	0.53
40:L3:68:HIS:CD2	40:L3:69:LYS:HG3	2.43	0.53
38:4:125:U:H2'	38:4:125:U:O2	2.08	0.53
78:Q2:10:THR:HA	78:Q2:20:HIS:CD2	2.99	0.53
1:2:558:U:O2'	1:2:559:C:O5'	2.25	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:C3:12:SER:HB3	1:6:956:C:OP2	335.89	0.53
36:5:322:U:H5''	36:5:323:A:OP1	2.09	0.53
4:S2:159:THR:HG21	1:6:1097:U:O3'	383.93	0.53
38:4:85:G:C8	38:4:85:G:H3'	2.44	0.53
37:7:2:G:O2'	37:7:23:A:N1	2.31	0.53
6:S4:19:LEU:HD22	1:6:788:A:H2'	390.14	0.53
86:2:2045:OHX:N4	86:2:2099:OHX:N3	2.56	0.53
45:L8:200:LEU:HD11	45:L8:211:LEU:HD21	5.87	0.53
18:C6:143:ARG:HH22	35:SM:84:LYS:HZ1	1.57	0.53
11:S9:168:ARG:HD3	11:S9:171:ARG:HH11	1.74	0.53
46:L9:77:ASN:HB3	46:L9:151:VAL:HG21	1.89	0.53
36:5:956:U:OP1	86:5:4152:OHX:N2	2.42	0.53
36:5:996:A:C2	36:5:1054:A:C4	2.96	0.53
1:2:393:C:H4'	1:2:1673:G:O2'	2.07	0.53
9:S7:98:ILE:HG12	9:S7:121:VAL:HG21	2.26	0.53
36:1:1778:G:O2'	36:1:1780:G:OP2	2.21	0.53
63:N7:104:PRO:O	63:N7:108:GLU:HG3	3.00	0.53
41:L4:22:LEU:HD11	41:L4:26:PHE:HB2	3.41	0.53
1:2:1776:A:H2'	1:2:1777:G:C8	2.43	0.53
1:2:229:U:H2'	1:2:230:C:C6	2.43	0.53
36:1:1408:G:P	68:O2:33:ARG:HH22	2.31	0.53
24:D2:18:GLU:OE1	24:D2:69:LEU:HB3	2.83	0.53
8:S6:105:ASP:OD2	8:S6:105:ASP:N	3.14	0.53
1:2:1472:C:OP1	7:S5:102:ARG:NH2	2.34	0.53
40:L3:296:THR:HG21	40:L3:357:LYS:O	2.11	0.53
1:6:991:G:OP2	86:6:2171:OHX:N2	2.42	0.53
2:S0:52:LYS:HB3	23:D1:82:VAL:HG22	1.91	0.53
47:M0:77:THR:HG22	47:M0:85:PHE:CZ	2.44	0.53
51:M5:68:ARG:NH1	51:M5:68:ARG:HG2	2.20	0.53
7:S5:35:GLN:C	7:S5:37:GLN:H	2.52	0.53
48:M1:137:ARG:HG2	37:7:28:C:H5''	307.12	0.53
70:O4:99:LYS:O	70:O4:103:LYS:HG2	2.10	0.53
78:Q2:71:ARG:HG3	78:Q2:71:ARG:NH1	2.64	0.53
42:L5:34:LYS:HE3	57:N1:30:TYR:CZ	2.43	0.53
6:S4:105:VAL:HG11	6:S4:245:LYS:H	2.39	0.53
20:C8:28:ILE:O	20:C8:32:LEU:HG	2.09	0.53
24:D2:17:ALA:HB2	24:D2:25:VAL:HG13	1.89	0.53
36:5:530:G:O6	86:5:3949:OHX:N3	2.42	0.53
86:5:4001:OHX:N6	86:5:4090:OHX:N2	2.57	0.53
36:1:2505:U:H2'	36:1:2506:U:H6	1.73	0.53
86:1:4023:OHX:N4	86:1:4061:OHX:N2	2.56	0.53
86:5:4201:OHX:N6	86:8:224:OHX:N5	2.56	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:624:G:H2'	1:6:625:C:C6	2.43	0.53
36:1:2883:U:H2'	36:1:2884:C:H6	1.72	0.53
2:S0:4:PRO:HB2	2:S0:7:PHE:HB2	1.89	0.53
36:1:696:C:HO2'	36:1:697:A:H8	1.57	0.53
5:S3:37:VAL:HG12	5:S3:50:ILE:HA	2.83	0.53
68:O2:50:ILE:O	68:O2:50:ILE:HG13	2.09	0.53
51:M5:106:VAL:HG11	51:M5:132:VAL:HG21	2.40	0.53
2:S0:169:SER:O	2:S0:173:ILE:HG12	2.15	0.53
36:1:1577:G:H2'	36:1:1578:C:O4'	2.08	0.53
36:5:882:A:H2'	36:5:883:A:H5''	1.91	0.53
47:M0:47:PRO:HB3	47:M0:171:TRP:CZ2	2.43	0.53
1:6:163:G:H8	1:6:163:G:O5'	1.92	0.53
41:L4:152:VAL:CG2	41:L4:172:VAL:HG21	2.38	0.53
71:O5:82:ALA:O	38:8:38:U:H5	64.91	0.53
1:2:959:U:C6	15:C3:61:THR:HB	2.44	0.53
36:1:1245:A:H3'	36:1:1246:G:H5''	1.90	0.53
36:5:93:C:OP2	36:5:2764:C:O2'	2.22	0.53
1:6:484:C:H42	1:6:503:G:H22	1.56	0.53
69:O3:59:VAL:O	69:O3:61:GLY:N	3.08	0.53
33:E1:136:LYS:O	33:E1:138:ARG:HB2	2.08	0.53
11:S9:118:LEU:HG	11:S9:158:PHE:CE1	2.44	0.53
43:L6:52:VAL:HG11	43:L6:65:ILE:HG13	1.91	0.53
16:C4:16:VAL:HG22	16:C4:33:LEU:HA	1.90	0.53
86:8:215:OHX:N5	86:8:223:OHX:N1	2.57	0.53
6:S4:193:GLY:O	6:S4:194:THR:OG1	2.26	0.53
86:1:4059:OHX:N4	86:1:4166:OHX:N1	2.56	0.53
41:L4:74:ILE:HD12	41:L4:75:PRO:HD2	5.04	0.53
36:5:2765:C:H2'	36:5:2766:U:C6	2.44	0.53
36:5:2771:U:O2'	36:5:2772:C:O5'	2.25	0.53
36:1:1577:G:H2'	36:1:1578:C:C1'	2.39	0.53
8:S6:48:TYR:CZ	8:S6:121:LEU:HD22	5.44	0.53
46:L9:174:LYS:HB2	76:Q0:127:LEU:HD11	3.15	0.53
15:C3:71:ILE:O	15:C3:75:LEU:HD12	3.20	0.53
63:N7:99:GLU:HG3	63:N7:100:THR:HG23	6.26	0.53
72:O6:53:TYR:HA	72:O6:56:ARG:NH1	2.24	0.53
36:1:786:A:H4'	36:1:787:G:H5'	1.89	0.53
38:8:103:G:O6	86:8:216:OHX:N5	2.41	0.53
1:2:1381:U:H1'	1:2:1516:A:N6	2.24	0.53
36:5:961:C:O2	86:5:4176:OHX:N4	2.42	0.53
59:N3:80:ARG:NE	59:N3:97:ASP:OD2	2.40	0.53
42:L5:119:TYR:CZ	42:L5:135:VAL:HG23	2.44	0.53
36:1:567:G:O6	86:1:4006:OHX:N1	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:703:G:H2'	1:2:704:C:H5'	1.90	0.53
46:L9:12:VAL:HG13	46:L9:16:VAL:HG22	2.53	0.53
12:C0:55:VAL:HA	12:C0:69:THR:HG23	1.91	0.53
86:5:4201:OHX:N4	86:8:224:OHX:N1	2.56	0.53
26:D4:122:GLY:O	26:D4:125:LEU:N	2.35	0.53
28:D6:18:VAL:HG21	28:D6:33:ASP:OD1	2.08	0.53
61:N5:136:ALA:O	61:N5:139:ILE:HG23	2.09	0.53
57:N1:82:ASN:O	65:N9:21:ILE:HA	2.08	0.53
40:L3:250:ALA:HB3	36:5:2880:U:H1'	224.13	0.53
24:D2:103:ILE:HA	24:D2:112:ASP:HA	1.90	0.53
49:M3:128:ARG:NH1	71:O5:109:ILE:O	3.43	0.53
61:N5:79:GLY:O	61:N5:81:ILE:HD12	3.66	0.53
51:M5:143:ARG:HH21	71:O5:92:LEU:HA	1.74	0.53
1:6:1752:U:OP2	86:6:2061:OHX:N5	2.41	0.53
57:N1:104:GLU:O	57:N1:108:ARG:HB2	2.09	0.53
36:5:1032:C:H5'	36:5:1033:U:OP2	2.09	0.53
36:1:2402:A:O2'	36:1:2403:G:OP2	2.24	0.53
3:S1:176:VAL:HG13	3:S1:184:LEU:HD22	4.54	0.53
42:L5:40:HIS:CD2	42:L5:42:ALA:H	2.18	0.53
1:2:1488:G:H5'	1:2:1489:U:OP1	2.09	0.53
71:O5:89:ARG:HD2	38:8:38:U:C4	69.87	0.53
69:O3:86:ARG:HH12	36:5:498:A:H5'	215.69	0.53
47:M0:4:ARG:CZ	47:M0:99:ILE:HD12	2.39	0.53
36:1:2303:A:OP1	77:Q1:23:ARG:NH2	2.41	0.53
86:5:4212:OHX:N4	86:5:4222:OHX:N3	2.56	0.53
36:1:2867:C:H5'	36:1:2867:C:C6	2.43	0.53
2:S0:200:ASP:HA	2:S0:203:PHE:CE1	2.71	0.53
34:SR:197:SER:HB2	34:SR:216:LYS:HB3	2.84	0.53
62:N6:37:LYS:H	62:N6:37:LYS:CE	2.25	0.53
39:L2:128:ARG:NH1	36:5:2177:G:OP2	198.48	0.53
43:L6:158:TYR:OH	50:M4:114:ASP:OD2	2.17	0.53
37:7:3:U:H2'	37:7:4:U:H6	1.72	0.53
9:S7:9:LEU:HD21	9:S7:17:GLU:HB3	2.67	0.53
36:1:516:A:O3'	44:L7:60:ARG:NH2	2.40	0.53
51:M5:16:SER:O	51:M5:20:ARG:HG2	2.09	0.53
1:2:924:A:O2'	1:2:987:G:OP1	2.27	0.53
36:5:1317:A:OP1	86:5:4097:OHX:N1	2.42	0.53
3:S1:131:ASP:HB3	3:S1:180:THR:HG23	1.91	0.53
38:4:85:G:O6	62:N6:112:ASP:HB3	2.09	0.53
62:N6:47:ALA:O	62:N6:122:LYS:NZ	2.42	0.53
28:D6:10:ARG:HB3	28:D6:34:LYS:HA	1.90	0.53
11:S9:162:SER:O	11:S9:165:GLY:N	4.00	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:S5:94:THR:HB	7:S5:114:ILE:HG13	1.91	0.53
7:S5:43:PHE:HB3	7:S5:46:TRP:HD1	5.92	0.53
9:S7:14:THR:OG1	9:S7:15:GLU:N	2.41	0.53
10:S8:8:ARG:HH21	10:S8:22:ARG:NH1	9.19	0.53
44:L7:73:GLY:O	57:N1:143:THR:HB	2.18	0.53
86:1:3943:OHX:N1	86:1:4200:OHX:N2	2.57	0.53
43:L6:47:PHE:CD1	43:L6:74:VAL:HG22	2.70	0.53
1:2:1235:C:C2	33:E1:138:ARG:NH2	2.77	0.53
2:S0:168:HIS:HB3	2:S0:203:PHE:CZ	2.64	0.53
1:2:839:U:C2'	1:2:840:U:H5'	2.39	0.53
52:M6:171:LYS:O	52:M6:175:THR:HG22	3.25	0.53
42:L5:226:TYR:HE2	42:L5:236:LEU:HD11	1.74	0.53
24:D2:37:PHE:CD2	24:D2:103:ILE:HD12	2.44	0.53
15:C3:37:ILE:HD13	15:C3:74:ILE:HD13	1.91	0.53
24:D2:41:MET:HG2	24:D2:129:VAL:HG21	2.63	0.53
1:6:1584:G:H22	1:6:1611:A:P	2.31	0.53
58:N2:22:PRO:HB2	58:N2:28:PHE:HB2	2.43	0.53
1:6:727:U:H2'	1:6:728:U:H6	1.73	0.53
41:L4:112:LYS:HG2	36:5:790:U:H4'	119.27	0.53
12:C0:16:PHE:HD2	12:C0:76:LEU:HD23	1.74	0.53
36:5:1237:G:H22	36:5:1251:A:H2	1.57	0.53
59:N3:129:VAL:O	59:N3:133:SER:OG	2.26	0.53
50:M4:92:GLU:OE2	50:M4:92:GLU:N	2.35	0.53
20:C8:42:TYR:HE2	20:C8:73:MET:HG3	3.73	0.52
19:C7:8:THR:HG21	1:6:1330:G:N2	420.55	0.52
42:L5:58:LYS:HD2	42:L5:93:THR:HG21	1.89	0.52
36:5:2397:A:C2	36:5:2873:U:H5'	2.44	0.52
42:L5:294:ALA:C	42:L5:296:GLN:H	2.10	0.52
11:S9:146:PHE:O	11:S9:147:MET:HB2	2.32	0.52
69:O3:59:VAL:HG23	69:O3:60:ARG:N	2.53	0.52
2:S0:147:THR:OG1	2:S0:159:ALA:HB1	2.09	0.52
34:SR:38:ARG:HA	34:SR:67:ILE:HG23	2.14	0.52
42:L5:261:THR:HG23	42:L5:264:GLN:NE2	2.23	0.52
57:N1:12:ARG:HD3	57:N1:13:TYR:CZ	2.55	0.52
2:S0:167:LYS:HG2	2:S0:168:HIS:CE1	2.44	0.52
36:5:1716:U:H5'	36:5:1716:U:C6	2.43	0.52
49:M3:124:ILE:HD11	49:M3:126:PHE:CZ	2.44	0.52
14:C2:55:GLY:HA2	14:C2:85:LYS:HE3	1.90	0.52
1:2:1258:U:H4'	12:C0:2:LEU:HD13	1.91	0.52
2:S0:175:TYR:HE1	2:S0:197:ILE:HG22	1.75	0.52
67:O1:13:THR:HG22	67:O1:72:ARG:CD	2.40	0.52
36:1:3294:A:H2'	36:1:3295:A:O4'	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
45:L8:71:VAL:HG22	45:L8:76:ALA:HB2	1.91	0.52
6:S4:187:ARG:NH2	1:6:753:A:H62	374.25	0.52
36:1:535:G:O6	86:1:4064:OHX:N3	2.41	0.52
55:M9:96:ILE:O	55:M9:100:ARG:HG3	2.09	0.52
36:1:926:A:H2'	36:1:927:C:C6	2.44	0.52
41:L4:290:ILE:HG23	54:M8:35:PHE:CE2	2.59	0.52
47:M0:202:LYS:HD3	37:7:64:A:N1	344.88	0.52
1:2:992:A:H2	1:2:1012:U:N3	2.01	0.52
1:2:959:U:H5'	29:D7:28:PRO:HB3	1.92	0.52
36:1:2097:U:H2'	36:1:2098:C:C6	2.44	0.52
22:D0:67:THR:HG21	31:D9:40:ARG:HB2	1.90	0.52
15:C3:23:PRO:O	15:C3:25:TRP:N	2.42	0.52
86:5:4011:OHX:N6	86:5:4198:OHX:N5	2.57	0.52
26:D4:35:VAL:O	26:D4:36:SER:HB3	2.09	0.52
59:N3:13:ILE:HG12	59:N3:53:SER:HB2	4.31	0.52
23:D1:71:ARG:HG3	23:D1:83:TRP:CZ2	2.64	0.52
61:N5:80:ASN:ND2	61:N5:126:LEU:HB2	2.24	0.52
36:5:1754:G:OP1	86:5:4076:OHX:N1	2.42	0.52
61:N5:92:LYS:HD2	36:5:1831:U:OP2	104.14	0.52
86:5:4094:OHX:N1	86:5:4234:OHX:N4	2.57	0.52
36:5:252:U:H4'	36:5:253:A:C5'	2.40	0.52
86:1:4208:OHX:N4	38:4:16:G:OP1	2.42	0.52
1:6:1133:A:H2'	1:6:1134:C:O4'	2.09	0.52
79:Q3:37:TYR:HB2	79:Q3:47:VAL:HB	1.91	0.52
1:2:108:A:H2'	1:2:109:G:C8	2.45	0.52
36:5:2112:U:H4'	36:5:2113:A:H5'	1.91	0.52
40:L3:129:ALA:O	36:5:3150:A:H5'	211.72	0.52
40:L3:331:ASN:OD1	40:L3:331:ASN:N	2.38	0.52
36:1:304:G:N3	36:1:304:G:H5'	2.24	0.52
1:6:946:U:H2'	1:6:947:U:C6	2.44	0.52
3:S1:173:THR:O	3:S1:177:GLN:NE2	2.42	0.52
62:N6:112:ASP:HB2	62:N6:115:ARG:H	1.75	0.52
36:1:830:A:H2'	36:1:831:G:O4'	2.09	0.52
42:L5:265:TYR:HE1	37:7:121:U:H5''	316.89	0.52
1:2:144:U:H5	8:S6:137:ARG:NH1	2.07	0.52
22:D0:105:GLN:HA	22:D0:108:ILE:HD13	7.47	0.52
38:8:77:A:H2'	38:8:78:G:O4'	2.10	0.52
69:O3:19:SER:HB3	36:5:1330:A:OP1	233.82	0.52
44:L7:24:GLU:O	44:L7:26:VAL:N	2.30	0.52
27:D5:61:SER:H	27:D5:64:VAL:HB	1.98	0.52
25:D3:50:LYS:HD3	25:D3:101:GLU:HG2	1.91	0.52
1:2:629:U:OP1	15:C3:127:ARG:NH2	2.42	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:5:1560:G:H2'	36:5:1561:G:C8	2.44	0.52
36:5:3027:A:H2'	36:5:3028:G:O4'	2.10	0.52
36:1:1688:U:H2'	36:1:1689:U:C6	2.45	0.52
52:M6:88:VAL:O	52:M6:90:HIS:N	2.43	0.52
36:5:2746:A:H2'	36:5:2747:A:O4'	2.10	0.52
1:2:767:U:H5	11:S9:142:ASN:OD1	1.91	0.52
36:5:629:U:H2'	36:5:630:A:C8	2.45	0.52
36:1:239:G:O6	86:1:4038:OHX:N3	2.42	0.52
36:1:3278:C:H2'	36:1:3278:C:O2	2.07	0.52
25:D3:37:ALA:O	25:D3:41:SER:HB3	3.40	0.52
70:O4:81:CYS:SG	70:O4:81:CYS:O	2.94	0.52
1:2:1588:G:OP1	86:2:2117:OHX:N3	2.42	0.52
36:1:3308:C:O2	53:M7:69:ARG:HD3	2.10	0.52
1:2:1102:G:OP2	25:D3:7:ARG:NH1	2.43	0.52
46:L9:8:GLN:NE2	46:L9:69:ARG:HG2	3.66	0.52
1:2:581:U:OP2	5:S3:143:ARG:NH1	2.42	0.52
7:S5:40:ILE:HG23	7:S5:42:LEU:HD22	1.92	0.52
8:S6:176:GLN:HG2	1:6:169:A:C5'	328.61	0.52
16:C4:122:PRO:O	16:C4:124:ASP:N	2.43	0.52
86:5:4011:OHX:N4	86:5:4198:OHX:N1	2.57	0.52
12:C0:49:LEU:HB3	12:C0:55:VAL:CG1	2.45	0.52
2:S0:140:ASN:HD22	4:S2:62:PRO:HD3	4.63	0.52
36:1:2697:A:H2'	36:1:2698:G:H8	1.74	0.52
86:1:4007:OHX:N6	86:1:4175:OHX:N5	2.56	0.52
40:L3:150:ARG:HG2	40:L3:150:ARG:HH11	2.38	0.52
1:2:482:U:H2'	1:2:483:A:C8	2.44	0.52
36:1:2401:A:O2'	41:L4:68:GLY:HA2	2.09	0.52
63:N7:5:LEU:HD23	63:N7:25:ILE:HD13	2.73	0.52
65:N9:16:ALA:O	65:N9:20:GLY:HA3	4.24	0.52
29:D7:61:THR:HG23	29:D7:62:ILE:O	2.08	0.52
51:M5:155:VAL:O	51:M5:162:ARG:NH2	2.38	0.52
8:S6:109:LEU:HD13	8:S6:111:LEU:HD21	1.90	0.52
36:1:2617:U:H5	36:1:2621:G:OP2	1.93	0.52
40:L3:315:GLY:HA2	36:5:3379:C:H4'	214.49	0.52
1:2:1492:A:HO2'	1:2:1493:A:H8	1.56	0.52
86:1:3955:OHX:N4	86:1:4041:OHX:N5	2.58	0.52
1:6:1572:G:H2'	1:6:1572:G:N3	2.24	0.52
6:S4:117:GLU:O	6:S4:119:ALA:N	2.95	0.52
29:D7:81:ARG:O	29:D7:82:LYS:HE3	3.82	0.52
36:5:3189:G:H2'	36:5:3190:C:O4'	2.09	0.52
1:6:653:C:H42	1:6:677:G:H1	1.56	0.52
36:5:112:U:O2'	36:5:113:C:OP2	2.27	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:M5:200:TRP:CE3	36:5:683:U:H5''	102.32	0.52
36:5:181:U:H1'	36:5:236:G:N2	2.25	0.52
78:Q2:17:CYS:SG	78:Q2:77:CYS:CB	3.13	0.52
1:2:1585:U:N3	1:2:1611:A:C2	2.69	0.52
36:1:2403:G:H22	36:1:2404:A:H62	1.57	0.52
41:L4:99:MET:CE	41:L4:102:PRO:HA	3.47	0.52
11:S9:96:VAL:HA	11:S9:99:LEU:HD22	1.92	0.52
36:1:2895:G:O2'	76:Q0:100:TYR:O	2.24	0.52
36:1:316:U:O2'	72:O6:30:LYS:HD2	2.08	0.52
34:SR:211:ILE:HG22	34:SR:223:TRP:CD1	2.42	0.52
48:M1:21:ILE:HG22	48:M1:23:VAL:HG22	1.91	0.52
14:C2:61:VAL:HA	14:C2:89:ILE:HG22	1.91	0.52
2:S0:118:PRO:HG2	2:S0:141:ILE:HD13	2.16	0.52
49:M3:64:LYS:HD3	49:M3:65:TYR:CE1	2.44	0.52
36:5:1307:G:C2	36:5:1308:A:C2	2.97	0.52
21:C9:117:SER:OG	21:C9:118:PRO:O	2.27	0.52
86:1:4036:OHX:N6	86:1:4048:OHX:N5	2.58	0.52
36:5:549:U:O4	86:5:4013:OHX:N4	2.43	0.52
36:1:3185:U:C6	52:M6:126:VAL:HG21	2.44	0.52
36:5:247:C:C2	36:5:248:U:H1'	2.44	0.52
36:1:2976:A:OP1	86:1:4123:OHX:N6	2.43	0.52
71:O5:44:ILE:O	71:O5:48:ARG:HG3	4.92	0.52
36:1:3275:U:H5''	69:O3:68:TRP:HZ2	1.74	0.52
34:SR:116:ASP:HB2	34:SR:117:LYS:HD2	1.92	0.52
36:5:2725:U:O4	86:5:3959:OHX:N1	2.42	0.52
36:1:2440:G:H1	36:1:2507:C:H42	1.58	0.52
36:5:1276:U:OP2	86:5:4007:OHX:N1	2.43	0.52
86:1:3964:OHX:N1	86:1:4143:OHX:N3	2.58	0.52
58:N2:33:TYR:CE2	58:N2:63:VAL:HG21	2.45	0.52
55:M9:154:ALA:O	55:M9:156:ASN:N	3.73	0.52
7:S5:188:LYS:HD2	7:S5:193:THR:HG22	4.45	0.52
31:D9:4:GLU:OE2	33:E1:145:HIS:NE2	6.08	0.52
36:1:929:A:H2'	36:1:930:U:C6	2.45	0.52
60:N4:52:THR:O	60:N4:56:ARG:HG3	2.10	0.52
41:L4:204:GLY:O	41:L4:246:ARG:NH1	2.52	0.52
36:5:2567:C:N4	36:5:2568:C:H41	2.08	0.52
1:2:1657:U:C2	86:2:2090:OHX:N1	2.78	0.52
86:2:2045:OHX:N2	86:2:2099:OHX:N5	2.58	0.52
36:5:621:A:H2'	36:5:622:A:C8	2.45	0.52
2:S0:56:LYS:HE2	2:S0:159:ALA:O	4.49	0.52
77:Q1:23:ARG:O	86:5:4001:OHX:N2	265.01	0.52
57:N1:32:LYS:NZ	57:N1:98:HIS:H	2.58	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:M5:91:GLU:O	51:M5:93:LYS:HE3	2.08	0.52
25:D3:100:ASP:O	25:D3:101:GLU:HB3	4.86	0.52
86:1:4036:OHX:N2	86:1:4048:OHX:N1	2.57	0.52
49:M3:73:ARG:NH2	36:5:77:A:N7	80.88	0.52
49:M3:87:ALA:O	49:M3:91:ARG:HG3	2.10	0.52
36:5:3227:A:C2'	36:5:3228:C:H5'	2.40	0.52
1:2:1672:G:H2'	1:2:1673:G:C8	2.44	0.52
36:5:2562:A:N6	36:5:2579:G:O2'	2.41	0.52
48:M1:40:LEU:HD23	48:M1:114:ILE:HD11	1.92	0.52
1:6:1071:U:H2'	1:6:1072:C:C6	2.44	0.52
1:2:692:C:H2'	1:2:693:U:O4'	2.10	0.52
1:6:1756:A:H8	1:6:1756:A:O5'	1.92	0.52
39:L2:241:ARG:HG2	36:5:2155:G:OP1	221.86	0.52
39:L2:83:HIS:CE1	39:L2:86:GLN:HB2	2.44	0.52
22:D0:36:ASN:HA	22:D0:39:SER:HB2	5.22	0.52
10:S8:105:ASP:O	10:S8:107:THR:N	2.38	0.52
23:D1:81:ASN:O	23:D1:82:VAL:HB	2.10	0.52
11:S9:27:GLU:OE1	11:S9:39:LYS:NZ	2.68	0.52
3:S1:29:TRP:CD1	3:S1:47:LEU:HG	2.44	0.52
66:O0:98:SER:OG	66:O0:99:ASP:N	2.43	0.52
36:5:3279:A:C2'	36:5:3280:U:H5'	2.40	0.52
14:C2:118:ALA:O	14:C2:120:VAL:N	2.43	0.52
45:L8:33:ASN:HA	36:5:2549:G:C2	211.93	0.52
26:D4:15:ASN:OD1	26:D4:17:LEU:HB2	4.66	0.52
23:D1:40:ASP:OD1	23:D1:44:ARG:HB2	2.23	0.52
36:5:437:G:H5''	36:5:438:A:OP2	2.09	0.52
86:5:4066:OHX:N1	86:5:4141:OHX:N2	2.58	0.52
1:6:485:A:C6	1:6:486:G:H1'	2.45	0.52
36:1:1845:G:O2'	73:O7:5:THR:HB	2.10	0.52
36:5:2875:U:H5	36:5:2945:G:O6	1.92	0.52
9:S7:58:LEU:HG	9:S7:88:ARG:HD2	1.91	0.52
36:1:3095:U:H2'	36:1:3096:C:C6	2.44	0.52
56:N0:42:TRP:O	56:N0:46:GLN:HG3	2.36	0.52
4:S2:88:LYS:HD3	4:S2:89:GLN:O	5.40	0.52
1:6:315:A:O2'	86:6:2160:OHX:N1	2.43	0.52
36:1:789:A:H2'	36:1:790:U:C6	2.45	0.52
29:D7:36:LYS:HB3	29:D7:42:ASN:O	3.10	0.52
40:L3:60:LEU:HD23	40:L3:67:PHE:HB3	1.92	0.52
32:E0:13:LYS:HB2	1:6:567:A:H4'	371.13	0.52
21:C9:86:ARG:HG3	21:C9:86:ARG:HH11	1.75	0.52
14:C2:103:LEU:HG	14:C2:116:VAL:HG13	4.34	0.52
36:1:662:U:H2'	36:1:663:C:C6	2.45	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
42:L5:120:LYS:NZ	42:L5:123:GLU:OE1	5.05	0.52
18:C6:82:ARG:HH12	18:C6:114:ARG:HB3	1.75	0.52
41:L4:144:LYS:HA	86:L4:404:OHX:N2	2.25	0.52
1:2:1488:G:H3'	1:2:1515:A:H61	1.74	0.52
46:L9:162:GLN:HG3	46:L9:163:GLN:N	2.79	0.52
1:2:1657:U:C4	86:2:2090:OHX:N4	2.78	0.52
6:S4:156:VAL:O	6:S4:157:ASN:HB2	2.10	0.52
1:2:192:U:O2'	1:2:193:U:O5'	2.27	0.52
1:6:193:U:C4	1:6:195:G:C8	2.98	0.52
61:N5:38:LEU:O	61:N5:39:LYS:HB2	4.61	0.52
36:1:121:A:C2	45:L8:129:PRO:HB3	2.45	0.52
1:6:488:G:N2	1:6:499:U:H3	2.07	0.52
3:S1:104:ASP:HA	3:S1:214:LYS:HE2	1.92	0.52
36:1:1540:U:OP1	86:1:4023:OHX:N1	2.42	0.52
36:1:2698:G:O2'	57:N1:12:ARG:HG3	2.10	0.52
55:M9:4:LEU:O	55:M9:7:GLN:HG2	5.01	0.52
1:2:840:U:O2'	1:2:841:U:H5"	2.09	0.52
44:L7:228:SER:HA	44:L7:232:ARG:NH2	2.86	0.52
9:S7:89:HIS:CD2	9:S7:165:LYS:HG2	4.27	0.52
86:5:4055:OHX:N3	86:5:4197:OHX:N4	2.57	0.52
29:D7:47:PHE:CE1	29:D7:49:HIS:HB2	2.47	0.52
5:S3:20:GLU:HG3	12:C0:61:TRP:CD2	2.45	0.52
73:O7:22:CYS:SG	73:O7:24:ARG:HB2	2.49	0.52
78:Q2:3:ASN:HB2	78:Q2:92:GLU:HG3	1.92	0.52
76:Q0:94:SER:HB2	76:Q0:122:ARG:O	2.09	0.52
28:D6:49:ALA:O	28:D6:53:LEU:N	2.42	0.52
65:N9:5:LYS:HE2	65:N9:8:THR:HB	2.25	0.52
36:1:2415:C:OP1	39:L2:2:GLY:HA2	2.10	0.52
8:S6:19:ASP:O	8:S6:20:ASP:HB2	2.10	0.52
11:S9:149:ARG:NE	1:6:765:G:N7	429.60	0.52
36:1:2528:G:N7	86:1:4186:OHX:N3	2.57	0.52
11:S9:83:VAL:HG23	11:S9:85:VAL:HG23	1.92	0.52
20:C8:6:GLN:O	27:D5:42:LEU:HD13	2.10	0.52
42:L5:113:LEU:HB3	42:L5:115:LEU:HD22	1.91	0.52
3:S1:62:LYS:O	3:S1:88:VAL:HB	2.32	0.52
36:5:2841:G:OP2	86:5:4136:OHX:N1	2.43	0.52
40:L3:238:LEU:HB3	40:L3:242:THR:HG21	2.15	0.52
37:3:3:U:H2'	37:3:4:U:C6	2.45	0.52
57:N1:127:GLN:HG3	36:5:1095:U:N3	261.66	0.52
4:S2:186:LYS:HD2	4:S2:189:GLN:OE1	4.51	0.52
43:L6:47:PHE:O	43:L6:50:LYS:HB2	2.20	0.52
44:L7:27:ALA:HA	44:L7:30:ARG:HB3	2.43	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:1507:G:N3	36:1:1507:G:H5'	2.24	0.52
20:C8:31:ALA:O	20:C8:34:THR:HG22	2.43	0.52
39:L2:13:GLY:HA2	39:L2:16:PHE:HB2	1.92	0.52
14:C2:40:GLY:HA3	14:C2:125:ASN:HB3	1.91	0.52
36:1:114:A:N1	36:1:266:A:O2'	2.39	0.52
73:O7:28:HIS:ND1	73:O7:31:LYS:HB2	2.25	0.52
40:L3:221:THR:HG22	40:L3:273:HIS:H	2.89	0.52
45:L8:67:ILE:CG2	45:L8:237:ILE:HD12	2.40	0.52
36:1:530:G:N7	86:1:3924:OHX:N6	2.58	0.52
21:C9:6:VAL:HG13	21:C9:66:TYR:CE1	2.45	0.52
36:1:3228:C:O2'	36:1:3229:G:OP2	2.26	0.52
1:6:248:U:OP1	86:6:2123:OHX:N3	2.43	0.52
1:6:425:A:H8	1:6:425:A:H5'	1.75	0.52
1:2:93:A:O2'	6:S4:4:GLY:HA3	2.10	0.52
36:5:1778:G:O2'	36:5:1780:G:OP2	2.26	0.52
37:7:77:G:N2	37:7:102:A:OP2	2.36	0.52
36:5:1414:G:O6	86:5:4145:OHX:N1	2.43	0.52
41:L4:148:ILE:HA	41:L4:149:PRO:C	2.40	0.52
1:2:1487:A:H2'	1:2:1488:G:C8	2.45	0.52
36:1:3206:C:O2	56:N0:155:ARG:NH1	2.43	0.52
36:5:3294:A:H2'	36:5:3295:A:O4'	2.10	0.52
55:M9:43:LYS:N	55:M9:43:LYS:HD2	4.68	0.52
22:D0:57:ARG:HG3	22:D0:89:ARG:CZ	2.40	0.52
63:N7:64:LYS:HD2	36:5:1812:G:O6	186.17	0.52
36:5:252:U:H4'	36:5:253:A:H5'	1.92	0.52
55:M9:154:ALA:O	55:M9:158:GLU:HG2	2.35	0.52
73:O7:31:LYS:O	73:O7:33:THR:HG22	2.10	0.52
6:S4:3:ARG:HB3	1:6:93:A:H1'	326.44	0.52
36:5:900:G:H1'	36:5:1589:A:N6	2.25	0.52
63:N7:27:LYS:HB3	63:N7:42:LEU:HB2	2.73	0.52
4:S2:179:VAL:O	4:S2:198:THR:OG1	2.33	0.52
62:N6:56:VAL:HG11	62:N6:104:LEU:HD13	1.91	0.52
7:S5:145:ASP:OD2	7:S5:146:THR:N	2.43	0.52
8:S6:78:THR:HG23	8:S6:92:ARG:HG2	1.92	0.52
1:6:166:C:OP2	86:6:2170:OHX:N4	2.43	0.52
73:O7:48:ASN:HA	73:O7:54:LYS:NZ	2.64	0.52
36:5:999:G:O2'	36:5:1000:C:H5'	2.09	0.52
19:C7:99:VAL:CB	19:C7:118:PRO:HB2	2.40	0.52
69:O3:23:ASN:OD1	69:O3:25:PRO:HD3	2.12	0.52
36:1:671:U:OP2	54:M8:57:ILE:HD12	2.10	0.52
1:2:1283:U:OP1	86:2:2115:OHX:N2	2.42	0.52
47:M0:76:MET:HE1	47:M0:138:VAL:HG11	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:D6:79:ILE:HA	28:D6:84:VAL:CB	2.37	0.51
27:D5:50:ILE:HG22	27:D5:51:LEU:HD12	1.91	0.51
1:2:1774:G:N7	77:Q1:4:LYS:NZ	2.58	0.51
3:S1:126:THR:CG2	3:S1:136:ARG:HE	2.40	0.51
9:S7:131:PHE:HB3	9:S7:132:PRO:CD	2.41	0.51
36:1:1765:U:H4'	36:1:1765:U:OP1	2.10	0.51
75:O9:15:LYS:O	75:O9:19:GLN:HG2	3.85	0.51
54:M8:96:PHE:CG	54:M8:97:PRO:HD2	2.63	0.51
23:D1:40:ASP:OD2	23:D1:44:ARG:NH2	2.43	0.51
40:L3:92:TYR:HB2	40:L3:157:VAL:HG22	1.92	0.51
36:1:2544:U:H2'	36:1:2545:C:C6	2.45	0.51
1:2:730:G:H21	1:2:731:C:H5'	1.75	0.51
36:1:1478:C:H2'	36:1:1479:U:C6	2.44	0.51
42:L5:226:TYR:CE1	42:L5:236:LEU:HD11	4.93	0.51
43:L6:176:PHE:HA	50:M4:114:ASP:HB2	2.82	0.51
11:S9:149:ARG:HH11	11:S9:149:ARG:HG2	4.59	0.51
1:6:595:G:H2'	1:6:596:C:C6	2.45	0.51
72:O6:33:ALA:O	72:O6:34:SER:HB3	2.16	0.51
40:L3:256:HIS:HA	40:L3:257:PRO:C	2.39	0.51
1:6:794:U:H4'	1:6:795:U:OP2	2.10	0.51
36:5:2927:C:H2'	36:5:2928:C:C6	2.45	0.51
1:6:1064:G:H2'	1:6:1065:A:C8	2.46	0.51
6:S4:10:LYS:HD3	1:6:381:C:OP1	359.23	0.51
67:O1:17:HIS:HB2	67:O1:69:TYR:HB3	1.92	0.51
7:S5:166:ARG:NH2	1:6:1163:A:O3'	347.96	0.51
5:S3:183:GLY:O	5:S3:184:ILE:HD13	3.20	0.51
1:2:416:A:H5'	1:2:417:A:N7	2.25	0.51
21:C9:7:ARG:HD2	1:6:1366:U:O2'	425.51	0.51
79:Q3:13:LYS:HE3	79:Q3:14:TYR:CZ	2.45	0.51
46:L9:37:ASN:OD1	46:L9:39:LYS:HB2	2.29	0.51
8:S6:154:ARG:HD3	1:6:78:A:C8	340.73	0.51
48:M1:137:ARG:HD3	37:7:28:C:OP1	304.17	0.51
48:M1:82:ARG:HG2	48:M1:112:LEU:HB2	1.91	0.51
6:S4:192:ILE:HG13	6:S4:243:GLY:HA3	2.54	0.51
36:1:715:A:H5''	64:N8:114:GLY:O	2.10	0.51
1:2:1248:C:H2'	1:2:1249:U:C6	2.44	0.51
39:L2:243:THR:OG1	36:5:2244:A:H5''	228.66	0.51
36:1:2355:G:H4'	53:M7:139:TYR:CE2	2.45	0.51
86:5:4066:OHX:N3	86:5:4141:OHX:N4	2.57	0.51
17:C5:15:HIS:O	17:C5:21:ASP:HA	2.09	0.51
61:N5:132:ALA:O	61:N5:135:ILE:HG22	2.11	0.51
39:L2:227:ARG:HG2	39:L2:239:ALA:HB2	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:C5:122:THR:CG2	1:6:1558:U:H3	367.71	0.51
11:S9:91:LYS:O	11:S9:92:LYS:HG2	2.10	0.51
36:5:726:G:H8	36:5:726:G:C5'	2.22	0.51
79:Q3:27:LYS:O	79:Q3:31:ILE:HG13	3.54	0.51
36:1:2118:C:H2'	36:1:2119:A:O4'	2.10	0.51
12:C0:24:LYS:HB2	12:C0:63:TYR:CE1	2.82	0.51
4:S2:40:LYS:HG3	4:S2:247:ALA:HB1	4.80	0.51
36:1:428:A:H2'	36:1:429:U:C6	2.45	0.51
36:1:1348:U:O2	36:1:1349:G:N2	2.43	0.51
1:6:558:U:H2'	1:6:558:U:O2	2.10	0.51
51:M5:135:VAL:HG13	51:M5:142:ILE:HG12	2.08	0.51
1:2:702:G:C6	1:2:737:A:N6	2.79	0.51
41:L4:145:ILE:O	41:L4:145:ILE:HG12	2.96	0.51
2:S0:41:ARG:HD2	2:S0:42:PRO:O	2.11	0.51
66:O0:17:VAL:HG11	66:O0:92:ILE:HD12	1.92	0.51
36:1:409:A:OP2	86:1:4060:OHX:N5	2.43	0.51
39:L2:224:THR:HG21	36:5:2201:G:N2	223.32	0.51
1:6:1227:A:H4'	1:6:1228:G:H5'	1.92	0.51
2:S0:136:ALA:HB1	2:S0:141:ILE:HB	1.92	0.51
26:D4:124:ARG:O	26:D4:127:LYS:HG3	2.10	0.51
52:M6:65:ASN:O	52:M6:68:ARG:HG2	2.10	0.51
5:S3:170:THR:HG22	5:S3:187:LYS:HA	2.84	0.51
1:2:584:C:H1'	32:E0:18:THR:HG21	1.91	0.51
86:1:3976:OHX:N6	86:1:4159:OHX:N2	2.58	0.51
12:C0:16:PHE:O	12:C0:88:PRO:HA	2.11	0.51
77:Q1:21:ARG:HD2	1:6:1654:G:OP1	282.85	0.51
36:1:3279:A:N6	36:1:3280:U:O4	2.43	0.51
8:S6:142:ARG:O	8:S6:146:GLY:N	2.43	0.51
41:L4:154:THR:O	41:L4:157:GLU:HG3	2.09	0.51
36:5:2425:G:H2'	36:5:2426:U:O4'	2.11	0.51
5:S3:107:PHE:O	5:S3:111:ASN:HB2	2.13	0.51
36:1:781:G:OP1	54:M8:151:ARG:HD2	2.11	0.51
42:L5:33:ARG:HD2	37:7:7:G:OP1	271.84	0.51
36:5:2530:G:H2'	36:5:2531:C:H5'	1.92	0.51
36:5:1232:C:C5	36:5:1261:G:H2'	2.45	0.51
86:5:3978:OHX:N6	86:5:4196:OHX:N5	2.59	0.51
21:C9:57:ARG:HH21	21:C9:80:TYR:HB3	1.73	0.51
86:5:3924:OHX:N5	38:8:17:A:OP1	2.43	0.51
1:2:647:G:H22	1:2:687:G:N2	2.07	0.51
37:3:22:A:H1'	42:L5:272:TYR:CZ	2.45	0.51
73:O7:14:LYS:HE2	75:O9:51:ILE:HG13	1.93	0.51
33:E1:121:CYS:HB3	33:E1:130:VAL:HG11	4.99	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
86:3:218:OHX:N2	86:3:223:OHX:N1	2.58	0.51
21:C9:100:ILE:O	21:C9:104:VAL:HG23	2.40	0.51
46:L9:84:LYS:CE	46:L9:191:LEU:HD13	2.41	0.51
42:L5:152:ARG:NH1	42:L5:152:ARG:HG3	2.43	0.51
36:1:1580:A:H4'	36:1:1581:C:O5'	2.11	0.51
86:1:4032:OHX:N4	86:1:4149:OHX:N3	2.57	0.51
46:L9:44:THR:HG22	36:5:3186:A:N3	326.77	0.51
36:1:2656:A:H4'	78:Q2:98:LYS:HD2	1.92	0.51
11:S9:37:LYS:HE2	1:6:594:A:OP2	413.65	0.51
72:O6:33:ALA:HB1	72:O6:38:LYS:HD2	4.20	0.51
36:1:520:U:O4	41:L4:349:THR:HG23	2.11	0.51
2:S0:101:ARG:NH2	1:6:1321:A:OP2	401.85	0.51
16:C4:131:GLY:O	16:C4:133:ARG:N	3.08	0.51
41:L4:118:LYS:O	41:L4:122:THR:HG23	2.10	0.51
10:S8:136:SER:HB3	10:S8:139:ALA:HB3	1.92	0.51
36:5:1667:A:H2'	36:5:1668:G:C8	2.45	0.51
36:5:742:G:N7	86:5:4003:OHX:N4	2.58	0.51
36:1:3041:U:OP1	59:N3:12:ARG:NH1	2.36	0.51
24:D2:36:LYS:O	24:D2:40:VAL:HG23	2.10	0.51
34:SR:276:PRO:HB2	34:SR:278:PHE:CE1	4.10	0.51
34:SR:198:ASN:O	34:SR:215:GLY:HA3	2.21	0.51
42:L5:107:ARG:HH21	42:L5:110:LEU:HD23	1.76	0.51
86:1:4084:OHX:N6	86:1:4153:OHX:N5	2.58	0.51
28:D6:38:ARG:HH21	28:D6:83:ILE:HG13	1.76	0.51
66:O0:99:ASP:N	66:O0:99:ASP:OD2	2.81	0.51
7:S5:43:PHE:HB3	7:S5:46:TRP:CD1	5.44	0.51
7:S5:184:PHE:CE2	1:6:1471:A:H5'	341.85	0.51
64:N8:115:LYS:HG3	36:5:715:A:C8	149.04	0.51
36:5:1328:C:H2'	36:5:1329:U:C6	2.45	0.51
65:N9:21:ILE:HG22	65:N9:22:LYS:N	3.46	0.51
1:2:1766:A:H5''	86:2:2093:OHX:N6	2.26	0.51
6:S4:3:ARG:NH1	1:6:93:A:O4'	326.24	0.51
36:5:1196:C:OP1	86:5:4235:OHX:N6	2.44	0.51
54:M8:76:ALA:HA	54:M8:79:LYS:HD2	4.27	0.51
25:D3:108:GLY:HA2	1:6:600:U:OP2	358.16	0.51
6:S4:240:LYS:HE2	6:S4:240:LYS:H	1.75	0.51
50:M4:47:ASP:CG	50:M4:55:ARG:HB2	2.92	0.51
40:L3:2:SER:O	36:5:2939:G:OP2	246.72	0.51
26:D4:29:HIS:CE1	26:D4:34:ASN:H	2.29	0.51
36:1:863:C:H2'	36:1:864:G:O4'	2.09	0.51
7:S5:162:VAL:HG22	7:S5:167:ARG:HG2	2.65	0.51
4:S2:178:ILE:HB	4:S2:185:LYS:HG2	3.53	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:8:78:G:H2'	38:8:79:A:O4'	2.09	0.51
12:C0:15:LEU:HD13	12:C0:21:VAL:HG23	1.93	0.51
12:C0:46:LEU:HA	12:C0:49:LEU:HB2	2.30	0.51
40:L3:323:MET:HE2	40:L3:356:LEU:HD11	3.87	0.51
36:5:998:A:O2'	36:5:999:G:H5'	2.11	0.51
36:5:2428:U:O4	86:5:4214:OHX:N5	2.43	0.51
36:1:112:U:O2'	36:1:113:C:OP2	2.26	0.51
71:O5:115:LYS:HB2	71:O5:115:LYS:NZ	2.26	0.51
36:1:191:U:H2'	36:1:192:C:C6	2.45	0.51
1:2:1274:C:C5	35:SM:96:ARG:HG3	2.45	0.51
3:S1:180:THR:HG22	3:S1:181:LEU:H	1.75	0.51
3:S1:183:GLN:O	3:S1:187:LYS:N	2.44	0.51
49:M3:166:ALA:N	64:N8:135:GLU:OE1	2.20	0.51
20:C8:140:THR:HA	20:C8:143:ARG:HH11	2.36	0.51
40:L3:232:ARG:HG2	40:L3:233:TRP:CD1	2.46	0.51
36:1:3112:G:O2'	46:L9:70:THR:HB	2.11	0.51
1:6:197:A:H2'	1:6:198:A:C8	2.46	0.51
26:D4:121:THR:CG2	26:D4:123:LYS:HB2	7.47	0.51
26:D4:112:LYS:O	26:D4:116:LYS:HG3	2.11	0.51
63:N7:23:VAL:HB	63:N7:43:VAL:HB	1.92	0.51
36:5:2799:A:H5''	36:5:2800:G:O5'	2.10	0.51
9:S7:58:LEU:N	9:S7:89:HIS:O	2.40	0.51
61:N5:105:VAL:HG13	61:N5:130:TYR:CG	4.69	0.51
36:5:2683:U:H2'	36:5:2684:C:H6	1.76	0.51
36:5:549:U:H2'	36:5:550:A:C8	2.45	0.51
36:1:904:A:OP2	73:O7:30:GLN:NE2	2.38	0.51
38:8:59:A:H5''	38:8:61:A:C8	2.45	0.51
33:E1:117:LEU:HB3	33:E1:118:ARG:HH11	1.74	0.51
36:5:806:A:H5''	36:5:936:A:H61	1.75	0.51
44:L7:92:ILE:HG13	54:M8:4:ASP:HB2	1.91	0.51
37:3:79:A:C2	37:3:102:A:C4	2.99	0.51
1:6:1268:G:H1'	1:6:1448:G:H5''	1.93	0.51
11:S9:89:ASP:HB2	11:S9:90:LYS:HD3	1.93	0.51
1:2:505:A:N3	1:2:505:A:H2'	2.24	0.51
1:2:16:G:H2'	1:2:17:C:C6	2.45	0.51
17:C5:19:GLY:N	20:C8:93:THR:O	2.44	0.51
86:5:3978:OHX:N4	86:5:4196:OHX:N3	2.59	0.51
27:D5:38:HIS:ND1	27:D5:70:LYS:HG2	6.60	0.51
42:L5:106:ALA:O	42:L5:110:LEU:HB2	2.11	0.51
14:C2:72:ILE:O	14:C2:76:GLU:HB2	2.37	0.51
13:C1:33:ARG:NH1	13:C1:53:TYR:O	3.33	0.51
16:C4:17:ALA:HB3	16:C4:81:VAL:HA	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
49:M3:59:ARG:HD3	36:5:73:C:C2	93.44	0.51
1:6:699:U:O4	86:6:2074:OHX:N1	2.43	0.51
36:1:1555:U:H5	36:1:1559:A:H61	1.58	0.51
1:2:1528:U:OP1	7:S5:109:LYS:HG2	2.11	0.51
45:L8:91:PHE:O	45:L8:95:ASN:HB2	2.11	0.51
74:O8:39:ARG:HH12	74:O8:63:LYS:HE2	9.35	0.51
34:SR:42:LEU:HB2	34:SR:61:PHE:HB2	1.93	0.51
62:N6:83:ASP:O	62:N6:84:LYS:HB2	2.36	0.51
36:5:2427:U:H2'	36:5:2428:U:C6	2.46	0.51
1:2:1590:G:OP1	21:C9:91:TYR:HB2	2.11	0.51
58:N2:89:LEU:HB3	58:N2:93:ILE:HD12	2.78	0.51
64:N8:90:TYR:CG	64:N8:100:PRO:HG3	2.46	0.51
63:N7:111:LYS:HE2	36:5:1629:U:O4	206.22	0.51
41:L4:217:LYS:HE2	36:5:210:U:O2	68.08	0.51
39:L2:116:VAL:HG23	39:L2:117:GLU:O	2.70	0.51
57:N1:56:PHE:CZ	57:N1:78:LYS:HD3	2.45	0.51
12:C0:11:ILE:HD12	12:C0:42:VAL:HA	1.91	0.51
18:C6:78:VAL:O	18:C6:81:ILE:HG12	2.41	0.51
36:1:551:A:O2'	36:1:552:G:O5'	2.28	0.51
1:6:846:G:H2'	1:6:847:A:C8	2.45	0.51
1:2:1180:C:O2'	17:C5:128:HIS:ND1	2.42	0.51
67:O1:75:ILE:HG12	67:O1:93:VAL:HG13	2.70	0.51
55:M9:28:GLU:O	55:M9:32:ILE:HG13	2.11	0.51
50:M4:47:ASP:OD1	50:M4:55:ARG:HB2	2.58	0.51
50:M4:49:PRO:HG3	50:M4:78:THR:HG23	3.41	0.51
36:1:2208:A:N1	86:1:4047:OHX:N4	2.59	0.51
19:C7:44:LYS:HG3	19:C7:47:ARG:HH12	2.83	0.51
11:S9:39:LYS:HB3	11:S9:43:TYR:CZ	2.58	0.51
1:6:648:G:C2	1:6:687:G:C2	2.98	0.51
71:O5:86:ARG:O	71:O5:90:ARG:HG2	2.23	0.51
53:M7:138:LYS:NZ	36:5:2356:A:OP1	147.40	0.51
47:M0:206:LEU:O	47:M0:210:ILE:HG13	2.11	0.51
86:5:4054:OHX:N3	86:5:4108:OHX:N5	2.59	0.51
48:M1:59:ILE:HD12	48:M1:65:ILE:HD11	2.17	0.51
12:C0:14:TYR:HE2	12:C0:21:VAL:HG22	1.76	0.51
22:D0:100:VAL:O	22:D0:104:THR:HG23	2.34	0.51
55:M9:23:TRP:HB2	55:M9:53:LYS:HD2	1.93	0.51
6:S4:185:GLY:H	6:S4:189:LEU:HD13	1.76	0.51
86:5:4094:OHX:N1	86:5:4234:OHX:N2	2.59	0.51
1:6:1350:U:H2'	1:6:1351:G:H8	1.74	0.51
36:1:2333:C:H2'	36:1:2334:U:O4'	2.11	0.51
1:2:1662:G:O2'	1:2:1663:G:H5'	2.11	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
44:L7:89:ILE:HG13	44:L7:214:TRP:CH2	2.46	0.51
1:2:611:U:OP1	25:D3:19:ARG:NH2	2.44	0.51
52:M6:143:THR:OG1	52:M6:150:GLU:OE2	2.73	0.51
62:N6:79:ALA:HB1	62:N6:98:ASN:HB3	1.92	0.51
36:5:3341:U:H5''	36:5:3342:A:OP2	2.10	0.51
66:O0:61:MET:HG3	66:O0:62:LEU:N	2.47	0.51
1:2:114:C:H5'	1:2:114:C:H6	1.76	0.51
9:S7:30:SER:O	9:S7:34:LEU:HB2	2.11	0.51
28:D6:19:LYS:NZ	1:6:944:A:OP2	295.69	0.51
40:L3:244:ARG:NH1	40:L3:244:ARG:HG2	2.26	0.51
1:6:291:G:H2'	1:6:292:U:C6	2.46	0.51
6:S4:36:HIS:ND1	6:S4:85:GLY:HA3	2.26	0.51
1:6:1482:C:OP2	1:6:1521:G:N1	2.42	0.51
52:M6:110:PRO:HA	52:M6:113:ASP:OD2	2.10	0.51
25:D3:70:LYS:HB3	25:D3:93:LEU:HD22	2.35	0.51
33:E1:130:VAL:HG11	33:E1:143:LYS:HG2	1.92	0.51
66:O0:13:LYS:HE3	66:O0:103:THR:HG21	2.12	0.51
36:5:2418:G:O6	86:5:4247:OHX:N2	2.44	0.51
41:L4:140:HIS:HA	41:L4:177:ASP:OD1	2.11	0.51
44:L7:110:ARG:NH2	54:M8:3:ILE:HD12	2.43	0.51
22:D0:105:GLN:HG3	22:D0:106:ILE:N	2.26	0.51
42:L5:64:ILE:HD12	42:L5:144:VAL:HG21	4.43	0.51
1:2:793:A:H5''	1:2:794:U:C6	2.46	0.51
36:5:135:C:H4'	36:5:136:G:OP2	2.10	0.51
36:5:3318:G:OP2	86:5:4138:OHX:N5	2.44	0.51
17:C5:33:PHE:O	17:C5:36:LEU:HD22	5.11	0.51
40:L3:313:HIS:O	40:L3:333:LYS:HE3	3.26	0.51
1:6:336:G:OP2	86:6:2155:OHX:N4	2.44	0.51
22:D0:46:GLU:CD	22:D0:52:LYS:HE2	2.32	0.51
36:1:2366:C:H5'	40:L3:259:HIS:NE2	2.26	0.51
39:L2:40:TYR:O	36:5:2550:U:H5	212.34	0.51
26:D4:50:ALA:HB1	26:D4:54:ALA:HB3	3.57	0.51
7:S5:29:ILE:HG21	18:C6:57:LEU:HD11	1.92	0.51
36:5:815:G:C6	36:5:906:A:C4	2.99	0.51
36:1:2636:A:H5''	36:1:2637:A:H5'	1.93	0.51
13:C1:22:ASN:ND2	13:C1:25:VAL:HG23	2.26	0.51
36:1:522:A:OP1	86:1:3948:OHX:N5	2.43	0.51
19:C7:37:GLU:HG3	34:SR:150:TRP:HE1	1.75	0.51
36:5:2239:G:N7	86:5:4190:OHX:N5	2.58	0.51
52:M6:18:ARG:NH2	36:5:1318:A:OP1	276.86	0.51
36:5:2935:U:H2'	36:5:2935:U:O2	2.11	0.51
36:1:3217:C:H2'	36:1:3217:C:O2	2.11	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:5:2195:C:OP2	86:5:4204:OHX:N4	2.44	0.51
36:1:1482:A:H4'	36:1:1483:G:OP2	2.10	0.51
6:S4:132:GLY:N	6:S4:136:VAL:O	2.81	0.51
3:S1:175:GLU:HG2	3:S1:193:ILE:CD1	4.29	0.50
1:2:734:A:H4'	1:2:735:C:H5'	1.93	0.50
63:N7:46:ILE:HD11	63:N7:48:ARG:C	2.30	0.50
63:N7:21:LYS:HE3	63:N7:47:GLU:O	2.10	0.50
1:2:1291:G:N2	1:2:1324:G:N2	2.59	0.50
28:D6:34:LYS:O	28:D6:35:ALA:HB3	4.45	0.50
49:M3:109:PHE:O	49:M3:113:VAL:HG23	2.10	0.50
18:C6:37:THR:O	18:C6:45:ARG:NH1	3.13	0.50
78:Q2:71:ARG:CG	78:Q2:71:ARG:HH11	2.72	0.50
35:SM:84:LYS:HG2	35:SM:86:ASN:H	1.76	0.50
1:2:711:U:H1'	1:2:712:G:C8	2.46	0.50
34:SR:70:ASP:OD1	34:SR:71:CYS:N	2.44	0.50
1:6:1081:A:H1'	1:6:1082:C:C5	2.46	0.50
36:1:3330:A:H5''	36:1:3330:A:H8	1.76	0.50
22:D0:80:GLU:HG3	31:D9:54:LYS:NZ	2.26	0.50
24:D2:104:LEU:HB2	24:D2:124:LYS:O	2.11	0.50
36:1:3269:U:H4'	36:1:3270:U:O5'	2.12	0.50
2:S0:184:LEU:O	2:S0:186:GLY:N	2.77	0.50
7:S5:129:PRO:O	7:S5:132:VAL:HB	2.56	0.50
51:M5:14:LYS:HE2	36:5:269:G:H5''	133.13	0.50
51:M5:14:LYS:HA	51:M5:19:LEU:HD23	2.20	0.50
36:1:900:G:H1'	36:1:1589:A:H61	1.76	0.50
36:5:1157:G:H2'	36:5:1158:A:O4'	2.11	0.50
1:2:796:A:OP2	86:2:2058:OHX:N6	2.44	0.50
36:5:3316:A:O2'	86:5:4249:OHX:N3	2.45	0.50
48:M1:8:PRO:CD	48:M1:9:MET:H	2.63	0.50
46:L9:143:GLU:O	46:L9:144:ILE:HG22	4.79	0.50
20:C8:54:LEU:H	20:C8:54:LEU:HD22	1.77	0.50
79:Q3:2:ALA:HB2	36:5:853:G:N7	251.15	0.50
20:C8:86:LEU:HG	20:C8:99:HIS:HB2	2.03	0.50
36:5:94:G:H2'	36:5:95:A:C8	2.46	0.50
53:M7:79:THR:HG22	53:M7:80:LYS:HG3	6.14	0.50
1:2:702:G:O6	1:2:737:A:N6	2.44	0.50
61:N5:115:ARG:NH1	61:N5:119:THR:OG1	2.44	0.50
28:D6:70:LYS:HE3	1:6:931:C:OP1	319.28	0.50
28:D6:10:ARG:NH1	28:D6:36:ILE:HA	2.27	0.50
57:N1:71:SER:HB3	57:N1:91:LEU:O	2.10	0.50
46:L9:163:GLN:HA	46:L9:166:ARG:HD2	1.93	0.50
75:O9:50:ASN:O	75:O9:51:ILE:HB	2.27	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:670:C:P	54:M8:147:ARG:NH2	2.84	0.50
4:S2:90:THR:HG23	4:S2:92:ALA:H	1.76	0.50
1:2:337:G:H3'	13:C1:133:LYS:HB2	1.93	0.50
56:N0:155:ARG:HD3	56:N0:172:TYR:CD2	2.46	0.50
26:D4:57:VAL:HB	26:D4:60:PHE:HE2	3.99	0.50
36:1:2443:A:N6	36:1:2504:U:C4	2.79	0.50
57:N1:12:ARG:HD3	57:N1:13:TYR:CE1	2.68	0.50
1:6:1657:U:HO2'	1:6:1658:G:P	2.29	0.50
36:1:1812:G:O2'	36:1:1818:U:H4'	2.11	0.50
86:1:3964:OHX:N5	86:1:4143:OHX:N6	2.59	0.50
77:Q1:16:LYS:NZ	1:6:1750:A:OP1	288.15	0.50
1:2:652:G:H1	1:2:682:C:H42	1.58	0.50
40:L3:46:PHE:CE2	40:L3:205:VAL:HG13	3.05	0.50
63:N7:36:HIS:CD2	63:N7:74:VAL:HG11	2.71	0.50
38:8:145:U:H2'	38:8:146:U:C6	2.46	0.50
55:M9:130:ASN:C	55:M9:132:PHE:H	2.13	0.50
86:1:3968:OHX:N3	86:1:4076:OHX:N4	2.58	0.50
68:O2:55:ILE:HB	36:5:947:G:H5'	187.40	0.50
4:S2:97:ARG:HB2	4:S2:118:ALA:O	2.17	0.50
50:M4:128:ARG:HG2	50:M4:132:LYS:HG3	1.94	0.50
3:S1:38:PHE:CD1	3:S1:73:LEU:HG	3.45	0.50
46:L9:109:ALA:O	46:L9:110:LYS:HB2	2.23	0.50
1:2:538:A:H8	1:2:543:C:N4	2.09	0.50
36:1:2396:G:OP1	36:1:2397:A:H4'	2.11	0.50
14:C2:66:VAL:HG11	14:C2:72:ILE:HG13	4.10	0.50
41:L4:271:LYS:HB2	41:L4:274:TYR:CB	2.60	0.50
12:C0:34:GLU:O	12:C0:35:ILE:HB	4.61	0.50
79:Q3:74:ALA:O	79:Q3:78:THR:HG22	2.54	0.50
40:L3:76:VAL:HG11	40:L3:323:MET:HE3	2.27	0.50
61:N5:105:VAL:HG13	61:N5:130:TYR:CD2	4.82	0.50
36:5:1232:C:H2'	36:5:1233:G:H8	1.76	0.50
86:5:4000:OHX:N2	86:5:4190:OHX:N1	2.60	0.50
19:C7:26:LEU:HD23	19:C7:58:MET:HB3	3.50	0.50
39:L2:69:TYR:OH	36:5:2557:A:OP1	192.05	0.50
40:L3:366:GLY:O	40:L3:368:GLY:N	2.87	0.50
36:1:2747:A:H5'	42:L5:175:HIS:HA	1.93	0.50
1:2:1031:U:H4'	1:2:1032:G:OP2	2.10	0.50
41:L4:286:VAL:HG11	54:M8:31:LYS:HD2	4.92	0.50
33:E1:98:VAL:HG22	33:E1:99:LYS:H	1.76	0.50
36:1:170:G:C4	36:1:250:U:O2	2.65	0.50
16:C4:20:TYR:HB3	16:C4:27:PHE:HB2	2.05	0.50
53:M7:182:ILE:HG22	53:M7:183:ALA:N	2.25	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
54:M8:178:ARG:HD2	64:N8:50:PRO:HB2	3.94	0.50
36:1:1567:U:H5	36:1:1568:U:C2	2.28	0.50
23:D1:1:MET:HG3	23:D1:10:GLU:HB3	1.93	0.50
1:6:577:G:N1	86:6:2159:OHX:N4	2.60	0.50
20:C8:42:TYR:HA	20:C8:85:PHE:HE1	1.76	0.50
36:5:1654:A:C2'	36:5:1655:G:H5''	2.37	0.50
36:5:2180:G:H2'	36:5:2181:C:C6	2.46	0.50
36:1:2896:A:H5'	36:1:2896:A:H8	1.76	0.50
20:C8:138:THR:OG1	1:6:1459:C:OP2	350.73	0.50
7:S5:43:PHE:H	7:S5:46:TRP:H	2.44	0.50
49:M3:76:THR:HG23	49:M3:101:ARG:NH1	2.41	0.50
3:S1:97:LEU:HB3	3:S1:232:HIS:CD2	4.32	0.50
18:C6:58:ASP:C	18:C6:60:PHE:H	2.15	0.50
49:M3:94:GLY:HA3	71:O5:116:TYR:OH	2.10	0.50
74:O8:4:GLU:HG2	74:O8:5:ILE:N	2.25	0.50
36:5:622:A:H2'	36:5:623:U:O4'	2.11	0.50
7:S5:161:ASP:O	30:D8:44:VAL:HA	2.11	0.50
1:2:260:U:O2'	1:2:261:U:OP1	2.29	0.50
10:S8:182:TYR:OH	10:S8:188:GLU:OE1	2.15	0.50
48:M1:16:LYS:HG2	48:M1:130:VAL:HG13	1.93	0.50
36:1:2177:G:OP2	39:L2:128:ARG:HD3	2.12	0.50
13:C1:57:LYS:NZ	1:6:326:G:OP1	290.54	0.50
64:N8:47:LYS:HE3	64:N8:48:TYR:CZ	4.62	0.50
45:L8:116:VAL:O	45:L8:118:GLU:N	2.59	0.50
36:1:3374:U:OP1	67:O1:17:HIS:ND1	2.38	0.50
19:C7:17:ILE:HG23	19:C7:58:MET:HE1	1.94	0.50
10:S8:2:GLY:HA2	1:6:1729:C:O2'	287.30	0.50
8:S6:214:LYS:HB3	8:S6:218:GLU:OE1	6.09	0.50
57:N1:14:MET:HE2	57:N1:15:PHE:CE2	2.46	0.50
34:SR:113:VAL:O	34:SR:155:ARG:NH1	2.44	0.50
69:O3:88:ASN:HB2	36:5:429:U:H4'	215.51	0.50
1:2:1226:A:O2'	1:2:1227:A:OP1	2.26	0.50
86:2:2076:OHX:N6	86:2:2163:OHX:N2	2.59	0.50
25:D3:132:LEU:O	25:D3:135:LEU:N	2.44	0.50
11:S9:119:ALA:O	11:S9:124:HIS:ND1	4.47	0.50
49:M3:191:ALA:O	49:M3:194:GLU:HB2	7.88	0.50
36:5:1470:U:H2'	36:5:1471:U:C6	2.46	0.50
36:1:2371:G:O6	86:1:3875:OHX:N3	2.44	0.50
50:M4:17:VAL:HG12	50:M4:72:LEU:HB3	1.92	0.50
13:C1:73:GLY:HA3	13:C1:86:ILE:HG23	5.32	0.50
1:2:1039:A:H5''	23:D1:62:ARG:NH2	2.25	0.50
36:1:2233:A:OP2	86:1:4047:OHX:N5	2.44	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:1698:G:O2'	1:6:1699:G:O5'	2.27	0.50
39:L2:217:GLN:O	39:L2:218:HIS:HB3	2.12	0.50
10:S8:36:THR:HG23	10:S8:96:LEU:O	2.11	0.50
16:C4:37:GLU:HA	1:6:895:G:O2'	259.36	0.50
46:L9:109:ALA:HB1	46:L9:111:PHE:CD2	2.47	0.50
42:L5:41:LYS:HB2	57:N1:68:THR:O	2.45	0.50
10:S8:196:LEU:HD22	10:S8:200:LYS:HD3	7.08	0.50
9:S7:71:HIS:CG	9:S7:131:PHE:HZ	2.29	0.50
86:5:4011:OHX:N3	86:5:4198:OHX:N1	2.59	0.50
1:2:709:C:C4	1:2:710:U:H1'	2.46	0.50
1:2:105:A:OP1	10:S8:18:ARG:NH1	2.44	0.50
53:M7:60:PHE:HB3	53:M7:64:ASN:HB3	1.92	0.50
64:N8:13:GLY:HA2	36:5:943:U:H3'	164.14	0.50
36:1:1556:C:O2'	36:1:2169:G:N1	2.44	0.50
40:L3:255:TRP:CD1	36:5:2395:G:H5''	216.48	0.50
8:S6:4:ASN:HA	8:S6:15:THR:HG22	1.94	0.50
1:2:1274:C:H5	35:SM:96:ARG:H	1.59	0.50
14:C2:60:VAL:HG22	14:C2:122:VAL:HG22	1.99	0.50
6:S4:15:PRO:HG2	6:S4:18:TRP:CE2	2.47	0.50
36:5:1367:G:HO2'	36:5:1368:U:H6	1.56	0.50
36:5:3237:U:H2'	36:5:3238:G:O4'	2.12	0.50
3:S1:146:GLN:O	3:S1:148:ASN:N	2.44	0.50
43:L6:107:ALA:O	43:L6:109:GLU:HG2	2.12	0.50
48:M1:133:ARG:HD2	48:M1:153:LYS:H	5.13	0.50
13:C1:76:VAL:HG12	13:C1:85:VAL:O	2.62	0.50
32:E0:53:LYS:HE2	32:E0:55:ARG:HD3	7.26	0.50
43:L6:58:LEU:HD12	43:L6:78:ARG:HD3	1.98	0.50
36:5:273:A:N7	86:5:4065:OHX:N3	2.60	0.50
2:S0:179:ARG:HD3	2:S0:183:ARG:NH1	2.20	0.50
40:L3:350:ALA:O	40:L3:351:LEU:HB2	2.11	0.50
66:O0:99:ASP:O	66:O0:101:LEU:N	2.86	0.50
52:M6:159:LYS:NZ	36:5:3243:A:OP1	267.43	0.50
14:C2:45:LEU:H	14:C2:120:VAL:HG23	5.08	0.50
10:S8:138:ASN:HD22	1:6:197:A:H61	279.46	0.50
36:1:2310:U:OP1	86:1:4142:OHX:N1	2.45	0.50
29:D7:37:CYS:HA	29:D7:77:THR:HG22	3.29	0.50
34:SR:25:THR:HA	34:SR:73:LEU:HD12	3.30	0.50
50:M4:38:ILE:HD11	56:N0:150:PHE:CE2	2.47	0.50
36:1:2505:U:H2'	36:1:2506:U:C6	2.46	0.50
1:6:1258:U:H5	1:6:1259:U:C2	2.30	0.50
6:S4:11:ARG:O	6:S4:12:LEU:HB2	2.12	0.50
17:C5:25:LEU:HA	17:C5:28:MET:HE2	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:D8:13:ILE:HD13	30:D8:31:GLU:HB2	1.94	0.50
46:L9:90:MET:HG2	46:L9:181:VAL:HG22	1.94	0.50
28:D6:12:LYS:HE2	28:D6:16:GLY:H	2.33	0.50
45:L8:130:TYR:CD1	45:L8:202:GLU:HB3	2.46	0.50
34:SR:115:ILE:HG13	34:SR:121:MET:O	2.93	0.50
38:4:14:C:H5'	53:M7:121:GLN:O	2.12	0.50
8:S6:148:SER:O	8:S6:151:ASP:HB2	3.73	0.50
26:D4:19:ALA:HB1	26:D4:81:GLU:OE2	3.40	0.50
45:L8:136:LEU:HD13	51:M5:3:ALA:CB	2.71	0.50
19:C7:71:PHE:HD1	19:C7:73:LEU:HB3	1.76	0.50
86:1:4071:OHX:N1	86:1:4118:OHX:N2	2.59	0.50
36:1:1547:G:P	51:M5:105:ARG:HH11	2.34	0.50
8:S6:2:LYS:HE2	8:S6:17:GLU:OE2	4.89	0.50
36:1:2225:U:H2'	36:1:2226:U:C6	2.47	0.50
2:S0:66:ALA:HB2	23:D1:37:ALA:HB2	2.01	0.50
25:D3:23:ARG:HH11	25:D3:23:ARG:CG	2.49	0.50
3:S1:173:THR:O	3:S1:177:GLN:HB2	6.11	0.50
28:D6:92:ARG:HD2	1:6:1796:C:OP2	344.90	0.50
8:S6:67:VAL:CG2	8:S6:99:GLY:HA2	2.55	0.50
66:O0:100:ILE:HD12	66:O0:101:LEU:HD23	1.93	0.50
2:S0:64:ILE:HG23	2:S0:73:VAL:HG11	2.51	0.50
36:1:1492:G:N7	75:O9:2:ALA:HB1	2.26	0.50
26:D4:20:ARG:HH11	26:D4:22:GLN:NE2	3.55	0.50
59:N3:81:GLN:O	59:N3:98:ASN:ND2	2.44	0.50
17:C5:22:LEU:HA	17:C5:25:LEU:HB2	3.02	0.50
1:2:1041:G:OP1	86:2:2150:OHX:N5	2.45	0.50
48:M1:28:ASP:OD2	48:M1:32:ARG:NH2	6.96	0.50
24:D2:11:LEU:HD12	24:D2:74:VAL:HB	1.93	0.50
36:1:239:G:O2'	36:1:240:U:OP1	2.26	0.50
36:1:861:C:H2'	36:1:862:U:C6	2.47	0.50
24:D2:73:GLY:HA3	24:D2:128:PHE:CZ	2.47	0.50
1:2:968:U:H2'	1:2:969:C:O4'	2.12	0.50
36:5:1919:G:N7	86:5:4072:OHX:N4	2.59	0.50
36:5:2592:G:H4'	36:5:2594:C:C2	2.47	0.50
2:S0:82:GLY:O	2:S0:86:VAL:HG22	2.11	0.50
36:5:1221:A:H3'	36:5:1222:G:H5'	1.94	0.50
18:C6:82:ARG:NH1	18:C6:114:ARG:O	3.10	0.50
1:6:540:G:O2'	1:6:542:A:H5'	2.11	0.50
9:S7:41:LEU:HD13	9:S7:70:PHE:CD1	2.47	0.50
76:Q0:77:ILE:HG22	76:Q0:78:ILE:N	2.26	0.50
36:5:1554:U:H4'	36:5:1555:U:OP1	2.10	0.50
36:5:1556:C:H2'	36:5:2169:G:N1	2.26	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
42:L5:155:THR:HA	42:L5:179:ARG:HA	1.93	0.50
86:1:4023:OHX:N6	86:1:4061:OHX:N2	2.60	0.50
2:S0:189:VAL:HG13	2:S0:190:ASP:N	2.26	0.50
53:M7:48:LEU:HB3	53:M7:88:VAL:HG13	1.93	0.50
52:M6:193:GLN:O	52:M6:196:ALA:HB3	2.11	0.50
86:1:3964:OHX:N1	86:1:4143:OHX:N4	2.60	0.50
11:S9:149:ARG:CZ	1:6:765:G:C5	429.05	0.50
86:5:4000:OHX:N4	86:5:4190:OHX:N3	2.60	0.50
36:1:3348:G:H1	36:1:3357:U:H3	1.58	0.50
50:M4:50:LYS:HD2	50:M4:91:CYS:SG	6.16	0.50
36:5:23:A:OP1	86:5:3906:OHX:N4	2.45	0.50
39:L2:181:LYS:NZ	36:5:860:G:O5'	212.84	0.50
49:M3:2:ALA:HB2	64:N8:31:GLY:O	2.12	0.50
36:5:256:G:H2'	36:5:257:U:C6	2.47	0.50
42:L5:256:THR:HG23	37:7:119:U:OP1	294.03	0.50
19:C7:52:GLY:HA3	1:6:1389:C:O2'	423.85	0.50
49:M3:47:ALA:HB1	49:M3:48:PRO:HD2	1.93	0.50
39:L2:215:ASN:HB2	36:5:2968:G:N7	216.99	0.50
4:S2:111:VAL:O	4:S2:136:VAL:HA	2.12	0.50
40:L3:138:ALA:O	40:L3:140:ASP:N	2.44	0.50
1:6:587:C:H2'	1:6:588:U:O4'	2.12	0.50
41:L4:319:LYS:O	41:L4:320:ASN:HB3	2.90	0.50
3:S1:133:TYR:CE1	3:S1:220:GLN:HB3	2.47	0.50
71:O5:101:THR:HG23	71:O5:103:LYS:H	1.77	0.50
10:S8:37:LYS:H	10:S8:59:ARG:H	1.60	0.50
1:6:1429:G:H2'	1:6:1430:U:C6	2.46	0.50
66:O0:13:LYS:O	66:O0:17:VAL:HG23	2.12	0.50
36:1:1240:A:H3'	36:1:1241:U:C5'	2.42	0.50
36:1:2339:C:P	59:N3:48:ARG:HG2	2.52	0.50
7:S5:159:ALA:HB3	7:S5:225:ARG:HB3	3.80	0.50
31:D9:34:TYR:OH	1:6:1487:A:OP1	420.00	0.50
11:S9:109:LEU:HB2	11:S9:146:PHE:CB	2.71	0.50
36:5:1688:U:H2'	36:5:1689:U:C5	2.46	0.50
28:D6:11:ASN:HB3	1:6:934:C:H6	332.77	0.50
36:1:307:A:O2'	36:1:2223:A:N3	2.39	0.50
3:S1:135:LEU:HD21	3:S1:217:LEU:HD12	6.40	0.50
36:1:1564:U:H2'	36:1:1565:G:H8	1.76	0.50
40:L3:332:ARG:O	40:L3:333:LYS:HB2	2.23	0.50
63:N7:78:ASN:OD1	66:O0:35:ARG:NH2	2.39	0.50
21:C9:112:GLY:O	21:C9:127:ASN:HB3	2.84	0.50
86:5:4055:OHX:N1	86:5:4197:OHX:N4	2.60	0.50
65:N9:20:GLY:O	65:N9:21:ILE:HB	2.59	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:956:U:OP1	86:1:4128:OHX:N1	2.45	0.50
39:L2:214:GLY:O	39:L2:215:ASN:HB2	4.58	0.50
69:O3:30:ILE:HB	69:O3:81:VAL:HG12	1.93	0.50
1:2:256:A:H2'	1:2:257:A:O4'	2.12	0.50
6:S4:98:ASN:ND2	6:S4:116:ASP:OD1	2.57	0.50
31:D9:24:CYS:HB2	1:6:1434:U:H4'	411.16	0.50
1:2:872:G:O6	86:2:2127:OHX:N3	2.45	0.50
63:N7:124:ALA:O	63:N7:126:LYS:N	2.70	0.50
1:6:1727:G:H2'	1:6:1728:A:C8	2.47	0.50
26:D4:132:ARG:C	26:D4:134:ALA:H	2.15	0.50
58:N2:104:ARG:NH2	36:5:1758:G:H5'	119.58	0.50
70:O4:58:ARG:HH11	70:O4:58:ARG:CG	2.24	0.50
14:C2:139:HIS:ND1	14:C2:139:HIS:O	2.45	0.50
11:S9:120:LYS:O	11:S9:120:LYS:HD3	4.83	0.50
52:M6:61:ALA:HA	52:M6:70:PRO:HD2	1.94	0.49
47:M0:174:THR:CG2	47:M0:176:LEU:H	2.11	0.49
11:S9:38:ASN:HB2	11:S9:41:GLU:HG3	1.93	0.49
18:C6:47:LYS:HZ1	18:C6:114:ARG:HD3	3.80	0.49
30:D8:9:LEU:HD13	30:D8:53:ILE:HG21	1.94	0.49
40:L3:169:THR:CG2	40:L3:171:LEU:H	2.33	0.49
34:SR:161:LYS:HD3	34:SR:164:ASP:HB3	1.93	0.49
1:2:569:C:H41	25:D3:69:ARG:NH1	2.10	0.49
1:6:1600:A:H4'	1:6:1601:G:OP1	2.11	0.49
1:2:197:A:H2'	1:2:198:A:C8	2.46	0.49
1:6:190:C:O2'	1:6:191:C:O5'	2.30	0.49
1:2:856:A:N7	9:S7:97:ARG:HB2	2.28	0.49
38:8:83:C:H4'	38:8:85:G:C2	2.47	0.49
36:1:1581:C:H2'	36:1:1582:C:C5'	2.42	0.49
24:D2:124:LYS:HE2	1:6:747:C:O2'	356.86	0.49
59:N3:66:LYS:O	59:N3:70:ARG:HG3	2.49	0.49
1:2:272:U:HO2'	1:2:273:G:H8	1.59	0.49
1:2:1535:U:O2'	1:2:1536:G:H5''	2.12	0.49
15:C3:11:ILE:HG12	15:C3:11:ILE:O	2.12	0.49
59:N3:80:ARG:NH1	59:N3:116:GLY:HA3	2.27	0.49
36:1:269:G:O6	86:1:4083:OHX:N3	2.45	0.49
74:O8:16:ARG:O	74:O8:18:ALA:N	3.36	0.49
47:M0:208:ASN:HA	47:M0:211:ARG:HD2	3.02	0.49
36:5:992:A:O2'	36:5:993:G:H5'	2.12	0.49
1:2:495:C:H3'	1:2:496:G:O4'	2.11	0.49
3:S1:56:SER:OG	3:S1:59:ASP:OD1	2.30	0.49
36:5:913:A:H2	36:5:2134:G:N3	2.10	0.49
66:O0:46:ALA:HB2	66:O0:72:GLY:H	1.76	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:1480:G:H4'	36:1:1481:A:OP1	2.12	0.49
41:L4:52:VAL:HG11	41:L4:99:MET:HE3	1.94	0.49
3:S1:125:VAL:HG11	3:S1:173:THR:HG22	2.79	0.49
47:M0:36:LEU:HD22	47:M0:73:ASN:ND2	3.04	0.49
17:C5:126:VAL:HG22	17:C5:127:ARG:H	2.52	0.49
36:5:2943:G:H2'	36:5:2944:U:O4'	2.11	0.49
11:S9:126:ARG:O	11:S9:130:THR:HG22	2.12	0.49
40:L3:347:SER:O	40:L3:348:ARG:HB3	2.12	0.49
1:2:1794:A:H1'	28:D6:79:ILE:HD13	1.93	0.49
86:5:3973:OHX:N1	86:5:4241:OHX:N2	2.60	0.49
57:N1:68:THR:HG22	57:N1:71:SER:O	2.77	0.49
1:6:1255:G:O2'	1:6:1256:A:O5'	2.29	0.49
1:2:856:A:H1'	9:S7:64:VAL:HG11	1.94	0.49
39:L2:130:SER:HA	39:L2:169:ILE:HG22	1.93	0.49
1:6:484:C:H42	1:6:503:G:N2	2.10	0.49
1:6:219:A:N6	1:6:843:U:C2	2.79	0.49
36:5:1764:U:H3'	36:5:1765:U:C5'	2.43	0.49
12:C0:49:LEU:O	12:C0:54:TYR:HB2	2.12	0.49
34:SR:38:ARG:HG2	34:SR:67:ILE:CG2	2.49	0.49
1:2:56:U:H4'	1:2:57:G:H5'	1.94	0.49
27:D5:60:VAL:HG22	27:D5:101:TYR:HB2	1.93	0.49
40:L3:56:ILE:CD1	40:L3:323:MET:HE1	3.72	0.49
5:S3:64:ARG:O	5:S3:66:ILE:N	2.49	0.49
67:O1:13:THR:HG22	67:O1:72:ARG:HH11	1.77	0.49
86:1:4059:OHX:N6	86:1:4166:OHX:N3	2.60	0.49
34:SR:267:PRO:HG2	34:SR:269:TYR:CE1	2.47	0.49
36:1:1722:U:OP1	55:M9:100:ARG:HD3	2.12	0.49
36:1:2655:U:OP2	78:Q2:2:VAL:HA	2.12	0.49
62:N6:102:SER:OG	62:N6:103:LYS:HE2	3.49	0.49
36:5:2822:U:OP2	86:5:3953:OHX:N1	2.45	0.49
74:O8:32:ASN:O	74:O8:34:ALA:N	2.45	0.49
11:S9:34:PHE:HD1	11:S9:111:THR:HG21	1.77	0.49
1:2:1351:G:C2	1:2:1375:A:C2	3.00	0.49
39:L2:24:GLN:OE1	39:L2:60:LYS:NZ	3.23	0.49
1:2:1171:A:H2'	1:2:1172:G:C8	2.46	0.49
36:5:1409:G:N7	86:5:4160:OHX:N6	2.60	0.49
5:S3:115:ILE:HD12	5:S3:116:ARG:H	4.80	0.49
52:M6:56:ASP:O	52:M6:59:ARG:HG2	2.19	0.49
21:C9:131:ASP:OD2	21:C9:134:ARG:NH1	4.41	0.49
6:S4:29:PRO:HD3	1:6:448:C:OP1	374.14	0.49
1:2:1553:G:O6	17:C5:43:ARG:HD3	2.12	0.49
36:1:2943:G:C8	40:L3:2:SER:N	2.80	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
41:L4:144:LYS:H	41:L4:144:LYS:HZ2	6.06	0.49
51:M5:183:THR:O	51:M5:184:LYS:HB2	2.12	0.49
36:1:1230:G:H2'	36:1:1231:A:H8	1.77	0.49
9:S7:67:LEU:HD13	9:S7:71:HIS:CE1	2.47	0.49
36:1:1752:A:OP2	86:1:4051:OHX:N5	2.45	0.49
39:L2:3:ARG:HD3	36:5:911:C:N4	178.67	0.49
1:2:583:C:OP1	86:2:2027:OHX:N3	2.45	0.49
36:1:3096:C:H2'	36:1:3097:C:C6	2.47	0.49
15:C3:127:ARG:NH2	1:6:629:U:OP1	308.95	0.49
36:5:3228:C:H4'	36:5:3229:G:O5'	2.11	0.49
36:5:420:G:OP1	36:5:420:G:OP2	2.30	0.49
36:1:2366:C:H5'	40:L3:259:HIS:HE2	1.77	0.49
36:5:1222:G:O6	86:5:4128:OHX:N1	2.46	0.49
7:S5:63:GLN:HB3	7:S5:88:PRO:HA	2.19	0.49
15:C3:115:LEU:HD22	15:C3:119:GLU:HG3	1.94	0.49
36:5:1734:G:O6	86:5:3969:OHX:N5	2.46	0.49
36:1:1629:U:P	63:N7:112:LYS:HE2	2.52	0.49
39:L2:156:LYS:NZ	36:5:2157:G:O3'	205.58	0.49
36:1:1192:C:O2	86:1:4054:OHX:N3	2.44	0.49
36:1:801:A:O2'	86:1:3985:OHX:N2	2.45	0.49
68:O2:41:VAL:HG12	68:O2:46:PHE:CD2	2.91	0.49
36:5:1769:G:C2	36:5:1770:G:C8	3.00	0.49
67:O1:83:GLU:O	67:O1:85:ALA:N	3.79	0.49
63:N7:135:ARG:HG2	63:N7:135:ARG:NH2	2.22	0.49
86:6:2060:OHX:N5	86:6:2147:OHX:N3	2.60	0.49
40:L3:35:ASP:OD1	40:L3:184:ASN:O	2.31	0.49
18:C6:82:ARG:HH12	18:C6:114:ARG:HB2	2.37	0.49
36:5:3121:U:H1'	36:5:3122:A:H5''	1.94	0.49
18:C6:41:PRO:O	18:C6:43:ILE:N	2.41	0.49
10:S8:8:ARG:HG3	10:S8:8:ARG:O	2.12	0.49
20:C8:56:LYS:HD2	20:C8:61:LEU:HD23	3.78	0.49
36:1:1104:G:O5'	36:1:1104:G:H8	1.95	0.49
23:D1:38:LYS:HD3	23:D1:51:VAL:HG23	1.94	0.49
36:1:1014:U:C2'	36:1:1015:U:H5''	2.42	0.49
3:S1:103:MET:HB3	3:S1:215:VAL:CG1	2.60	0.49
10:S8:147:ALA:C	10:S8:149:SER:H	2.69	0.49
72:O6:93:ILE:O	72:O6:97:SER:HB3	2.12	0.49
38:8:62:C:O2	86:8:219:OHX:N1	2.45	0.49
36:5:1595:U:C2	36:5:1596:C:C5	3.00	0.49
67:O1:13:THR:CG2	67:O1:72:ARG:HH11	2.25	0.49
56:N0:46:GLN:HG2	56:N0:51:VAL:O	2.11	0.49
59:N3:133:SER:O	86:6:2118:OHX:N3	295.85	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:4:10:A:H2'	38:4:11:C:C6	2.47	0.49
19:C7:60:ARG:NH1	1:6:1401:A:OP1	412.80	0.49
47:M0:31:ILE:HG13	47:M0:32:ARG:N	2.27	0.49
9:S7:23:ALA:O	9:S7:27:LEU:HG	2.12	0.49
41:L4:255:PHE:O	41:L4:258:LEU:HB2	2.40	0.49
36:1:784:A:C6	54:M8:93:ILE:HG22	2.48	0.49
86:1:3980:OHX:N5	86:1:4158:OHX:N2	2.60	0.49
36:5:8:C:H2'	36:5:9:U:O4'	2.12	0.49
3:S1:171:ILE:HD13	3:S1:196:GLU:HG2	1.95	0.49
1:2:990:C:H2'	1:2:991:G:O4'	2.12	0.49
36:5:1072:G:H2'	36:5:1073:U:H6	1.77	0.49
86:6:2060:OHX:N2	86:6:2147:OHX:N6	2.60	0.49
2:S0:9:LEU:HD23	2:S0:54:TRP:CG	2.48	0.49
8:S6:31:ARG:HH11	8:S6:34:GLN:NE2	2.92	0.49
1:6:1491:U:H5'	1:6:1492:A:OP1	2.11	0.49
56:N0:171:PHE:O	56:N0:172:TYR:C	4.20	0.49
36:1:190:U:H2'	62:N6:60:ARG:NH2	2.26	0.49
12:C0:32:HIS:CD2	12:C0:35:ILE:HB	2.47	0.49
28:D6:44:ILE:HD12	28:D6:45:VAL:N	2.27	0.49
33:E1:135:HIS:HB3	1:6:1250:U:O2'	432.65	0.49
44:L7:96:PRO:HB2	44:L7:99:PRO:HD2	1.95	0.49
70:O4:16:ARG:HH11	70:O4:16:ARG:CG	3.66	0.49
1:2:2:A:C2	4:S2:170:ILE:HD12	2.47	0.49
9:S7:140:VAL:HG22	9:S7:150:GLN:HG2	3.77	0.49
36:1:2437:G:N2	36:1:2511:A:H1'	2.27	0.49
4:S2:53:ILE:HD11	4:S2:73:LEU:HD22	1.94	0.49
41:L4:220:ARG:NH1	36:5:211:A:OP1	74.93	0.49
34:SR:102:ARG:NH2	1:6:1341:A:O2'	459.09	0.49
36:5:419:G:N7	86:8:214:OHX:N3	2.61	0.49
36:5:2635:A:H4'	36:5:2636:A:O5'	2.12	0.49
42:L5:50:ARG:NH2	42:L5:147:ASP:OD2	2.37	0.49
73:O7:16:HIS:HA	73:O7:27:PHE:O	2.47	0.49
47:M0:51:HIS:CD2	57:N1:160:ILE:HG23	2.46	0.49
52:M6:8:VAL:HG13	52:M6:34:VAL:HG22	2.50	0.49
39:L2:225:ILE:O	39:L2:238:ILE:O	4.80	0.49
36:1:2611:U:H2'	36:1:2612:U:C6	2.47	0.49
15:C3:89:TYR:CE2	15:C3:150:VAL:HG22	2.47	0.49
7:S5:41:LYS:O	7:S5:67:PRO:HB2	2.12	0.49
49:M3:57:VAL:HG12	49:M3:58:VAL:H	1.78	0.49
36:1:174:C:H2'	36:1:175:C:C6	2.47	0.49
35:SM:70:ASN:O	35:SM:74:LYS:HD3	2.12	0.49
36:5:595:G:N1	36:5:609:G:H5''	2.28	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:C6:12:LYS:HE2	18:C6:17:THR:HB	4.22	0.49
36:1:2790:A:OP2	54:M8:181:SER:HB3	2.12	0.49
53:M7:127:ARG:HD2	36:5:1505:C:OP1	128.92	0.49
36:1:92:G:OP2	36:1:93:C:H5'	2.12	0.49
36:1:156:G:OP2	72:O6:25:LYS:HB3	2.12	0.49
1:2:1102:G:P	24:D2:76:SER:HB2	2.53	0.49
1:2:1291:G:H8	1:2:1291:G:O5'	1.96	0.49
1:2:1173:C:OP1	20:C8:132:ARG:NH1	2.46	0.49
74:O8:62:ALA:O	74:O8:66:ILE:HG13	2.13	0.49
9:S7:41:LEU:HB3	9:S7:70:PHE:CE1	2.47	0.49
11:S9:129:ILE:HA	11:S9:134:ILE:CG1	4.18	0.49
1:2:1786:G:P	16:C4:136:ARG:HH22	2.35	0.49
36:1:709:A:P	54:M8:179:ARG:HH22	2.32	0.49
36:1:1352:A:H1'	36:1:1353:U:O5'	2.13	0.49
11:S9:118:LEU:HD23	11:S9:158:PHE:CZ	4.02	0.49
36:1:1615:C:H2'	36:1:1616:U:C6	2.48	0.49
1:6:825:U:O2'	1:6:826:U:OP2	2.24	0.49
36:1:2880:U:H1'	40:L3:250:ALA:HB3	1.93	0.49
15:C3:15:ALA:HB2	29:D7:20:LYS:HG3	1.93	0.49
57:N1:105:PHE:O	57:N1:108:ARG:N	2.45	0.49
36:5:789:A:H2'	36:5:790:U:C6	2.47	0.49
73:O7:48:ASN:OD1	73:O7:54:LYS:NZ	2.45	0.49
57:N1:56:PHE:CE1	57:N1:78:LYS:HD3	2.47	0.49
36:5:2726:C:O2'	36:5:2727:A:H2'	2.13	0.49
45:L8:203:VAL:HG13	45:L8:204:ARG:O	2.12	0.49
43:L6:98:VAL:HA	43:L6:101:PHE:CD2	2.49	0.49
55:M9:115:ILE:HG12	55:M9:119:LEU:HD23	1.95	0.49
36:5:731:U:H2'	36:5:732:C:H6	1.77	0.49
36:1:898:U:H2'	36:1:899:U:O4'	2.13	0.49
66:O0:45:ALA:HB3	66:O0:48:THR:HG22	1.94	0.49
1:2:1055:U:O4	86:2:2166:OHX:N3	2.46	0.49
36:5:926:A:H2'	36:5:927:C:C6	2.47	0.49
30:D8:60:GLU:O	30:D8:62:GLU:N	5.14	0.49
36:1:1460:A:H2'	36:1:1461:A:H8	1.77	0.49
54:M8:24:VAL:HG23	54:M8:25:TYR:CD2	2.47	0.49
1:6:496:G:O6	1:6:497:G:N2	2.42	0.49
36:1:1658:G:H2'	36:1:1659:U:C6	2.48	0.49
50:M4:121:MET:HE1	36:5:3215:A:O5'	275.42	0.49
39:L2:209:HIS:HD2	39:L2:211:HIS:N	2.01	0.49
38:4:68:G:OP2	86:O7:103:OHX:N6	2.45	0.49
1:6:647:G:H22	1:6:687:G:H1	1.61	0.49
1:6:453:U:O2	1:6:453:U:H3'	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:S2:67:GLN:O	4:S2:71:THR:HG23	3.86	0.49
1:6:542:A:H1'	1:6:543:C:OP1	2.13	0.49
8:S6:13:GLN:OE1	1:6:151:G:N2	311.12	0.49
41:L4:292:SER:OG	41:L4:293:SER:N	2.45	0.49
36:1:2513:U:H2'	36:1:2592:G:N1	2.25	0.49
34:SR:22:SER:OG	34:SR:69:GLN:O	4.51	0.49
41:L4:35:VAL:HG13	41:L4:235:LEU:HD11	2.49	0.49
1:6:918:U:H2'	1:6:919:A:C8	2.46	0.49
36:1:1580:A:H5'	36:1:2522:G:N7	2.27	0.49
6:S4:195:ILE:O	6:S4:209:HIS:O	4.61	0.49
15:C3:151:ASN:O	86:C3:202:OHX:N6	2.46	0.49
69:O3:15:SER:OG	69:O3:16:TYR:O	2.29	0.49
34:SR:90:ARG:NH1	34:SR:99:THR:OG1	2.45	0.49
86:1:3955:OHX:N2	86:1:4041:OHX:N6	2.61	0.49
1:2:1282:U:OP1	86:2:2115:OHX:N5	2.46	0.49
45:L8:162:LEU:HA	51:M5:7:LEU:HD11	1.94	0.49
13:C1:10:GLU:HG2	1:6:327:U:H1'	270.97	0.49
1:2:1022:C:H4'	1:2:1125:A:H61	1.76	0.49
5:S3:162:GLN:HG3	1:6:1333:C:H4'	429.18	0.49
11:S9:65:LYS:HA	11:S9:70:LEU:HG	1.93	0.49
36:1:2539:C:H5'	36:1:2541:U:O4	2.13	0.49
62:N6:12:ARG:HG2	36:5:215:G:OP1	88.01	0.49
42:L5:131:LEU:HD22	42:L5:131:LEU:H	1.77	0.49
1:2:217:A:OP1	1:2:217:A:H2'	2.13	0.49
43:L6:18:LEU:N	43:L6:18:LEU:HD22	2.28	0.49
50:M4:40:ASP:HA	56:N0:143:PHE:CE1	3.07	0.49
36:1:2405:C:O2	36:1:2819:A:N1	2.46	0.49
9:S7:174:ASN:O	9:S7:178:GLY:N	2.45	0.49
1:2:79:C:H4'	8:S6:173:PRO:O	2.12	0.49
1:2:699:U:H2'	1:2:700:C:C6	2.48	0.49
86:1:4084:OHX:N4	86:1:4153:OHX:N1	2.59	0.49
1:2:886:U:O2'	16:C4:121:VAL:O	2.29	0.49
47:M0:210:ILE:HG12	47:M0:217:PHE:CE2	2.48	0.49
24:D2:23:ARG:HB2	29:D7:4:VAL:HG12	5.23	0.49
62:N6:125:LYS:O	62:N6:126:LEU:HG	2.12	0.49
20:C8:91:ASP:HB3	20:C8:95:GLY:H	2.04	0.49
1:2:445:A:H1'	1:2:525:A:OP1	2.13	0.49
36:1:1554:U:C2	36:1:1555:U:C5	3.00	0.49
59:N3:68:GLU:CD	59:N3:68:GLU:H	2.15	0.49
34:SR:61:PHE:HD1	34:SR:92:TRP:CE3	2.43	0.49
11:S9:92:LYS:HB2	11:S9:95:TYR:HD2	8.66	0.49
54:M8:41:ASP:HB2	54:M8:42:ALA:H	4.47	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:S7:115:SER:O	9:S7:116:ARG:HB2	2.37	0.49
9:S7:73:VAL:O	9:S7:75:THR:N	2.54	0.49
46:L9:29:GLY:HA3	46:L9:82:VAL:HG13	1.95	0.49
68:O2:19:ARG:HH22	36:5:1433:A:P	164.13	0.49
1:6:30:G:H2'	1:6:31:C:C6	2.46	0.49
60:N4:34:SER:HA	60:N4:37:ALA:HB3	1.95	0.49
36:5:1749:A:H8	36:5:1749:A:OP1	1.95	0.49
12:C0:87:VAL:O	12:C0:89:ALA:N	4.39	0.49
36:1:981:U:HO2'	36:1:982:C:P	2.36	0.49
6:S4:49:ARG:HG3	6:S4:50:ASN:N	4.17	0.49
11:S9:40:LYS:HA	11:S9:43:TYR:HB2	1.94	0.49
3:S1:48:VAL:HG21	3:S1:61:LEU:HD13	7.06	0.49
24:D2:119:LYS:HG2	1:6:687:G:H5''	394.03	0.49
1:6:894:U:H2'	1:6:895:G:C8	2.48	0.49
36:1:155:G:O2'	72:O6:27:SER:HB3	2.12	0.49
42:L5:270:LYS:HD3	37:7:2:G:H4'	321.75	0.49
1:6:1255:G:O2'	1:6:1256:A:H8	1.96	0.49
1:6:162:A:H2'	1:6:163:G:C8	2.47	0.49
17:C5:37:ALA:O	17:C5:42:ARG:NH1	4.48	0.49
56:N0:115:ARG:NH1	36:5:1296:C:H5'	292.21	0.49
36:5:1555:U:H5'	36:5:1556:C:OP2	2.13	0.49
36:5:132:C:C2'	36:5:133:U:H5''	2.42	0.49
34:SR:37:SER:OG	34:SR:38:ARG:N	2.59	0.49
21:C9:84:LYS:HE3	1:6:1563:C:OP1	380.78	0.49
46:L9:31:ARG:HH21	46:L9:188:THR:HG22	1.78	0.49
55:M9:52:LYS:HG2	55:M9:52:LYS:O	2.78	0.49
1:6:230:C:N3	1:6:235:G:N2	2.50	0.49
1:2:1516:A:O2'	1:2:1517:U:H5'	2.13	0.49
57:N1:105:PHE:CE2	36:5:1062:A:H4'	244.89	0.49
36:1:3228:C:H4'	36:1:3229:G:O5'	2.12	0.49
1:2:474:A:O2'	11:S9:37:LYS:HE2	2.13	0.49
13:C1:46:LYS:HE2	1:6:846:G:H21	310.88	0.49
9:S7:30:SER:HB3	9:S7:34:LEU:HD12	1.94	0.49
51:M5:47:LYS:HE3	51:M5:51:LEU:HD11	2.37	0.49
43:L6:109:GLU:CD	43:L6:109:GLU:H	5.00	0.49
75:O9:4:GLN:HG2	36:5:1588:A:C2	127.64	0.49
49:M3:119:TYR:O	49:M3:123:ILE:HG23	2.12	0.49
49:M3:162:ASN:ND2	49:M3:164:GLU:HB2	3.38	0.49
36:5:1176:C:H2'	36:5:1177:G:N2	2.28	0.49
36:1:3291:G:O2'	36:1:3292:A:H5'	2.12	0.49
20:C8:49:LYS:NZ	20:C8:79:TYR:O	2.45	0.49
67:O1:40:ALA:O	67:O1:43:HIS:O	4.91	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
61:N5:63:ILE:O	61:N5:63:ILE:HD13	2.13	0.49
36:5:90:C:C2'	36:5:91:G:H5'	2.43	0.49
49:M3:15:ARG:CZ	36:5:96:G:H5''	152.17	0.49
6:S4:29:PRO:O	6:S4:30:ARG:HB3	4.62	0.49
55:M9:20:ARG:HG3	36:5:1875:G:OP2	138.24	0.49
8:S6:160:ARG:NH2	1:6:68:A:OP1	345.58	0.49
47:M0:33:ILE:HD11	47:M0:36:LEU:HG	1.93	0.49
42:L5:57:ASN:C	42:L5:58:LYS:HG2	2.34	0.49
42:L5:106:ALA:HB2	42:L5:166:ALA:HA	1.95	0.49
42:L5:273:ARG:O	42:L5:273:ARG:HG2	2.84	0.49
41:L4:203:ARG:NH1	41:L4:226:GLU:OE2	2.77	0.49
71:O5:6:ALA:O	71:O5:9:LEU:N	2.46	0.49
59:N3:120:LYS:H	59:N3:137:VAL:HG23	1.78	0.49
10:S8:8:ARG:C	10:S8:9:HIS:O	2.49	0.49
36:1:2585:G:C6	61:N5:24:LEU:HD13	2.48	0.49
36:1:1765:U:H2'	36:1:1766:G:H8	1.78	0.49
75:O9:9:ILE:HG22	75:O9:13:MET:CE	2.43	0.49
24:D2:23:ARG:NH1	24:D2:65:LEU:O	2.46	0.49
42:L5:146:LEU:HD13	42:L5:148:ILE:CD1	4.30	0.49
1:6:219:A:H2'	1:6:831:U:O2	2.13	0.49
36:1:2662:G:H2'	36:1:2663:G:C8	2.48	0.49
62:N6:39:LEU:HD22	62:N6:43:TYR:CE2	2.95	0.49
36:1:3103:A:OP2	86:1:4170:OHX:N3	2.46	0.49
14:C2:54:ARG:NH1	14:C2:56:GLU:OE2	2.44	0.49
1:6:1657:U:H4'	1:6:1658:G:OP2	2.13	0.49
1:2:138:A:N6	1:2:266:A:H61	2.11	0.49
9:S7:161:GLN:O	9:S7:165:LYS:HE3	2.13	0.49
2:S0:93:THR:HG21	2:S0:181:VAL:HG21	2.20	0.49
36:5:1192:C:H41	36:5:1302:A:P	2.35	0.49
9:S7:17:GLU:OE2	9:S7:46:ILE:N	3.05	0.49
86:1:4071:OHX:N5	86:1:4118:OHX:N6	2.60	0.49
36:5:2591:A:O2'	36:5:2592:G:H5'	2.13	0.49
36:1:2714:G:H4'	36:1:2715:A:O5'	2.13	0.49
36:5:1631:C:H5''	36:5:1632:A:H5''	1.94	0.49
1:2:1316:G:H2'	1:2:1317:C:C6	2.48	0.49
57:N1:57:TYR:OH	57:N1:87:LYS:HD2	2.13	0.49
36:5:378:A:N7	36:5:391:A:H2	2.11	0.49
50:M4:22:LEU:HB3	50:M4:64:VAL:HG13	2.76	0.49
36:1:1481:A:OP1	36:1:1481:A:O4'	2.30	0.48
53:M7:69:ARG:HG2	53:M7:79:THR:CG2	3.97	0.48
10:S8:36:THR:HA	10:S8:58:LEU:O	4.84	0.48
32:E0:28:LYS:HD3	1:6:542:A:N1	430.85	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:C4:12:GLN:HB3	16:C4:77:THR:OG1	2.12	0.48
41:L4:292:SER:O	41:L4:293:SER:OG	2.26	0.48
4:S2:99:LYS:HA	4:S2:117:THR:HA	2.43	0.48
33:E1:144:CYS:SG	33:E1:147:VAL:HG22	2.53	0.48
11:S9:171:ARG:HH11	11:S9:174:ARG:HD3	3.99	0.48
36:1:2244:A:H5''	39:L2:243:THR:OG1	2.12	0.48
68:O2:126:LEU:O	68:O2:128:LEU:N	2.44	0.48
73:O7:8:PHE:HA	73:O7:11:ARG:HD3	3.17	0.48
86:1:4023:OHX:N3	86:1:4061:OHX:N1	2.61	0.48
38:4:79:A:O3'	38:4:80:A:H4'	2.13	0.48
86:1:4032:OHX:N4	86:1:4149:OHX:N1	2.61	0.48
36:1:2319:U:O4	86:1:4043:OHX:N2	2.46	0.48
36:5:2436:U:H3	36:5:2511:A:H62	1.61	0.48
40:L3:227:GLU:HG3	40:L3:270:ARG:HB3	4.81	0.48
24:D2:110:ILE:HD13	24:D2:126:LEU:HD11	1.95	0.48
79:Q3:35:ALA:HB3	79:Q3:37:TYR:CE2	3.12	0.48
1:2:1366:U:O2'	21:C9:7:ARG:HD2	2.12	0.48
36:5:69:C:H2'	36:5:70:A:O4'	2.13	0.48
36:1:900:G:H1'	36:1:1589:A:N6	2.28	0.48
50:M4:17:VAL:HG22	50:M4:36:VAL:O	2.12	0.48
62:N6:59:VAL:HG22	62:N6:103:LYS:O	5.91	0.48
1:6:1336:A:OP1	86:6:2178:OHX:N1	2.46	0.48
18:C6:93:HIS:HA	18:C6:97:VAL:HG23	2.15	0.48
26:D4:104:SER:HB3	26:D4:107:GLN:HG3	1.95	0.48
58:N2:20:SER:O	58:N2:24:GLU:HG2	2.54	0.48
36:5:1912:U:N3	36:5:2122:G:OP2	2.40	0.48
20:C8:101:LEU:O	20:C8:104:ASN:HB3	2.46	0.48
64:N8:12:ARG:HH22	36:5:661:G:P	150.87	0.48
2:S0:122:ILE:HG23	2:S0:144:ILE:HB	2.88	0.48
64:N8:24:LYS:N	64:N8:24:LYS:HD3	4.55	0.48
70:O4:22:VAL:HG12	70:O4:30:LEU:HD22	1.95	0.48
36:1:1170:A:OP2	86:1:3962:OHX:N3	2.46	0.48
25:D3:23:ARG:HG3	25:D3:23:ARG:NH1	2.42	0.48
65:N9:24:PRO:HD2	65:N9:25:LYS:H	3.50	0.48
1:2:1555:A:OP1	17:C5:47:ARG:HD3	2.12	0.48
36:1:3353:G:O2'	36:1:3354:U:OP1	2.31	0.48
1:2:142:G:N2	1:2:173:A:C2	2.73	0.48
36:1:45:A:OP2	51:M5:85:THR:HG21	2.13	0.48
11:S9:134:ILE:HD13	11:S9:141:VAL:O	2.91	0.48
1:2:213:A:OP2	86:2:2116:OHX:N2	2.46	0.48
52:M6:68:ARG:HH12	36:5:2988:C:P	215.84	0.48
1:6:485:A:C5	1:6:486:G:H1'	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:2443:A:O2'	36:1:2444:C:OP2	2.27	0.48
6:S4:120:SER:O	6:S4:164:LEU:HB2	2.94	0.48
41:L4:191:LYS:HG2	41:L4:194:TYR:CZ	2.48	0.48
45:L8:214:LEU:HA	45:L8:214:LEU:HD12	1.81	0.48
52:M6:72:HIS:O	52:M6:74:ARG:HD3	2.46	0.48
36:5:863:C:H2'	36:5:864:G:O4'	2.13	0.48
41:L4:26:PHE:CD1	41:L4:130:ALA:HB2	3.17	0.48
36:5:2111:G:H4'	36:5:2112:U:OP2	2.13	0.48
48:M1:9:MET:HG3	48:M1:9:MET:O	2.13	0.48
86:2:2076:OHX:N3	86:2:2163:OHX:N5	2.61	0.48
5:S3:115:ILE:HG21	35:SM:110:TRP:HA	1.94	0.48
36:1:2578:U:OP1	86:1:4151:OHX:N5	2.46	0.48
42:L5:15:ARG:CZ	36:5:1003:A:H1'	290.76	0.48
19:C7:66:VAL:HB	19:C7:69:ILE:HD11	1.95	0.48
36:5:2697:A:H2'	36:5:2698:G:C8	2.49	0.48
1:6:250:C:H5'	1:6:250:C:H6	1.78	0.48
10:S8:151:LYS:HD3	10:S8:151:LYS:O	2.13	0.48
36:1:2777:G:H5'	36:1:2779:A:OP2	2.14	0.48
78:Q2:17:CYS:HG	78:Q2:74:CYS:HG	1.46	0.48
36:1:2207:A:C2'	36:1:2208:A:H5'	2.43	0.48
36:1:3272:C:O2	43:L6:80:ASN:HB2	2.13	0.48
36:1:3166:C:N4	36:1:3284:G:H1	2.01	0.48
3:S1:131:ASP:CG	3:S1:180:THR:HB	5.43	0.48
1:2:779:U:OP2	1:2:780:A:H2	1.96	0.48
3:S1:141:ALA:HB1	3:S1:207:LEU:HD13	5.34	0.48
37:3:49:G:O6	42:L5:58:LYS:NZ	2.31	0.48
36:1:357:A:OP2	86:O9:101:OHX:N4	2.46	0.48
41:L4:151:VAL:HG12	41:L4:152:VAL:H	2.51	0.48
1:6:140:A:H4'	1:6:140:A:OP2	2.13	0.48
36:5:3000:A:H2'	36:5:3001:C:C6	2.48	0.48
36:1:1951:C:H5'	36:1:1952:G:OP1	2.13	0.48
57:N1:100:LYS:C	57:N1:102:ARG:H	2.15	0.48
46:L9:13:PRO:HD2	46:L9:16:VAL:CG2	2.42	0.48
59:N3:11:PHE:CD1	59:N3:88:ARG:HD2	2.47	0.48
1:2:1236:A:C1'	33:E1:138:ARG:HH22	2.27	0.48
34:SR:201:THR:HB	34:SR:242:SER:HA	1.95	0.48
40:L3:303:LYS:HD2	40:L3:361:THR:HG21	1.94	0.48
1:6:737:A:H2'	1:6:738:G:H8	1.79	0.48
45:L8:165:PHE:HA	72:O6:47:ILE:HD13	2.20	0.48
5:S3:34:TYR:OH	5:S3:37:VAL:HG22	2.44	0.48
6:S4:187:ARG:HH22	1:6:753:A:H62	374.94	0.48
29:D7:80:ARG:HG2	29:D7:81:ARG:N	2.29	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
78:Q2:3:ASN:HA	78:Q2:92:GLU:O	2.13	0.48
5:S3:172:THR:HA	5:S3:184:ILE:O	2.20	0.48
49:M3:2:ALA:N	64:N8:33:GLY:O	4.53	0.48
36:5:585:A:H2'	36:5:586:C:C6	2.48	0.48
68:O2:115:LEU:HB2	68:O2:117:ILE:HD12	2.53	0.48
36:1:591:G:H4'	36:1:592:A:OP1	2.13	0.48
10:S8:115:ALA:O	10:S8:143:TRP:NE1	3.00	0.48
1:6:358:U:O2'	1:6:360:A:H5''	2.14	0.48
39:L2:79:ASN:O	39:L2:82:VAL:HG13	2.39	0.48
1:6:1650:U:H2'	1:6:1651:A:C8	2.49	0.48
68:O2:18:LYS:HB3	68:O2:30:GLU:HG2	3.06	0.48
36:5:847:A:H2'	36:5:848:A:C8	2.48	0.48
49:M3:106:GLN:HB3	72:O6:18:THR:OG1	2.59	0.48
36:1:2887:A:H2'	36:1:2887:A:N3	2.27	0.48
1:6:1450:U:OP2	86:6:2128:OHX:N4	2.46	0.48
41:L4:342:LYS:NZ	44:L7:56:GLU:OE2	2.25	0.48
36:1:1664:G:H2'	36:1:1665:C:C6	2.48	0.48
1:6:577:G:H3'	1:6:577:G:H8	1.78	0.48
20:C8:41:ARG:HD3	1:6:1565:C:OP1	369.60	0.48
47:M0:77:THR:HG22	47:M0:85:PHE:HZ	1.79	0.48
39:L2:193:ARG:NH2	36:5:2181:C:H5''	196.33	0.48
36:5:2209:U:O4	86:5:3962:OHX:N4	2.46	0.48
22:D0:72:ASN:ND2	1:6:1429:G:H21	385.97	0.48
36:1:863:C:OP1	86:1:3886:OHX:N5	2.46	0.48
1:2:1795:U:O4	28:D6:9:GLY:HA2	2.13	0.48
73:O7:66:TYR:OH	73:O7:73:ARG:NH2	2.71	0.48
1:6:538:A:H2	1:6:540:G:N2	2.12	0.48
40:L3:233:TRP:CD1	40:L3:265:ALA:HB1	2.49	0.48
1:2:169:A:OP1	8:S6:137:ARG:HG3	2.13	0.48
36:1:1231:A:OP2	86:1:4089:OHX:N5	2.46	0.48
1:2:190:C:O2'	1:2:191:C:H5'	2.13	0.48
2:S0:69:ASN:HB3	2:S0:71:GLU:OE2	2.14	0.48
19:C7:104:ASN:HA	19:C7:107:SER:HB3	4.17	0.48
2:S0:185:ARG:N	23:D1:45:ALA:H	2.69	0.48
66:O0:34:LEU:HD23	66:O0:59:TYR:HB3	1.96	0.48
42:L5:152:ARG:CG	42:L5:152:ARG:HH11	2.50	0.48
1:6:825:U:O2'	1:6:826:U:P	2.71	0.48
17:C5:21:ASP:N	17:C5:21:ASP:OD1	2.46	0.48
54:M8:176:ARG:NH1	64:N8:46:ASP:OD2	2.55	0.48
36:5:1192:C:H5	86:5:4091:OHX:N4	2.11	0.48
63:N7:22:LYS:HD3	63:N7:129:TRP:CZ3	2.48	0.48
36:1:1672:U:O2'	36:1:1673:G:H5'	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:7:64:A:H5'	37:7:65:G:H5''	1.94	0.48
71:O5:21:LEU:HD11	71:O5:55:LEU:HD21	1.95	0.48
36:1:2655:U:H4'	36:1:2656:A:O4'	2.13	0.48
78:Q2:3:ASN:O	36:5:2655:U:H2'	238.96	0.48
36:1:3279:A:C6	36:1:3280:U:C4	3.02	0.48
52:M6:18:ARG:O	52:M6:22:VAL:HG13	2.19	0.48
77:Q1:16:LYS:O	77:Q1:20:VAL:HG23	2.21	0.48
36:1:1498:A:H2'	36:1:1499:C:C6	2.48	0.48
7:S5:134:VAL:O	7:S5:138:THR:HG23	2.37	0.48
17:C5:85:ILE:HD11	17:C5:116:LEU:HD23	1.94	0.48
36:1:1798:A:H2'	36:1:1799:A:C8	2.47	0.48
36:5:3157:U:H3'	36:5:3158:G:C5'	2.43	0.48
31:D9:22:ARG:HG2	31:D9:37:ASN:O	2.28	0.48
63:N7:16:GLY:O	63:N7:18:TYR:N	2.57	0.48
6:S4:71:LYS:HB2	6:S4:75:LYS:O	2.14	0.48
38:4:154:C:H2'	38:4:155:A:O4'	2.14	0.48
51:M5:71:ARG:NH2	36:5:32:U:O3'	140.88	0.48
20:C8:38:VAL:HG12	20:C8:42:TYR:CD2	2.48	0.48
3:S1:77:GLU:O	3:S1:80:SER:OG	3.94	0.48
1:2:1642:G:O3'	77:Q1:9:ARG:NH2	2.46	0.48
1:2:700:C:H42	1:2:738:G:H1	1.61	0.48
10:S8:58:LEU:HD21	1:6:1676:U:H5''	272.00	0.48
10:S8:61:GLU:HG3	10:S8:77:ARG:HD2	5.31	0.48
18:C6:115:THR:O	18:C6:117:LEU:N	3.65	0.48
86:5:4187:OHX:N1	86:5:4189:OHX:N2	2.61	0.48
42:L5:41:LYS:HA	42:L5:41:LYS:HE3	3.37	0.48
1:2:219:A:H5'	1:2:831:U:O2'	2.13	0.48
9:S7:64:VAL:HG22	9:S7:94:ALA:HB1	2.37	0.48
1:6:1590:G:H2'	1:6:1591:C:C6	2.48	0.48
22:D0:96:PRO:O	22:D0:100:VAL:HG23	2.18	0.48
86:5:4212:OHX:N1	86:5:4222:OHX:N5	2.60	0.48
1:2:1477:G:H2'	1:2:1478:G:H8	1.76	0.48
86:1:3976:OHX:N5	86:1:4159:OHX:N1	2.62	0.48
73:O7:30:GLN:NE2	36:5:904:A:OP2	148.74	0.48
51:M5:73:ARG:HG2	51:M5:75:VAL:HG22	3.15	0.48
36:1:1874:A:H5''	55:M9:18:GLY:HA3	1.95	0.48
1:2:1435:G:N7	12:C0:25:LYS:HE3	2.28	0.48
1:6:1318:G:N7	86:6:2165:OHX:N5	2.61	0.48
8:S6:119:GLN:HG3	8:S6:120:GLU:H	1.78	0.48
86:7:219:OHX:N3	86:7:224:OHX:N6	2.61	0.48
1:2:850:A:H5'	55:M9:165:LYS:HG2	1.95	0.48
36:1:1080:A:OP2	42:L5:140:ARG:NH2	2.46	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
42:L5:45:ASN:O	42:L5:47:PRO:HD3	2.31	0.48
1:2:1163:A:N6	1:2:1164:G:C6	2.81	0.48
55:M9:163:ARG:HH21	55:M9:163:ARG:HG3	4.43	0.48
49:M3:42:ARG:HH21	49:M3:51:LEU:HD22	5.31	0.48
1:2:1553:G:N2	1:2:1555:A:H3'	2.29	0.48
3:S1:129:THR:OG1	3:S1:131:ASP:O	3.04	0.48
47:M0:36:LEU:HD13	47:M0:87:LEU:HD13	1.95	0.48
18:C6:113:ASP:CG	18:C6:115:THR:H	2.17	0.48
8:S6:135:PRO:HB2	8:S6:141:ILE:HG12	2.48	0.48
46:L9:69:ARG:HD3	46:L9:72:LYS:HD3	1.96	0.48
66:O0:15:ALA:O	66:O0:19:LYS:HG2	2.76	0.48
14:C2:62:LEU:HA	14:C2:120:VAL:HA	1.95	0.48
6:S4:104:ASP:OD2	6:S4:108:ARG:HB2	2.14	0.48
6:S4:104:ASP:HB3	6:S4:105:VAL:H	1.44	0.48
57:N1:139:ARG:NH2	57:N1:139:ARG:HG2	4.77	0.48
86:2:2116:OHX:N5	86:C1:201:OHX:N3	2.61	0.48
47:M0:4:ARG:NH2	47:M0:99:ILE:HD12	2.29	0.48
1:6:1417:A:H2'	1:6:1418:G:O4'	2.14	0.48
36:1:2535:A:H3'	36:1:2536:A:C8	2.49	0.48
1:2:248:U:H4'	13:C1:36:LYS:HD3	1.94	0.48
21:C9:33:TYR:OH	21:C9:103:LYS:HD2	2.13	0.48
39:L2:133:TYR:HB3	39:L2:168:VAL:HG12	1.95	0.48
43:L6:129:GLU:O	43:L6:130:ILE:HG12	4.77	0.48
61:N5:136:ALA:HB1	61:N5:141:TYR:CE1	2.49	0.48
36:1:2407:C:H2'	36:1:2408:U:C6	2.48	0.48
86:1:4059:OHX:N2	86:1:4166:OHX:N1	2.61	0.48
36:1:695:C:O2'	36:1:696:C:H5'	2.13	0.48
21:C9:6:VAL:HG13	21:C9:66:TYR:CZ	2.85	0.48
1:2:1390:U:O2	1:2:1412:G:H1'	2.13	0.48
16:C4:57:PRO:HB3	16:C4:100:ALA:HB2	1.95	0.48
86:1:3973:OHX:N1	38:4:31:G:OP2	2.46	0.48
36:5:3131:U:H2'	36:5:3132:C:C6	2.48	0.48
1:6:1050:G:O6	86:6:2195:OHX:N4	2.46	0.48
21:C9:25:GLN:HG2	21:C9:27:LYS:H	1.78	0.48
36:1:2094:C:H2'	36:1:2095:G:H8	1.77	0.48
38:8:26:U:H2'	38:8:27:U:C6	2.48	0.48
1:6:517:U:O4	86:6:2102:OHX:N4	2.47	0.48
1:2:607:G:H5'	1:2:613:G:N2	2.29	0.48
36:5:1014:U:H3	36:5:1036:A:H61	1.58	0.48
74:O8:77:ARG:O	74:O8:78:LEU:HB2	2.13	0.48
7:S5:192:GLU:OE2	27:D5:63:SER:OG	3.51	0.48
19:C7:96:SER:HA	19:C7:97:ASN:HA	1.52	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:1489:U:H5'	1:6:1494:C:H1'	1.95	0.48
1:2:1625:C:OP1	4:S2:91:ARG:NH2	2.47	0.48
36:1:1932:A:H5'	36:1:1933:A:OP2	2.13	0.48
66:O0:25:LEU:HD22	66:O0:90:VAL:HG22	2.25	0.48
66:O0:40:LYS:HD3	66:O0:93:LEU:O	2.22	0.48
36:5:1886:A:O4'	36:5:3307:A:H5'	2.14	0.48
1:2:778:G:C8	1:2:783:G:C2	3.01	0.48
86:1:4084:OHX:N4	86:1:4153:OHX:N3	2.61	0.48
53:M7:128:ARG:HG2	53:M7:136:ILE:HG21	4.70	0.48
28:D6:87:ARG:HD2	1:6:1797:A:N1	345.32	0.48
36:1:2897:A:H2'	36:1:2899:C:C5'	2.43	0.48
56:N0:1:MET:HA	56:N0:4:PHE:CZ	5.71	0.48
46:L9:49:ASN:OD1	46:L9:51:GLN:N	2.71	0.48
46:L9:12:VAL:HB	46:L9:51:GLN:HA	1.95	0.48
16:C4:24:ASN:O	16:C4:25:ASP:HB2	2.13	0.48
45:L8:101:THR:HG22	45:L8:104:GLU:HB2	1.96	0.48
44:L7:121:LYS:O	44:L7:121:LYS:HD3	2.13	0.48
36:1:1447:G:H3'	53:M7:67:ILE:HD11	1.95	0.48
2:S0:189:VAL:HG13	2:S0:190:ASP:H	1.78	0.48
86:5:4201:OHX:N2	86:8:224:OHX:N1	2.61	0.48
34:SR:74:THR:HG23	34:SR:79:TYR:HB2	1.94	0.48
68:O2:33:ARG:HH22	36:5:1408:G:P	160.48	0.48
86:1:3980:OHX:N1	86:1:4158:OHX:N4	2.62	0.48
1:2:263:C:H4'	1:2:292:U:H5'	1.95	0.48
41:L4:72:ALA:O	41:L4:76:ARG:NH1	2.60	0.48
33:E1:103:LEU:HA	33:E1:105:TYR:HD2	2.74	0.48
52:M6:121:PRO:HA	52:M6:124:LEU:HD22	2.16	0.48
36:1:2713:U:O2'	78:Q2:8:ARG:NH1	2.47	0.48
36:1:2623:G:C5	36:1:2624:G:C5	3.01	0.48
1:6:706:A:H2'	1:6:707:A:O4'	2.14	0.48
39:L2:104:LEU:HG	39:L2:136:ILE:HD11	1.95	0.48
50:M4:32:LEU:HD11	50:M4:94:TRP:CG	2.49	0.48
36:5:318:A:OP1	86:5:3955:OHX:N5	2.46	0.48
36:1:1506:A:H1'	36:1:1848:G:O6	2.13	0.48
47:M0:3:ARG:CZ	47:M0:63:GLU:HG3	2.53	0.48
36:5:1072:G:H2'	36:5:1073:U:C6	2.48	0.48
40:L3:345:ASN:OD1	40:L3:347:SER:HB2	2.13	0.48
46:L9:41:ILE:O	46:L9:42:ASP:HB2	2.13	0.48
18:C6:79:TYR:HA	18:C6:82:ARG:HD3	1.94	0.48
3:S1:49:ASN:O	3:S1:57:ALA:HB2	2.14	0.48
36:5:314:U:O4	86:5:4189:OHX:N5	2.46	0.48
28:D6:34:LYS:NZ	1:6:1793:G:N7	323.86	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:542:A:OP1	1:6:544:A:C4	2.66	0.48
7:S5:64:VAL:CG1	7:S5:89:ILE:HD11	4.59	0.48
1:6:1595:U:N3	1:6:1600:A:C2	2.72	0.48
48:M1:109:HIS:O	48:M1:112:LEU:HD23	2.57	0.48
2:S0:74:VAL:HG23	2:S0:118:PRO:HB3	1.94	0.48
36:1:263:C:H2'	36:1:264:G:O4'	2.14	0.48
26:D4:57:VAL:HG13	26:D4:60:PHE:HE2	1.78	0.48
53:M7:139:TYR:CE2	36:5:2355:G:H4'	147.67	0.48
86:5:4001:OHX:N6	86:5:4090:OHX:N5	2.62	0.48
43:L6:40:LEU:HB3	43:L6:84:VAL:HG13	2.68	0.48
36:1:2401:A:O3'	41:L4:68:GLY:HA2	2.14	0.48
53:M7:88:VAL:O	53:M7:92:GLN:HG3	3.69	0.48
86:1:4036:OHX:N2	86:1:4048:OHX:N5	2.62	0.48
40:L3:10:ARG:NH2	40:L3:14:LEU:HD21	2.28	0.48
46:L9:161:LEU:O	46:L9:164:ILE:HG22	2.13	0.48
36:1:1260:A:H1'	36:1:1280:C:H1'	1.95	0.48
86:1:4056:OHX:N2	86:1:4163:OHX:N4	2.62	0.48
36:1:3227:A:C2'	36:1:3228:C:H5'	2.43	0.48
6:S4:4:GLY:HA3	1:6:93:A:O2'	330.53	0.48
54:M8:151:ARG:HD2	36:5:781:G:OP1	161.53	0.48
36:1:1547:G:OP1	51:M5:105:ARG:HD3	2.12	0.48
9:S7:22:GLN:HA	9:S7:25:VAL:HG23	1.96	0.48
55:M9:35:ALA:O	55:M9:36:ASN:ND2	6.01	0.48
36:1:3233:C:H2'	36:1:3234:A:C8	2.49	0.48
17:C5:51:SER:C	17:C5:53:PRO:HD2	3.94	0.48
63:N7:54:THR:HG22	63:N7:57:HIS:CE1	3.30	0.48
56:N0:132:THR:O	56:N0:133:ALA:HB3	2.13	0.48
1:2:1115:U:OP1	77:Q1:14:LYS:NZ	2.43	0.48
36:5:627:U:H2'	36:5:628:A:C8	2.49	0.48
25:D3:111:GLY:O	25:D3:121:ARG:HD2	5.60	0.48
1:6:613:G:H4'	1:6:614:C:OP1	2.13	0.48
1:2:623:A:OP1	86:2:2158:OHX:N4	2.47	0.48
2:S0:206:ASP:N	2:S0:207:PRO:HA	4.04	0.48
36:1:1157:G:H2'	36:1:1158:A:O4'	2.14	0.48
4:S2:58:LEU:HD11	4:S2:236:PRO:HG2	1.95	0.48
36:5:567:G:H2'	36:5:568:G:C8	2.48	0.48
36:5:1214:U:H2'	36:5:1215:U:C6	2.48	0.48
36:5:3352:U:O4'	36:5:3353:G:C2	2.66	0.48
1:6:1392:U:H2'	1:6:1393:C:C6	2.49	0.48
1:6:1561:U:H4'	1:6:1599:C:H4'	1.95	0.48
1:6:1699:G:H22	1:6:1702:A:H5''	1.78	0.48
7:S5:59:VAL:O	7:S5:61:TYR:N	3.87	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:S9:163:PRO:C	11:S9:165:GLY:H	2.14	0.48
7:S5:64:VAL:HG12	7:S5:65:ARG:HD3	1.95	0.48
1:2:1370:U:H4'	1:2:1371:A:H5'	1.96	0.48
15:C3:16:ILE:HG13	15:C3:62:GLN:HE22	4.26	0.48
4:S2:230:TRP:CD2	24:D2:68:ARG:HD3	2.49	0.48
1:2:397:A:O3'	10:S8:50:GLY:HA2	2.13	0.48
1:2:1570:A:OP1	86:2:2155:OHX:N5	2.47	0.48
11:S9:171:ARG:CZ	11:S9:174:ARG:HD3	4.45	0.48
26:D4:15:ASN:HD22	26:D4:22:GLN:NE2	2.97	0.48
44:L7:150:LYS:HD3	44:L7:244:ASN:ND2	2.28	0.48
16:C4:115:ILE:HG21	28:D6:44:ILE:HG21	7.00	0.48
86:5:4066:OHX:N3	86:5:4141:OHX:N6	2.62	0.48
36:5:1152:G:OP2	36:5:1152:G:H8	1.96	0.48
1:2:717:C:N4	1:2:720:G:H22	2.11	0.48
2:S0:92:HIS:HB3	2:S0:182:LEU:HD11	2.43	0.48
36:5:1614:C:H2'	36:5:1615:C:C6	2.48	0.48
61:N5:105:VAL:HG11	61:N5:126:LEU:HD22	2.28	0.48
54:M8:102:ALA:HA	54:M8:122:ILE:O	2.13	0.48
54:M8:126:GLN:O	54:M8:130:ARG:HG3	2.14	0.48
40:L3:152:LYS:HG3	40:L3:192:VAL:HG11	1.94	0.48
51:M5:178:HIS:ND1	36:5:69:C:OP1	117.13	0.48
20:C8:83:ALA:HA	20:C8:86:LEU:HD22	2.11	0.48
49:M3:58:VAL:HG13	36:5:75:G:H5''	88.13	0.48
1:2:939:A:H2'	1:2:940:A:C8	2.48	0.48
1:6:1236:A:H2'	1:6:1237:G:C8	2.48	0.48
25:D3:13:ARG:O	25:D3:17:VAL:HG23	2.13	0.48
36:1:690:A:H4'	36:1:691:A:OP1	2.14	0.48
36:1:1063:G:N7	36:1:1097:G:H2'	2.28	0.48
1:2:97:C:H2'	1:2:98:U:C6	2.49	0.48
1:6:1360:A:H3'	1:6:1361:U:H4'	1.96	0.48
1:2:1081:A:H2'	1:2:1083:G:N7	2.29	0.48
52:M6:23:VAL:O	52:M6:27:LEU:HG	2.13	0.48
5:S3:217:ILE:O	5:S3:218:LEU:HB2	2.51	0.48
36:1:371:G:O6	86:1:4183:OHX:N4	2.47	0.48
36:5:1390:A:N3	36:5:1390:A:H5'	2.29	0.48
35:SM:75:ASP:N	35:SM:75:ASP:OD1	3.17	0.48
67:O1:11:GLU:HG2	67:O1:74:ARG:HB2	1.96	0.48
20:C8:40:ARG:HB3	21:C9:45:MET:SD	2.54	0.48
3:S1:133:TYR:CG	3:S1:181:LEU:HD11	2.49	0.48
28:D6:94:ASN:OD1	28:D6:96:ALA:HB3	2.54	0.48
42:L5:269:SER:CB	37:7:1:G:H21	317.77	0.48
7:S5:64:VAL:HG13	7:S5:89:ILE:HD11	4.35	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
71:O5:85:THR:HB	71:O5:88:LEU:HD12	1.94	0.48
13:C1:94:ILE:HD12	25:D3:16:ARG:HD2	1.96	0.48
15:C3:33:VAL:HA	15:C3:36:GLN:HB2	1.96	0.48
16:C4:125:SER:OG	16:C4:126:THR:N	2.76	0.48
9:S7:74:GLN:HG2	9:S7:131:PHE:HD2	4.81	0.48
36:5:1094:U:O2'	36:5:1095:U:H3'	2.14	0.48
2:S0:163:ASN:C	2:S0:165:ARG:H	2.17	0.48
4:S2:173:PRO:O	4:S2:176:SER:OG	2.17	0.48
46:L9:84:LYS:HA	46:L9:188:THR:HG23	1.96	0.48
13:C1:36:LYS:NZ	13:C1:59:PRO:O	2.43	0.48
36:1:1471:U:H2'	36:1:1472:U:C6	2.48	0.48
86:5:4094:OHX:N3	86:5:4234:OHX:N6	2.62	0.48
29:D7:63:LEU:HD23	29:D7:63:LEU:HA	1.94	0.48
24:D2:67:GLY:O	24:D2:69:LEU:N	3.57	0.48
36:1:2366:C:H5'	40:L3:259:HIS:CE1	2.49	0.48
86:2:2076:OHX:N4	86:2:2163:OHX:N2	2.61	0.48
36:1:861:C:H2'	36:1:862:U:H6	1.78	0.48
1:6:1309:C:O2'	1:6:1401:A:N1	2.39	0.48
36:5:595:G:C8	36:5:609:G:C6	3.02	0.48
42:L5:11:ALA:O	42:L5:15:ARG:HG3	2.14	0.48
36:5:2696:A:H2'	36:5:2697:A:C8	2.49	0.48
6:S4:71:LYS:O	6:S4:90:ILE:HA	2.91	0.48
36:1:1063:G:C6	36:1:1097:G:C5	3.02	0.48
1:2:67:A:C2	1:2:69:G:H1'	2.49	0.48
36:1:889:U:H2'	36:1:890:C:O4'	2.14	0.48
68:O2:24:ARG:HD3	68:O2:25:TYR:CZ	2.57	0.48
51:M5:69:GLY:O	36:5:290:G:H4'	145.89	0.48
3:S1:128:LYS:HE3	3:S1:132:ASP:HB3	1.96	0.48
1:2:1160:A:H2'	1:2:1161:C:C6	2.48	0.48
74:O8:12:LEU:HA	74:O8:12:LEU:HD12	4.52	0.48
55:M9:10:LEU:HD23	55:M9:41:ILE:HD13	1.96	0.48
5:S3:134:CYS:N	5:S3:157:LEU:HD11	2.29	0.48
36:5:415:G:OP2	86:5:4219:OHX:N4	2.47	0.48
41:L4:326:ARG:O	44:L7:41:ARG:NH2	3.34	0.48
50:M4:84:LYS:O	50:M4:87:ALA:HB3	2.13	0.48
36:1:2939:G:OP2	40:L3:2:SER:O	2.32	0.47
63:N7:46:ILE:HD11	63:N7:49:TYR:HA	1.96	0.47
2:S0:10:THR:OG1	2:S0:12:GLU:HG2	2.13	0.47
7:S5:68:ILE:HD13	7:S5:69:PHE:N	5.31	0.47
1:2:144:U:H5	8:S6:137:ARG:HH12	1.62	0.47
52:M6:156:LEU:HD13	36:5:3243:A:C8	264.01	0.47
1:2:1402:G:OP1	19:C7:10:LYS:NZ	2.44	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:5:1109:U:H2'	36:5:1110:U:O4'	2.14	0.47
61:N5:39:LYS:HG3	36:5:13:A:H4'	120.29	0.47
74:O8:5:ILE:HG22	74:O8:54:LEU:HD13	2.56	0.47
36:1:73:C:C2	49:M3:59:ARG:HD3	2.49	0.47
40:L3:211:GLN:HE21	40:L3:284:ARG:HA	1.79	0.47
56:N0:71:LYS:O	56:N0:73:LYS:HE2	2.14	0.47
40:L3:81:THR:O	40:L3:81:THR:CG2	2.72	0.47
86:5:4201:OHX:N6	86:8:224:OHX:N3	2.61	0.47
36:1:1389:G:OP2	86:1:3976:OHX:N4	2.47	0.47
86:1:3976:OHX:N5	86:1:4159:OHX:N2	2.62	0.47
12:C0:48:SER:O	12:C0:52:LYS:HG2	2.14	0.47
39:L2:70:ARG:NH1	39:L2:72:ARG:HE	5.64	0.47
49:M3:91:ARG:NH2	49:M3:97:VAL:O	2.47	0.47
34:SR:16:HIS:ND1	34:SR:39:ASP:OD2	2.38	0.47
86:1:3964:OHX:N5	86:1:4143:OHX:N3	2.62	0.47
7:S5:34:GLN:HG2	18:C6:57:LEU:HD13	1.95	0.47
86:2:2076:OHX:N3	86:2:2163:OHX:N1	2.62	0.47
12:C0:59:PHE:CZ	12:C0:62:GLN:HA	2.49	0.47
74:O8:9:LYS:NZ	74:O8:13:GLU:OE2	2.31	0.47
1:2:755:A:H2'	1:2:756:A:C8	2.49	0.47
36:1:1863:G:N1	36:1:1866:C:OP2	2.39	0.47
36:5:1252:A:H2'	36:5:1253:U:H5'	1.95	0.47
38:8:67:U:O4	86:8:225:OHX:N3	2.47	0.47
36:5:2950:G:C5	36:5:2979:U:C4	3.02	0.47
36:1:3224:G:O6	86:1:3897:OHX:N4	2.47	0.47
1:2:912:U:H4'	1:2:913:G:H2'	1.94	0.47
1:6:1031:U:H4'	1:6:1032:G:OP2	2.14	0.47
36:5:1571:A:H1'	36:5:1572:U:C5	2.49	0.47
64:N8:91:LEU:HD13	64:N8:121:VAL:HG21	1.95	0.47
46:L9:67:ALA:HA	46:L9:70:THR:HG23	1.96	0.47
14:C2:88:LEU:O	14:C2:89:ILE:HB	2.37	0.47
36:1:38:U:H4'	64:N8:32:ARG:HD2	1.95	0.47
56:N0:1:MET:O	56:N0:2:ALA:HB2	2.13	0.47
36:5:437:G:OP2	36:5:437:G:H8	1.96	0.47
48:M1:54:VAL:HG11	48:M1:57:PHE:CD2	2.49	0.47
66:O0:34:LEU:HD21	66:O0:42:ILE:HG21	3.43	0.47
86:1:4007:OHX:N3	86:1:4175:OHX:N1	2.62	0.47
52:M6:36:VAL:HB	52:M6:108:ILE:HB	4.63	0.47
53:M7:52:LEU:HD13	53:M7:88:VAL:HG11	2.05	0.47
9:S7:164:TYR:OH	9:S7:165:LYS:HE2	2.14	0.47
86:1:3968:OHX:N5	86:1:4076:OHX:N1	2.62	0.47
8:S6:206:ALA:O	8:S6:210:GLN:HG3	2.53	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
86:2:2076:OHX:N6	86:2:2163:OHX:N5	2.61	0.47
10:S8:140:GLU:HA	10:S8:143:TRP:HB2	3.18	0.47
1:2:1157:A:H2'	1:2:1160:A:N7	2.29	0.47
51:M5:27:VAL:HB	51:M5:122:ASN:ND2	2.29	0.47
52:M6:77:SER:HB2	52:M6:104:VAL:HG12	1.96	0.47
6:S4:155:LYS:NZ	1:6:244:A:OP1	345.97	0.47
36:5:36:C:H2'	36:5:37:U:H5'	1.96	0.47
48:M1:71:VAL:CG1	48:M1:75:LYS:HE3	6.12	0.47
1:2:1638:G:P	35:SM:94:HIS:HE2	2.37	0.47
36:5:766:U:H4'	36:5:767:U:O5'	2.13	0.47
1:6:1478:G:H2'	1:6:1479:A:O4'	2.13	0.47
3:S1:168:ILE:HG12	3:S1:197:ILE:HD12	1.96	0.47
2:S0:183:ARG:NH2	2:S0:191:ARG:O	2.48	0.47
64:N8:8:THR:HG21	36:5:662:U:OP1	149.76	0.47
1:2:158:U:HO2'	1:2:159:U:H3'	1.80	0.47
22:D0:72:ASN:N	22:D0:72:ASN:OD1	2.47	0.47
25:D3:102:VAL:HG12	25:D3:127:VAL:HA	2.55	0.47
7:S5:57:SER:HB3	30:D8:53:ILE:HB	1.96	0.47
37:3:121:U:H5''	42:L5:265:TYR:HE1	1.80	0.47
8:S6:68:LEU:HD13	8:S6:68:LEU:HA	1.63	0.47
36:1:1110:U:O4	86:1:3983:OHX:N5	2.47	0.47
36:1:3118:C:H4'	76:Q0:106:ARG:NH2	2.23	0.47
1:2:1561:U:H2'	1:2:1562:G:H8	1.80	0.47
1:2:488:G:OP1	1:2:488:G:H4'	2.14	0.47
37:3:4:U:H2'	37:3:5:G:H8	1.75	0.47
45:L8:108:ARG:O	45:L8:112:GLU:HG2	2.14	0.47
36:5:1329:U:O2'	36:5:1330:A:P	2.72	0.47
12:C0:14:TYR:CE2	12:C0:21:VAL:HG22	2.49	0.47
68:O2:119:VAL:O	68:O2:122:PRO:HD3	2.27	0.47
86:1:4023:OHX:N6	86:1:4061:OHX:N5	2.62	0.47
1:6:820:U:H2'	1:6:820:U:H6	1.36	0.47
36:1:3218:A:H5''	36:1:3219:G:C4	2.49	0.47
25:D3:100:ASP:OD2	25:D3:142:LYS:NZ	2.68	0.47
86:1:4065:OHX:N3	86:1:4177:OHX:N1	2.62	0.47
1:6:71:A:H2'	1:6:72:A:O4'	2.15	0.47
1:6:800:U:H2'	1:6:801:G:C8	2.47	0.47
1:6:1230:A:H8	1:6:1258:U:C5	2.32	0.47
6:S4:26:CYS:HB2	6:S4:27:TYR:CD2	5.07	0.47
39:L2:14:SER:OG	39:L2:15:ILE:N	2.47	0.47
17:C5:122:THR:HG21	1:6:1455:G:OP1	370.59	0.47
54:M8:122:ILE:HD11	54:M8:130:ARG:CZ	3.27	0.47
36:1:1345:G:N7	86:1:3964:OHX:N4	2.62	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:S5:166:ARG:O	7:S5:170:GLN:HB2	2.14	0.47
1:2:600:U:OP2	25:D3:108:GLY:HA2	2.14	0.47
36:5:3056:U:OP2	86:5:3941:OHX:N2	2.48	0.47
34:SR:260:ILE:HB	34:SR:274:LEU:HD12	2.77	0.47
40:L3:57:VAL:HG23	40:L3:358:TRP:HE3	1.79	0.47
35:SM:22:PRO:HB3	48:M1:38:GLU:OE1	2.13	0.47
26:D4:77:ASN:O	26:D4:78:SER:HB3	2.93	0.47
56:N0:77:VAL:HG11	56:N0:106:LEU:HG	4.41	0.47
1:2:1473:U:O2	1:2:1473:U:H2'	2.13	0.47
27:D5:81:ARG:HB2	27:D5:81:ARG:HH11	4.06	0.47
1:2:1727:G:H2'	1:2:1728:A:C8	2.48	0.47
42:L5:196:ARG:NH2	42:L5:237:GLU:OE2	2.47	0.47
36:1:846:A:H2'	36:1:847:A:O4'	2.14	0.47
2:S0:154:GLU:HA	23:D1:63:GLY:HA2	1.96	0.47
36:5:2403:G:C2	36:5:2404:A:N7	2.78	0.47
1:6:577:G:H3'	1:6:577:G:C8	2.50	0.47
25:D3:103:LEU:HB2	25:D3:126:LYS:HB2	2.48	0.47
14:C2:46:ARG:HH12	1:6:1253:U:P	455.02	0.47
55:M9:101:VAL:HG13	55:M9:104:ARG:HH12	1.77	0.47
36:5:2897:A:H2'	36:5:2899:C:H5''	1.96	0.47
1:6:1542:G:H22	1:6:1568:C:H1'	1.79	0.47
38:4:151:C:C4	61:N5:24:LEU:HD11	2.50	0.47
7:S5:123:VAL:O	27:D5:58:ARG:HD2	2.14	0.47
26:D4:40:LEU:O	26:D4:44:LEU:HD12	2.99	0.47
44:L7:96:PRO:O	44:L7:100:ARG:HB2	2.33	0.47
86:5:4066:OHX:N5	86:5:4141:OHX:N6	2.62	0.47
3:S1:149:GLN:HE22	3:S1:154:SER:HB2	1.77	0.47
36:5:1018:G:H2'	36:5:1019:G:O4'	2.15	0.47
53:M7:64:ASN:HA	53:M7:67:ILE:HG12	1.97	0.47
34:SR:242:SER:O	34:SR:292:LEU:HD21	2.14	0.47
60:N4:4:GLU:HG2	60:N4:30:ARG:HD3	1.96	0.47
86:1:4056:OHX:N2	86:1:4163:OHX:N1	2.62	0.47
55:M9:90:PRO:HG2	55:M9:93:VAL:CG2	3.19	0.47
36:5:181:U:H1'	36:5:236:G:H22	1.79	0.47
11:S9:36:LEU:O	32:E0:33:ARG:HG3	2.14	0.47
40:L3:261:MET:HE2	52:M6:64:PHE:HA	1.95	0.47
3:S1:147:ALA:O	3:S1:148:ASN:HB3	2.13	0.47
36:1:1856:C:H2'	36:1:1857:C:H6	1.80	0.47
3:S1:36:SER:HB2	3:S1:231:LEU:HB3	1.96	0.47
36:5:2298:U:O4	36:5:2923:U:H5	1.97	0.47
64:N8:128:ARG:HB3	72:O6:8:ALA:CB	3.17	0.47
36:5:736:A:H2'	36:5:737:G:O4'	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:2561:A:HO2'	36:1:2562:A:H8	1.61	0.47
39:L2:206:PRO:HG3	39:L2:213:GLY:HA2	3.72	0.47
36:5:2505:U:H2'	36:5:2506:U:C4	2.48	0.47
36:1:534:U:O2	56:N0:146:LYS:HA	2.14	0.47
1:6:681:U:H4'	1:6:682:C:OP1	2.14	0.47
1:2:373:G:O6	86:2:2160:OHX:N6	2.48	0.47
36:1:817:A:H8	73:O7:15:SER:HG	1.61	0.47
47:M0:36:LEU:HD12	47:M0:87:LEU:HB3	2.88	0.47
36:1:2960:C:H2'	36:1:2961:G:C8	2.49	0.47
1:6:916:U:H5''	1:6:917:U:OP2	2.14	0.47
47:M0:193:ASP:OD1	36:5:1010:G:N2	336.02	0.47
47:M0:24:ARG:NH1	47:M0:24:ARG:HG3	2.26	0.47
1:2:819:G:N3	1:2:820:U:H5	2.12	0.47
2:S0:73:VAL:O	2:S0:95:ALA:HA	2.14	0.47
17:C5:68:PRO:HG2	17:C5:71:GLU:OE2	2.14	0.47
4:S2:139:ILE:CD1	4:S2:191:ALA:HB1	2.44	0.47
86:2:2116:OHX:N6	86:C1:201:OHX:N3	2.63	0.47
11:S9:171:ARG:HE	11:S9:174:ARG:CB	5.45	0.47
16:C4:102:LEU:HD11	28:D6:45:VAL:HG12	2.85	0.47
64:N8:66:ALA:HA	64:N8:69:TRP:N	3.89	0.47
2:S0:139:VAL:CG2	4:S2:62:PRO:HG3	2.82	0.47
36:5:1952:G:H1	36:5:2094:C:N4	2.09	0.47
36:1:2573:G:N7	86:1:4002:OHX:N1	2.62	0.47
36:5:1818:U:H2'	36:5:1819:U:C6	2.48	0.47
36:1:2535:A:N6	36:1:2544:U:H3	2.10	0.47
52:M6:15:LEU:HD21	52:M6:125:ARG:HG3	2.03	0.47
41:L4:138:ARG:NH2	41:L4:240:PRO:HB2	2.57	0.47
21:C9:117:SER:HB2	21:C9:123:ARG:HB2	1.96	0.47
61:N5:135:ILE:O	61:N5:139:ILE:HG22	2.15	0.47
36:5:1081:U:HO2'	36:5:1082:U:C5'	2.27	0.47
1:6:1645:G:H22	1:6:1756:A:H2	1.60	0.47
8:S6:210:GLN:HG2	8:S6:214:LYS:HZ2	1.79	0.47
42:L5:54:ARG:NH2	42:L5:147:ASP:OD1	2.31	0.47
36:5:731:U:H2'	36:5:732:C:C6	2.50	0.47
1:2:1332:C:O2'	5:S3:162:GLN:HB3	2.14	0.47
1:2:749:U:H2'	1:2:750:U:C6	2.49	0.47
86:1:4016:OHX:N6	70:O4:64:THR:O	2.48	0.47
86:1:3873:OHX:N2	73:O7:46:SER:OG	2.48	0.47
44:L7:145:ARG:HA	44:L7:185:ILE:HD13	2.07	0.47
1:6:1432:U:H4'	1:6:1433:G:H5''	1.97	0.47
36:1:707:U:H2'	36:1:708:G:H5''	1.96	0.47
3:S1:175:GLU:O	3:S1:187:LYS:NZ	2.44	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:S1:70:LEU:HD21	3:S1:79:HIS:CG	2.50	0.47
63:N7:121:ARG:HG3	63:N7:121:ARG:HH11	1.80	0.47
47:M0:193:ASP:OD2	47:M0:198:LYS:NZ	5.46	0.47
53:M7:136:ILE:O	53:M7:137:ASN:ND2	2.54	0.47
28:D6:82:ARG:NH2	1:6:1152:A:OP1	329.19	0.47
1:2:538:A:H8	1:2:543:C:C4	2.32	0.47
14:C2:46:ARG:HD2	1:6:1255:G:O6	455.04	0.47
66:O0:16:LEU:HD12	66:O0:98:SER:N	2.29	0.47
12:C0:22:VAL:HB	12:C0:32:HIS:NE2	8.00	0.47
1:2:177:U:H1'	8:S6:191:ARG:NH1	2.29	0.47
6:S4:62:LYS:HE3	6:S4:66:MET:HG2	6.66	0.47
46:L9:189:GLU:O	46:L9:191:LEU:N	2.48	0.47
36:1:3281:U:H2'	36:1:3282:U:C6	2.48	0.47
1:2:1450:U:H2'	1:2:1451:C:H6	1.78	0.47
1:2:720:G:O2'	1:2:721:U:H5'	2.15	0.47
20:C8:88:ARG:NH2	20:C8:91:ASP:OD2	2.88	0.47
1:6:1697:G:H8	1:6:1705:C:C2	2.32	0.47
39:L2:77:ILE:CD1	39:L2:128:ARG:HB3	2.48	0.47
86:5:3991:OHX:N4	38:8:112:U:O2	2.48	0.47
9:S7:89:HIS:CG	9:S7:165:LYS:HG2	4.09	0.47
40:L3:152:LYS:HE3	40:L3:192:VAL:HG22	1.97	0.47
1:2:1175:U:H2'	1:2:1176:G:H8	1.80	0.47
15:C3:11:ILE:O	15:C3:12:SER:HB2	2.14	0.47
1:6:653:C:N4	1:6:677:G:H1	2.13	0.47
39:L2:40:TYR:HA	39:L2:91:GLY:HA3	1.97	0.47
1:6:1237:G:H2'	1:6:1238:A:C8	2.49	0.47
36:5:1949:G:H1	36:5:2097:U:H3	1.62	0.47
70:O4:55:SER:OG	70:O4:69:HIS:HB3	2.13	0.47
36:1:3314:A:OP1	40:L3:174:LYS:HB2	2.14	0.47
36:5:1246:G:O2'	36:5:1264:G:OP2	2.28	0.47
39:L2:90:ALA:HB2	39:L2:101:VAL:HG13	2.14	0.47
42:L5:22:ARG:HG2	42:L5:28:THR:OG1	2.14	0.47
44:L7:241:LYS:NZ	36:5:576:C:OP1	275.25	0.47
1:6:1685:G:H1	1:6:1716:C:H42	1.62	0.47
43:L6:170:LYS:HB3	43:L6:172:HIS:CE1	2.50	0.47
52:M6:29:ASN:OD1	69:O3:14:LEU:HD22	2.15	0.47
9:S7:104:ARG:H	9:S7:104:ARG:HG2	1.35	0.47
36:5:850:U:H2'	36:5:851:C:C6	2.50	0.47
36:1:980:A:H2'	36:1:981:U:C6	2.49	0.47
64:N8:21:ARG:HD2	36:5:1369:A:H5''	185.17	0.47
74:O8:46:ARG:HH21	74:O8:51:LEU:HB2	2.24	0.47
1:2:894:U:H2'	1:2:895:G:H8	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
64:N8:6:THR:CG2	64:N8:8:THR:HG23	2.39	0.47
11:S9:122:VAL:O	11:S9:125:ALA:HB3	2.13	0.47
44:L7:229:PHE:CD1	44:L7:229:PHE:C	3.08	0.47
36:1:1815:U:O2'	36:1:1816:A:OP2	2.28	0.47
41:L4:9:HIS:HE1	41:L4:146:PRO:HB2	1.78	0.47
1:2:542:A:H2'	1:2:543:C:H3'	1.95	0.47
44:L7:165:ASP:OD2	44:L7:166:ASN:N	2.85	0.47
36:5:357:A:OP2	86:5:4207:OHX:N5	2.47	0.47
7:S5:89:ILE:HD12	7:S5:90:ILE:N	2.43	0.47
36:1:839:C:H4'	36:1:1724:U:H2'	1.96	0.47
21:C9:28:LEU:O	21:C9:29:GLU:HB2	2.15	0.47
1:6:199:G:HO2'	1:6:200:A:H8	1.61	0.47
2:S0:120:LEU:HD12	2:S0:121:VAL:H	1.79	0.47
41:L4:271:LYS:HB2	41:L4:274:TYR:HB3	2.01	0.47
16:C4:99:GLN:NE2	28:D6:44:ILE:O	3.61	0.47
47:M0:86:HIS:ND1	47:M0:139:ARG:NH1	2.58	0.47
36:5:2752:U:O2	86:5:4230:OHX:N3	2.48	0.47
20:C8:4:VAL:HG21	27:D5:82:HIS:ND1	3.13	0.47
1:2:720:G:H2'	1:2:720:G:N3	2.30	0.47
21:C9:33:TYR:O	21:C9:35:ASP:N	3.44	0.47
1:2:900:A:OP1	16:C4:43:THR:OG1	2.25	0.47
36:5:2951:G:O2'	36:5:2952:G:H5'	2.14	0.47
47:M0:7:ARG:NH1	36:5:2828:G:OP1	269.99	0.47
36:5:1915:A:H2'	36:5:1916:U:C6	2.50	0.47
5:S3:64:ARG:NH1	5:S3:68:GLU:OE1	2.87	0.47
54:M8:67:ILE:HG12	54:M8:81:VAL:HG21	1.97	0.47
34:SR:79:TYR:HE1	34:SR:100:TYR:HE1	2.53	0.47
36:1:3227:A:H2'	36:1:3228:C:H5'	1.95	0.47
1:2:93:A:H1'	6:S4:3:ARG:HB3	1.97	0.47
45:L8:67:ILE:HG22	45:L8:237:ILE:HB	1.96	0.47
43:L6:97:ASN:O	43:L6:98:VAL:HB	2.15	0.47
9:S7:116:ARG:HE	9:S7:116:ARG:HB2	1.57	0.47
10:S8:70:GLU:OE2	10:S8:117:TYR:OH	2.99	0.47
10:S8:115:ALA:O	10:S8:117:TYR:N	3.95	0.47
86:7:219:OHX:N5	86:7:224:OHX:N2	2.62	0.47
1:6:1360:A:C4	1:6:1361:U:H1'	2.50	0.47
1:2:912:U:H4'	1:2:913:G:O5'	2.15	0.47
29:D7:72:LYS:NZ	29:D7:72:LYS:HB2	3.76	0.47
1:6:654:C:H2'	1:6:655:G:C8	2.49	0.47
38:8:74:U:O2	86:8:218:OHX:N5	2.47	0.47
42:L5:257:GLU:O	42:L5:258:LYS:HB2	2.13	0.47
36:1:230:U:H2'	36:1:231:G:O4'	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:D9:10:HIS:CG	31:D9:11:PRO:HD2	2.50	0.47
73:O7:76:ASN:O	73:O7:79:GLN:HG3	2.26	0.47
36:5:3160:U:H2'	36:5:3161:C:C6	2.50	0.47
60:N4:22:VAL:HG22	60:N4:28:ILE:HG12	1.96	0.47
51:M5:160:GLU:OE1	51:M5:160:GLU:N	2.87	0.47
31:D9:5:ASN:OD1	31:D9:7:TRP:NE1	2.44	0.47
36:5:3159:C:H2'	36:5:3160:U:C6	2.50	0.47
1:2:1017:U:H2'	1:2:1018:U:C6	2.49	0.47
29:D7:19:HIS:CE1	29:D7:21:LEU:H	3.02	0.47
3:S1:122:GLU:HG2	3:S1:140:ILE:HG13	1.97	0.47
64:N8:103:ASP:OD1	64:N8:106:ALA:HB2	2.14	0.47
46:L9:85:GLY:O	46:L9:186:PHE:HA	2.36	0.47
47:M0:205:SER:O	47:M0:209:ASN:HB2	2.15	0.47
36:5:3263:G:O6	86:5:4119:OHX:N2	2.48	0.47
36:1:1374:G:O6	64:N8:10:LYS:NZ	2.47	0.47
1:2:142:G:O5'	1:2:142:G:H8	1.98	0.47
2:S0:79:ARG:O	2:S0:83:GLN:HG3	2.97	0.47
41:L4:93:MET:HB2	36:5:658:G:N2	145.98	0.47
36:1:621:A:O2'	86:1:4167:OHX:N1	2.48	0.47
1:2:161:U:OP2	8:S6:87:ARG:NH2	2.48	0.47
36:5:2209:U:H4'	36:5:2210:G:OP1	2.14	0.47
56:N0:12:ARG:HD2	56:N0:22:PRO:HG2	3.81	0.47
46:L9:162:GLN:HB2	46:L9:179:ILE:O	2.15	0.47
36:1:2418:G:O6	86:1:4122:OHX:N1	2.48	0.47
41:L4:182:LEU:CD1	41:L4:223:PRO:HG2	2.45	0.47
7:S5:222:LYS:HA	7:S5:225:ARG:NH1	3.73	0.47
19:C7:4:VAL:HA	1:6:1402:G:OP1	405.72	0.47
18:C6:10:PHE:CE2	1:6:1379:C:H5'	433.07	0.47
23:D1:39:VAL:HB	23:D1:44:ARG:O	2.15	0.47
45:L8:26:LEU:HD12	45:L8:26:LEU:H	1.79	0.47
86:5:4023:OHX:N4	86:5:4215:OHX:N3	2.63	0.47
36:5:1348:U:C6	36:5:1355:A:C5	3.03	0.47
1:6:1472:C:H2'	1:6:1535:U:O4	2.14	0.47
36:5:1561:G:H1	36:5:1578:C:N4	2.12	0.47
71:O5:59:ASN:O	71:O5:63:ARG:HG2	4.05	0.47
34:SR:205:SER:OG	34:SR:207:ASP:OD2	2.61	0.47
73:O7:32:LYS:HA	73:O7:32:LYS:HD3	1.69	0.47
58:N2:54:VAL:HG13	58:N2:67:SER:HB2	3.28	0.47
6:S4:159:THR:HG23	6:S4:173:ILE:HD13	1.97	0.47
36:1:1509:A:H2'	36:1:1510:G:C8	2.49	0.47
67:O1:25:PHE:HB3	67:O1:65:LYS:HG3	4.70	0.47
36:1:1611:G:H2'	36:1:1612:A:O4'	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:422:G:OP1	86:2:2043:OHX:N6	2.48	0.47
64:N8:84:GLU:O	64:N8:87:ARG:HB2	2.72	0.47
34:SR:157:VAL:HB	34:SR:168:THR:HG22	3.17	0.47
1:6:992:A:H5'	1:6:992:A:H8	1.80	0.47
51:M5:109:ARG:NH1	38:8:141:C:OP1	120.94	0.47
63:N7:15:ARG:HD2	63:N7:79:HIS:CD2	2.92	0.47
20:C8:35:ILE:HB	20:C8:38:VAL:CG2	2.45	0.47
36:5:2836:C:O2	36:5:2836:C:O4'	2.28	0.47
13:C1:108:PRO:HG2	13:C1:134:THR:O	2.70	0.47
56:N0:137:ARG:HD3	36:5:1213:G:OP1	325.22	0.47
3:S1:63:GLY:HA2	3:S1:88:VAL:O	2.14	0.47
3:S1:30:PHE:HB3	3:S1:96:LEU:HD22	3.66	0.47
7:S5:167:ARG:HH21	30:D8:55:VAL:HG21	3.93	0.47
71:O5:89:ARG:HD2	38:8:38:U:O4	69.60	0.47
37:3:19:C:H2'	37:3:20:A:H8	1.79	0.47
2:S0:71:GLU:HA	2:S0:95:ALA:N	2.30	0.47
17:C5:69:GLU:OE1	86:C5:201:OHX:N2	2.48	0.47
86:2:2045:OHX:N4	86:2:2099:OHX:N6	2.63	0.47
39:L2:55:GLY:O	39:L2:56:ALA:HB3	4.64	0.47
74:O8:17:ARG:O	74:O8:19:ASP:N	2.41	0.47
2:S0:167:LYS:HB3	2:S0:168:HIS:H	1.62	0.47
7:S5:109:LYS:O	7:S5:113:ILE:HG13	2.31	0.47
6:S4:11:ARG:HB2	6:S4:27:TYR:C	2.57	0.47
63:N7:4:PHE:O	63:N7:5:LEU:HB2	4.54	0.47
4:S2:53:ILE:HG12	4:S2:73:LEU:HD22	3.98	0.47
1:2:1789:G:OP2	16:C4:132:ARG:NH2	2.41	0.47
2:S0:101:ARG:HG3	2:S0:102:PHE:N	2.29	0.47
86:1:3968:OHX:N6	86:1:4076:OHX:N2	2.63	0.47
11:S9:121:SER:HB3	11:S9:124:HIS:H	2.59	0.47
49:M3:162:ASN:HD21	49:M3:164:GLU:HB2	2.66	0.47
1:6:652:G:N2	1:6:683:C:C2	2.82	0.47
38:4:26:U:H2'	38:4:27:U:C6	2.50	0.47
39:L2:30:ARG:NH2	39:L2:33:ASP:OD2	2.63	0.47
36:5:701:G:H2'	36:5:702:C:C6	2.49	0.47
36:5:1438:U:H2'	36:5:1439:U:C6	2.49	0.47
44:L7:137:GLY:HA3	44:L7:236:ILE:HB	1.96	0.47
36:1:1926:C:H5'	36:1:1927:G:C5	2.49	0.47
56:N0:39:SER:OG	37:7:98:C:OP1	285.12	0.47
76:Q0:93:LYS:HB3	76:Q0:103:LEU:O	2.15	0.47
25:D3:88:PRO:O	25:D3:89:ASN:HB2	2.15	0.47
2:S0:125:ASP:HB3	2:S0:128:SER:HB2	2.66	0.47
32:E0:39:LEU:O	32:E0:43:ARG:HB2	2.42	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
79:Q3:84:ARG:O	79:Q3:88:GLU:HG3	2.89	0.47
7:S5:103:ASN:HA	7:S5:106:LYS:HD2	1.97	0.47
36:5:1049:C:H2'	36:5:1050:U:C6	2.50	0.47
36:1:2404:A:N3	36:1:2404:A:H2'	2.30	0.47
39:L2:202:VAL:HG23	39:L2:211:HIS:HB3	1.96	0.47
47:M0:36:LEU:CD1	47:M0:87:LEU:HB3	3.15	0.47
1:2:927:C:H1'	16:C4:125:SER:CB	2.45	0.47
1:2:1424:A:H1'	4:S2:92:ALA:HB1	1.97	0.47
35:SM:68:ARG:HG2	1:6:1460:A:OP1	337.04	0.47
54:M8:64:VAL:O	54:M8:96:PHE:HE2	1.98	0.47
16:C4:81:VAL:HG22	16:C4:115:ILE:HB	1.97	0.47
72:O6:9:ILE:HA	72:O6:13:LYS:HD3	2.73	0.47
47:M0:156:ARG:HG2	47:M0:163:GLN:CG	2.86	0.47
86:2:2096:OHX:N3	86:2:2109:OHX:N1	2.62	0.47
59:N3:13:ILE:CG2	59:N3:85:TRP:CD1	2.98	0.47
73:O7:13:ASN:O	36:5:817:A:C4	140.07	0.47
27:D5:85:LYS:HG3	27:D5:86:GLU:N	2.33	0.47
79:Q3:75:ALA:HA	79:Q3:78:THR:HG23	2.31	0.47
1:2:717:C:H2'	1:2:718:U:H5''	1.98	0.47
34:SR:238:ASP:OD2	34:SR:258:THR:OG1	2.36	0.47
1:6:76:A:H3'	86:6:2192:OHX:N1	2.30	0.47
45:L8:105:LYS:HG3	45:L8:109:LEU:HD23	4.39	0.47
14:C2:125:ASN:CG	35:SM:168:GLU:H	6.05	0.47
67:O1:13:THR:CG2	67:O1:72:ARG:HH21	5.73	0.47
54:M8:123:THR:OG1	54:M8:125:ASP:OD2	2.24	0.47
1:2:1762:A:C1'	1:2:1783:C:H5'	2.45	0.47
24:D2:11:LEU:O	24:D2:15:ASN:HB2	2.84	0.47
7:S5:100:ASN:O	7:S5:102:ARG:N	2.47	0.47
51:M5:102:ALA:O	51:M5:106:VAL:HG13	2.15	0.47
59:N3:80:ARG:HH12	59:N3:116:GLY:HA3	1.79	0.47
36:1:191:U:H5'	36:1:191:U:H6	1.79	0.47
1:2:1274:C:C5	35:SM:95:SER:HA	2.50	0.47
36:5:926:A:H2'	36:5:927:C:H6	1.80	0.47
36:5:1013:G:H2'	36:5:1014:U:O4'	2.16	0.47
42:L5:99:TYR:CD2	42:L5:199:ILE:HG12	3.02	0.47
9:S7:39:ARG:NH2	55:M9:185:LEU:HD22	2.85	0.47
49:M3:157:ARG:HH12	64:N8:146:GLU:CD	2.39	0.47
1:6:1503:A:H2'	1:6:1504:G:O4'	2.14	0.47
1:2:1029:U:O4	86:2:2170:OHX:N3	2.48	0.47
1:6:1241:G:H2'	1:6:1242:A:O4'	2.14	0.47
36:1:1227:C:H5'	36:1:1228:C:OP2	2.15	0.47
35:SM:43:ASP:OD1	35:SM:45:SER:OG	2.79	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
66:O0:73:GLY:O	66:O0:76:GLU:HG2	2.15	0.47
66:O0:87:VAL:HB	36:5:1728:G:O2'	250.66	0.47
27:D5:74:SER:OG	1:6:1534:G:OP2	344.90	0.47
36:1:1645:U:C2'	36:1:1646:G:H5'	2.45	0.47
36:1:1674:G:OP2	86:1:3952:OHX:N2	2.48	0.47
42:L5:48:LYS:HZ1	36:5:2749:G:P	242.34	0.47
6:S4:37:LYS:HB2	6:S4:40:GLU:HG2	1.97	0.47
36:5:2960:C:H2'	36:5:2961:G:C8	2.50	0.47
55:M9:142:ILE:O	55:M9:146:LYS:HG2	4.67	0.47
79:Q3:3:LYS:HE2	79:Q3:3:LYS:HB3	1.57	0.47
52:M6:83:ALA:CB	36:5:1313:G:H5'	258.82	0.47
4:S2:59:HIS:CE1	4:S2:238:SER:HA	3.50	0.47
6:S4:212:ASP:OD1	6:S4:214:LEU:N	2.48	0.47
3:S1:70:LEU:HD13	3:S1:79:HIS:CG	3.67	0.46
1:6:470:A:OP2	86:6:2103:OHX:N1	2.48	0.46
20:C8:5:VAL:O	27:D5:42:LEU:HB2	3.58	0.46
86:5:3973:OHX:N1	86:5:4241:OHX:N1	2.63	0.46
40:L3:169:THR:HG23	40:L3:171:LEU:HG	2.35	0.46
1:2:320:U:H2'	1:2:321:C:C6	2.51	0.46
11:S9:171:ARG:HA	11:S9:174:ARG:HB2	2.59	0.46
35:SM:34:LYS:HA	35:SM:34:LYS:HD3	3.84	0.46
52:M6:60:LYS:CE	36:5:1307:G:H5''	250.83	0.46
17:C5:18:ARG:HG2	20:C8:92:ILE:HA	1.95	0.46
73:O7:2:GLY:O	73:O7:7:SER:HB3	2.16	0.46
36:5:1016:C:OP1	36:5:1016:C:C6	2.68	0.46
6:S4:54:TYR:OH	6:S4:97:GLU:OE2	2.30	0.46
1:2:1762:A:H1'	1:2:1783:C:H5'	1.97	0.46
34:SR:63:GLY:HA2	1:6:1341:A:OP1	451.29	0.46
1:2:1217:A:C8	1:2:1217:A:H5'	2.49	0.46
5:S3:21:LEU:HD22	5:S3:25:PHE:CE2	2.50	0.46
6:S4:3:ARG:NH1	1:6:399:A:N3	322.80	0.46
86:1:4071:OHX:N5	86:1:4118:OHX:N2	2.63	0.46
64:N8:29:PRO:O	64:N8:31:GLY:N	2.48	0.46
1:2:1389:C:O2'	19:C7:52:GLY:HA3	2.15	0.46
1:2:1746:A:H2'	1:2:1747:G:O4'	2.15	0.46
36:5:2541:U:H4'	36:5:2542:U:OP1	2.16	0.46
3:S1:23:PRO:O	3:S1:26:ARG:HB3	2.44	0.46
36:1:2419:A:H2'	36:1:2420:C:C6	2.50	0.46
25:D3:54:LEU:HD11	25:D3:75:GLN:HB2	1.97	0.46
36:1:2186:U:OP2	39:L2:200:ARG:HD2	2.14	0.46
64:N8:27:LYS:HE2	64:N8:27:LYS:HB3	1.98	0.46
67:O1:34:LYS:HE2	67:O1:34:LYS:HB2	4.57	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:S7:185:ILE:HG22	9:S7:186:PRO:HD2	1.97	0.46
36:5:1310:G:N7	86:5:4026:OHX:N4	2.62	0.46
8:S6:56:ASN:ND2	8:S6:60:GLY:O	2.49	0.46
36:1:3187:A:H5''	50:M4:8:LYS:HD2	1.96	0.46
36:5:508:U:H2'	36:5:509:U:C6	2.50	0.46
36:5:239:G:N7	86:5:4131:OHX:N5	2.63	0.46
70:O4:81:CYS:O	70:O4:82:ALA:HB3	2.15	0.46
23:D1:1:MET:O	23:D1:9:VAL:HG12	2.15	0.46
11:S9:38:ASN:HB3	11:S9:40:LYS:H	1.80	0.46
39:L2:192:LYS:HB3	39:L2:193:ARG:NH2	2.30	0.46
1:2:1507:G:O6	86:2:2147:OHX:N5	2.48	0.46
36:1:1245:A:C3'	36:1:1246:G:H5''	2.46	0.46
1:6:188:A:H2'	1:6:189:C:O4'	2.15	0.46
20:C8:145:ARG:HE	20:C8:145:ARG:HA	4.66	0.46
79:Q3:50:GLY:O	79:Q3:51:ALA:HB3	2.15	0.46
86:5:4001:OHX:N3	86:5:4090:OHX:N5	2.63	0.46
34:SR:13:LEU:HB3	34:SR:45:TRP:CZ3	2.50	0.46
40:L3:230:THR:OG1	40:L3:247:ARG:HB3	2.14	0.46
51:M5:91:GLU:OE2	86:5:3921:OHX:N4	166.30	0.46
86:1:4088:OHX:N2	86:1:4157:OHX:N4	2.62	0.46
24:D2:80:ASN:OD1	24:D2:124:LYS:HG2	2.15	0.46
43:L6:51:ARG:NH1	50:M4:114:ASP:OD2	2.56	0.46
66:O0:86:ARG:NH1	79:Q3:44:LYS:HG2	2.31	0.46
36:5:3358:U:H2'	36:5:3359:A:H8	1.81	0.46
40:L3:221:THR:HG22	40:L3:272:TYR:N	2.81	0.46
36:5:741:U:H2'	36:5:742:G:O4'	2.15	0.46
39:L2:181:LYS:HZ3	36:5:860:G:P	214.59	0.46
34:SR:205:SER:HB3	34:SR:210:LEU:HB2	1.97	0.46
7:S5:126:ASP:HB3	7:S5:127:GLN:H	1.50	0.46
1:6:872:G:H2'	1:6:873:U:O4'	2.14	0.46
22:D0:97:VAL:HG13	22:D0:98:GLN:H	2.35	0.46
24:D2:28:ARG:HA	24:D2:29:PRO:HA	1.66	0.46
75:O9:41:ARG:HH22	36:5:1517:G:P	97.92	0.46
1:6:1045:C:C2	1:6:1074:G:C2	3.02	0.46
1:6:276:C:H1'	1:6:277:U:H5	1.80	0.46
56:N0:84:ARG:HG3	36:5:1295:G:OP1	294.47	0.46
28:D6:60:PRO:C	28:D6:62:TYR:H	2.18	0.46
1:2:1498:G:H5''	21:C9:72:GLY:HA3	1.97	0.46
41:L4:84:ARG:O	41:L4:87:GLN:HG3	2.74	0.46
36:1:59:G:H2'	38:4:33:A:O2'	2.15	0.46
43:L6:68:PRO:HG2	43:L6:71:VAL:CG2	3.69	0.46
36:5:2403:G:H5'	36:5:2871:G:H5'	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
71:O5:101:THR:CG2	71:O5:104:GLN:H	2.39	0.46
1:2:702:G:C6	1:2:737:A:C6	3.03	0.46
7:S5:73:THR:HG23	18:C6:114:ARG:HB3	4.34	0.46
7:S5:59:VAL:C	7:S5:61:TYR:H	2.89	0.46
11:S9:53:ARG:O	11:S9:57:ARG:HG3	2.15	0.46
1:2:1759:C:O2'	36:1:2263:C:H4'	2.15	0.46
16:C4:124:ASP:O	16:C4:125:SER:HB2	2.15	0.46
17:C5:119:PHE:HA	35:SM:57:ASN:ND2	2.49	0.46
1:2:1595:U:H5	1:2:1596:C:C5	2.34	0.46
26:D4:27:VAL:HG11	26:D4:35:VAL:HG11	1.97	0.46
86:2:2096:OHX:N6	86:2:2109:OHX:N5	2.63	0.46
36:1:2683:U:H2'	36:1:2684:C:H6	1.80	0.46
20:C8:27:LYS:O	20:C8:31:ALA:N	2.75	0.46
1:2:356:G:OP2	86:2:2037:OHX:N6	2.48	0.46
36:1:1811:G:H2'	36:1:1812:G:O4'	2.15	0.46
5:S3:29:LEU:HD21	5:S3:69:LEU:HD21	2.85	0.46
12:C0:23:ALA:O	12:C0:24:LYS:HB3	4.61	0.46
20:C8:87:ASN:OD1	20:C8:99:HIS:HA	2.51	0.46
57:N1:160:ILE:HD12	57:N1:160:ILE:HA	1.72	0.46
36:1:1433:A:P	68:O2:19:ARG:HH22	2.38	0.46
51:M5:109:ARG:HD3	51:M5:109:ARG:HA	1.77	0.46
25:D3:86:PHE:O	25:D3:88:PRO:HD3	2.16	0.46
1:2:1560:U:O4'	1:2:1560:U:O2	2.31	0.46
47:M0:145:LYS:NZ	47:M0:167:LEU:HD11	2.31	0.46
47:M0:47:PRO:HB3	47:M0:171:TRP:CE2	2.50	0.46
50:M4:55:ARG:NH2	50:M4:77:ARG:HA	2.31	0.46
36:5:1876:U:H6	36:5:1876:U:H5''	1.80	0.46
10:S8:38:ILE:HA	10:S8:60:ILE:O	2.30	0.46
46:L9:40:HIS:ND1	46:L9:41:ILE:HG13	4.50	0.46
20:C8:15:LEU:HD21	20:C8:59:GLY:HA2	3.43	0.46
64:N8:77:LYS:HB3	64:N8:80:THR:OG1	2.16	0.46
36:1:99:A:H5''	51:M5:194:GLN:OE1	2.16	0.46
36:1:2104:A:OP2	55:M9:81:ARG:NH2	2.39	0.46
1:6:195:G:H2'	1:6:196:G:H5''	1.96	0.46
59:N3:54:LEU:HD11	59:N3:119:GLY:HA3	2.51	0.46
53:M7:74:LYS:NZ	36:5:3310:A:OP1	186.42	0.46
1:6:831:U:OP2	1:6:831:U:H6	1.98	0.46
52:M6:65:ASN:HB3	52:M6:68:ARG:HD3	2.13	0.46
67:O1:19:ARG:HD3	67:O1:35:GLU:CG	2.47	0.46
5:S3:72:LEU:HD22	12:C0:65:TYR:HD1	1.99	0.46
78:Q2:61:LYS:HE2	78:Q2:63:LYS:O	2.16	0.46
86:1:4007:OHX:N4	86:1:4175:OHX:N1	2.62	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:799:A:H5''	6:S4:201:HIS:CD2	2.50	0.46
36:5:1560:G:H1	36:5:1579:C:H42	1.64	0.46
29:D7:63:LEU:O	29:D7:74:SER:N	2.44	0.46
24:D2:105:THR:HG23	24:D2:110:ILE:CG1	2.82	0.46
45:L8:74:THR:HB	45:L8:230:LYS:HZ1	1.80	0.46
63:N7:105:SER:HA	63:N7:108:GLU:HG3	1.97	0.46
11:S9:149:ARG:HG2	1:6:765:G:O6	434.24	0.46
36:5:25:U:O4	86:5:3906:OHX:N6	2.49	0.46
3:S1:35:PRO:HB3	3:S1:231:LEU:HD11	4.41	0.46
6:S4:159:THR:HG21	6:S4:227:VAL:O	2.41	0.46
36:1:2426:U:H2'	36:1:2427:U:C6	2.51	0.46
7:S5:95:ASN:O	7:S5:98:MET:HG2	2.14	0.46
25:D3:62:LYS:HD2	25:D3:118:PRO:HB3	1.98	0.46
48:M1:47:GLN:HG2	48:M1:67:VAL:HG12	1.97	0.46
39:L2:80:GLU:HG3	79:Q3:66:GLY:HA2	1.97	0.46
47:M0:200:LEU:HD12	47:M0:213:PHE:HB2	3.84	0.46
1:2:1252:C:O4'	33:E1:133:ALA:HB2	2.14	0.46
72:O6:77:LEU:HD23	36:5:294:U:H4'	146.55	0.46
58:N2:37:LEU:O	58:N2:41:ILE:HG13	2.26	0.46
1:2:1051:G:O2'	1:2:1052:U:P	2.73	0.46
25:D3:98:GLU:O	25:D3:99:ASN:HB2	2.27	0.46
1:6:570:A:H5''	1:6:571:G:OP2	2.15	0.46
42:L5:68:THR:HG22	42:L5:70:THR:H	1.80	0.46
61:N5:44:PRO:O	61:N5:45:LYS:HB2	4.37	0.46
6:S4:180:LEU:HD13	6:S4:228:ILE:HD11	3.14	0.46
36:1:1940:G:H2'	36:1:1941:C:O4'	2.16	0.46
36:1:2206:G:H1	36:1:2237:C:H42	1.63	0.46
2:S0:179:ARG:HD3	2:S0:183:ARG:NE	3.57	0.46
33:E1:126:CYS:O	33:E1:128:ALA:N	2.47	0.46
20:C8:126:ARG:HB3	20:C8:133:VAL:HG23	1.97	0.46
7:S5:112:ARG:HD3	1:6:1529:C:OP1	373.95	0.46
14:C2:97:LEU:HD12	14:C2:118:ALA:HB3	3.14	0.46
44:L7:110:ARG:CZ	54:M8:3:ILE:HD12	2.56	0.46
49:M3:93:ILE:HA	49:M3:93:ILE:HD13	1.60	0.46
13:C1:80:MET:HB3	13:C1:83:THR:O	3.06	0.46
53:M7:88:VAL:O	53:M7:92:GLN:HG2	2.16	0.46
1:2:901:G:C6	1:2:902:G:C6	3.04	0.46
39:L2:70:ARG:NH2	36:5:2522:G:C6	175.41	0.46
36:1:2947:G:N3	40:L3:250:ALA:HB1	2.30	0.46
68:O2:11:LYS:O	68:O2:13:HIS:N	2.47	0.46
24:D2:74:VAL:O	24:D2:75:ILE:HD13	2.95	0.46
40:L3:62:ARG:O	40:L3:68:HIS:HB2	2.76	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
63:N7:104:PRO:O	63:N7:108:GLU:HG2	2.16	0.46
15:C3:74:ILE:O	15:C3:78:ASN:ND2	3.17	0.46
1:6:263:C:H4'	1:6:292:U:H5'	1.97	0.46
55:M9:163:ARG:HD3	1:6:813:U:C6	305.23	0.46
1:2:622:A:OP2	86:2:2158:OHX:N1	2.49	0.46
68:O2:24:ARG:HG2	68:O2:25:TYR:CZ	2.72	0.46
43:L6:68:PRO:HG2	43:L6:71:VAL:HG21	3.24	0.46
19:C7:2:GLY:N	1:6:1312:A:OP1	392.18	0.46
36:5:985:U:H2'	36:5:986:U:H6	1.80	0.46
1:2:102:U:O4	1:2:360:A:H2'	2.16	0.46
21:C9:15:ILE:HD11	21:C9:63:ARG:HD3	3.18	0.46
36:1:1683:A:OP2	58:N2:85:LYS:HE2	2.15	0.46
36:5:435:C:H2'	36:5:436:A:O4'	2.14	0.46
34:SR:106:HIS:CD2	34:SR:110:VAL:HG22	2.85	0.46
1:2:1240:U:OP2	86:2:2145:OHX:N1	2.49	0.46
1:2:808:U:H2'	1:2:809:A:C8	2.51	0.46
46:L9:122:LYS:HG2	46:L9:123:ILE:N	3.22	0.46
40:L3:80:ASP:OD2	40:L3:314:TYR:OH	2.70	0.46
37:3:39:C:N3	48:M1:70:THR:HG23	2.30	0.46
1:2:604:A:OP2	86:2:2169:OHX:N5	2.48	0.46
36:1:806:A:H5''	36:1:936:A:H61	1.81	0.46
1:2:1615:C:O2'	1:2:1616:G:OP2	2.32	0.46
36:1:818:C:N3	36:1:920:A:H5'	2.31	0.46
41:L4:229:ASN:OD1	41:L4:231:ALA:N	2.36	0.46
37:3:24:A:H2'	37:3:25:G:O4'	2.16	0.46
4:S2:246:GLU:HG2	4:S2:246:GLU:H	1.62	0.46
63:N7:17:ARG:HG2	70:O4:73:SER:O	2.15	0.46
51:M5:96:ARG:HD3	36:5:31:C:H4'	125.24	0.46
3:S1:69:CYS:CB	16:C4:114:ARG:HD3	3.19	0.46
24:D2:77:PRO:HG3	25:D3:7:ARG:O	2.16	0.46
1:6:1255:G:H4'	1:6:1256:A:OP1	2.15	0.46
51:M5:31:ARG:HG3	51:M5:129:TYR:OH	3.44	0.46
16:C4:81:VAL:HG13	16:C4:115:ILE:HG23	3.14	0.46
36:1:715:A:H4'	36:1:716:A:OP1	2.15	0.46
74:O8:4:GLU:HG2	74:O8:5:ILE:H	1.80	0.46
36:5:1235:U:C4'	36:5:1236:G:H5'	2.45	0.46
1:6:104:A:H61	1:6:308:C:H5'	1.81	0.46
26:D4:105:ARG:O	26:D4:109:LYS:HG3	2.16	0.46
42:L5:279:LYS:O	42:L5:279:LYS:HD3	2.16	0.46
36:1:1555:U:H5''	36:1:1556:C:OP2	2.16	0.46
36:1:1947:G:OP1	55:M9:136:ARG:NH1	2.49	0.46
24:D2:7:LEU:HD22	24:D2:11:LEU:HG	2.12	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:2655:U:C5	78:Q2:4:VAL:HG12	2.50	0.46
41:L4:71:VAL:HG13	41:L4:76:ARG:NH1	2.30	0.46
39:L2:104:LEU:O	39:L2:107:VAL:HG22	2.39	0.46
6:S4:159:THR:HB	6:S4:227:VAL:HG23	2.03	0.46
36:1:2970:C:H4'	36:1:2971:A:N1	2.31	0.46
53:M7:4:TYR:CE1	53:M7:16:SER:HB2	2.60	0.46
40:L3:168:LYS:O	40:L3:319:ASN:ND2	2.37	0.46
1:6:968:U:H2'	1:6:969:C:O4'	2.15	0.46
1:2:859:A:C6	15:C3:73:ARG:HD3	2.49	0.46
36:5:1349:G:H2'	36:5:1350:A:C8	2.51	0.46
34:SR:111:MET:N	34:SR:125:GLY:O	2.90	0.46
36:1:1796:G:H5''	36:1:1797:A:OP1	2.16	0.46
1:2:516:G:OP2	86:2:2071:OHX:N6	2.48	0.46
33:E1:134:ASN:H	1:6:1251:U:H4'	443.14	0.46
36:5:3094:A:H2'	36:5:3095:U:C6	2.51	0.46
1:2:1427:A:OP2	35:SM:93:ARG:NH1	2.49	0.46
22:D0:32:LYS:H	22:D0:32:LYS:HD2	4.30	0.46
36:1:3154:C:C2	36:1:3157:U:O4	2.68	0.46
1:2:1194:A:OP2	22:D0:75:GLY:N	2.48	0.46
16:C4:84:ARG:HA	16:C4:119:THR:HG22	1.97	0.46
1:6:470:A:H8	1:6:470:A:C5'	2.28	0.46
1:2:1482:C:OP2	1:2:1521:G:N1	2.45	0.46
42:L5:244:HIS:O	42:L5:248:ARG:HG3	2.15	0.46
63:N7:50:PRO:HD3	63:N7:68:ILE:HG12	1.96	0.46
41:L4:144:LYS:O	41:L4:144:LYS:HE3	2.15	0.46
86:5:4187:OHX:N1	86:5:4189:OHX:N4	2.64	0.46
72:O6:58:ILE:HG22	72:O6:90:MET:CG	3.03	0.46
36:1:2261:G:O6	86:1:3937:OHX:N4	2.48	0.46
46:L9:171:ASP:HA	36:5:2899:C:C5	323.69	0.46
4:S2:178:ILE:HD12	4:S2:189:GLN:HG3	1.97	0.46
74:O8:17:ARG:HG2	74:O8:19:ASP:OD2	3.56	0.46
59:N3:17:LEU:HD21	59:N3:98:ASN:ND2	2.31	0.46
42:L5:184:ASP:OD2	42:L5:187:THR:OG1	6.40	0.46
1:6:486:G:H4'	1:6:486:G:OP1	2.15	0.46
5:S3:38:GLU:OE1	5:S3:40:ARG:NE	2.49	0.46
24:D2:83:ILE:O	24:D2:86:ILE:HG12	2.16	0.46
16:C4:29:HIS:HB3	16:C4:41:ARG:HG3	1.97	0.46
29:D7:50:ALA:O	29:D7:52:THR:N	2.46	0.46
48:M1:32:ARG:O	48:M1:36:VAL:HG23	2.15	0.46
86:1:4056:OHX:N5	86:1:4163:OHX:N3	2.63	0.46
7:S5:29:ILE:HA	7:S5:30:PRO:HD3	1.95	0.46
1:2:1091:A:H5''	1:2:1091:A:N3	2.31	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:C7:71:PHE:HE1	19:C7:73:LEU:HD22	1.80	0.46
36:5:3156:U:O2'	36:5:3157:U:O2	2.33	0.46
39:L2:109:GLU:HG3	1:6:922:G:H4'	242.86	0.46
44:L7:143:THR:HG22	44:L7:241:LYS:HE3	1.97	0.46
50:M4:134:ALA:C	50:M4:136:ALA:H	2.45	0.46
36:1:3084:C:H2'	36:1:3085:G:O4'	2.15	0.46
40:L3:307:PRO:HD3	40:L3:311:PHE:CE2	2.88	0.46
15:C3:85:PRO:HG2	15:C3:129:TYR:CE2	2.63	0.46
1:6:1053:G:N7	86:6:2196:OHX:N4	2.63	0.46
86:5:4033:OHX:N3	86:5:4081:OHX:N6	2.64	0.46
10:S8:154:SER:O	10:S8:158:SER:HB3	3.53	0.46
36:1:1221:A:H3'	36:1:1222:G:C5'	2.45	0.46
1:2:142:G:O5'	1:2:142:G:C8	2.68	0.46
7:S5:143:ARG:NH1	7:S5:218:GLU:OE1	2.49	0.46
53:M7:25:SER:HB3	53:M7:28:ASN:HB2	2.61	0.46
34:SR:178:VAL:HB	34:SR:192:PHE:HB2	2.19	0.46
36:1:291:C:OP1	51:M5:68:ARG:NH1	2.49	0.46
47:M0:24:ARG:O	47:M0:25:ALA:HB3	4.59	0.46
54:M8:147:ARG:NH2	36:5:670:C:OP1	162.87	0.46
71:O5:84:LYS:HB3	71:O5:85:THR:H	1.47	0.46
36:5:2101:C:H2'	36:5:2102:U:H6	1.81	0.46
4:S2:186:LYS:HA	4:S2:186:LYS:HD2	2.57	0.46
30:D8:26:THR:H	30:D8:44:VAL:HG22	2.65	0.46
39:L2:172:GLY:HA3	79:Q3:67:GLY:HA2	3.77	0.46
67:O1:19:ARG:HB3	67:O1:35:GLU:HG2	1.97	0.46
36:1:2442:G:H2'	36:1:2443:A:H5''	1.97	0.46
36:1:735:A:H2'	36:1:736:A:H8	1.78	0.46
86:5:4212:OHX:N2	86:5:4222:OHX:N5	2.63	0.46
1:2:1445:G:N2	33:E1:90:LYS:O	2.49	0.46
33:E1:94:LYS:HB3	33:E1:95:HIS:H	1.50	0.46
72:O6:97:SER:OG	72:O6:98:ARG:N	2.49	0.46
49:M3:16:LYS:HE3	36:5:49:A:OP1	134.22	0.46
1:2:1606:C:H2'	1:2:1607:G:C8	2.51	0.46
40:L3:222:LYS:HG2	40:L3:223:GLY:N	2.30	0.46
1:2:386:G:OP2	10:S8:25:ARG:NH2	2.48	0.46
1:2:1662:G:C2'	1:2:1663:G:H5'	2.46	0.46
38:8:145:U:H2'	38:8:146:U:H6	1.80	0.46
11:S9:117:GLY:O	11:S9:119:ALA:N	2.48	0.46
54:M8:41:ASP:OD1	54:M8:41:ASP:C	2.54	0.46
36:1:598:A:OP1	44:L7:41:ARG:NH1	2.48	0.46
45:L8:106:LYS:O	45:L8:110:THR:HG23	4.45	0.46
36:5:3216:G:H3'	36:5:3219:G:N3	2.31	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:M5:56:LYS:NZ	51:M5:145:ASP:OD2	2.96	0.46
4:S2:188:LEU:HD13	4:S2:196:VAL:HG11	2.03	0.46
34:SR:108:SER:OG	34:SR:109:ASP:N	2.46	0.46
35:SM:35:ALA:O	35:SM:37:VAL:N	2.98	0.46
1:6:1078:C:H2'	1:6:1079:U:C6	2.51	0.46
17:C5:64:LYS:HG3	17:C5:73:PRO:HG3	1.97	0.46
36:5:2581:U:O2'	36:5:2582:C:H5'	2.15	0.46
41:L4:104:LYS:HD2	41:L4:106:TRP:CZ2	2.57	0.46
8:S6:193:LEU:HA	8:S6:193:LEU:HD23	1.76	0.46
36:5:1507:G:H5'	36:5:1507:G:N3	2.31	0.46
36:1:1454:A:OP2	86:1:4210:OHX:N6	2.49	0.46
68:O2:99:ASN:N	68:O2:99:ASN:OD1	2.63	0.46
64:N8:7:LYS:HA	64:N8:7:LYS:HD3	1.79	0.46
77:Q1:15:ARG:HG3	77:Q1:15:ARG:HH11	4.53	0.46
1:2:1748:G:O6	86:2:2105:OHX:N4	2.49	0.46
7:S5:117:THR:HG22	7:S5:121:ILE:HD11	1.98	0.46
1:2:1649:G:N7	86:2:2052:OHX:N1	2.64	0.46
36:5:1066:G:OP1	86:5:4226:OHX:N2	2.49	0.46
39:L2:204:MET:HE3	39:L2:209:HIS:HB2	1.97	0.46
37:7:23:A:H2'	37:7:24:A:C8	2.51	0.46
57:N1:68:THR:HG21	36:5:2736:A:O2'	226.27	0.46
20:C8:127:HIS:CD2	20:C8:133:VAL:HG11	3.56	0.46
25:D3:12:ALA:O	25:D3:16:ARG:HB2	4.07	0.46
36:1:1231:A:OP2	86:1:4089:OHX:N6	2.49	0.46
1:2:830:U:H2'	1:2:830:U:O2	2.15	0.46
6:S4:192:ILE:HD13	6:S4:238:LEU:HD22	1.97	0.46
39:L2:114:SER:HB2	39:L2:169:ILE:CD1	2.45	0.46
45:L8:94:PHE:CE2	45:L8:200:LEU:HG	2.51	0.46
36:5:3165:A:C6	36:5:3286:G:C6	3.04	0.46
1:2:1490:C:H1'	1:2:1491:U:O4'	2.15	0.46
19:C7:23:LYS:O	19:C7:24:LEU:HB2	2.16	0.46
1:6:1673:G:O5'	1:6:1673:G:H8	1.98	0.46
36:1:308:A:H5'	36:1:2223:A:O2'	2.16	0.46
53:M7:41:LEU:HD21	53:M7:95:LEU:HD22	1.98	0.46
2:S0:193:GLN:C	2:S0:195:TRP:H	2.19	0.46
61:N5:105:VAL:HG11	61:N5:126:LEU:HD13	3.02	0.46
36:1:1831:U:OP2	61:N5:92:LYS:HD2	2.16	0.46
36:1:1831:U:O2'	38:4:114:G:OP1	2.21	0.46
36:5:209:A:H4'	36:5:211:A:C8	2.51	0.46
78:Q2:2:VAL:HA	36:5:2655:U:OP2	240.91	0.46
36:1:1659:U:H2'	36:1:1660:C:C6	2.51	0.46
1:2:1332:C:O5'	1:2:1332:C:H6	1.99	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:S8:117:TYR:CD1	10:S8:150:ALA:HB2	2.51	0.46
1:2:1157:A:H3'	1:2:1157:A:C8	2.51	0.46
1:2:808:U:O4	1:2:809:A:N6	2.49	0.46
4:S2:243:TYR:HB3	4:S2:246:GLU:HG3	2.19	0.46
36:5:3013:U:H2'	36:5:3014:U:C6	2.50	0.46
36:1:3192:U:H2'	36:1:3193:C:C6	2.50	0.46
36:1:2158:A:H5'	36:1:2160:G:O4'	2.15	0.46
18:C6:55:VAL:HG21	18:C6:105:LEU:HG	2.20	0.46
46:L9:88:TYR:CE2	46:L9:184:LYS:HG2	2.51	0.46
1:6:1175:U:H2'	1:6:1176:G:C8	2.51	0.46
34:SR:232:TYR:HE1	34:SR:234:LEU:HD11	1.81	0.46
35:SM:52:PRO:O	35:SM:54:PRO:HD3	5.22	0.46
17:C5:72:LYS:H	17:C5:72:LYS:HG2	3.10	0.46
55:M9:116:ASP:OD1	55:M9:116:ASP:N	4.05	0.46
73:O7:65:ARG:HG3	73:O7:65:ARG:HH11	1.80	0.46
35:SM:97:THR:C	35:SM:99:LYS:H	2.18	0.46
49:M3:129:ASN:CG	49:M3:130:GLY:H	3.84	0.46
37:7:106:U:H2'	37:7:107:C:O4'	2.16	0.46
41:L4:299:ILE:HG22	41:L4:300:ARG:O	2.16	0.46
56:N0:13:ARG:HA	56:N0:56:GLY:HA2	1.98	0.46
22:D0:71:PRO:HB3	31:D9:41:GLN:HG2	2.55	0.46
1:2:647:G:N2	1:2:687:G:N2	2.64	0.46
20:C8:132:ARG:HG3	20:C8:138:THR:HG22	1.98	0.46
40:L3:116:ARG:HG2	40:L3:175:LYS:CA	2.44	0.46
86:2:2045:OHX:N2	86:2:2099:OHX:N6	2.64	0.46
45:L8:108:ARG:HA	45:L8:111:LYS:HD2	3.44	0.46
86:2:2096:OHX:N4	86:2:2109:OHX:N2	2.64	0.46
59:N3:15:LEU:HD23	59:N3:53:SER:HB3	1.97	0.46
86:5:4066:OHX:N1	86:5:4141:OHX:N4	2.64	0.46
86:1:3995:OHX:N1	86:1:4034:OHX:N2	2.64	0.46
36:1:2533:G:H2'	36:1:2534:G:O4'	2.15	0.46
36:1:307:A:H2'	36:1:308:A:C8	2.50	0.46
6:S4:199:GLU:OE2	6:S4:209:HIS:NE2	2.46	0.46
60:N4:5:ILE:HD12	60:N4:10:GLY:HA2	1.98	0.46
17:C5:31:GLU:HG3	17:C5:32:ASP:N	2.29	0.46
9:S7:89:HIS:ND1	9:S7:168:SER:OG	2.31	0.46
3:S1:143:THR:HB	3:S1:205:PHE:HE1	1.80	0.46
34:SR:80:ALA:O	34:SR:91:LEU:HD12	2.16	0.46
42:L5:215:ASP:OD1	42:L5:218:ARG:HG3	2.15	0.46
42:L5:176:SER:OG	36:5:2747:A:OP1	244.68	0.46
36:1:2617:U:H3'	65:N9:3:LYS:HD3	1.98	0.46
41:L4:119:ARG:HA	41:L4:122:THR:HG23	2.57	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
41:L4:315:LYS:NZ	36:5:609:G:OP2	240.29	0.46
36:1:1856:C:H2'	36:1:1857:C:C6	2.50	0.46
56:N0:146:LYS:HE3	36:5:535:G:P	360.65	0.46
36:1:1509:A:O2'	36:1:1510:G:H5'	2.15	0.46
36:1:1785:U:H2'	36:1:1786:G:C8	2.51	0.46
36:1:1886:A:O4'	36:1:3307:A:H5'	2.16	0.46
27:D5:88:ILE:O	27:D5:104:ALA:N	2.49	0.46
86:2:2172:OHX:N3	86:2:2173:OHX:N4	2.64	0.46
1:2:1266:U:H2'	1:2:1267:G:C8	2.51	0.46
1:2:147:A:H2'	1:2:148:A:O4'	2.16	0.46
36:1:2298:U:O4	36:1:2923:U:H5	1.99	0.46
34:SR:183:LEU:HD23	34:SR:183:LEU:HA	1.80	0.46
37:3:40:C:O2'	48:M1:72:ARG:HD2	2.16	0.46
18:C6:59:LYS:HB2	18:C6:59:LYS:HE2	1.78	0.46
45:L8:169:LEU:HD23	45:L8:169:LEU:HA	2.02	0.46
1:6:492:A:H2'	1:6:493:U:H5''	1.98	0.46
68:O2:60:ASN:OD1	68:O2:62:LYS:HB2	2.15	0.46
36:1:3181:C:O2'	52:M6:164:SER:OG	2.29	0.45
3:S1:220:GLN:H	3:S1:220:GLN:HG3	1.47	0.45
47:M0:76:MET:CE	47:M0:138:VAL:HG11	2.46	0.45
37:3:27:A:P	42:L5:57:ASN:H	2.39	0.45
36:1:2513:U:H4'	36:1:2514:U:OP1	2.16	0.45
1:2:218:A:HO2'	1:2:219:A:P	2.32	0.45
36:1:2112:U:H5''	60:N4:44:LYS:NZ	2.30	0.45
6:S4:104:ASP:HB2	6:S4:108:ARG:H	1.81	0.45
22:D0:65:ILE:HD11	31:D9:36:LEU:HD21	1.98	0.45
5:S3:211:PRO:HG3	19:C7:20:TYR:CE1	2.51	0.45
61:N5:38:LEU:CD1	61:N5:40:LEU:HD13	2.45	0.45
45:L8:25:PRO:HG2	45:L8:27:THR:HB	1.98	0.45
64:N8:66:ALA:HB1	64:N8:69:TRP:HB2	4.33	0.45
31:D9:30:LEU:HA	31:D9:39:CYS:HA	2.19	0.45
66:O0:30:THR:HB	66:O0:91:SER:HB2	1.98	0.45
51:M5:5:LYS:NZ	51:M5:8:GLU:OE1	3.99	0.45
1:2:584:C:OP2	86:2:2027:OHX:N6	2.49	0.45
36:1:3079:U:OP1	36:1:3079:U:H6	1.99	0.45
40:L3:81:THR:HB	40:L3:321:PHE:HA	1.97	0.45
6:S4:121:TYR:HA	6:S4:164:LEU:HG	1.98	0.45
6:S4:179:LYS:N	6:S4:194:THR:O	2.50	0.45
1:6:234:G:H2'	1:6:235:G:O4'	2.16	0.45
36:5:1363:A:OP2	86:5:4197:OHX:N3	2.49	0.45
1:2:1783:C:H2'	1:2:1784:C:C6	2.50	0.45
86:1:4059:OHX:N2	86:1:4166:OHX:N5	2.63	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:846:G:H2'	1:6:847:A:H8	1.81	0.45
13:C1:46:LYS:HA	13:C1:46:LYS:HD2	2.41	0.45
66:O0:77:LEU:O	66:O0:81:VAL:HG22	2.27	0.45
36:1:1517:G:P	75:O9:41:ARG:HH22	2.39	0.45
36:1:1795:U:H4'	36:1:1796:G:C4	2.51	0.45
61:N5:58:ASP:O	61:N5:62:VAL:HG23	2.16	0.45
1:2:1754:A:O2'	86:2:2059:OHX:N5	2.48	0.45
74:O8:22:THR:HG22	74:O8:74:LYS:HB3	4.26	0.45
74:O8:30:LYS:HD2	74:O8:40:GLN:NE2	3.00	0.45
62:N6:74:TYR:CE1	62:N6:77:LYS:HD2	4.84	0.45
1:2:1781:A:H2'	1:2:1782:A:O4'	2.16	0.45
1:6:1218:G:O6	1:6:1444:A:H2'	2.16	0.45
46:L9:103:ILE:HG12	46:L9:136:PHE:CE2	2.52	0.45
46:L9:138:THR:O	46:L9:139:ASN:ND2	2.39	0.45
36:1:2558:U:O2'	36:1:2559:U:H5'	2.16	0.45
36:5:577:C:H2'	36:5:579:G:H5''	1.97	0.45
3:S1:226:GLY:HA2	36:5:2536:A:H4'	257.56	0.45
57:N1:119:ALA:HB2	57:N1:126:VAL:HG13	2.02	0.45
36:5:953:G:H2'	36:5:1117:G:H5''	1.99	0.45
68:O2:61:LYS:HD3	36:5:1339:C:OP1	193.89	0.45
23:D1:60:ARG:HA	23:D1:65:SER:HB2	2.18	0.45
15:C3:105:ASN:C	15:C3:107:LYS:H	2.20	0.45
36:5:2403:G:N7	36:5:2870:C:H4'	2.31	0.45
70:O4:81:CYS:SG	70:O4:84:CYS:SG	3.13	0.45
3:S1:142:PHE:O	3:S1:207:LEU:HA	2.22	0.45
3:S1:48:VAL:HG22	3:S1:64:ARG:NH2	3.28	0.45
39:L2:226:SER:N	36:5:2202:C:H5''	208.99	0.45
36:5:2897:A:H2'	36:5:2899:C:H5'	1.97	0.45
4:S2:42:GLY:HA2	4:S2:68:ILE:HD11	1.97	0.45
1:2:1788:G:P	16:C4:127:ARG:HH12	2.39	0.45
11:S9:109:LEU:HB2	11:S9:146:PHE:HB2	3.24	0.45
1:2:61:A:C8	1:2:269:G:O2'	2.64	0.45
16:C4:136:ARG:HD2	1:6:1769:U:O2	303.41	0.45
12:C0:32:HIS:CG	12:C0:33:GLU:H	3.34	0.45
28:D6:44:ILE:HD12	28:D6:45:VAL:HG22	1.97	0.45
86:5:4066:OHX:N5	86:5:4141:OHX:N2	2.64	0.45
1:2:649:U:O2'	1:2:650:U:H6	2.00	0.45
36:5:1481:A:C2'	36:5:1858:A:N3	2.79	0.45
33:E1:83:LYS:O	33:E1:84:VAL:HG12	2.17	0.45
27:D5:82:HIS:O	27:D5:84:GLU:N	3.38	0.45
53:M7:31:GLU:CG	53:M7:60:PHE:HA	3.47	0.45
2:S0:188:LEU:HB3	2:S0:189:VAL:H	1.57	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
86:1:4065:OHX:N4	86:1:4177:OHX:N2	2.64	0.45
36:1:1553:U:H4'	36:1:1554:U:H5'	1.98	0.45
36:5:655:C:H2'	36:5:656:A:C8	2.51	0.45
69:O3:49:ILE:HD11	69:O3:71:VAL:N	2.31	0.45
1:2:987:G:C2	39:L2:249:SER:HB2	2.52	0.45
55:M9:158:GLU:HG2	55:M9:158:GLU:H	2.11	0.45
21:C9:6:VAL:HB	21:C9:14:PHE:CE1	2.50	0.45
51:M5:44:ARG:HH22	36:5:269:G:P	125.81	0.45
1:2:1316:G:H2'	1:2:1317:C:H6	1.81	0.45
86:2:2172:OHX:N5	86:2:2173:OHX:N1	2.65	0.45
55:M9:180:LYS:HA	55:M9:183:ALA:HB3	1.98	0.45
61:N5:86:VAL:HG12	61:N5:120:LYS:HB3	1.99	0.45
54:M8:62:VAL:O	54:M8:87:VAL:HA	2.42	0.45
8:S6:14:LYS:HG2	8:S6:16:PHE:CE2	4.46	0.45
36:5:566:G:N7	86:5:4130:OHX:N5	2.65	0.45
36:1:2659:G:N7	86:1:3883:OHX:N5	2.64	0.45
44:L7:191:VAL:O	44:L7:191:VAL:HG12	2.16	0.45
18:C6:87:LYS:HB3	18:C6:87:LYS:HE2	2.15	0.45
36:1:2571:U:H2'	36:1:2571:U:OP1	2.16	0.45
36:1:107:A:OP1	49:M3:39:ARG:NH1	2.47	0.45
42:L5:90:HIS:NE2	42:L5:229:ASP:OD2	3.05	0.45
36:5:1064:A:H4'	36:5:1065:A:O5'	2.16	0.45
16:C4:119:THR:HA	16:C4:120:PRO:HD2	2.24	0.45
41:L4:16:THR:HG22	41:L4:18:ASN:HB3	1.99	0.45
40:L3:35:ASP:OD2	40:L3:37:ARG:HD2	2.31	0.45
36:1:2767:U:P	86:1:4136:OHX:N2	2.89	0.45
36:5:298:U:H5''	36:5:299:G:H5'	1.97	0.45
40:L3:169:THR:HG23	40:L3:171:LEU:H	1.95	0.45
8:S6:63:MET:HE1	8:S6:106:LEU:HD13	2.87	0.45
39:L2:147:ARG:NH2	39:L2:155:LYS:HG3	5.13	0.45
36:1:410:U:O4	86:1:4060:OHX:N2	2.50	0.45
13:C1:101:GLU:OE1	25:D3:16:ARG:NH2	3.61	0.45
36:1:3121:U:H1'	36:1:3122:A:H5''	1.97	0.45
40:L3:53:MET:HE3	36:5:3048:A:H5''	233.16	0.45
42:L5:95:TRP:CH2	42:L5:161:GLY:HA2	2.51	0.45
22:D0:105:GLN:HG3	22:D0:106:ILE:H	1.80	0.45
22:D0:108:ILE:H	22:D0:108:ILE:HG13	1.60	0.45
40:L3:102:LEU:HD23	40:L3:102:LEU:N	2.28	0.45
44:L7:47:ARG:NH2	44:L7:179:LEU:HD11	2.79	0.45
36:5:2093:A:O2'	36:5:2094:C:O4'	2.24	0.45
26:D4:112:LYS:NZ	1:6:57:G:OP1	345.52	0.45
30:D8:66:LEU:HA	30:D8:66:LEU:HD23	1.73	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
40:L3:147:GLU:OE1	40:L3:150:ARG:NH2	4.86	0.45
36:1:3065:G:O6	86:1:4138:OHX:N6	2.48	0.45
36:1:2877:G:H2'	36:1:2878:G:O4'	2.16	0.45
55:M9:15:VAL:HG11	55:M9:52:LYS:HG3	1.97	0.45
36:1:1362:G:H2'	36:1:1363:A:C8	2.52	0.45
36:5:2440:G:H2'	36:5:2441:A:C8	2.51	0.45
14:C2:131:ASP:HB2	14:C2:132:GLU:CD	2.37	0.45
6:S4:222:LEU:O	6:S4:225:VAL:N	2.47	0.45
36:1:2407:C:H2'	36:1:2408:U:H6	1.81	0.45
54:M8:120:GLU:OE2	54:M8:130:ARG:NH2	2.73	0.45
38:8:1:A:OP1	86:8:214:OHX:N5	2.50	0.45
36:1:3088:G:H2'	36:1:3089:C:O4'	2.16	0.45
1:2:1347:U:O2	1:2:1516:A:H5'	2.17	0.45
73:O7:24:ARG:NH1	36:5:361:A:OP1	120.91	0.45
1:6:794:U:H3'	1:6:795:U:H5'	1.98	0.45
51:M5:44:ARG:HB2	51:M5:47:LYS:HB3	2.27	0.45
36:5:595:G:H1	36:5:609:G:H5''	1.81	0.45
68:O2:19:ARG:HD2	68:O2:28:VAL:CG1	2.90	0.45
63:N7:54:THR:OG1	63:N7:55:LYS:N	2.50	0.45
78:Q2:40:LYS:HE3	78:Q2:44:ASP:OD2	2.17	0.45
36:1:2383:C:H5'	52:M6:71:PHE:CE2	2.52	0.45
6:S4:246:LEU:HD21	6:S4:254:ARG:CZ	2.46	0.45
36:5:2883:U:OP2	86:5:4061:OHX:N4	2.50	0.45
1:6:1154:G:N7	86:6:2135:OHX:N2	2.65	0.45
4:S2:187:LEU:HD12	4:S2:211:LEU:HD22	5.32	0.45
42:L5:24:ARG:NH2	37:7:13:A:N3	293.75	0.45
36:1:1915:A:H2'	36:1:1916:U:C6	2.51	0.45
21:C9:108:LEU:HA	21:C9:111:ILE:HG22	1.98	0.45
36:5:2585:G:C2	38:8:151:C:H5	2.35	0.45
60:N4:17:ARG:HD3	60:N4:17:ARG:HA	1.73	0.45
6:S4:33:ALA:O	1:6:121:U:H1'	351.99	0.45
86:2:2084:OHX:N6	86:2:2086:OHX:N5	2.65	0.45
1:6:180:A:H2'	1:6:181:A:O4'	2.16	0.45
7:S5:76:ARG:NH2	18:C6:120:ASP:OD1	2.49	0.45
18:C6:129:PHE:CE1	22:D0:78:THR:HA	2.79	0.45
36:1:29:C:H4'	36:1:62:A:H4'	1.98	0.45
36:1:3139:A:H2'	36:1:3140:G:O4'	2.17	0.45
36:5:708:G:H5''	36:5:708:G:H8	1.81	0.45
15:C3:80:LEU:HD12	15:C3:80:LEU:HA	3.15	0.45
64:N8:62:HIS:O	64:N8:62:HIS:CG	2.81	0.45
55:M9:13:SER:OG	55:M9:38:ARG:NH2	2.49	0.45
36:1:3257:C:H2'	36:1:3258:U:O4'	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:1738:U:H2'	1:2:1739:C:C6	2.51	0.45
36:5:3154:C:O2	36:5:3154:C:H2'	2.17	0.45
36:1:505:G:OP1	41:L4:320:ASN:ND2	2.39	0.45
20:C8:11:PHE:CD1	27:D5:41:ILE:HD13	4.12	0.45
3:S1:51:SER:HB3	3:S1:57:ALA:H	2.80	0.45
36:1:315:C:OP2	72:O6:28:TYR:OH	2.30	0.45
25:D3:7:ARG:HG2	25:D3:7:ARG:HH11	1.81	0.45
36:1:330:G:OP2	86:1:4046:OHX:N2	2.49	0.45
1:2:542:A:HO2'	1:2:542:A:H8	1.63	0.45
21:C9:105:LEU:O	21:C9:109:GLU:HG3	5.19	0.45
48:M1:23:VAL:HG13	48:M1:29:ARG:HH11	1.81	0.45
7:S5:42:LEU:HB2	7:S5:46:TRP:O	2.16	0.45
41:L4:141:ARG:CZ	41:L4:180:LYS:HD3	2.68	0.45
41:L4:226:GLU:CD	41:L4:246:ARG:HH22	2.46	0.45
51:M5:180:PHE:O	51:M5:184:LYS:HB2	2.16	0.45
59:N3:120:LYS:H	59:N3:137:VAL:CG2	2.30	0.45
9:S7:74:GLN:HG2	9:S7:131:PHE:CD2	4.87	0.45
36:1:1495:U:H5	36:1:1835:A:C2	2.35	0.45
41:L4:269:SER:C	41:L4:271:LYS:H	2.16	0.45
19:C7:34:LEU:HD22	19:C7:38:ILE:HD13	5.16	0.45
26:D4:60:PHE:CD1	26:D4:71:GLY:HA3	2.51	0.45
16:C4:99:GLN:HG3	28:D6:46:GLU:OE2	3.21	0.45
36:1:2746:A:C6	42:L5:148:ILE:HD12	2.50	0.45
6:S4:62:LYS:HE3	6:S4:66:MET:CG	7.12	0.45
2:S0:160:ILE:HA	2:S0:161:PRO:HD2	1.95	0.45
23:D1:36:VAL:HG11	23:D1:78:LEU:HD13	1.98	0.45
44:L7:221:LYS:O	44:L7:228:SER:O	5.06	0.45
60:N4:23:ARG:NH2	60:N4:25:ASP:OD2	2.48	0.45
36:1:627:U:H4'	36:1:1399:A:O2'	2.17	0.45
10:S8:26:LYS:O	10:S8:29:LEU:HB3	2.17	0.45
10:S8:29:LEU:C	10:S8:29:LEU:HD23	2.37	0.45
53:M7:36:ILE:HG12	53:M7:44:ALA:HB1	1.98	0.45
22:D0:51:VAL:O	22:D0:52:LYS:HB2	4.19	0.45
14:C2:74:LEU:HD11	33:E1:106:TYR:CD1	2.50	0.45
9:S7:46:ILE:HG12	9:S7:60:ILE:HA	2.00	0.45
9:S7:96:ARG:CZ	9:S7:124:LYS:HB3	2.57	0.45
25:D3:132:LEU:O	25:D3:136:TRP:N	2.78	0.45
68:O2:43:ARG:NH1	36:5:1368:U:H5'	194.07	0.45
36:1:2225:U:H2'	36:1:2226:U:H6	1.79	0.45
36:1:847:A:H2'	36:1:848:A:C8	2.51	0.45
36:5:2505:U:H2'	36:5:2506:U:C5	2.51	0.45
64:N8:84:GLU:HA	64:N8:87:ARG:HB2	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
50:M4:8:LYS:HB3	50:M4:9:ALA:H	1.55	0.45
34:SR:200:ASN:N	34:SR:214:ALA:O	2.72	0.45
40:L3:106:TRP:HB2	40:L3:133:TYR:CE2	2.51	0.45
36:5:2217:U:H2'	36:5:2218:G:H8	1.81	0.45
21:C9:40:SER:OG	21:C9:96:ALA:HA	2.16	0.45
34:SR:112:SER:HB2	34:SR:153:GLN:HA	2.01	0.45
59:N3:74:MET:SD	59:N3:102:ILE:HD13	2.57	0.45
76:Q0:88:LYS:HB3	76:Q0:88:LYS:HE3	4.22	0.45
2:S0:111:ILE:HA	2:S0:111:ILE:HD12	1.71	0.45
57:N1:75:ILE:HG22	57:N1:88:ARG:HD2	1.98	0.45
1:6:658:C:H5'	1:6:659:C:OP2	2.16	0.45
21:C9:77:ASN:OD1	21:C9:101:ASN:ND2	2.49	0.45
16:C4:87:GLY:O	16:C4:90:ARG:HB2	2.16	0.45
42:L5:269:SER:O	42:L5:270:LYS:HB2	4.64	0.45
42:L5:270:LYS:HG2	37:7:2:G:H5'	319.67	0.45
1:2:1683:C:HO2'	1:2:1684:U:P	2.37	0.45
36:5:1564:U:H2'	36:5:1565:G:C8	2.52	0.45
44:L7:152:GLY:O	44:L7:163:LEU:HG	2.17	0.45
36:5:2101:C:H2'	36:5:2102:U:C6	2.51	0.45
5:S3:210:GLU:HA	5:S3:211:PRO:HD3	2.06	0.45
58:N2:100:THR:O	58:N2:101:ASN:HB2	2.17	0.45
4:S2:178:ILE:HB	4:S2:185:LYS:HE3	1.98	0.45
74:O8:17:ARG:NH2	74:O8:52:TYR:OH	3.66	0.45
1:2:420:A:H2'	1:2:421:A:O4'	2.17	0.45
3:S1:105:PHE:CD2	3:S1:213:ARG:HA	2.52	0.45
34:SR:33:LEU:O	34:SR:45:TRP:HD1	1.99	0.45
46:L9:84:LYS:HA	46:L9:188:THR:HB	4.25	0.45
31:D9:21:CYS:HA	31:D9:30:LEU:HD21	3.18	0.45
5:S3:195:SER:HB2	5:S3:200:LYS:HG2	5.47	0.45
43:L6:42:LEU:HD23	43:L6:84:VAL:HG22	2.46	0.45
1:6:56:U:H4'	1:6:57:G:H5'	1.97	0.45
13:C1:6:THR:HB	13:C1:9:SER:HB3	1.98	0.45
2:S0:172:LEU:HD22	2:S0:176:LEU:HG	1.98	0.45
86:5:4201:OHX:N2	86:8:224:OHX:N5	2.64	0.45
36:5:1560:G:C6	36:5:1580:A:N6	2.85	0.45
42:L5:55:PHE:CZ	42:L5:158:ARG:HG3	2.52	0.45
61:N5:76:VAL:HG22	61:N5:81:ILE:O	2.16	0.45
41:L4:157:GLU:HB3	41:L4:211:GLU:O	2.17	0.45
33:E1:117:LEU:HB3	33:E1:118:ARG:NH1	2.30	0.45
11:S9:119:ALA:HA	11:S9:124:HIS:HD2	1.80	0.45
7:S5:41:LYS:HB3	7:S5:41:LYS:HE2	2.74	0.45
36:5:2960:C:OP1	86:5:3972:OHX:N5	2.50	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
57:N1:54:HIS:CD2	36:5:2724:U:H4'	229.90	0.45
40:L3:84:VAL:HG13	40:L3:162:VAL:HB	2.00	0.45
52:M6:31:GLN:HG3	52:M6:33:ILE:HD12	1.99	0.45
1:2:943:C:N4	28:D6:15:ARG:HG2	2.31	0.45
67:O1:23:VAL:O	67:O1:28:ARG:NH1	2.47	0.45
1:2:1057:U:H1'	1:2:1058:U:H2'	1.99	0.45
54:M8:145:ASN:ND2	36:5:746:A:OP1	176.97	0.45
14:C2:24:ILE:O	14:C2:26:ASP:N	2.50	0.45
8:S6:21:GLU:O	8:S6:25:ARG:HB2	2.17	0.45
28:D6:90:GLU:CD	28:D6:90:GLU:H	3.26	0.45
36:1:2516:U:O2'	36:1:2595:A:N6	2.47	0.45
6:S4:125:LYS:HB2	6:S4:226:PHE:CE2	2.92	0.45
23:D1:80:LYS:O	23:D1:81:ASN:HB2	2.17	0.45
16:C4:117:ASP:OD1	16:C4:118:VAL:N	2.49	0.45
78:Q2:50:PHE:O	86:Q2:503:OHX:N2	2.49	0.45
61:N5:115:ARG:NH1	61:N5:115:ARG:HG3	2.21	0.45
6:S4:86:PHE:O	6:S4:87:MET:HB2	2.16	0.45
66:O0:18:ILE:HG13	66:O0:23:TYR:CE1	2.67	0.45
1:2:830:U:O2'	1:2:831:U:OP2	2.31	0.45
43:L6:2:SER:HA	68:O2:81:ASP:OD2	2.67	0.45
66:O0:10:ILE:HD13	66:O0:104:LEU:HD21	5.17	0.45
24:D2:24:GLN:NE2	29:D7:3:LEU:O	5.24	0.45
44:L7:177:GLY:O	44:L7:178:ILE:HB	2.16	0.45
1:6:219:A:C6	1:6:843:U:H1'	2.52	0.45
36:1:3039:C:OP1	59:N3:88:ARG:NH2	2.50	0.45
59:N3:13:ILE:HG13	59:N3:14:SER:N	4.70	0.45
17:C5:18:ARG:NH2	17:C5:38:PRO:HG3	2.55	0.45
36:1:1554:U:O2'	36:1:1582:C:H5	1.98	0.45
40:L3:56:ILE:HG12	40:L3:356:LEU:HD22	2.40	0.45
45:L8:41:GLN:HG3	45:L8:44:ARG:NH1	2.31	0.45
17:C5:123:TYR:HD2	17:C5:124:THR:O	1.98	0.45
54:M8:100:THR:HG23	54:M8:120:GLU:HB3	2.35	0.45
36:1:655:C:H2'	36:1:656:A:H8	1.80	0.45
5:S3:34:TYR:HE2	5:S3:37:VAL:HG13	2.11	0.45
36:1:551:A:C4	36:1:552:G:C8	3.05	0.45
1:6:272:U:O2'	1:6:273:G:OP2	2.28	0.45
7:S5:122:ASN:ND2	7:S5:126:ASP:O	4.03	0.45
3:S1:116:LYS:HB3	3:S1:117:TRP:H	1.65	0.45
65:N9:33:LYS:NZ	36:5:2722:U:OP1	203.66	0.45
7:S5:25:LEU:H	7:S5:25:LEU:HD22	1.81	0.45
86:6:2067:OHX:N3	86:6:2075:OHX:N5	2.65	0.45
36:5:10:C:O2'	36:5:1558:A:N6	2.46	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:S3:203:PRO:HB3	1:6:1332:C:H4'	428.09	0.45
16:C4:88:GLY:O	16:C4:92:LYS:NZ	8.29	0.45
35:SM:47:ALA:HB2	36:1:2678:A:C8	2.51	0.45
40:L3:107:ALA:HA	40:L3:199:PHE:CD2	2.50	0.45
8:S6:164:LYS:HB3	8:S6:167:LYS:O	2.42	0.45
4:S2:54:GLU:OE1	23:D1:11:LEU:HB2	2.59	0.45
42:L5:150:LEU:HD23	42:L5:150:LEU:HA	1.75	0.45
71:O5:73:LYS:HA	71:O5:73:LYS:HD2	5.18	0.45
57:N1:83:ARG:HD2	57:N1:85:LEU:HD21	1.98	0.45
10:S8:184:LEU:HD12	10:S8:184:LEU:HA	1.83	0.45
1:2:1469:A:H2'	1:2:1470:C:C6	2.52	0.45
47:M0:175:ASN:O	47:M0:176:LEU:HB2	4.71	0.45
49:M3:46:ILE:HG22	49:M3:49:ARG:CB	3.59	0.45
2:S0:179:ARG:O	2:S0:183:ARG:HD3	3.38	0.45
36:1:2943:G:P	40:L3:2:SER:HB2	2.56	0.45
18:C6:54:LEU:HD21	18:C6:112:TYR:CE1	3.68	0.45
3:S1:88:VAL:HG11	3:S1:96:LEU:HD12	1.96	0.45
1:2:1433:G:C8	31:D9:41:GLN:HG2	2.51	0.45
24:D2:119:LYS:HB2	24:D2:121:VAL:HG22	4.33	0.45
46:L9:105:GLU:OE2	46:L9:108:GLY:HA2	2.17	0.45
2:S0:58:VAL:O	2:S0:62:ARG:HB2	2.16	0.45
7:S5:59:VAL:O	7:S5:60:ASP:HB2	2.17	0.45
42:L5:269:SER:O	37:7:22:A:N1	324.42	0.45
7:S5:45:LYS:HD3	7:S5:45:LYS:HA	1.37	0.45
35:SM:23:LYS:HD2	35:SM:23:LYS:HA	3.67	0.45
1:2:144:U:O2'	1:2:145:A:H8	1.99	0.45
36:5:3364:C:OP1	86:5:3942:OHX:N1	2.50	0.45
1:2:830:U:O2'	1:2:831:U:H6	1.98	0.45
22:D0:48:HIS:O	22:D0:48:HIS:CG	2.70	0.45
14:C2:45:LEU:O	14:C2:49:THR:HG23	2.21	0.45
3:S1:126:THR:HG22	3:S1:136:ARG:HB2	1.99	0.45
42:L5:95:TRP:HZ3	42:L5:156:GLY:O	8.18	0.45
19:C7:106:THR:O	19:C7:110:VAL:HG23	2.17	0.45
72:O6:26:ILE:HG13	72:O6:26:ILE:H	1.51	0.45
2:S0:33:GLN:C	2:S0:34:GLU:HG2	2.37	0.45
45:L8:140:VAL:O	45:L8:144:GLU:HG3	2.25	0.45
43:L6:5:LYS:O	43:L6:6:ALA:HB2	2.16	0.45
1:6:716:C:H2'	1:6:717:C:O4'	2.17	0.45
86:1:4088:OHX:N6	86:1:4157:OHX:N4	2.64	0.45
86:1:4065:OHX:N6	86:1:4177:OHX:N5	2.65	0.45
1:6:73:U:H2'	1:6:74:U:C6	2.50	0.45
36:5:1781:C:H2'	36:5:1782:U:H6	1.79	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:385:A:H2'	36:1:386:A:H8	1.80	0.45
61:N5:106:ASP:O	61:N5:127:THR:HG23	2.16	0.45
51:M5:73:ARG:O	51:M5:75:VAL:N	4.19	0.45
36:5:2439:A:N6	36:5:2508:U:H3	2.14	0.45
42:L5:119:TYR:CE1	42:L5:135:VAL:HG23	2.52	0.45
12:C0:7:ASP:O	12:C0:11:ILE:HG12	2.16	0.45
1:6:1122:G:O6	86:6:2162:OHX:N6	2.50	0.45
1:2:383:G:N7	86:2:2131:OHX:N4	2.64	0.45
15:C3:124:ARG:NH2	1:6:967:A:OP2	320.18	0.45
1:6:53:G:H2'	1:6:54:C:O4'	2.16	0.45
5:S3:10:LYS:HG3	5:S3:11:LEU:HD23	2.13	0.45
36:1:1879:A:H4'	36:1:1880:U:OP2	2.15	0.45
1:6:994:G:O2'	1:6:995:A:H5'	2.17	0.45
1:2:477:A:H61	1:2:511:A:H61	1.64	0.45
36:5:2137:U:C6	36:5:2141:U:C4	3.05	0.45
36:5:2606:G:N3	36:5:2606:G:H2'	2.31	0.45
50:M4:31:LYS:HD3	50:M4:51:ALA:HB1	3.57	0.45
47:M0:142:ASP:CG	47:M0:178:ARG:HH22	2.70	0.45
1:6:591:A:H2'	1:6:592:A:C8	2.51	0.45
4:S2:140:ARG:HD2	23:D1:10:GLU:OE1	4.55	0.45
1:6:1699:G:H2'	1:6:1700:C:H5'	1.97	0.45
28:D6:73:TYR:CE2	28:D6:83:ILE:HD12	10.09	0.45
7:S5:43:PHE:N	7:S5:46:TRP:H	2.77	0.45
40:L3:265:ALA:C	40:L3:266:ARG:HG2	2.46	0.45
10:S8:197:THR:C	10:S8:199:LYS:H	2.20	0.45
35:SM:83:LYS:CE	1:6:1178:G:H4'	340.38	0.45
36:1:1230:G:N2	36:1:1279:C:N3	2.55	0.45
36:5:1947:G:N2	36:5:2102:U:C2	2.85	0.45
36:1:1246:G:H2'	36:1:1247:U:O4'	2.17	0.45
76:Q0:114:LYS:HG2	76:Q0:115:CYS:N	2.37	0.45
36:1:1426:C:H4'	41:L4:40:THR:HB	1.99	0.45
36:1:3046:A:H2'	36:1:3047:U:O4'	2.17	0.45
1:2:1300:A:P	4:S2:99:LYS:HZ1	2.39	0.45
18:C6:143:ARG:HH22	35:SM:84:LYS:NZ	2.14	0.45
86:2:2116:OHX:N2	86:C1:201:OHX:N4	2.64	0.45
5:S3:164:VAL:O	5:S3:168:ILE:HG13	2.16	0.45
20:C8:52:VAL:HG13	20:C8:61:LEU:HD21	3.25	0.45
24:D2:23:ARG:NH1	24:D2:66:ASN:HA	2.52	0.45
15:C3:91:LEU:HB3	15:C3:122:ILE:HG12	1.98	0.45
34:SR:154:VAL:HG12	34:SR:171:SER:CB	2.46	0.45
86:5:4212:OHX:N4	86:5:4222:OHX:N6	2.64	0.45
43:L6:54:TYR:HA	43:L6:65:ILE:HD12	5.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:416:A:H4'	1:6:417:A:OP2	2.16	0.45
25:D3:142:LYS:HA	25:D3:143:PRO:HD3	1.82	0.45
2:S0:35:PRO:C	2:S0:37:VAL:H	2.20	0.45
1:2:380:U:H5	11:S9:5:PRO:CA	2.29	0.45
43:L6:176:PHE:C	50:M4:114:ASP:H	3.39	0.45
46:L9:124:ARG:HG2	46:L9:164:ILE:HG13	1.99	0.45
51:M5:58:GLY:HA3	51:M5:142:ILE:HD13	1.98	0.45
48:M1:153:LYS:HG2	48:M1:153:LYS:O	5.12	0.45
86:1:4071:OHX:N1	86:1:4118:OHX:N4	2.65	0.45
86:1:4071:OHX:N3	86:1:4118:OHX:N6	2.64	0.45
69:O3:70:LYS:HE2	36:5:585:A:OP1	241.99	0.45
31:D9:7:TRP:O	31:D9:8:PHE:HB2	2.15	0.45
69:O3:2:ALA:HB2	36:5:3216:G:OP2	265.69	0.45
36:1:2320:A:H2	79:Q3:16:VAL:HG13	1.81	0.45
7:S5:120:ILE:O	7:S5:124:LEU:HD13	3.79	0.45
46:L9:7:GLU:OE2	46:L9:54:LYS:HE3	2.17	0.45
52:M6:122:GLN:NE2	36:5:1181:U:H2'	273.04	0.45
10:S8:66:SER:O	10:S8:183:ILE:HG23	5.91	0.45
38:8:121:U:O2'	38:8:122:U:H5'	2.17	0.45
36:1:3173:G:C2	69:O3:96:ALA:HB2	2.52	0.45
77:Q1:2:ARG:HD3	1:6:1772:C:OP1	314.76	0.45
1:2:1509:C:H2'	1:2:1510:U:O4'	2.16	0.45
71:O5:49:LYS:HD2	71:O5:49:LYS:N	2.31	0.45
3:S1:55:LYS:HD3	3:S1:55:LYS:HA	2.07	0.45
1:6:1096:C:H6	1:6:1096:C:H2'	1.56	0.45
1:6:478:A:C2	1:6:511:A:C2	3.05	0.45
4:S2:140:ARG:NH2	4:S2:226:THR:OG1	3.87	0.45
3:S1:164:ILE:O	3:S1:168:ILE:HG13	2.48	0.45
28:D6:84:VAL:HG22	28:D6:85:ARG:N	2.30	0.45
52:M6:110:PRO:C	52:M6:112:TYR:N	3.03	0.45
62:N6:45:ILE:HD12	62:N6:119:ILE:HG23	1.99	0.45
71:O5:78:LYS:HA	71:O5:81:ARG:CD	2.44	0.45
28:D6:36:ILE:HD11	28:D6:83:ILE:HG22	1.99	0.45
28:D6:87:ARG:HB3	28:D6:91:ASP:HB2	1.99	0.45
4:S2:148:LEU:HA	23:D1:4:ASP:HB2	1.98	0.45
73:O7:69:HIS:ND1	73:O7:72:ARG:NH2	2.66	0.45
1:6:1595:U:H3'	1:6:1596:C:O2	2.17	0.45
35:SM:77:THR:O	35:SM:79:SER:N	3.60	0.45
74:O8:59:ALA:O	74:O8:62:ALA:HB3	2.20	0.45
4:S2:37:PRO:HA	4:S2:65:GLU:OE1	2.45	0.45
68:O2:77:ALA:HB3	68:O2:81:ASP:OD2	2.38	0.45
10:S8:8:ARG:CD	10:S8:21:PHE:HB3	2.45	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:D4:57:VAL:HB	26:D4:60:PHE:CE2	4.90	0.45
36:1:716:A:N6	64:N8:117:ARG:HG3	2.32	0.45
36:1:3242:G:H2'	40:L3:154:TYR:CE1	2.52	0.45
86:2:2096:OHX:N6	86:2:2109:OHX:N2	2.65	0.45
46:L9:87:LYS:NZ	46:L9:191:LEU:HD21	16.41	0.45
45:L8:166:LEU:HD23	45:L8:166:LEU:HA	2.14	0.45
51:M5:70:ASN:HD21	51:M5:93:LYS:HE3	3.28	0.45
72:O6:62:ARG:HH22	72:O6:98:ARG:NH1	2.14	0.45
22:D0:87:HIS:HB3	22:D0:89:ARG:NH1	2.32	0.45
5:S3:58:VAL:O	5:S3:66:ILE:HG12	2.17	0.45
44:L7:158:LYS:CG	44:L7:159:GLN:H	2.28	0.45
1:6:713:A:H2'	1:6:714:G:H5''	1.99	0.45
9:S7:9:LEU:HB3	9:S7:10:SER:H	2.92	0.45
86:5:4000:OHX:N6	86:5:4190:OHX:N3	2.65	0.45
86:2:2076:OHX:N4	86:2:2163:OHX:N1	2.64	0.45
1:2:494:U:O2'	1:2:495:C:O5'	2.32	0.45
49:M3:107:GLU:OE2	72:O6:18:THR:HG23	2.17	0.45
28:D6:62:TYR:CG	28:D6:63:ALA:N	2.95	0.45
86:5:4033:OHX:N1	86:5:4081:OHX:N4	2.64	0.45
48:M1:72:ARG:NH2	37:7:40:C:O2	307.29	0.45
36:5:2882:U:H2'	36:5:2883:U:C6	2.52	0.45
34:SR:44:SER:O	34:SR:58:VAL:HG13	3.58	0.45
36:5:495:G:H2'	36:5:496:C:O4'	2.16	0.45
36:5:807:A:H61	36:5:934:G:H22	1.64	0.45
36:1:938:C:OP1	36:1:963:G:H5'	2.17	0.45
12:C0:6:GLU:O	12:C0:10:LYS:HD3	3.49	0.45
6:S4:160:VAL:HG13	6:S4:169:ILE:HG23	2.89	0.45
48:M1:106:ILE:O	48:M1:106:ILE:HG12	2.16	0.45
5:S3:127:MET:HE2	5:S3:155:GLY:HA3	1.99	0.45
36:1:1758:G:H1	36:1:1767:C:H42	1.65	0.45
36:1:3362:A:H2'	36:1:3363:U:O4'	2.17	0.45
20:C8:35:ILE:HB	20:C8:38:VAL:HG21	1.99	0.45
8:S6:173:PRO:O	1:6:79:C:H4'	344.83	0.45
1:6:1698:G:N2	1:6:1699:G:C8	2.85	0.45
17:C5:40:ARG:NH2	1:6:1552:U:O4	393.57	0.45
36:5:1655:G:C8	36:5:1655:G:C5'	3.00	0.45
1:2:732:G:C6	86:2:2130:OHX:N3	2.85	0.45
86:1:4084:OHX:N2	86:1:4153:OHX:N5	2.65	0.45
7:S5:59:VAL:HG12	7:S5:60:ASP:H	3.04	0.45
36:5:283:G:O6	36:5:304:G:H1'	2.17	0.45
1:6:1567:U:C5	1:6:1568:C:C4	3.05	0.45
2:S0:61:ALA:HA	2:S0:64:ILE:HD12	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S0:90:ALA:HB1	2:S0:95:ALA:O	2.41	0.45
11:S9:143:ILE:HG22	11:S9:145:SER:H	1.82	0.45
3:S1:41:ARG:NH2	3:S1:97:LEU:HD11	2.32	0.45
86:5:4054:OHX:N4	86:5:4108:OHX:N1	2.65	0.45
70:O4:8:ARG:HB2	70:O4:34:HIS:CD2	2.81	0.45
86:2:2116:OHX:N5	86:C1:201:OHX:N1	2.65	0.45
11:S9:171:ARG:NH1	11:S9:174:ARG:HG3	2.32	0.45
28:D6:23:CYS:CB	28:D6:74:CYS:HB3	2.45	0.45
1:6:674:C:H2'	1:6:675:U:C6	2.51	0.45
44:L7:96:PRO:HG2	44:L7:99:PRO:HG2	2.99	0.45
9:S7:44:LYS:HE2	9:S7:44:LYS:HB3	2.43	0.45
63:N7:10:VAL:HB	63:N7:83:THR:CG2	2.46	0.45
2:S0:30:GLN:NE2	2:S0:149:LEU:HD13	2.32	0.45
6:S4:26:CYS:HB2	6:S4:27:TYR:CE2	5.08	0.45
17:C5:28:MET:O	17:C5:32:ASP:HB2	2.17	0.45
4:S2:165:VAL:HA	4:S2:201:ASN:O	2.17	0.45
63:N7:99:GLU:HG3	63:N7:100:THR:N	3.25	0.45
1:2:986:G:H2'	1:2:987:G:O4'	2.17	0.45
13:C1:86:ILE:HD13	13:C1:86:ILE:HG21	1.99	0.45
86:1:4071:OHX:N3	86:1:4118:OHX:N4	2.64	0.45
12:C0:25:LYS:HD2	12:C0:59:PHE:CZ	2.51	0.45
31:D9:5:ASN:C	31:D9:7:TRP:H	2.21	0.45
36:5:2537:U:HO2'	36:5:2538:U:C4'	2.28	0.45
1:6:276:C:H1'	1:6:277:U:C5	2.52	0.45
36:1:1792:C:H2'	36:1:1795:U:C5	2.52	0.45
36:1:3174:A:OP1	69:O3:97:SER:OG	2.28	0.45
1:6:319:U:H1'	1:6:323:A:C4	2.52	0.45
65:N9:38:LYS:HD2	36:5:1076:C:H4'	214.40	0.45
39:L2:44:ILE:HG23	39:L2:87:PHE:CE1	3.01	0.45
1:6:333:A:C6	1:6:334:G:C6	3.05	0.45
2:S0:103:THR:HA	2:S0:104:PRO:HD3	1.74	0.45
36:5:240:U:O2'	36:5:241:G:H8	2.00	0.45
29:D7:17:ARG:HD3	1:6:1070:C:H4'	370.11	0.45
15:C3:99:ARG:O	15:C3:103:GLU:HG2	2.16	0.45
16:C4:135:ARG:HG3	1:6:1007:C:H5''	296.68	0.45
16:C4:112:ILE:HB	28:D6:57:SER:OG	2.16	0.45
36:1:701:G:H2'	36:1:702:C:C6	2.52	0.45
38:8:157:U:H2'	38:8:158:U:C6	2.52	0.45
36:1:537:A:H2'	36:1:538:G:O4'	2.17	0.45
36:1:3030:G:N7	86:1:4077:OHX:N6	2.65	0.45
40:L3:306:THR:HG22	40:L3:310:GLY:HA2	1.97	0.45
47:M0:152:LEU:HA	47:M0:152:LEU:HD23	2.11	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
62:N6:108:LYS:HA	62:N6:108:LYS:HD3	4.73	0.45
36:1:1887:A:OP2	86:1:3896:OHX:N4	2.50	0.45
1:2:1278:G:H2'	1:2:1279:C:O4'	2.17	0.45
41:L4:42:VAL:HG12	41:L4:236:LEU:HD21	1.98	0.45
36:1:2403:G:C2	36:1:2404:A:N7	2.83	0.44
36:1:2206:G:C2	36:1:2207:A:C8	3.05	0.44
11:S9:93:LEU:HA	11:S9:96:VAL:CG1	2.38	0.44
25:D3:130:VAL:O	25:D3:131:SER:CB	2.71	0.44
42:L5:4:GLN:CD	42:L5:4:GLN:H	2.17	0.44
42:L5:270:LYS:O	42:L5:273:ARG:HD2	3.92	0.44
36:1:1109:U:H2'	36:1:1110:U:O4'	2.17	0.44
33:E1:126:CYS:HB3	33:E1:130:VAL:HG21	1.99	0.44
55:M9:106:LEU:HD12	55:M9:106:LEU:HA	1.95	0.44
16:C4:122:PRO:C	16:C4:124:ASP:N	2.70	0.44
4:S2:139:ILE:HD12	4:S2:191:ALA:HB1	1.99	0.44
1:6:1591:C:H2'	1:6:1592:A:C8	2.52	0.44
20:C8:13:HIS:O	20:C8:14:ILE:HG22	3.27	0.44
44:L7:151:ARG:HD2	44:L7:244:ASN:ND2	2.32	0.44
47:M0:99:ILE:HG13	47:M0:100:ASN:N	2.32	0.44
42:L5:184:ASP:HB3	42:L5:187:THR:HG23	1.98	0.44
67:O1:5:LYS:HA	67:O1:89:LEU:HD21	1.99	0.44
36:5:2947:G:H4'	36:5:2947:G:OP2	2.17	0.44
36:5:2510:U:O2'	36:5:2511:A:H5''	2.16	0.44
2:S0:22:THR:HA	2:S0:169:SER:OG	2.34	0.44
51:M5:143:ARG:HH21	71:O5:92:LEU:HD23	1.82	0.44
1:2:1492:A:O2'	1:2:1493:A:H8	1.99	0.44
11:S9:117:GLY:C	11:S9:119:ALA:H	2.21	0.44
55:M9:109:TYR:HB3	55:M9:115:ILE:HG12	5.08	0.44
26:D4:104:SER:HB3	26:D4:107:GLN:CG	2.47	0.44
17:C5:77:ARG:HB3	17:C5:102:PHE:CE1	2.94	0.44
6:S4:180:LEU:N	6:S4:229:GLY:O	2.89	0.44
57:N1:88:ARG:NH2	65:N9:33:LYS:HB3	2.32	0.44
10:S8:31:ARG:HH21	10:S8:48:THR:HG22	2.20	0.44
42:L5:98:ALA:O	42:L5:162:ALA:HA	2.56	0.44
1:2:929:A:N6	1:2:930:A:C6	2.85	0.44
37:7:58:C:OP1	86:7:217:OHX:N3	2.51	0.44
36:5:2191:U:H2'	36:5:2192:C:O4'	2.17	0.44
38:4:37:A:H5''	38:4:39:G:O4'	2.17	0.44
55:M9:99:LEU:O	55:M9:103:ARG:HB2	2.17	0.44
36:1:422:A:C2	36:1:2363:A:H4'	2.53	0.44
48:M1:63:GLU:O	48:M1:64:LYS:HB2	2.16	0.44
18:C6:127:LYS:HE2	18:C6:132:LYS:O	4.64	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:C6:127:LYS:HA	18:C6:134:ALA:HA	1.99	0.44
1:2:549:G:C2	1:2:550:A:C8	3.05	0.44
36:5:2437:G:H2'	36:5:2438:A:O4'	2.17	0.44
36:5:3291:G:H2'	36:5:3292:A:C8	2.52	0.44
57:N1:73:GLY:HA2	57:N1:89:LEU:O	2.28	0.44
36:1:378:A:N7	36:1:391:A:H2	2.15	0.44
36:5:144:A:N6	36:5:145:G:C2	2.85	0.44
40:L3:296:THR:HB	40:L3:299:ASP:HB2	1.99	0.44
3:S1:133:TYR:CZ	3:S1:181:LEU:HD12	5.20	0.44
36:1:412:G:OP1	53:M7:62:ARG:NH1	2.50	0.44
18:C6:82:ARG:NH1	18:C6:114:ARG:HB2	2.95	0.44
6:S4:87:MET:SD	6:S4:123:LEU:HB2	2.58	0.44
7:S5:61:TYR:HD2	7:S5:164:PRO:HB2	2.68	0.44
6:S4:72:VAL:HG23	6:S4:77:ARG:HB2	1.98	0.44
48:M1:23:VAL:HG11	48:M1:29:ARG:HG2	1.99	0.44
1:6:542:A:N7	1:6:543:C:H2'	2.32	0.44
4:S2:65:GLU:O	4:S2:68:ILE:HB	2.17	0.44
15:C3:28:LEU:HB3	15:C3:29:SER:H	1.58	0.44
45:L8:78:PHE:CD2	45:L8:179:ILE:HD13	2.52	0.44
1:2:639:U:P	9:S7:117:THR:HG1	2.38	0.44
39:L2:52:SER:HB3	39:L2:191:LEU:HD12	5.51	0.44
36:5:92:G:H5'	36:5:93:C:C5'	2.45	0.44
16:C4:102:LEU:CD1	28:D6:45:VAL:HG12	2.92	0.44
64:N8:74:ASN:CB	64:N8:76:ASP:HB2	2.46	0.44
86:2:2096:OHX:N4	86:2:2109:OHX:N1	2.65	0.44
36:5:1880:U:H2'	36:5:1881:A:O4'	2.16	0.44
1:2:1113:A:H4'	1:2:1114:G:OP1	2.17	0.44
36:1:2443:A:N6	36:1:2503:G:C2	2.86	0.44
36:1:2662:G:H2'	36:1:2663:G:H8	1.82	0.44
51:M5:8:GLU:HG3	51:M5:50:ARG:NH1	4.04	0.44
1:2:1067:C:H2'	1:2:1068:C:C6	2.48	0.44
14:C2:125:ASN:ND2	35:SM:169:ALA:H	5.52	0.44
36:1:3095:U:H2'	36:1:3096:C:H6	1.81	0.44
5:S3:64:ARG:O	5:S3:67:ASN:HB2	2.16	0.44
29:D7:59:CYS:O	29:D7:61:THR:N	2.75	0.44
41:L4:209:TYR:O	41:L4:230:VAL:HG22	2.47	0.44
2:S0:57:LEU:HG	2:S0:177:LEU:HD23	1.99	0.44
63:N7:80:LEU:O	63:N7:82:PRO:HD3	2.87	0.44
41:L4:22:LEU:HA	41:L4:23:PRO:HD3	1.94	0.44
9:S7:60:ILE:HD12	9:S7:92:PHE:CE2	2.53	0.44
50:M4:89:ALA:HB1	50:M4:92:GLU:CD	2.37	0.44
36:1:1722:U:H1'	55:M9:96:ILE:HG12	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:594:A:H4'	1:6:595:G:H5'	1.98	0.44
1:2:755:A:HO2'	1:2:756:A:P	2.40	0.44
52:M6:83:ALA:HB1	36:5:1313:G:H5'	259.25	0.44
24:D2:6:VAL:HG22	24:D2:29:PRO:HD2	1.99	0.44
1:2:603:U:H2'	1:2:604:A:H8	1.82	0.44
66:O0:53:LYS:HZ1	36:5:2552:C:H5	242.96	0.44
1:2:489:C:H2'	1:2:490:C:C6	2.52	0.44
38:8:109:A:C2'	38:8:110:C:H5'	2.47	0.44
47:M0:9:TYR:CG	47:M0:97:LEU:HD13	2.52	0.44
50:M4:20:VAL:HG22	50:M4:66:THR:OG1	2.17	0.44
73:O7:63:ARG:O	73:O7:68:LYS:HE3	3.89	0.44
68:O2:20:HIS:CG	68:O2:42:VAL:HG21	2.52	0.44
42:L5:194:LEU:HD23	42:L5:194:LEU:HA	2.12	0.44
36:1:3222:U:H6	36:1:3222:U:H5''	1.81	0.44
68:O2:64:LYS:HE2	68:O2:65:PHE:CZ	2.52	0.44
23:D1:74:GLN:HB2	23:D1:79:LEU:HB2	1.99	0.44
15:C3:114:ARG:NH1	15:C3:114:ARG:HG2	2.36	0.44
1:2:1459:C:N4	20:C8:139:LYS:HE2	2.31	0.44
86:3:218:OHX:N2	86:3:223:OHX:N5	2.65	0.44
1:6:542:A:OP1	1:6:544:A:C5	2.71	0.44
39:L2:96:LEU:O	79:Q3:87:ARG:HD3	2.25	0.44
7:S5:31:GLU:O	7:S5:35:GLN:HB2	2.16	0.44
62:N6:52:ARG:O	62:N6:53:ASP:HB2	4.46	0.44
1:6:1540:G:C6	1:6:1541:G:C4	3.05	0.44
2:S0:69:ASN:HB3	2:S0:71:GLU:OE1	2.64	0.44
36:1:1062:A:N3	57:N1:130:ARG:NH2	2.58	0.44
20:C8:28:ILE:HG13	20:C8:56:LYS:O	5.28	0.44
36:1:716:A:C6	64:N8:117:ARG:HG3	2.53	0.44
36:1:149:U:OP2	51:M5:49:ARG:NH2	2.48	0.44
1:2:1236:A:O4'	33:E1:138:ARG:NH2	2.50	0.44
36:1:2303:A:P	77:Q1:23:ARG:NH2	2.90	0.44
22:D0:22:ILE:HD12	22:D0:118:VAL:HA	1.98	0.44
42:L5:261:THR:OG1	42:L5:264:GLN:HG3	2.17	0.44
36:1:736:A:H2'	36:1:737:G:O4'	2.16	0.44
47:M0:22:TYR:CZ	36:5:1048:A:H2'	268.27	0.44
28:D6:11:ASN:HB3	1:6:934:C:C6	333.63	0.44
40:L3:335:ILE:HG13	40:L3:336:VAL:N	2.41	0.44
36:5:1715:A:H4'	36:5:1716:U:OP1	2.18	0.44
86:1:4065:OHX:N3	86:1:4177:OHX:N5	2.65	0.44
36:1:1580:A:H5'	36:1:2522:G:C5	2.53	0.44
12:C0:2:LEU:HB3	12:C0:3:MET:H	4.19	0.44
40:L3:55:THR:O	40:L3:56:ILE:HD12	2.16	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:D9:54:LYS:HB3	31:D9:54:LYS:HE3	1.72	0.44
14:C2:38:HIS:O	14:C2:125:ASN:ND2	2.50	0.44
61:N5:132:ALA:HA	61:N5:135:ILE:HG22	2.02	0.44
39:L2:227:ARG:NH2	36:5:2161:G:O3'	202.07	0.44
38:8:104:A:C8	38:8:105:A:C8	3.05	0.44
58:N2:82:LYS:NZ	36:5:1686:U:O4	163.58	0.44
49:M3:35:ARG:NH1	36:5:685:G:OP1	81.86	0.44
71:O5:21:LEU:HD22	71:O5:25:LYS:HE3	2.08	0.44
58:N2:33:TYR:HE2	58:N2:63:VAL:HG21	1.80	0.44
36:5:2426:U:H2'	36:5:2427:U:C6	2.53	0.44
36:5:72:C:C2	36:5:74:G:H1'	2.53	0.44
45:L8:130:TYR:HD1	45:L8:202:GLU:HB3	1.82	0.44
21:C9:132:LEU:O	21:C9:135:ILE:HG13	2.17	0.44
6:S4:71:LYS:HB3	6:S4:76:VAL:HA	2.00	0.44
86:7:219:OHX:N5	86:7:224:OHX:N6	2.66	0.44
56:N0:77:VAL:HG21	56:N0:94:ILE:HD12	1.98	0.44
21:C9:63:ARG:O	21:C9:67:MET:HE3	2.17	0.44
4:S2:188:LEU:HA	4:S2:188:LEU:HD23	1.94	0.44
37:7:113:C:C4	37:7:114:U:C4	3.06	0.44
14:C2:59:LEU:HA	14:C2:87:PRO:HB2	2.00	0.44
34:SR:206:PRO:HG2	34:SR:247:PRO:HA	3.56	0.44
30:D8:18:ARG:HD3	30:D8:25:VAL:O	2.17	0.44
1:2:350:U:O2	1:2:352:A:C6	2.70	0.44
11:S9:78:ARG:HG3	11:S9:79:ARG:N	2.52	0.44
79:Q3:80:ARG:HE	79:Q3:80:ARG:HB2	2.78	0.44
36:1:1591:G:H5''	70:O4:37:LYS:NZ	2.32	0.44
2:S0:13:ASP:HA	2:S0:16:LEU:HD12	1.99	0.44
53:M7:39:TRP:O	53:M7:114:VAL:HG12	2.17	0.44
36:5:114:A:N1	36:5:266:A:O2'	2.41	0.44
47:M0:19:LYS:HG3	47:M0:26:VAL:CG2	4.49	0.44
36:1:3019:U:O4	86:1:3993:OHX:N4	2.51	0.44
36:5:3384:U:H2'	36:5:3385:U:C6	2.52	0.44
39:L2:179:LEU:O	39:L2:180:LEU:HB2	2.17	0.44
36:1:980:A:H2'	36:1:981:U:C1'	2.47	0.44
63:N7:17:ARG:O	63:N7:19:ALA:N	2.51	0.44
2:S0:59:LEU:HD12	23:D1:79:LEU:HD21	5.65	0.44
1:6:82:U:H2'	1:6:83:G:O4'	2.18	0.44
1:2:646:C:H2'	1:2:647:G:C8	2.53	0.44
8:S6:141:ILE:HG21	8:S6:153:VAL:HG13	1.99	0.44
28:D6:6:ALA:N	1:6:1796:C:C5	344.93	0.44
6:S4:77:ARG:HH11	6:S4:77:ARG:HG3	4.05	0.44
36:1:2771:U:H4'	78:Q2:15:LYS:NZ	2.32	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:2098:C:H2'	36:1:2099:A:C8	2.43	0.44
73:O7:55:ARG:NH1	36:5:353:G:O6	113.12	0.44
54:M8:162:ALA:HA	54:M8:163:PRO:HD2	1.53	0.44
49:M3:122:LYS:HA	71:O5:120:ALA:HA	2.00	0.44
42:L5:76:ALA:CB	42:L5:109:THR:HG22	2.69	0.44
10:S8:49:ARG:O	10:S8:52:ASN:ND2	2.78	0.44
12:C0:8:ARG:HD2	12:C0:12:HIS:CE1	2.52	0.44
47:M0:99:ILE:HG22	47:M0:123:HIS:HB2	1.99	0.44
36:5:284:A:H4'	36:5:285:A:N3	2.33	0.44
66:O0:42:ILE:HD11	66:O0:67:VAL:HG22	1.99	0.44
36:1:3066:U:H2'	36:1:3067:C:C6	2.53	0.44
51:M5:75:VAL:HA	51:M5:76:PRO:HD3	1.75	0.44
34:SR:133:VAL:HG12	34:SR:141:LEU:HD12	2.67	0.44
29:D7:74:SER:O	29:D7:76:GLY:N	2.50	0.44
36:1:2366:C:OP1	40:L3:259:HIS:NE2	2.43	0.44
18:C6:57:LEU:H	18:C6:57:LEU:HD12	4.18	0.44
36:1:2712:U:H2'	36:1:2713:U:C6	2.52	0.44
36:5:1046:A:H2'	36:5:1049:C:C5	2.52	0.44
36:1:3006:A:C2	36:1:3141:A:C4	3.05	0.44
1:2:1301:U:H2'	1:2:1302:U:O4'	2.17	0.44
36:1:2358:A:H2'	36:1:2359:C:O4'	2.18	0.44
33:E1:86:THR:HG23	33:E1:87:THR:H	4.30	0.44
36:5:2115:G:H22	36:5:2120:A:H1'	1.83	0.44
78:Q2:31:GLY:HA3	36:5:2767:U:O3'	192.40	0.44
36:1:2191:U:H2'	36:1:2192:C:O4'	2.18	0.44
1:2:1511:U:H2'	1:2:1512:G:C8	2.52	0.44
1:2:1422:A:C2	1:2:1423:U:C2	3.05	0.44
6:S4:45:ILE:HA	6:S4:61:VAL:HG11	1.99	0.44
59:N3:93:LEU:H	59:N3:93:LEU:HD23	2.10	0.44
9:S7:110:GLN:HB3	9:S7:110:GLN:HE21	4.41	0.44
36:1:374:A:N3	36:1:376:G:H5''	2.31	0.44
14:C2:95:LYS:HA	14:C2:117:GLY:HA2	3.64	0.44
36:1:1480:G:O2'	36:1:1871:U:O4	2.28	0.44
2:S0:55:GLU:OE2	23:D1:80:LYS:N	2.37	0.44
27:D5:43:ASP:HB2	27:D5:46:LYS:HG3	1.98	0.44
4:S2:82:ASN:OD1	4:S2:83:ILE:N	2.50	0.44
28:D6:10:ARG:HD3	28:D6:34:LYS:HA	2.69	0.44
1:6:542:A:C8	1:6:543:C:H5'	2.51	0.44
7:S5:43:PHE:CE2	7:S5:90:ILE:HG21	2.67	0.44
62:N6:3:LYS:HD2	62:N6:8:VAL:HG22	1.99	0.44
36:1:2282:U:O2	36:1:2310:U:H4'	2.16	0.44
1:2:1595:U:N3	1:2:1600:A:C2	2.81	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:M5:150:TRP:CZ3	51:M5:151:ILE:HG12	2.53	0.44
86:5:4001:OHX:N3	86:5:4090:OHX:N1	2.66	0.44
86:5:4001:OHX:N4	86:5:4090:OHX:N1	2.66	0.44
36:5:1815:U:O2'	36:5:1816:A:P	2.75	0.44
11:S9:157:ASP:OD2	11:S9:158:PHE:N	2.51	0.44
36:1:1035:G:H3'	36:1:1036:A:H8	1.83	0.44
17:C5:12:PHE:CE2	48:M1:85:LYS:HE2	6.93	0.44
1:2:25:C:H2'	1:2:25:C:H6	1.66	0.44
1:2:591:A:H2'	1:2:592:A:H8	1.82	0.44
86:1:4023:OHX:N3	86:1:4061:OHX:N5	2.65	0.44
36:5:1029:G:H2'	36:5:1030:A:H8	1.82	0.44
40:L3:305:ILE:HG12	40:L3:321:PHE:CZ	2.52	0.44
36:1:1556:C:H2'	36:1:2169:G:N2	2.32	0.44
74:O8:36:LYS:HG2	74:O8:37:PRO:HD2	2.00	0.44
34:SR:16:HIS:O	34:SR:308:ASN:HB3	2.54	0.44
36:5:420:G:O5'	36:5:420:G:OP1	2.35	0.44
5:S3:18:TYR:CE1	5:S3:37:VAL:HG23	2.52	0.44
11:S9:31:ALA:HA	11:S9:36:LEU:HD12	2.00	0.44
38:8:46:G:O2'	38:8:61:A:N1	2.43	0.44
36:1:269:G:H5'	51:M5:120:TRP:CE3	2.52	0.44
42:L5:160:PHE:HA	42:L5:163:LEU:HB3	2.36	0.44
1:6:1039:A:O2'	1:6:1040:G:OP2	2.30	0.44
6:S4:18:TRP:HE3	6:S4:20:LEU:HD11	1.83	0.44
36:5:1409:G:O6	86:5:4160:OHX:N6	2.51	0.44
49:M3:57:VAL:HG13	49:M3:147:ILE:CG2	2.47	0.44
86:7:219:OHX:N3	86:7:224:OHX:N4	2.66	0.44
3:S1:35:PRO:HB2	3:S1:36:SER:H	1.52	0.44
31:D9:6:VAL:O	31:D9:8:PHE:N	4.50	0.44
38:4:141:C:OP1	51:M5:109:ARG:NH1	2.49	0.44
27:D5:74:SER:HA	27:D5:77:ARG:NH2	2.46	0.44
1:2:1498:G:C2'	1:2:1499:G:H5'	2.47	0.44
36:5:986:U:OP2	86:5:4146:OHX:N2	2.51	0.44
36:1:2971:A:N3	36:1:2971:A:H3'	2.33	0.44
6:S4:45:ILE:HB	6:S4:80:THR:HG23	2.41	0.44
6:S4:61:VAL:HG12	6:S4:65:LEU:HD12	1.98	0.44
37:7:110:G:C6	37:7:111:U:C4	3.06	0.44
86:5:4127:OHX:N4	86:5:4144:OHX:N2	2.66	0.44
1:2:751:G:H2'	1:2:752:A:H8	1.83	0.44
1:6:231:U:H2'	1:6:232:U:H5''	1.99	0.44
53:M7:116:HIS:HB3	53:M7:149:VAL:HB	2.00	0.44
70:O4:65:VAL:HG12	70:O4:70:LYS:HE2	3.17	0.44
6:S4:13:ALA:O	6:S4:39:ARG:NH2	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:5:2846:U:O2'	86:5:4052:OHX:N1	2.51	0.44
18:C6:9:THR:HA	1:6:1340:U:O4	434.71	0.44
33:E1:88:PRO:HA	33:E1:89:LYS:HA	4.68	0.44
43:L6:15:VAL:HG23	68:O2:5:PRO:HG2	5.36	0.44
39:L2:5:ILE:HG22	39:L2:208:ASP:O	2.16	0.44
1:2:975:C:H5''	15:C3:109:LYS:HE3	1.98	0.44
36:5:929:A:H2'	36:5:930:U:C6	2.53	0.44
40:L3:121:ASN:O	40:L3:125:SER:HB3	2.18	0.44
4:S2:123:GLY:HA2	4:S2:126:ARG:NH1	2.33	0.44
6:S4:131:LEU:HD22	6:S4:131:LEU:HA	1.82	0.44
1:6:137:U:H2'	1:6:137:U:H6	1.49	0.44
36:5:249:U:OP2	36:5:249:U:H2'	2.18	0.44
36:1:1127:G:O5'	36:1:1127:G:H8	2.00	0.44
1:6:1398:U:H4'	1:6:1399:C:OP2	2.16	0.44
22:D0:37:VAL:O	22:D0:41:ILE:HD13	2.17	0.44
36:5:83:U:OP2	86:5:4205:OHX:N4	2.51	0.44
45:L8:177:TYR:CZ	45:L8:222:PHE:O	4.66	0.44
7:S5:205:SER:C	7:S5:207:THR:H	2.21	0.44
50:M4:45:LEU:HD12	50:M4:56:GLN:O	2.17	0.44
1:2:1557:U:OP2	1:2:1559:A:O2'	2.18	0.44
49:M3:46:ILE:HD12	49:M3:49:ARG:NH1	2.52	0.44
36:1:1940:G:N2	36:1:3362:A:C8	2.83	0.44
7:S5:164:PRO:HA	7:S5:167:ARG:HG3	3.34	0.44
64:N8:75:LEU:O	64:N8:77:LYS:N	2.77	0.44
66:O0:17:VAL:CG2	66:O0:100:ILE:HG12	2.48	0.44
41:L4:135:VAL:O	41:L4:140:HIS:HB2	2.17	0.44
21:C9:23:GLN:HG2	21:C9:55:TYR:CG	2.53	0.44
1:2:1537:C:N4	86:2:2155:OHX:N6	2.66	0.44
56:N0:169:SER:OG	56:N0:171:PHE:HB3	2.70	0.44
41:L4:49:ALA:HA	41:L4:109:TRP:CZ2	2.63	0.44
1:2:1769:U:O2	16:C4:136:ARG:HD2	2.17	0.44
86:2:2116:OHX:N2	86:C1:201:OHX:N1	2.66	0.44
13:C1:18:HIS:O	86:C1:201:OHX:N6	2.50	0.44
36:1:1422:G:H21	43:L6:5:LYS:HZ3	1.66	0.44
47:M0:74:LYS:HE3	47:M0:74:LYS:HB2	1.81	0.44
36:5:1329:U:H6	36:5:1329:U:O5'	2.01	0.44
1:2:73:U:H4'	1:2:74:U:OP1	2.18	0.44
59:N3:81:GLN:O	59:N3:82:ALA:CB	2.65	0.44
9:S7:44:LYS:HZ3	9:S7:95:GLU:HG2	1.79	0.44
9:S7:44:LYS:NZ	9:S7:95:GLU:OE2	4.20	0.44
42:L5:155:THR:HB	42:L5:179:ARG:HA	2.23	0.44
86:1:4007:OHX:N6	86:1:4175:OHX:N2	2.66	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:1445:G:C5	33:E1:91:ILE:HB	2.53	0.44
36:5:1348:U:C5	36:5:1355:A:C5	3.06	0.44
35:SM:46:LYS:HA	36:5:1018:G:H4'	325.42	0.44
32:E0:17:GLN:OE1	1:6:563:U:H4'	383.42	0.44
40:L3:286:GLY:HA3	40:L3:321:PHE:CZ	2.52	0.44
22:D0:34:LEU:HD21	22:D0:89:ARG:HD2	4.03	0.44
6:S4:118:GLU:HA	6:S4:121:TYR:CE1	2.84	0.44
26:D4:126:ALA:O	26:D4:129:VAL:HG12	2.18	0.44
36:1:1579:C:N4	36:1:1580:A:H62	2.16	0.44
39:L2:245:LEU:HD12	39:L2:245:LEU:HA	2.38	0.44
21:C9:118:PRO:O	21:C9:119:LYS:HB2	2.17	0.44
6:S4:179:LYS:O	6:S4:194:THR:O	2.35	0.44
9:S7:164:TYR:HD2	9:S7:164:TYR:H	1.63	0.44
36:1:7:C:H5''	45:L8:193:LYS:HB3	1.99	0.44
1:2:287:G:O2'	1:2:288:A:P	2.75	0.44
45:L8:116:VAL:HG21	45:L8:123:GLN:HA	1.99	0.44
1:2:417:A:H4'	1:2:418:G:O5'	2.16	0.44
36:1:781:G:N7	86:1:3945:OHX:N5	2.65	0.44
36:1:1460:A:H2'	36:1:1461:A:C8	2.52	0.44
1:6:922:G:H2'	1:6:923:A:H8	1.83	0.44
39:L2:104:LEU:O	39:L2:139:HIS:HE1	2.01	0.44
68:O2:24:ARG:HD3	68:O2:25:TYR:OH	2.40	0.44
39:L2:213:GLY:CA	36:5:2967:A:H5''	205.80	0.44
34:SR:128:ASP:O	34:SR:130:THR:HG23	2.16	0.44
1:6:1216:C:O2'	1:6:1444:A:N1	2.47	0.44
40:L3:306:THR:OG1	40:L3:316:GLU:O	2.22	0.44
36:1:1029:G:H2'	36:1:1030:A:C8	2.52	0.44
25:D3:57:LEU:HD22	32:E0:4:VAL:HG12	1.99	0.44
1:2:1393:C:H2'	1:2:1394:G:O4'	2.17	0.44
36:5:2656:A:H4'	36:5:2657:A:OP1	2.17	0.44
1:6:348:U:O4	86:6:2163:OHX:N4	2.51	0.44
48:M1:107:ASP:HA	48:M1:124:GLY:HA2	1.99	0.44
13:C1:54:ILE:HD13	13:C1:54:ILE:HA	1.88	0.44
79:Q3:45:LYS:HE3	79:Q3:45:LYS:HB2	1.57	0.44
42:L5:271:LYS:HD3	42:L5:271:LYS:HA	4.24	0.44
69:O3:44:TYR:HA	69:O3:47:LYS:HG3	2.29	0.44
34:SR:272:ASP:OD1	34:SR:273:ASP:N	2.51	0.44
79:Q3:10:ILE:HD12	36:5:837:A:H1'	230.44	0.44
36:1:650:C:H2'	36:1:651:G:C8	2.52	0.44
36:5:408:A:N6	38:8:15:G:H1'	2.32	0.44
1:2:283:U:H5''	8:S6:188:ARG:HD3	1.99	0.44
47:M0:29:SER:HA	47:M0:125:LEU:HD12	2.27	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
59:N3:125:LEU:HB3	59:N3:126:TRP:CD1	2.88	0.44
2:S0:52:LYS:NZ	23:D1:82:VAL:O	2.42	0.44
1:6:1699:G:N1	1:6:1701:A:H5''	2.33	0.44
3:S1:129:THR:OG1	3:S1:131:ASP:OD1	6.96	0.44
1:2:1433:G:H2'	1:2:1434:U:C6	2.52	0.44
2:S0:9:LEU:HD13	2:S0:10:THR:O	2.61	0.44
8:S6:31:ARG:NH1	8:S6:34:GLN:HE22	3.46	0.44
7:S5:37:GLN:CG	18:C6:53:LEU:HD13	2.66	0.44
71:O5:85:THR:O	71:O5:89:ARG:HB2	2.39	0.44
37:3:20:A:C4	37:3:60:G:N2	2.85	0.44
72:O6:57:LEU:HB2	72:O6:90:MET:HE3	4.70	0.44
71:O5:86:ARG:HG3	71:O5:90:ARG:CZ	2.71	0.44
36:5:3000:A:H2'	36:5:3001:C:H6	1.82	0.44
55:M9:81:ARG:HG3	55:M9:88:ARG:CZ	2.48	0.44
14:C2:118:ALA:HA	1:6:1227:A:H3'	462.76	0.44
1:6:189:C:C2'	1:6:190:C:H5'	2.48	0.44
27:D5:58:ARG:HA	27:D5:103:ARG:HB2	5.74	0.44
11:S9:109:LEU:HD13	11:S9:129:ILE:HD13	1.99	0.44
70:O4:8:ARG:CG	70:O4:8:ARG:HH11	2.30	0.44
49:M3:65:TYR:OH	36:5:700:C:OP1	109.22	0.44
1:6:830:U:C2'	1:6:831:U:H5'	2.47	0.44
1:6:833:U:OP2	86:6:2202:OHX:N5	2.50	0.44
86:2:2096:OHX:N3	86:2:2109:OHX:N5	2.66	0.44
22:D0:20:ILE:O	22:D0:94:GLU:HA	5.74	0.44
43:L6:40:LEU:HD13	43:L6:84:VAL:HG11	2.07	0.44
52:M6:108:ILE:HA	52:M6:109:PRO:HD2	2.18	0.44
36:1:383:G:O6	86:1:4065:OHX:N2	2.51	0.44
36:1:2138:A:HO2'	73:O7:2:GLY:N	2.16	0.44
36:5:2308:C:O2	86:5:4238:OHX:N1	2.51	0.44
10:S8:152:ILE:HD13	10:S8:157:GLU:OE1	2.17	0.44
13:C1:3:THR:HG1	13:C1:82:ARG:NE	2.16	0.44
13:C1:57:LYS:HB2	13:C1:110:HIS:NE2	2.33	0.44
36:1:1818:U:H3'	36:1:1819:U:H5''	2.00	0.44
1:2:902:G:O5'	1:2:902:G:H8	2.01	0.44
36:1:2882:U:H2'	36:1:2883:U:C6	2.53	0.44
40:L3:340:LYS:HE3	40:L3:340:LYS:HB3	4.59	0.44
2:S0:177:LEU:O	2:S0:181:VAL:HG22	3.56	0.44
73:O7:33:THR:HA	73:O7:39:TYR:O	2.18	0.44
36:5:999:G:C6	36:5:1000:C:N4	2.85	0.44
54:M8:57:ILE:HG21	54:M8:57:ILE:HD13	1.69	0.44
86:5:4000:OHX:N2	86:5:4190:OHX:N5	2.65	0.44
36:5:2594:C:H6	36:5:2594:C:OP2	2.01	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
74:O8:11:PHE:O	74:O8:15:THR:HG23	2.41	0.44
40:L3:367:LYS:HZ1	60:N4:34:SER:H	4.43	0.44
68:O2:89:THR:HG22	68:O2:117:ILE:HG12	2.00	0.44
10:S8:137:LYS:O	10:S8:140:GLU:N	3.28	0.44
6:S4:71:LYS:CB	6:S4:76:VAL:HA	2.48	0.44
1:2:755:A:H2'	1:2:756:A:H8	1.83	0.44
36:5:1049:C:H2'	36:5:1050:U:H6	1.81	0.44
36:5:1313:G:O6	86:5:4161:OHX:N6	2.50	0.44
51:M5:141:ALA:O	51:M5:145:ASP:HB2	2.69	0.44
10:S8:184:LEU:HB3	10:S8:189:LEU:HB2	2.06	0.44
49:M3:144:THR:HG21	71:O5:118:ILE:HG21	2.16	0.44
36:1:945:C:H2'	36:1:946:U:C6	2.53	0.44
39:L2:183:GLY:O	39:L2:186:PHE:HB3	2.18	0.44
1:6:1408:G:H2'	1:6:1409:G:O4'	2.18	0.44
36:1:343:U:H1'	41:L4:95:ARG:HG3	1.98	0.44
72:O6:74:LYS:HG3	72:O6:80:PHE:CD2	3.92	0.44
42:L5:286:VAL:O	42:L5:290:ILE:HG12	2.18	0.44
70:O4:10:ARG:O	36:5:1488:G:O2'	139.62	0.44
36:5:2973:G:C2'	36:5:2974:U:H5'	2.48	0.44
14:C2:78:LEU:HA	14:C2:78:LEU:HD23	1.88	0.44
15:C3:76:LYS:HB3	15:C3:76:LYS:HE3	1.75	0.44
69:O3:58:GLU:HA	69:O3:62:SER:O	2.31	0.44
21:C9:57:ARG:HH11	21:C9:57:ARG:CG	2.30	0.44
41:L4:142:VAL:HB	41:L4:145:ILE:HD13	2.81	0.44
86:5:4187:OHX:N5	86:5:4189:OHX:N2	2.65	0.44
70:O4:41:ARG:HG2	70:O4:56:THR:HG21	2.08	0.44
29:D7:29:ARG:CG	29:D7:29:ARG:HH11	2.25	0.44
1:2:819:G:O6	1:2:853:G:C6	2.71	0.44
51:M5:183:THR:HG23	51:M5:183:THR:O	2.18	0.44
19:C7:34:LEU:HD22	19:C7:38:ILE:CD1	4.65	0.44
59:N3:86:ARG:HA	59:N3:91:VAL:O	2.18	0.44
34:SR:26:SER:OG	34:SR:75:ALA:O	2.33	0.44
36:5:2406:C:H2'	36:5:2407:C:C6	2.53	0.44
22:D0:21:LYS:HA	22:D0:94:GLU:HG2	2.73	0.44
1:6:72:A:H5'	1:6:73:U:OP2	2.17	0.44
36:5:2896:A:C8	36:5:2896:A:H5''	2.52	0.44
86:1:4059:OHX:N4	86:1:4166:OHX:N3	2.65	0.44
41:L4:156:LEU:HD22	41:L4:215:ILE:HD13	1.99	0.44
63:N7:97:SER:HB3	63:N7:99:GLU:HG2	3.13	0.44
42:L5:135:VAL:HG12	42:L5:136:GLU:H	3.15	0.44
86:1:3964:OHX:N2	86:1:4143:OHX:N4	2.66	0.44
1:6:93:A:H4'	1:6:94:U:OP2	2.18	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:D4:54:ALA:HB2	26:D4:79:VAL:HG22	2.00	0.44
45:L8:136:LEU:HD11	45:L8:162:LEU:O	2.18	0.44
1:6:271:A:H5'	1:6:272:U:OP2	2.17	0.44
17:C5:85:ILE:HG22	17:C5:112:LEU:HD23	2.28	0.44
36:5:507:U:H2'	36:5:508:U:C6	2.53	0.44
36:1:806:A:C4	36:1:936:A:C2	3.06	0.44
36:5:2584:G:H3'	36:5:2585:G:H4'	1.99	0.44
30:D8:18:ARG:NH1	1:6:1616:G:H4'	363.93	0.44
1:6:964:U:H4'	1:6:965:U:O4'	2.18	0.44
15:C3:54:LEU:HB3	15:C3:60:VAL:CG1	3.19	0.44
58:N2:59:ASP:OD1	58:N2:60:GLY:N	4.78	0.44
60:N4:86:SER:C	60:N4:88:ASP:H	2.21	0.44
56:N0:131:LYS:HB2	56:N0:134:ASP:OD2	2.18	0.44
21:C9:16:ASN:HA	21:C9:56:LYS:HZ3	4.03	0.44
36:1:3385:U:H2'	36:1:3386:G:O4'	2.18	0.44
1:2:82:U:H2'	1:2:83:G:O4'	2.18	0.44
36:1:600:G:N7	86:1:4100:OHX:N1	2.65	0.44
1:2:130:C:O2'	1:2:131:C:OP1	2.24	0.44
36:1:606:C:O2'	36:1:607:A:N3	2.50	0.44
1:6:532:U:H2'	1:6:533:U:O4'	2.17	0.44
2:S0:76:ILE:HB	2:S0:123:VAL:HG22	1.99	0.44
19:C7:77:GLU:HG2	19:C7:80:ARG:HH21	7.42	0.44
8:S6:23:ARG:O	8:S6:26:VAL:HG23	2.17	0.44
13:C1:109:VAL:CG2	13:C1:139:VAL:HG23	2.47	0.44
1:2:871:G:O2'	29:D7:66:PRO:HB2	2.17	0.44
1:2:1096:C:O2	1:2:1096:C:H2'	2.16	0.44
4:S2:49:LYS:HA	4:S2:49:LYS:HD3	2.22	0.44
8:S6:158:ILE:HA	8:S6:158:ILE:HD12	1.63	0.44
1:2:637:C:OP1	24:D2:32:LYS:HG3	2.17	0.44
36:5:2167:A:H2'	36:5:2168:A:C8	2.53	0.44
23:D1:3:ASN:OD1	23:D1:7:GLN:HB2	2.81	0.44
68:O2:71:HIS:CE1	68:O2:118:LYS:HD3	2.94	0.44
40:L3:299:ASP:O	40:L3:300:ARG:HB2	2.17	0.44
36:5:2309:A:H4'	86:5:4196:OHX:N4	2.33	0.44
17:C5:126:VAL:HG13	17:C5:127:ARG:N	2.21	0.44
1:2:705:U:H2'	1:2:706:A:C8	2.52	0.44
86:5:4187:OHX:N5	86:5:4189:OHX:N6	2.66	0.44
36:1:96:G:P	64:N8:34:MET:HB2	2.58	0.44
6:S4:102:VAL:HG23	6:S4:182:TYR:OH	2.79	0.44
48:M1:29:ARG:HE	48:M1:29:ARG:HB2	3.45	0.44
51:M5:194:GLN:H	51:M5:194:GLN:HG2	1.58	0.44
4:S2:175:GLY:HA3	11:S9:53:ARG:NH2	2.80	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:595:G:C8	36:1:609:G:C6	3.05	0.44
59:N3:120:LYS:N	59:N3:137:VAL:HG23	2.33	0.44
9:S7:71:HIS:CG	9:S7:131:PHE:CZ	3.06	0.44
36:1:2115:G:H22	36:1:2120:A:H1'	1.82	0.44
75:O9:5:LYS:NZ	36:5:1493:G:N7	116.10	0.44
39:L2:56:ALA:HB2	39:L2:130:SER:CB	3.15	0.44
11:S9:129:ILE:HA	11:S9:134:ILE:HG12	4.81	0.44
15:C3:118:ILE:O	15:C3:122:ILE:HG13	2.17	0.44
2:S0:147:THR:O	2:S0:161:PRO:HA	2.34	0.44
30:D8:12:VAL:HA	30:D8:30:VAL:HG12	1.98	0.44
48:M1:108:GLU:HA	48:M1:122:ILE:HG23	2.40	0.44
1:2:1445:G:C4	33:E1:91:ILE:HB	2.53	0.44
72:O6:98:ARG:HB3	72:O6:99:ARG:H	4.40	0.44
59:N3:33:ASN:HD22	59:N3:63:LYS:HB2	3.79	0.44
14:C2:52:LEU:C	14:C2:54:ARG:H	2.21	0.44
63:N7:3:LYS:O	63:N7:5:LEU:N	2.51	0.44
51:M5:73:ARG:O	51:M5:74:PRO:O	2.36	0.44
54:M8:166:LEU:O	54:M8:167:SER:CB	4.15	0.44
76:Q0:85:LEU:HD23	76:Q0:85:LEU:HA	1.88	0.44
42:L5:114:GLY:C	42:L5:116:ASP:N	2.72	0.44
36:1:3275:U:C5'	69:O3:68:TRP:HZ2	2.30	0.44
22:D0:39:SER:HA	22:D0:42:VAL:HG12	1.99	0.44
36:5:1232:C:H2'	36:5:1233:G:C8	2.52	0.44
86:5:4000:OHX:N6	86:5:4190:OHX:N5	2.66	0.44
49:M3:54:LEU:HG	49:M3:119:TYR:CD1	2.52	0.44
2:S0:122:ILE:HA	2:S0:144:ILE:O	2.18	0.44
39:L2:212:GLY:O	39:L2:213:GLY:C	3.49	0.44
1:2:373:G:N7	86:2:2160:OHX:N6	2.66	0.44
9:S7:39:ARG:N	9:S7:40:PRO:HD2	2.33	0.44
19:C7:33:ARG:HD2	34:SR:109:ASP:OD2	2.59	0.44
13:C1:131:ILE:HB	13:C1:135:VAL:HG12	2.64	0.44
67:O1:51:LEU:HD22	67:O1:55:LEU:HD12	1.99	0.44
36:1:2197:C:N4	36:1:2241:U:H2'	2.33	0.44
1:6:1511:U:H2'	1:6:1512:G:C8	2.52	0.44
34:SR:84:SER:OG	34:SR:85:TRP:N	2.98	0.44
1:2:446:A:N6	1:2:461:G:H21	2.16	0.44
56:N0:109:ASP:OD1	56:N0:113:ARG:NH1	2.50	0.44
49:M3:188:ARG:NH1	49:M3:192:GLU:OE1	2.50	0.44
9:S7:155:ASP:OD2	9:S7:156:SER:N	2.91	0.44
68:O2:32:TRP:HB3	36:5:1407:A:H5'	171.62	0.44
36:1:3136:G:OP2	86:1:4103:OHX:N6	2.50	0.44
1:2:1080:U:H6	1:2:1080:U:OP2	2.01	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:D1:69:LEU:HA	23:D1:69:LEU:HD23	1.96	0.44
65:N9:28:LYS:HD3	65:N9:28:LYS:HA	1.57	0.44
56:N0:40:ARG:HA	56:N0:40:ARG:HD2	1.74	0.44
52:M6:38:ALA:O	52:M6:41:LEU:HB2	2.18	0.44
52:M6:46:GLU:OE2	52:M6:134:LYS:HE3	2.17	0.44
47:M0:116:ARG:NH2	36:5:2617:U:O3'	228.24	0.44
34:SR:228:LYS:HE3	34:SR:228:LYS:HB2	1.79	0.44
46:L9:26:LYS:HA	46:L9:35:THR:HG22	2.00	0.44
62:N6:16:ARG:NH2	38:8:23:U:OP1	88.22	0.44
48:M1:89:TYR:HB3	48:M1:169:ALA:CB	2.47	0.44
43:L6:80:ASN:HB2	36:5:3272:C:O2	248.31	0.43
1:2:1555:A:OP2	17:C5:47:ARG:NH2	2.51	0.43
1:2:733:A:H4'	1:2:734:A:C5	2.53	0.43
20:C8:11:PHE:HD2	20:C8:59:GLY:HA3	1.80	0.43
27:D5:41:ILE:O	27:D5:75:LEU:HD13	2.18	0.43
18:C6:54:LEU:HD22	18:C6:54:LEU:HA	1.85	0.43
41:L4:338:LYS:HA	41:L4:338:LYS:HD3	3.51	0.43
26:D4:34:ASN:OD1	1:6:521:A:O2'	428.19	0.43
1:6:1636:C:C2	1:6:1765:A:N6	2.86	0.43
36:5:1573:G:C5	36:5:1574:C:H1'	2.53	0.43
48:M1:21:ILE:HG12	48:M1:125:MET:HB3	4.44	0.43
41:L4:180:LYS:HE3	41:L4:180:LYS:HB3	1.71	0.43
33:E1:108:VAL:HA	33:E1:113:LYS:O	2.18	0.43
51:M5:172:ARG:NH1	36:5:29:C:O3'	106.01	0.43
22:D0:83:GLU:OE1	22:D0:85:ARG:NE	2.80	0.43
37:3:5:G:OP1	48:M1:143:ARG:NH2	2.42	0.43
86:5:4011:OHX:N4	86:5:4198:OHX:N2	2.66	0.43
86:2:2116:OHX:N6	86:C1:201:OHX:N4	2.66	0.43
76:Q0:78:ILE:HG12	76:Q0:83:LYS:HD2	2.00	0.43
29:D7:3:LEU:HD23	29:D7:3:LEU:HA	1.66	0.43
41:L4:170:LYS:HG3	41:L4:175:HIS:HB2	2.00	0.43
1:6:675:U:H2'	1:6:676:G:C8	2.53	0.43
55:M9:4:LEU:HD22	55:M9:7:GLN:HG3	4.96	0.43
27:D5:60:VAL:HG13	27:D5:101:TYR:HB2	2.09	0.43
59:N3:33:ASN:ND2	59:N3:64:LYS:HD3	2.33	0.43
36:5:2875:U:H2'	36:5:2876:C:O5'	2.17	0.43
36:5:1811:G:H2'	36:5:1812:G:O4'	2.18	0.43
36:1:22:G:H1'	38:4:104:A:N3	2.33	0.43
48:M1:10:ARG:HB3	48:M1:152:HIS:CE1	3.53	0.43
54:M8:93:ILE:HG23	36:5:784:A:C6	151.07	0.43
9:S7:115:SER:OG	9:S7:115:SER:O	2.60	0.43
38:4:141:C:H5'	51:M5:109:ARG:HD2	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
64:N8:126:LYS:HA	64:N8:146:GLU:O	2.51	0.43
1:2:943:C:H42	28:D6:15:ARG:HG2	1.83	0.43
36:5:1255:C:H2'	36:5:1256:G:H8	1.83	0.43
25:D3:63:GLN:HA	25:D3:65:ASN:N	2.33	0.43
42:L5:108:ARG:CZ	42:L5:253:PHE:HB2	2.47	0.43
40:L3:20:LYS:HD3	36:5:3139:A:H4'	223.02	0.43
36:1:1607:U:O2'	36:1:1608:C:H5'	2.18	0.43
1:2:245:U:O4	86:2:2094:OHX:N5	2.51	0.43
73:O7:84:SER:O	73:O7:85:LYS:HB2	2.18	0.43
36:5:2409:G:H4'	36:5:2410:U:OP2	2.18	0.43
36:1:674:G:O4'	41:L4:117:GLU:HG3	2.18	0.43
61:N5:108:LEU:HA	61:N5:108:LEU:HD23	1.91	0.43
36:1:1876:U:H5''	36:1:1876:U:H6	1.82	0.43
78:Q2:83:LEU:HA	78:Q2:83:LEU:HD23	1.80	0.43
20:C8:108:LYS:HA	20:C8:108:LYS:HD3	3.45	0.43
41:L4:324:LEU:O	41:L4:327:LEU:O	2.59	0.43
36:1:2402:A:C2	36:1:2871:G:C6	3.06	0.43
41:L4:57:GLY:HA3	41:L4:98:ARG:N	2.58	0.43
40:L3:137:TYR:O	40:L3:139:GLN:N	3.34	0.43
1:2:1553:G:O2'	31:D9:14:TYR:OH	2.30	0.43
40:L3:2:SER:O	40:L3:3:HIS:CB	2.76	0.43
86:1:4135:OHX:N5	86:1:4167:OHX:N6	2.66	0.43
1:2:647:G:N2	1:2:687:G:H22	2.16	0.43
61:N5:115:ARG:HD3	61:N5:121:LYS:HE2	2.00	0.43
28:D6:36:ILE:HD12	28:D6:36:ILE:N	5.22	0.43
1:2:1681:A:H1'	8:S6:66:GLY:HA2	1.99	0.43
20:C8:139:LYS:O	20:C8:143:ARG:NH1	2.69	0.43
72:O6:45:ARG:NH2	72:O6:54:GLU:OE1	2.52	0.43
36:1:2263:C:OP1	86:1:3990:OHX:N1	2.51	0.43
1:2:65:A:OP1	8:S6:176:GLN:NE2	2.42	0.43
4:S2:41:LEU:HD13	4:S2:68:ILE:HD13	2.76	0.43
36:5:2102:U:H2'	36:5:2103:U:C6	2.52	0.43
16:C4:122:PRO:C	16:C4:124:ASP:H	2.44	0.43
35:SM:57:ASN:O	35:SM:61:ILE:HG22	6.03	0.43
2:S0:90:ALA:HA	2:S0:95:ALA:HB3	2.11	0.43
66:O0:10:ILE:HA	66:O0:10:ILE:HD12	2.37	0.43
35:SM:84:LYS:HG2	35:SM:86:ASN:N	2.33	0.43
54:M8:150:VAL:HA	54:M8:153:PHE:CD1	2.52	0.43
54:M8:161:LYS:O	54:M8:162:ALA:CB	2.64	0.43
47:M0:48:LEU:O	47:M0:139:ARG:HA	2.17	0.43
19:C7:13:SER:CB	19:C7:54:THR:HG22	2.60	0.43
12:C0:21:VAL:HG12	12:C0:66:TYR:HD2	2.98	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:488:G:H21	1:6:499:U:H3	1.65	0.43
73:O7:8:PHE:HD2	36:5:1845:G:O2'	152.62	0.43
51:M5:93:LYS:O	51:M5:94:TYR:HB3	2.18	0.43
72:O6:59:ASP:O	72:O6:63:ASN:HB2	2.49	0.43
40:L3:4:ARG:O	40:L3:5:LYS:HB2	2.18	0.43
6:S4:95:THR:CG2	6:S4:97:GLU:HG2	6.47	0.43
71:O5:30:GLU:O	71:O5:34:GLN:HG3	2.76	0.43
61:N5:103:TYR:O	61:N5:105:VAL:HG23	2.96	0.43
1:6:1620:C:H2'	1:6:1621:U:C6	2.53	0.43
54:M8:122:ILE:HG22	54:M8:123:THR:O	2.97	0.43
57:N1:105:PHE:O	57:N1:109:VAL:HG23	2.18	0.43
1:2:1274:C:H41	35:SM:95:SER:HA	1.83	0.43
36:1:860:G:OP1	79:Q3:17:ARG:NH1	2.51	0.43
11:S9:108:ARG:HB2	11:S9:111:THR:HG23	4.28	0.43
21:C9:131:ASP:O	21:C9:135:ILE:HG23	2.97	0.43
5:S3:162:GLN:HG3	1:6:1333:C:C4'	428.71	0.43
36:1:1546:A:N7	51:M5:71:ARG:NH1	2.66	0.43
1:2:1637:C:O2'	35:SM:94:HIS:HE1	2.01	0.43
1:6:1504:G:H2'	1:6:1505:A:C8	2.53	0.43
36:5:2542:U:H1'	36:5:2543:U:C5	2.52	0.43
36:5:2581:U:H2'	36:5:2582:C:C6	2.53	0.43
36:1:3364:C:H2'	36:1:3365:U:C6	2.53	0.43
11:S9:101:VAL:HG23	11:S9:102:GLU:OE2	3.18	0.43
1:2:625:C:H2'	1:2:626:U:C6	2.53	0.43
41:L4:361:HIS:O	56:N0:28:ARG:NH2	2.71	0.43
36:1:1370:G:H5''	64:N8:18:GLY:O	2.18	0.43
1:6:1014:G:H2'	1:6:1015:U:O4'	2.19	0.43
7:S5:175:LEU:HD23	7:S5:197:GLU:HG3	2.39	0.43
36:5:3167:A:H2'	36:5:3168:A:O4'	2.17	0.43
36:5:1932:A:H5'	36:5:1933:A:OP2	2.18	0.43
18:C6:139:GLN:NE2	1:6:1465:C:OP1	353.71	0.43
4:S2:229:LEU:HD23	23:D1:23:ILE:HD11	2.66	0.43
36:1:815:G:C6	36:1:906:A:C4	3.06	0.43
36:1:2574:G:H2'	36:1:2575:G:H8	1.82	0.43
22:D0:43:LYS:HA	22:D0:43:LYS:HD2	1.65	0.43
40:L3:320:ASP:OD2	40:L3:320:ASP:N	2.50	0.43
65:N9:54:LEU:HD23	65:N9:54:LEU:HA	1.87	0.43
36:1:279:U:H2'	36:1:280:U:C6	2.53	0.43
36:5:2344:U:H2'	36:5:2345:A:C8	2.53	0.43
64:N8:14:HIS:C	64:N8:15:VAL:O	3.80	0.43
47:M0:61:SER:HB2	47:M0:63:GLU:HG2	1.99	0.43
36:1:2402:A:OP2	86:1:4092:OHX:N6	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:346:C:OP1	41:L4:52:VAL:HG22	2.18	0.43
10:S8:96:LEU:HD13	10:S8:179:CYS:SG	2.59	0.43
18:C6:115:THR:HG22	18:C6:116:LEU:N	5.15	0.43
3:S1:91:VAL:HG23	3:S1:96:LEU:HB3	2.00	0.43
7:S5:92:ARG:HH11	7:S5:92:ARG:CG	2.89	0.43
28:D6:73:TYR:CZ	28:D6:82:ARG:HD2	2.54	0.43
37:7:23:A:C6	37:7:24:A:C6	3.07	0.43
18:C6:45:ARG:HG2	18:C6:49:TYR:CE2	2.53	0.43
86:5:4093:OHX:N5	86:5:4199:OHX:N1	2.65	0.43
36:1:3115:C:O2'	36:1:3117:C:N4	2.45	0.43
35:SM:82:THR:HB	35:SM:83:LYS:H	1.40	0.43
33:E1:113:LYS:HD2	33:E1:113:LYS:H	1.82	0.43
36:1:1276:U:OP1	86:1:4089:OHX:N4	2.52	0.43
2:S0:120:LEU:HD12	2:S0:142:PRO:O	2.18	0.43
10:S8:10:LYS:HG2	13:C1:133:LYS:HE3	2.12	0.43
1:2:1571:C:OP2	86:2:2155:OHX:N1	2.51	0.43
33:E1:146:SER:OG	1:6:1234:A:H4'	436.02	0.43
41:L4:332:LYS:HE3	36:5:599:C:OP1	272.97	0.43
36:5:1098:A:C2'	36:5:1099:A:H5'	2.49	0.43
46:L9:13:PRO:HG2	46:L9:16:VAL:HG11	3.55	0.43
36:5:2093:A:H3'	36:5:2093:A:N3	2.34	0.43
52:M6:16:VAL:HG23	52:M6:42:ASN:O	2.19	0.43
1:2:1383:G:OP1	22:D0:87:HIS:ND1	2.42	0.43
17:C5:28:MET:HE3	17:C5:33:PHE:HB2	2.56	0.43
1:6:1621:U:C2	1:6:1622:G:C8	3.06	0.43
16:C4:45:GLY:HA2	16:C4:54:GLU:HG2	2.16	0.43
6:S4:222:LEU:HB3	6:S4:223:ASN:H	1.64	0.43
1:2:1734:U:O2'	1:2:1735:U:H5'	2.19	0.43
36:5:3259:U:H6	36:5:3259:U:C5'	2.31	0.43
2:S0:7:PHE:HZ	23:D1:43:GLY:HA2	2.74	0.43
36:1:1576:G:N7	36:1:1577:G:C6	2.87	0.43
1:2:1166:A:H2'	1:2:1167:G:O4'	2.18	0.43
76:Q0:127:LEU:HD13	76:Q0:128:LYS:HG2	2.00	0.43
73:O7:22:CYS:SG	73:O7:24:ARG:HG3	3.56	0.43
21:C9:5:SER:OG	21:C9:7:ARG:HG3	3.05	0.43
19:C7:71:PHE:CD1	19:C7:73:LEU:HB3	2.53	0.43
8:S6:2:LYS:HB3	8:S6:108:VAL:HG13	3.00	0.43
36:1:1486:G:O6	86:1:3980:OHX:N5	2.51	0.43
36:1:2612:U:H2'	36:1:2613:U:O4'	2.18	0.43
32:E0:43:ARG:HH12	1:6:590:C:H5''	417.96	0.43
3:S1:23:PRO:O	3:S1:27:LYS:HG2	2.18	0.43
3:S1:153:HIS:HE1	1:6:1045:C:OP1	335.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:D6:61:GLU:O	28:D6:62:TYR:HB3	2.26	0.43
57:N1:54:HIS:CE1	57:N1:55:LYS:HG2	4.39	0.43
36:5:2973:G:H2'	36:5:2974:U:H5'	2.00	0.43
5:S3:224:ASP:OD1	34:SR:228:LYS:HD2	2.19	0.43
36:5:3390:G:C2'	36:5:3391:A:H5'	2.49	0.43
47:M0:188:GLY:O	47:M0:190:VAL:N	2.51	0.43
8:S6:126:ASP:CG	8:S6:127:THR:N	3.39	0.43
11:S9:7:THR:HG21	1:6:758:U:OP1	383.62	0.43
63:N7:107:ARG:NH2	36:5:1635:G:OP1	210.64	0.43
1:6:1441:C:H2'	1:6:1442:U:C6	2.52	0.43
41:L4:283:THR:HB	41:L4:285:ASP:H	2.11	0.43
36:1:553:U:H2'	36:1:554:A:O4'	2.17	0.43
36:1:2606:G:H2'	36:1:2606:G:N3	2.33	0.43
34:SR:248:ASN:OD1	34:SR:248:ASN:N	2.51	0.43
40:L3:128:LYS:HB3	40:L3:128:LYS:HE2	2.28	0.43
57:N1:79:MET:HB3	57:N1:84:TYR:CE2	2.53	0.43
36:1:546:C:H5'	36:1:547:G:O4'	2.18	0.43
41:L4:311:HIS:NE2	41:L4:314:LYS:HA	2.34	0.43
1:6:1124:A:O2'	1:6:1125:A:H5'	2.18	0.43
70:O4:74:ARG:CD	70:O4:85:VAL:HG21	4.10	0.43
1:2:1587:A:H2'	1:2:1588:G:H8	1.82	0.43
10:S8:58:LEU:O	10:S8:59:ARG:HB2	2.18	0.43
40:L3:35:ASP:CG	40:L3:37:ARG:HD2	2.87	0.43
28:D6:85:ARG:HD3	28:D6:85:ARG:HA	1.57	0.43
27:D5:42:LEU:O	27:D5:44:GLN:N	2.51	0.43
18:C6:44:LEU:O	18:C6:47:LYS:HB2	2.17	0.43
63:N7:47:GLU:CD	63:N7:69:LYS:HE2	2.39	0.43
1:2:1515:A:OP2	5:S3:7:LYS:HB2	2.18	0.43
48:M1:25:GLU:OE2	48:M1:29:ARG:HD2	2.19	0.43
1:2:579:A:C2	5:S3:143:ARG:HG3	2.42	0.43
7:S5:33:VAL:O	7:S5:37:GLN:HB2	2.18	0.43
1:2:452:A:H3'	1:2:453:U:C5	2.54	0.43
1:2:887:A:C1'	16:C4:122:PRO:HB3	2.45	0.43
6:S4:126:VAL:CG2	6:S4:156:VAL:HA	2.52	0.43
6:S4:191:ARG:CZ	6:S4:245:LYS:HD2	4.17	0.43
20:C8:142:GLY:O	20:C8:145:ARG:HD2	2.17	0.43
2:S0:162:CYS:HB3	2:S0:163:ASN:H	1.51	0.43
12:C0:33:GLU:H	12:C0:33:GLU:CD	2.21	0.43
20:C8:28:ILE:HG13	20:C8:28:ILE:H	4.33	0.43
64:N8:65:GLN:O	64:N8:66:ALA:CB	2.65	0.43
74:O8:19:ASP:N	74:O8:19:ASP:OD2	2.88	0.43
36:1:3274:A:H2'	53:M7:171:ARG:NH1	2.34	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:1597:C:H2'	36:1:1598:G:C8	2.53	0.43
46:L9:188:THR:HG22	46:L9:189:GLU:N	4.94	0.43
36:1:2341:A:P	40:L3:247:ARG:HH22	2.42	0.43
36:5:1816:A:O2'	36:5:1817:G:OP1	2.32	0.43
66:O0:30:THR:O	66:O0:34:LEU:N	2.95	0.43
36:5:1480:G:N2	36:5:1872:C:C5	2.86	0.43
27:D5:82:HIS:O	27:D5:85:LYS:HB3	2.19	0.43
78:Q2:65:THR:OG1	78:Q2:87:ARG:NH1	2.49	0.43
86:1:4088:OHX:N6	86:1:4157:OHX:N3	2.66	0.43
1:2:443:C:OP2	26:D4:105:ARG:HB3	2.18	0.43
40:L3:361:THR:HG23	40:L3:371:GLN:O	2.17	0.43
36:5:65:A:C4	36:5:110:G:N7	2.86	0.43
36:1:564:G:H2'	36:1:565:U:C6	2.54	0.43
86:1:4056:OHX:N5	86:1:4163:OHX:N1	2.67	0.43
45:L8:123:GLN:O	45:L8:125:ALA:N	4.45	0.43
1:6:1363:U:O2'	1:6:1364:G:H5'	2.18	0.43
71:O5:47:VAL:O	71:O5:51:ILE:HG13	2.45	0.43
25:D3:135:LEU:HA	25:D3:135:LEU:HD23	2.38	0.43
36:5:67:A:OP1	86:5:3955:OHX:N6	2.52	0.43
42:L5:22:ARG:NH2	42:L5:28:THR:OG1	2.50	0.43
15:C3:73:ARG:HD3	1:6:859:A:C5	331.33	0.43
68:O2:64:LYS:HD3	68:O2:65:PHE:CE2	3.09	0.43
36:5:1394:A:H4'	36:5:1420:C:H4'	2.01	0.43
69:O3:38:PRO:HD2	69:O3:39:GLN:OE1	2.18	0.43
38:8:124:G:OP2	86:8:222:OHX:N2	2.52	0.43
36:1:2367:A:H2'	36:1:2368:A:O4'	2.18	0.43
76:Q0:113:ARG:NH1	36:5:1298:C:O3'	291.31	0.43
1:2:1178:G:H2'	1:2:1179:G:O4'	2.19	0.43
36:5:1483:G:C8	36:5:1485:G:C8	3.06	0.43
36:1:2850:G:O6	86:1:4079:OHX:N6	2.51	0.43
29:D7:67:THR:HG22	29:D7:68:GLY:H	1.82	0.43
20:C8:18:LEU:HA	20:C8:18:LEU:HD13	1.82	0.43
57:N1:31:LEU:HD23	57:N1:31:LEU:HA	2.30	0.43
18:C6:102:LYS:HB3	18:C6:102:LYS:HE2	2.59	0.43
34:SR:10:ARG:HD3	34:SR:10:ARG:HA	3.73	0.43
48:M1:17:LEU:HD21	48:M1:19:LEU:HD21	2.01	0.43
1:2:66:U:O3'	8:S6:171:LYS:NZ	2.50	0.43
3:S1:131:ASP:O	3:S1:133:TYR:N	2.44	0.43
36:1:3186:A:O2'	46:L9:42:ASP:HA	2.18	0.43
46:L9:162:GLN:NE2	76:Q0:89:TYR:CD1	3.20	0.43
36:1:20:A:P	71:O5:90:ARG:NH1	2.92	0.43
59:N3:48:ARG:HG3	36:5:2339:C:OP2	246.99	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:S1:157:GLN:O	3:S1:160:HIS:HB2	4.11	0.43
41:L4:222:VAL:HA	41:L4:223:PRO:HD3	1.82	0.43
36:1:1246:G:H8	36:1:1246:G:OP1	2.02	0.43
36:5:3194:C:H2'	36:5:3195:U:H3'	2.01	0.43
1:2:498:G:O2'	1:2:499:U:O5'	2.34	0.43
1:6:119:A:H1'	1:6:397:A:C5	2.53	0.43
86:2:2161:OHX:N5	11:S9:8:TYR:O	2.52	0.43
36:5:3163:A:N6	36:5:3164:C:H42	2.17	0.43
36:5:1556:C:H2'	36:5:2169:G:H1	1.84	0.43
36:5:438:A:C8	36:5:439:C:C5	3.03	0.43
78:Q2:63:LYS:HD2	78:Q2:87:ARG:NH2	2.33	0.43
86:1:4088:OHX:N5	86:1:4157:OHX:N1	2.66	0.43
1:6:74:U:H3'	1:6:75:U:H3'	2.00	0.43
1:2:1484:G:O4'	1:2:1607:G:H4'	2.19	0.43
54:M8:176:ARG:HA	54:M8:182:LYS:O	2.18	0.43
1:6:901:G:N1	1:6:902:G:C6	2.86	0.43
63:N7:64:LYS:HB2	63:N7:64:LYS:HE2	4.15	0.43
36:5:208:C:H2'	36:5:209:A:O4'	2.19	0.43
42:L5:211:LEU:HA	42:L5:211:LEU:HD23	1.69	0.43
71:O5:105:ARG:O	71:O5:109:ILE:HG13	3.07	0.43
34:SR:267:PRO:HD2	34:SR:269:TYR:HE1	2.96	0.43
8:S6:110:ALA:O	8:S6:111:LEU:HD23	2.18	0.43
42:L5:163:LEU:HD11	42:L5:175:HIS:CG	2.53	0.43
36:5:1366:A:C2	36:5:1367:G:C4	3.06	0.43
68:O2:24:ARG:HG2	68:O2:25:TYR:CE2	2.66	0.43
36:5:1525:G:C6	36:5:1526:U:O4	2.72	0.43
9:S7:122:HIS:HA	9:S7:125:ILE:HD12	2.01	0.43
28:D6:30:ILE:HG13	28:D6:31:PRO:HD2	2.18	0.43
1:2:1168:U:H2'	1:2:1169:G:H5'	2.01	0.43
36:5:279:U:H2'	36:5:280:U:C6	2.53	0.43
47:M0:115:MET:HB2	36:5:2865:U:OP1	239.62	0.43
40:L3:380:MET:HE3	36:5:3369:G:C6	226.49	0.43
6:S4:57:ASN:HB2	6:S4:60:GLU:H	1.98	0.43
36:5:2953:U:H2'	36:5:2954:U:H2'	2.01	0.43
36:1:345:G:H2'	38:4:25:G:O2'	2.18	0.43
42:L5:49:TYR:CD1	42:L5:66:SER:HB3	2.53	0.43
1:2:1061:A:H2'	1:2:1062:A:H5'	2.00	0.43
36:1:1256:G:O6	36:1:1261:G:N2	2.50	0.43
34:SR:159:ASN:OD1	34:SR:163:ASP:HA	3.53	0.43
41:L4:82:THR:O	41:L4:82:THR:OG1	2.35	0.43
17:C5:110:GLU:H	17:C5:110:GLU:CD	2.46	0.43
1:6:862:A:H4'	1:6:863:A:O5'	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:S8:76:THR:HB	10:S8:105:ASP:HB2	2.01	0.43
36:1:2854:U:P	47:M0:3:ARG:HH22	2.40	0.43
65:N9:23:LYS:HB3	65:N9:24:PRO:CD	2.68	0.43
48:M1:92:ARG:O	48:M1:95:ASN:HB2	2.42	0.43
36:1:2184:U:OP1	39:L2:209:HIS:HE1	2.01	0.43
3:S1:131:ASP:N	3:S1:131:ASP:OD1	4.28	0.43
3:S1:193:ILE:O	3:S1:197:ILE:HG12	2.19	0.43
1:2:1410:A:H5''	18:C6:118:ILE:HD13	2.00	0.43
25:D3:56:LYS:NZ	25:D3:96:VAL:O	3.71	0.43
11:S9:162:SER:HA	11:S9:163:PRO:HD2	2.47	0.43
7:S5:37:GLN:CD	18:C6:53:LEU:HD22	2.39	0.43
36:1:2260:U:H2'	36:1:2261:G:O4'	2.19	0.43
45:L8:152:LEU:HB3	45:L8:180:VAL:HG11	2.00	0.43
15:C3:16:ILE:HG13	15:C3:62:GLN:NE2	4.40	0.43
36:5:2840:C:H2'	36:5:2841:G:O4'	2.19	0.43
48:M1:12:LEU:HD12	48:M1:131:MET:HE3	2.01	0.43
18:C6:143:ARG:HB3	18:C6:143:ARG:HE	1.66	0.43
12:C0:32:HIS:NE2	12:C0:35:ILE:HG13	2.34	0.43
36:5:118:U:C5	36:5:119:U:C4	3.06	0.43
18:C6:128:LYS:HE3	1:6:1417:A:O2'	397.04	0.43
1:6:1157:A:H2'	1:6:1160:A:N7	2.33	0.43
22:D0:20:ILE:HD12	22:D0:100:VAL:HG21	3.92	0.43
78:Q2:63:LYS:HD2	78:Q2:87:ARG:CZ	2.49	0.43
36:5:3245:A:H2	36:5:3246:G:N1	2.17	0.43
36:5:956:U:H2'	36:5:957:C:C6	2.53	0.43
49:M3:124:ILE:O	49:M3:124:ILE:HG12	2.18	0.43
36:5:1506:A:H1'	36:5:1848:G:C6	2.53	0.43
21:C9:125:SER:OG	21:C9:128:GLY:N	2.52	0.43
86:5:4140:OHX:N4	86:5:4181:OHX:N1	2.67	0.43
40:L3:250:ALA:HB1	36:5:2947:G:N3	218.79	0.43
1:6:751:G:C2	1:6:752:A:C4	3.06	0.43
1:2:1192:C:H5'	18:C6:142:TYR:HA	2.01	0.43
9:S7:96:ARG:HB3	1:6:856:A:N6	365.68	0.43
51:M5:178:HIS:HD1	51:M5:178:HIS:H	1.98	0.43
63:N7:84:ARG:HA	66:O0:62:LEU:HD21	2.00	0.43
2:S0:65:ALA:O	2:S0:66:ALA:HB3	3.01	0.43
86:1:3980:OHX:N1	86:1:4158:OHX:N2	2.67	0.43
5:S3:162:GLN:OE1	5:S3:165:ASN:ND2	2.40	0.43
42:L5:140:ARG:HB2	36:5:1080:A:OP1	229.25	0.43
33:E1:103:LEU:HA	33:E1:103:LEU:HD23	1.69	0.43
5:S3:216:PRO:HB2	5:S3:217:ILE:H	1.56	0.43
17:C5:64:LYS:HA	17:C5:73:PRO:HB3	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
48:M1:26:SER:HB3	48:M1:63:GLU:HG2	2.36	0.43
39:L2:180:LEU:HG	79:Q3:26:VAL:HG21	2.33	0.43
21:C9:16:ASN:OD1	21:C9:56:LYS:NZ	3.06	0.43
1:2:130:C:HO2'	1:2:131:C:P	2.37	0.43
44:L7:116:PHE:HB2	44:L7:199:ASN:OD1	2.53	0.43
34:SR:245:PHE:O	34:SR:294:TRP:CD1	2.72	0.43
36:5:3018:C:C4	36:5:3019:U:C4	3.07	0.43
24:D2:107:SER:HA	1:6:804:A:C8	367.79	0.43
39:L2:236:GLY:N	36:5:2183:A:O2'	205.62	0.43
53:M7:26:PHE:HE1	53:M7:120:ASN:HA	1.83	0.43
36:5:2206:G:O2'	36:5:2207:A:H5'	2.19	0.43
1:6:322:G:OP1	86:6:2107:OHX:N5	2.52	0.43
36:1:608:A:C4	43:L6:22:ARG:NH1	2.87	0.43
1:6:636:A:O2'	1:6:637:C:H5'	2.19	0.43
9:S7:101:LYS:HD3	1:6:638:U:O2'	362.53	0.43
36:5:2816:G:C8	36:5:2869:U:H3'	2.53	0.43
9:S7:137:GLY:HA3	9:S7:153:LEU:HD12	2.73	0.43
1:6:848:C:H2'	1:6:849:C:C6	2.54	0.43
38:4:73:U:OP1	62:N6:24:SER:OG	2.28	0.43
71:O5:31:LEU:HD12	71:O5:31:LEU:HA	1.89	0.43
36:1:1390:A:H5'	36:1:1390:A:N3	2.33	0.43
22:D0:77:LYS:HG2	22:D0:77:LYS:H	1.59	0.43
29:D7:8:LEU:HA	29:D7:8:LEU:HD23	1.86	0.43
46:L9:169:ASN:O	46:L9:170:LYS:HG2	2.19	0.43
45:L8:150:LEU:HD23	45:L8:176:PRO:HB2	2.80	0.43
1:2:459:G:O2'	1:2:460:A:OP1	2.32	0.43
3:S1:158:SER:O	3:S1:162:ARG:HG3	2.18	0.43
5:S3:97:SER:O	5:S3:101:GLN:HG2	2.82	0.43
58:N2:13:LYS:NZ	36:5:1676:A:OP1	156.99	0.43
36:5:3275:U:O3'	36:5:3276:G:C2	2.71	0.43
36:5:3362:A:H2'	36:5:3363:U:O4'	2.19	0.43
36:5:1876:U:C6	36:5:1876:U:C5'	3.01	0.43
11:S9:93:LEU:O	11:S9:96:VAL:HG22	2.19	0.43
3:S1:39:GLU:HB3	3:S1:73:LEU:O	2.18	0.43
74:O8:46:ARG:NH1	74:O8:47:GLY:O	2.51	0.43
36:1:3353:G:O2'	36:1:3356:G:H5'	2.18	0.43
18:C6:116:LEU:HA	18:C6:116:LEU:HD23	4.53	0.43
62:N6:122:LYS:HE2	62:N6:122:LYS:HB3	1.83	0.43
49:M3:3:ILE:HG12	64:N8:34:MET:CE	2.48	0.43
1:2:1513:G:O2'	1:2:1515:A:N3	2.41	0.43
1:2:321:C:N4	1:2:1667:A:OP1	2.51	0.43
73:O7:69:HIS:O	73:O7:73:ARG:HG3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
72:O6:55:ARG:O	72:O6:58:ILE:HD13	2.54	0.43
21:C9:23:GLN:HG2	21:C9:55:TYR:CD2	2.54	0.43
49:M3:101:ARG:HB2	36:5:76:G:N7	84.83	0.43
61:N5:49:LYS:O	61:N5:50:ALA:HB3	2.19	0.43
36:5:1806:A:H2'	36:5:1807:G:O4'	2.19	0.43
56:N0:4:PHE:O	56:N0:100:VAL:HG22	2.18	0.43
19:C7:13:SER:HA	19:C7:54:THR:HG22	2.00	0.43
5:S3:163:PRO:O	5:S3:167:PHE:N	2.50	0.43
36:1:2242:A:H5''	39:L2:244:GLY:HA3	2.01	0.43
42:L5:184:ASP:OD1	42:L5:187:THR:HG22	2.19	0.43
1:2:712:G:H2'	1:2:713:A:O4'	2.18	0.43
36:1:884:A:OP1	73:O7:5:THR:CG2	2.67	0.43
36:1:2718:U:OP2	86:1:3987:OHX:N3	2.51	0.43
1:2:1247:U:H5''	33:E1:94:LYS:O	2.18	0.43
19:C7:23:LYS:H	34:SR:216:LYS:HE2	1.84	0.43
49:M3:126:PHE:CD1	49:M3:133:PRO:HG2	2.54	0.43
14:C2:52:LEU:HD13	14:C2:85:LYS:HZ1	1.83	0.43
43:L6:21:THR:HB	36:5:612:U:OP1	227.48	0.43
16:C4:18:ARG:HB2	16:C4:18:ARG:HE	4.28	0.43
46:L9:2:LYS:HA	46:L9:60:GLY:O	2.18	0.43
1:2:901:G:N2	16:C4:54:GLU:OE1	2.52	0.43
36:5:2947:G:N2	36:5:2948:C:C2	2.86	0.43
1:2:1244:A:HO2'	1:2:1245:G:P	2.40	0.43
1:2:1144:U:H2'	1:2:1145:U:C6	2.54	0.43
1:2:230:C:H2'	1:2:231:U:H5''	2.00	0.43
36:1:1486:G:H21	70:O4:6:THR:HG22	1.83	0.43
70:O4:22:VAL:CG1	70:O4:30:LEU:HD13	2.82	0.43
53:M7:4:TYR:CZ	53:M7:18:ARG:HG3	2.69	0.43
34:SR:232:TYR:OH	34:SR:265:LEU:HD22	5.50	0.43
36:1:3174:A:C6	36:1:3175:U:C4	3.07	0.43
33:E1:89:LYS:HD2	33:E1:89:LYS:HA	1.76	0.43
52:M6:14:HIS:O	52:M6:41:LEU:HD12	2.26	0.43
7:S5:81:ARG:HD3	7:S5:82:PHE:CE2	2.54	0.43
44:L7:125:GLU:OE1	44:L7:128:LYS:HE3	2.19	0.43
36:1:2250:G:O2'	36:1:2251:G:H5'	2.19	0.43
6:S4:23:LEU:O	6:S4:24:SER:OG	2.61	0.43
6:S4:64:ILE:HG13	26:D4:18:LEU:HG	2.00	0.43
1:2:328:A:H2'	1:2:329:G:O4'	2.18	0.43
1:2:1604:U:C4	1:2:1605:G:N7	2.87	0.43
48:M1:141:ARG:O	48:M1:145:LYS:HE2	2.18	0.43
36:1:3049:A:C2	40:L3:75:ALA:HB2	2.54	0.43
15:C3:20:ARG:HD3	24:D2:56:HIS:CD2	5.63	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
43:L6:90:LYS:HB2	43:L6:90:LYS:HE3	4.23	0.43
57:N1:27:LEU:HD22	57:N1:27:LEU:HA	1.80	0.43
1:2:179:A:H2'	1:2:180:A:O4'	2.19	0.43
36:5:2709:C:H2'	36:5:2710:C:C6	2.54	0.43
46:L9:45:PHE:CD1	46:L9:55:VAL:HG12	2.54	0.43
16:C4:84:ARG:HG2	16:C4:85:ALA:O	2.19	0.43
47:M0:76:MET:HE3	47:M0:148:VAL:HA	2.01	0.43
36:1:2960:C:H2'	36:1:2961:G:H8	1.82	0.43
1:6:470:A:H8	1:6:470:A:H5''	1.83	0.43
42:L5:111:GLN:C	42:L5:113:LEU:H	2.22	0.43
3:S1:61:LEU:HG	3:S1:64:ARG:HH21	1.84	0.43
1:6:1429:G:H2'	1:6:1430:U:H6	1.82	0.43
28:D6:4:LYS:HG3	28:D6:4:LYS:O	2.18	0.43
1:2:1682:U:O2'	1:2:1683:C:H5'	2.19	0.43
36:5:1565:G:N2	36:5:1566:A:H1'	2.34	0.43
46:L9:171:ASP:CG	46:L9:173:ARG:HH11	2.22	0.43
36:1:1355:A:H4'	36:1:1356:U:O5'	2.17	0.43
36:5:2573:G:H3'	36:5:2574:G:H5''	2.00	0.43
20:C8:119:ILE:HA	20:C8:119:ILE:HD12	3.09	0.43
5:S3:8:LYS:HG2	22:D0:63:LEU:HD21	2.67	0.43
19:C7:34:LEU:HD23	19:C7:34:LEU:HA	1.77	0.43
48:M1:166:LYS:C	48:M1:168:ASP:H	2.82	0.43
10:S8:114:GLU:HG2	10:S8:120:THR:HA	2.01	0.43
24:D2:17:ALA:HB2	24:D2:25:VAL:CG1	2.47	0.43
1:6:837:G:H2'	1:6:838:G:C8	2.54	0.43
30:D8:44:VAL:HG21	30:D8:48:VAL:CG2	2.92	0.43
45:L8:156:ASP:O	45:L8:183:LYS:HE3	6.80	0.43
23:D1:36:VAL:O	23:D1:51:VAL:N	2.51	0.43
22:D0:104:THR:HG21	22:D0:116:VAL:HG21	1.99	0.43
43:L6:52:VAL:CG1	43:L6:65:ILE:HG13	2.59	0.43
64:N8:42:ARG:HH21	36:5:2799:A:H1'	193.49	0.43
17:C5:15:HIS:HB3	17:C5:22:LEU:CD2	2.48	0.43
86:5:4034:OHX:N2	86:5:4117:OHX:N4	2.66	0.43
52:M6:127:LEU:HD22	56:N0:156:VAL:HG23	2.01	0.43
29:D7:61:THR:OG1	29:D7:62:ILE:N	3.42	0.43
36:1:246:U:H2'	36:1:247:C:C6	2.53	0.43
32:E0:13:LYS:HE2	1:6:566:C:O2	375.12	0.43
21:C9:66:TYR:HA	21:C9:124:ILE:HB	2.00	0.43
1:6:94:U:H2'	1:6:95:G:O4'	2.19	0.43
51:M5:11:GLN:HG2	51:M5:44:ARG:HH21	1.82	0.43
68:O2:55:ILE:HB	36:5:947:G:C5'	187.88	0.43
19:C7:26:LEU:HD22	19:C7:59:LYS:HA	2.41	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:1649:G:H2'	1:6:1650:U:C6	2.54	0.43
1:6:1317:C:H2'	1:6:1318:G:O4'	2.17	0.43
3:S1:140:ILE:O	3:S1:210:ILE:HA	2.18	0.43
19:C7:33:ARG:HG3	34:SR:127:ARG:NH1	2.34	0.43
46:L9:88:TYR:CE2	46:L9:184:LYS:HE2	2.53	0.43
34:SR:232:TYR:CE1	34:SR:234:LEU:HD11	2.54	0.43
86:2:2084:OHX:N6	86:2:2086:OHX:N2	2.66	0.43
36:5:2192:C:H2'	36:5:2193:U:O4'	2.19	0.43
53:M7:105:LYS:HB3	53:M7:107:LEU:HD13	2.23	0.43
1:2:485:A:H2'	1:2:486:G:O4'	2.18	0.43
36:1:2703:A:OP2	42:L5:23:ARG:NH1	2.48	0.43
37:3:58:C:H2'	37:3:59:U:H6	1.84	0.43
36:1:3383:G:H2'	36:1:3384:U:H6	1.83	0.43
1:2:1222:C:H2'	1:2:1223:A:O4'	2.19	0.43
45:L8:242:ALA:HA	45:L8:245:LYS:HD3	3.29	0.43
19:C7:81:LYS:HB2	19:C7:81:LYS:HE3	1.70	0.43
60:N4:57:LYS:HE3	60:N4:57:LYS:HB2	1.82	0.43
61:N5:57:LEU:HD12	61:N5:57:LEU:HA	1.79	0.43
5:S3:142:LEU:HD12	5:S3:142:LEU:HA	1.86	0.43
42:L5:177:GLU:HG3	42:L5:177:GLU:H	1.61	0.43
36:5:1226:G:H2'	36:5:1227:C:C6	2.53	0.43
78:Q2:14:GLY:O	78:Q2:16:THR:N	2.52	0.43
23:D1:74:GLN:HE21	23:D1:74:GLN:HB3	2.93	0.43
3:S1:172:LEU:O	3:S1:176:VAL:HG23	2.19	0.43
53:M7:112:LEU:HA	53:M7:112:LEU:HD12	1.99	0.43
11:S9:110:GLN:NE2	11:S9:122:VAL:O	2.51	0.43
62:N6:115:ARG:O	62:N6:119:ILE:HG13	2.19	0.43
53:M7:28:ASN:O	53:M7:32:THR:HG23	2.59	0.43
51:M5:68:ARG:HH11	36:5:291:C:P	145.41	0.43
86:5:4093:OHX:N6	86:5:4199:OHX:N2	2.66	0.43
38:8:142:C:H2'	38:8:143:U:C6	2.54	0.43
41:L4:140:HIS:CG	41:L4:247:PHE:HB2	2.96	0.43
1:2:1561:U:H4'	1:2:1599:C:H4'	2.01	0.43
33:E1:109:ASP:HB2	33:E1:113:LYS:HD3	2.00	0.43
1:6:1228:G:H4'	1:6:1228:G:OP2	2.19	0.43
1:2:885:G:H2'	1:2:886:U:C6	2.53	0.43
1:6:1198:G:OP1	1:6:1199:G:H1'	2.18	0.43
61:N5:24:LEU:HB3	61:N5:25:LYS:H	2.57	0.43
1:2:473:A:H4'	1:2:768:C:O2	2.19	0.43
1:2:1600:A:O2'	1:2:1602:C:N4	2.51	0.43
54:M8:2:GLY:O	54:M8:3:ILE:HD13	2.50	0.43
45:L8:33:ASN:HD22	45:L8:33:ASN:C	4.66	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:1533:C:H4'	1:6:1539:G:C6	2.53	0.43
36:1:1845:G:H8	36:1:1845:G:H5''	1.84	0.43
36:1:2544:U:H2'	36:1:2545:C:H6	1.84	0.43
13:C1:36:LYS:HE2	13:C1:59:PRO:O	4.42	0.43
36:5:3242:G:H21	36:5:3245:A:H5''	1.83	0.43
32:E0:14:VAL:HA	32:E0:17:GLN:HG2	2.13	0.43
26:D4:53:ASP:OD1	26:D4:96:LEU:HD21	2.55	0.43
36:1:1615:C:H2'	36:1:1616:U:H6	1.84	0.43
6:S4:194:THR:OG1	6:S4:195:ILE:N	2.50	0.43
1:6:138:A:H62	1:6:266:A:H61	1.66	0.43
61:N5:105:VAL:HG21	61:N5:135:ILE:HG13	2.51	0.43
36:5:541:U:O4	86:5:4013:OHX:N3	2.52	0.43
39:L2:15:ILE:HD12	39:L2:15:ILE:HA	4.63	0.43
36:1:2529:A:C2	36:1:2582:C:C2	3.06	0.43
34:SR:100:TYR:HA	34:SR:100:TYR:HD2	2.53	0.43
1:2:1015:U:H5''	1:2:1016:C:OP2	2.18	0.43
1:6:727:U:H2'	1:6:728:U:C6	2.53	0.43
36:5:2425:G:H2'	36:5:2426:U:C6	2.53	0.43
36:1:860:G:C6	39:L2:181:LYS:HB3	2.54	0.43
6:S4:71:LYS:HA	6:S4:76:VAL:O	2.19	0.43
36:5:2287:C:C5	36:5:2298:U:C2	3.07	0.43
36:1:1925:U:O2'	36:1:1927:G:N7	2.50	0.43
70:O4:67:LYS:HA	70:O4:70:LYS:HE3	2.01	0.43
64:N8:18:GLY:O	36:5:1370:G:H5''	175.35	0.43
47:M0:115:MET:HB3	36:5:2618:G:C5	237.87	0.43
48:M1:171:VAL:HG13	48:M1:172:LEU:N	2.34	0.43
45:L8:65:LEU:HD12	51:M5:25:VAL:HG13	1.99	0.43
1:6:1518:C:OP2	86:6:2143:OHX:N1	2.52	0.43
39:L2:149:ARG:HH22	39:L2:253:GLN:CB	7.09	0.43
10:S8:122:GLY:O	86:S8:302:OHX:N6	2.51	0.43
1:6:1085:G:N2	1:6:1088:A:OP2	2.46	0.43
36:5:48:A:O4'	36:5:50:U:C6	2.72	0.43
36:1:1621:A:H2'	36:1:1622:U:C6	2.54	0.43
34:SR:240:VAL:HG22	34:SR:256:THR:HG22	2.00	0.43
34:SR:29:GLN:H	34:SR:29:GLN:HG2	1.54	0.43
3:S1:54:LEU:HD23	3:S1:54:LEU:HA	2.27	0.43
36:5:825:U:H6	36:5:825:U:O5'	2.01	0.43
36:1:743:C:O2	54:M8:141:ARG:HD2	2.18	0.43
36:5:1500:G:H2'	36:5:1501:U:O4'	2.19	0.43
36:1:2208:A:C2	86:1:4047:OHX:N6	2.87	0.43
8:S6:169:TYR:HE2	8:S6:171:LYS:HD2	7.94	0.43
36:1:2939:G:C2'	36:1:2940:A:H5'	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:S8:59:ARG:O	10:S8:60:ILE:HG13	2.42	0.43
27:D5:43:ASP:N	27:D5:46:LYS:HD2	2.33	0.43
36:5:314:U:H2'	36:5:315:C:C6	2.54	0.43
72:O6:25:LYS:HG3	72:O6:28:TYR:CE2	3.09	0.43
28:D6:87:ARG:NH2	28:D6:94:ASN:O	2.39	0.43
36:1:291:C:OP2	51:M5:128:LYS:NZ	2.52	0.43
42:L5:41:LYS:HA	42:L5:41:LYS:HD2	1.62	0.43
13:C1:5:LEU:HD23	13:C1:7:VAL:HA	7.90	0.43
7:S5:37:GLN:NE2	18:C6:53:LEU:HD13	2.33	0.43
4:S2:227:PRO:HA	4:S2:230:TRP:CD1	2.54	0.43
1:6:1568:C:H2'	1:6:1568:C:H6	1.57	0.43
35:SM:61:ILE:HG13	35:SM:61:ILE:H	1.61	0.43
36:1:1759:C:H2'	36:1:1760:A:O4'	2.19	0.43
56:N0:155:ARG:HH21	56:N0:172:TYR:H	4.20	0.43
57:N1:39:ILE:HD12	57:N1:102:ARG:NE	3.71	0.43
11:S9:145:SER:O	11:S9:146:PHE:C	2.91	0.43
58:N2:100:THR:HA	36:5:1677:G:OP1	141.22	0.43
36:5:1807:G:C6	36:5:1808:G:N1	2.86	0.43
72:O6:26:ILE:HD13	36:5:155:G:H1'	87.89	0.43
36:1:3316:A:OP1	36:1:3318:G:N2	2.52	0.43
24:D2:24:GLN:OE1	29:D7:4:VAL:HA	2.19	0.43
48:M1:54:VAL:O	48:M1:56:THR:N	2.49	0.43
1:2:72:A:C2	1:2:73:U:C4	3.06	0.43
59:N3:13:ILE:HD11	59:N3:81:GLN:OE1	6.39	0.43
62:N6:39:LEU:HD22	62:N6:43:TYR:HE2	2.19	0.43
24:D2:114:GLU:HG2	24:D2:118:ARG:NH2	5.25	0.43
39:L2:77:ILE:HD12	39:L2:128:ARG:HB3	2.63	0.43
20:C8:26:ILE:HG13	20:C8:27:LYS:N	2.31	0.43
36:5:1895:A:O2'	36:5:3053:G:H4'	2.18	0.43
36:5:1015:U:P	36:5:1016:C:OP1	2.77	0.43
86:5:4034:OHX:N5	86:5:4117:OHX:N3	2.67	0.43
9:S7:112:ARG:NH2	1:6:639:U:OP1	364.40	0.43
67:O1:46:THR:HG23	67:O1:47:ASP:H	3.70	0.43
36:5:1258:U:O2	36:5:1260:A:C8	2.71	0.43
9:S7:43:PHE:HB2	9:S7:61:PHE:O	2.19	0.43
36:5:171:G:N2	36:5:248:U:O2	2.52	0.43
74:O8:78:LEU:HD13	74:O8:78:LEU:HA	1.69	0.43
52:M6:23:VAL:HG11	52:M6:84:LEU:HD11	2.01	0.43
73:O7:29:VAL:O	73:O7:32:LYS:HD3	2.77	0.43
66:O0:78:GLY:HA2	66:O0:87:VAL:HG13	2.01	0.43
77:Q1:15:ARG:HG3	77:Q1:15:ARG:NH1	4.91	0.43
36:1:2192:C:H2'	36:1:2193:U:O4'	2.18	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:1397:U:C5	1:6:1399:C:C2	3.07	0.43
1:6:225:A:O2'	1:6:226:A:H5'	2.19	0.43
72:O6:40:VAL:O	72:O6:44:VAL:HG23	2.19	0.43
34:SR:147:HIS:CD2	34:SR:179:LYS:HD2	2.53	0.43
52:M6:98:ALA:O	52:M6:101:ARG:HB2	2.18	0.43
41:L4:188:ARG:NH1	36:5:1382:G:OP2	113.37	0.43
1:6:1628:U:H2'	1:6:1629:G:C8	2.54	0.43
36:1:2284:C:H5''	36:1:2285:C:OP2	2.18	0.43
41:L4:3:ARG:HH21	41:L4:3:ARG:HG2	1.84	0.43
36:5:2985:C:H2'	36:5:2986:U:C6	2.54	0.43
5:S3:212:LYS:HD2	5:S3:212:LYS:HA	4.63	0.43
36:1:1237:G:H2'	36:1:1237:G:N3	2.34	0.43
36:1:3116:G:H2'	36:1:3116:G:N3	2.34	0.43
13:C1:30:ARG:HG2	13:C1:30:ARG:H	4.68	0.43
68:O2:31:ASN:OD1	68:O2:31:ASN:N	2.55	0.43
21:C9:47:PRO:HA	1:6:1477:G:O2'	375.64	0.43
39:L2:177:LYS:HB2	79:Q3:29:LEU:HD13	2.32	0.43
1:2:867:G:P	15:C3:3:ARG:NH1	2.92	0.43
36:1:1487:G:H1	36:1:1855:U:H3	1.67	0.43
36:5:1796:G:O6	86:5:4225:OHX:N5	2.51	0.43
16:C4:50:ALA:C	16:C4:52:ARG:N	2.91	0.42
41:L4:193:LYS:HE3	41:L4:193:LYS:HB2	1.60	0.42
3:S1:133:TYR:CE2	3:S1:181:LEU:HD12	4.88	0.42
3:S1:181:LEU:H	3:S1:181:LEU:HD13	1.84	0.42
2:S0:179:ARG:O	2:S0:183:ARG:HG3	2.19	0.42
3:S1:57:ALA:O	3:S1:61:LEU:HB2	5.90	0.42
37:3:73:C:C5	56:N0:13:ARG:NH1	2.87	0.42
28:D6:40:ALA:HB3	28:D6:69:ASN:ND2	2.34	0.42
8:S6:98:ARG:HD3	8:S6:99:GLY:N	2.34	0.42
41:L4:150:LEU:HD11	41:L4:172:VAL:HG13	2.01	0.42
19:C7:105:GLN:O	19:C7:109:LEU:N	2.76	0.42
52:M6:156:LEU:HD23	52:M6:156:LEU:HA	1.89	0.42
1:6:1228:G:H2'	1:6:1228:G:N3	2.34	0.42
36:1:1245:A:N6	36:1:1272:C:O2'	2.52	0.42
9:S7:131:PHE:CD2	9:S7:132:PRO:HD3	3.02	0.42
48:M1:12:LEU:HD12	48:M1:162:TRP:CG	4.20	0.42
3:S1:232:HIS:HB3	3:S1:233:GLY:H	3.12	0.42
19:C7:104:ASN:O	19:C7:106:THR:HG22	6.45	0.42
11:S9:167:ALA:O	11:S9:168:ARG:HB2	2.49	0.42
24:D2:23:ARG:CB	29:D7:4:VAL:HG12	5.72	0.42
1:2:300:A:O2'	1:2:301:A:H5'	2.19	0.42
40:L3:91:GLY:O	40:L3:102:LEU:HD23	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:2572:C:O2'	36:1:2573:G:C8	2.72	0.42
57:N1:17:ARG:HH11	57:N1:17:ARG:HG2	3.66	0.42
36:1:1177:G:H5'	69:O3:18:ARG:NH1	2.34	0.42
73:O7:11:ARG:HG2	36:5:817:A:O2'	148.59	0.42
32:E0:18:THR:HA	32:E0:19:PRO:HD2	2.31	0.42
34:SR:201:THR:CB	34:SR:242:SER:HA	2.49	0.42
52:M6:78:ARG:HG3	52:M6:78:ARG:NH1	2.98	0.42
36:1:612:U:H2'	36:1:613:G:C8	2.54	0.42
49:M3:16:LYS:NZ	36:5:98:G:OP1	133.44	0.42
56:N0:42:TRP:NE1	56:N0:53:LYS:HG3	2.34	0.42
65:N9:21:ILE:C	65:N9:22:LYS:HZ3	6.11	0.42
54:M8:99:THR:HB	54:M8:100:THR:H	1.43	0.42
54:M8:86:THR:CG2	54:M8:105:ARG:HB2	2.62	0.42
36:5:945:C:H2'	36:5:946:U:H6	1.83	0.42
45:L8:230:LYS:HD2	45:L8:230:LYS:HA	1.71	0.42
57:N1:104:GLU:HG3	57:N1:105:PHE:N	2.81	0.42
36:1:535:G:C6	36:1:555:U:N3	2.86	0.42
6:S4:117:GLU:C	6:S4:119:ALA:H	2.40	0.42
1:2:693:U:H5'	1:2:694:U:C5'	2.48	0.42
40:L3:221:THR:HB	40:L3:273:HIS:H	1.84	0.42
36:5:1231:A:H5''	36:5:1232:C:H5'	1.99	0.42
1:6:876:G:H1'	1:6:944:A:O4'	2.19	0.42
1:2:682:C:H2'	1:2:683:C:O4'	2.19	0.42
1:6:29:U:H2'	1:6:30:G:H8	1.84	0.42
36:5:3157:U:H3'	36:5:3158:G:H4'	2.01	0.42
42:L5:126:GLU:HA	42:L5:196:ARG:HD2	3.06	0.42
35:SM:43:ASP:HA	35:SM:44:PRO:HD3	2.50	0.42
36:1:2427:U:H2'	36:1:2428:U:C6	2.53	0.42
59:N3:102:ILE:HG13	59:N3:110:LYS:HB3	2.01	0.42
1:6:357:G:OP2	86:6:2075:OHX:N6	2.51	0.42
38:8:123:G:OP2	86:8:222:OHX:N6	2.52	0.42
36:5:1434:G:H5''	36:5:1437:C:C5	2.53	0.42
1:6:1334:U:H2'	1:6:1335:U:C6	2.54	0.42
37:3:67:G:H2'	37:3:68:C:O4'	2.20	0.42
6:S4:244:ILE:HA	6:S4:244:ILE:HD12	2.80	0.42
6:S4:89:VAL:O	6:S4:99:PHE:O	4.71	0.42
36:1:3165:A:H61	36:1:3285:C:H42	1.66	0.42
42:L5:58:LYS:HD2	42:L5:93:THR:OG1	2.19	0.42
1:2:699:U:OP2	1:2:733:A:N6	2.52	0.42
1:2:732:G:H2'	1:2:732:G:N3	2.34	0.42
10:S8:38:ILE:CD1	10:S8:80:GLY:HA2	2.49	0.42
10:S8:42:ARG:HB3	10:S8:59:ARG:HB2	2.37	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:755:A:O2'	1:6:756:A:OP1	2.37	0.42
52:M6:113:ASP:OD2	52:M6:113:ASP:N	2.52	0.42
1:6:1152:A:O2'	1:6:1153:G:H5'	2.18	0.42
1:2:542:A:O2'	1:2:543:C:O5'	2.37	0.42
11:S9:3:ARG:H	11:S9:3:ARG:HD3	2.96	0.42
5:S3:113:LEU:HD23	5:S3:113:LEU:HA	1.84	0.42
35:SM:77:THR:C	35:SM:79:SER:N	3.31	0.42
36:5:3174:A:N6	36:5:3278:C:C2	2.87	0.42
36:1:1355:A:H5'	36:1:1357:G:H1'	2.01	0.42
16:C4:23:PHE:HE2	16:C4:91:THR:HG21	1.84	0.42
49:M3:94:GLY:HA3	71:O5:116:TYR:CZ	2.54	0.42
45:L8:25:PRO:HB2	45:L8:26:LEU:H	1.49	0.42
59:N3:86:ARG:HB2	59:N3:92:PHE:CE1	2.53	0.42
2:S0:139:VAL:HG22	4:S2:62:PRO:HG3	2.43	0.42
36:5:1814:A:OP1	86:5:4178:OHX:N3	2.52	0.42
36:5:59:G:H4'	36:5:60:A:H4'	2.00	0.42
1:2:533:U:C4'	26:D4:33:ALA:HB2	2.49	0.42
2:S0:200:ASP:OD2	2:S0:203:PHE:HE1	2.58	0.42
36:1:2295:A:H5'	59:N3:61:THR:HG21	2.01	0.42
4:S2:125:ILE:O	4:S2:129:ILE:HG13	2.20	0.42
40:L3:303:LYS:NZ	40:L3:361:THR:HB	2.47	0.42
61:N5:106:ASP:HB2	61:N5:130:TYR:CE1	2.54	0.42
46:L9:113:GLU:HA	46:L9:124:ARG:O	2.56	0.42
34:SR:269:TYR:CE2	34:SR:271:VAL:HG22	2.54	0.42
1:2:229:U:H2'	1:2:230:C:H6	1.83	0.42
36:1:112:U:O2'	36:1:113:C:P	2.77	0.42
36:1:1483:G:C8	36:1:1485:G:C8	3.07	0.42
17:C5:85:ILE:HA	17:C5:89:MET:SD	2.59	0.42
36:1:2094:C:H2'	36:1:2095:G:C8	2.53	0.42
42:L5:68:THR:HB	42:L5:71:GLY:O	2.23	0.42
86:5:4033:OHX:N1	86:5:4081:OHX:N2	2.66	0.42
34:SR:109:ASP:HB2	34:SR:127:ARG:HD2	2.00	0.42
36:5:1340:G:H2'	36:5:1341:U:H6	1.84	0.42
14:C2:58:LEU:HA	14:C2:87:PRO:HG3	3.35	0.42
72:O6:74:LYS:HD2	72:O6:80:PHE:HD2	1.83	0.42
21:C9:93:HIS:O	21:C9:94:ILE:HD12	2.19	0.42
1:2:480:G:N2	1:2:509:G:H1'	2.34	0.42
1:6:1425:A:O2'	1:6:1426:C:H5'	2.19	0.42
41:L4:262:TRP:O	41:L4:276:LEU:HD11	3.16	0.42
36:5:3087:A:H2'	36:5:3088:G:O4'	2.19	0.42
45:L8:220:ALA:HA	45:L8:224:ASP:OD2	2.19	0.42
37:3:113:C:H2'	37:3:114:U:O4'	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:C5:79:HIS:O	17:C5:81:ARG:N	2.62	0.42
1:2:698:U:O4	86:2:2097:OHX:N3	2.51	0.42
36:1:810:A:H2'	36:1:811:U:C6	2.55	0.42
32:E0:36:LYS:HD3	32:E0:36:LYS:HA	3.21	0.42
2:S0:32:HIS:ND1	2:S0:32:HIS:O	2.52	0.42
52:M6:138:LEU:HA	52:M6:138:LEU:HD12	1.68	0.42
34:SR:123:ILE:HG13	34:SR:123:ILE:H	1.70	0.42
45:L8:84:ARG:CZ	45:L8:84:ARG:HB3	2.49	0.42
32:E0:41:THR:HA	32:E0:45:VAL:HB	2.00	0.42
1:2:1186:U:O4	1:2:1200:G:N2	2.45	0.42
1:6:1586:A:H2'	1:6:1587:A:O4'	2.18	0.42
36:1:634:C:H5'	69:O3:21:ARG:O	2.19	0.42
53:M7:69:ARG:HD3	36:5:3309:G:H1'	185.78	0.42
40:L3:3:HIS:HD2	36:5:2939:G:OP2	249.58	0.42
36:1:1631:C:OP2	63:N7:48:ARG:NH2	2.48	0.42
63:N7:46:ILE:HD13	63:N7:49:TYR:HA	2.96	0.42
61:N5:121:LYS:HD2	61:N5:123:TYR:CZ	2.58	0.42
13:C1:97:TYR:O	13:C1:99:ARG:HG2	2.19	0.42
28:D6:37:LYS:HD3	28:D6:70:LYS:HZ3	1.83	0.42
33:E1:143:LYS:HD3	1:6:1254:U:OP1	457.26	0.42
54:M8:94:PHE:CZ	64:N8:119:PRO:HD3	2.85	0.42
18:C6:45:ARG:O	18:C6:48:VAL:HG12	2.19	0.42
71:O5:82:ALA:O	38:8:38:U:C5	65.80	0.42
36:1:1949:G:OP2	55:M9:135:LYS:NZ	2.52	0.42
55:M9:104:ARG:HH22	55:M9:135:LYS:HD2	1.84	0.42
74:O8:41:THR:HG21	74:O8:62:ALA:CB	2.49	0.42
1:6:1:U:H1'	1:6:369:A:C8	2.55	0.42
36:1:637:C:H2'	36:1:638:C:H6	1.81	0.42
49:M3:101:ARG:HA	36:5:76:G:O6	87.67	0.42
1:6:192:U:H1'	1:6:193:U:C4	2.54	0.42
35:SM:68:ARG:HD2	35:SM:68:ARG:C	3.31	0.42
45:L8:108:ARG:NH1	36:5:121:A:C4	96.18	0.42
64:N8:96:LYS:HB3	64:N8:97:GLU:H	1.75	0.42
38:4:52:A:H62	75:O9:27:ILE:CD1	2.30	0.42
5:S3:167:PHE:O	5:S3:190:ARG:HG2	2.48	0.42
23:D1:38:LYS:HE3	23:D1:38:LYS:HB2	4.80	0.42
1:2:325:G:H4'	13:C1:80:MET:HE2	2.00	0.42
36:5:1151:U:H3'	36:5:1152:G:C8	2.54	0.42
72:O6:97:SER:O	72:O6:99:ARG:N	2.52	0.42
40:L3:4:ARG:HG3	40:L3:4:ARG:NH1	3.77	0.42
21:C9:118:PRO:C	21:C9:120:GLY:H	2.24	0.42
36:1:2873:U:H5	36:1:2941:A:H2	1.67	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
45:L8:109:LEU:O	45:L8:113:ALA:N	2.36	0.42
59:N3:40:LYS:O	59:N3:41:GLY:C	3.21	0.42
36:5:109:A:H4'	36:5:110:G:H5'	2.00	0.42
29:D7:62:ILE:HD12	29:D7:62:ILE:HA	2.83	0.42
86:2:2167:OHX:N1	86:2:2168:OHX:N3	2.67	0.42
36:1:3033:A:H2'	36:1:3034:C:H6	1.83	0.42
36:5:111:C:O2'	36:5:112:U:H5'	2.19	0.42
40:L3:19:ARG:HG3	40:L3:273:HIS:NE2	2.34	0.42
36:5:900:G:H1'	36:5:1589:A:H61	1.84	0.42
43:L6:98:VAL:HA	43:L6:101:PHE:HD2	1.84	0.42
18:C6:97:VAL:HG12	18:C6:98:ASP:H	2.01	0.42
1:2:622:A:H4'	1:2:623:A:OP1	2.19	0.42
5:S3:132:LYS:HB3	5:S3:189:MET:HG3	2.23	0.42
3:S1:116:LYS:HE2	3:S1:117:TRP:CZ2	5.97	0.42
86:5:4033:OHX:N3	86:5:4081:OHX:N4	2.67	0.42
1:2:131:C:O2'	1:2:132:U:OP1	2.33	0.42
1:6:5:U:H2'	1:6:6:G:H8	1.83	0.42
41:L4:10:SER:OG	41:L4:14:GLU:HG3	4.87	0.42
48:M1:60:ARG:HH11	48:M1:60:ARG:HB2	1.84	0.42
36:5:1801:U:H2'	36:5:1802:C:C6	2.55	0.42
36:1:146:U:H5'	36:1:148:G:O4'	2.18	0.42
34:SR:4:ASN:HA	34:SR:318:ALA:HB2	2.01	0.42
1:2:1313:A:H2'	1:2:1315:U:H5'	2.00	0.42
36:1:1719:G:OP1	55:M9:110:ARG:NH2	2.53	0.42
39:L2:61:VAL:HG22	39:L2:63:PHE:CE1	5.90	0.42
36:5:192:C:H2'	36:5:193:C:C6	2.55	0.42
61:N5:113:LEU:C	61:N5:113:LEU:HD12	2.40	0.42
30:D8:50:GLU:O	30:D8:51:ASN:HB2	2.19	0.42
36:1:1908:A:H8	36:1:1908:A:O5'	2.00	0.42
43:L6:55:LEU:HA	43:L6:55:LEU:HD23	1.88	0.42
6:S4:124:GLY:HA2	6:S4:142:HIS:CE1	2.81	0.42
41:L4:89:ALA:O	41:L4:90:PHE:O	4.45	0.42
36:1:3214:U:C2'	50:M4:121:MET:HE1	2.41	0.42
21:C9:57:ARG:HG3	21:C9:57:ARG:NH1	2.45	0.42
36:1:1073:U:O2'	65:N9:49:GLY:HA3	2.19	0.42
1:2:702:G:C2	1:2:703:G:H1'	2.55	0.42
36:1:1815:U:H1'	36:1:1816:A:O5'	2.19	0.42
27:D5:70:LYS:HB3	27:D5:71:ILE:HG13	2.01	0.42
18:C6:115:THR:O	18:C6:115:THR:OG1	2.37	0.42
53:M7:136:ILE:HD12	53:M7:136:ILE:HG23	2.72	0.42
46:L9:92:TYR:HD2	46:L9:179:ILE:HG23	6.14	0.42
11:S9:3:ARG:N	11:S9:3:ARG:HD3	2.67	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
66:O0:17:VAL:HG21	66:O0:100:ILE:HD13	3.35	0.42
41:L4:62:ALA:HB2	41:L4:77:VAL:HA	2.02	0.42
37:3:28:C:OP1	48:M1:137:ARG:HD3	2.19	0.42
41:L4:182:LEU:HA	41:L4:182:LEU:HD13	3.49	0.42
36:1:3106:A:H2'	36:1:3107:U:O4'	2.19	0.42
61:N5:23:ALA:O	61:N5:24:LEU:HB2	4.63	0.42
11:S9:171:ARG:O	11:S9:175:ARG:HB2	2.19	0.42
62:N6:91:ASN:C	62:N6:93:ALA:H	2.40	0.42
22:D0:96:PRO:HG2	22:D0:99:ILE:HG22	2.01	0.42
9:S7:44:LYS:HG3	9:S7:63:PRO:HD3	2.02	0.42
20:C8:4:VAL:HG21	27:D5:82:HIS:CG	3.17	0.42
64:N8:133:LEU:HD13	64:N8:137:LYS:HE3	2.01	0.42
24:D2:89:TRP:HE3	24:D2:93:LEU:HD22	3.10	0.42
2:S0:175:TYR:OH	2:S0:195:TRP:HB3	3.12	0.42
14:C2:40:GLY:O	14:C2:124:LYS:N	2.51	0.42
13:C1:57:LYS:HB2	13:C1:110:HIS:CE1	2.54	0.42
67:O1:80:ASN:OD1	67:O1:81:GLU:N	2.53	0.42
24:D2:105:THR:HG23	24:D2:110:ILE:HG12	2.02	0.42
1:2:1165:G:C6	1:2:1166:A:C6	3.07	0.42
73:O7:48:ASN:HA	73:O7:54:LYS:HZ1	3.07	0.42
23:D1:62:ARG:NH2	1:6:1039:A:H5''	380.95	0.42
75:O9:4:GLN:HG2	36:5:1588:A:C6	126.87	0.42
36:5:1252:A:H2	36:5:1263:A:C2	2.38	0.42
3:S1:117:TRP:O	3:S1:153:HIS:O	2.60	0.42
36:1:2970:C:H4'	36:1:2971:A:C2	2.54	0.42
36:5:2881:C:H2'	36:5:2882:U:C6	2.55	0.42
6:S4:65:LEU:HD23	6:S4:70:VAL:HG13	2.50	0.42
34:SR:316:MET:C	34:SR:318:ALA:H	4.74	0.42
36:5:422:A:C2	36:5:2363:A:H4'	2.55	0.42
44:L7:211:SER:O	44:L7:213:GLY:N	2.51	0.42
46:L9:4:ILE:CD1	56:N0:148:LEU:HD11	2.49	0.42
38:4:24:G:OP2	62:N6:13:ARG:HD3	2.19	0.42
11:S9:11:THR:O	11:S9:44:ARG:HG3	2.18	0.42
36:5:2512:C:N4	36:5:2513:U:O4	2.53	0.42
2:S0:105:GLY:O	2:S0:112:THR:HG21	2.18	0.42
78:Q2:89:LYS:HB2	36:5:2653:C:OP1	237.44	0.42
7:S5:99:MET:HG3	7:S5:180:ARG:NH2	2.34	0.42
36:1:2565:U:H2'	36:1:2566:C:C6	2.54	0.42
36:5:80:G:H2'	36:5:81:C:C6	2.54	0.42
49:M3:67:ARG:HG3	49:M3:67:ARG:H	1.65	0.42
54:M8:11:LYS:HB3	54:M8:11:LYS:HE3	1.84	0.42
36:5:959:C:OP2	36:5:960:U:C5	2.73	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
43:L6:60:ASP:O	43:L6:61:ASN:HB2	2.24	0.42
72:O6:4:LYS:HD2	72:O6:14:GLY:HA3	2.30	0.42
43:L6:82:ARG:NH1	69:O3:106:ASN:HB2	3.96	0.42
86:6:2121:OHX:N4	86:6:2171:OHX:N1	2.67	0.42
36:1:1073:U:H1'	65:N9:50:THR:HG22	2.00	0.42
3:S1:144:ARG:HB3	3:S1:208:GLN:HG2	3.21	0.42
41:L4:91:GLY:O	41:L4:94:CYS:HB2	2.56	0.42
3:S1:61:LEU:HD22	3:S1:61:LEU:H	1.83	0.42
28:D6:8:ASN:HB2	28:D6:9:GLY:H	2.28	0.42
75:O9:48:LYS:HD2	75:O9:48:LYS:HA	2.15	0.42
1:2:1519:U:H2'	1:2:1520:U:C5	2.54	0.42
36:1:638:C:H2'	36:1:639:G:C8	2.54	0.42
42:L5:34:LYS:HE3	57:N1:30:TYR:OH	2.19	0.42
38:4:41:A:O2'	73:O7:59:THR:HB	2.18	0.42
10:S8:10:LYS:HG2	13:C1:133:LYS:CE	2.72	0.42
45:L8:241:LYS:HB2	36:5:2586:G:C5	184.74	0.42
42:L5:146:LEU:HD13	42:L5:148:ILE:HD11	4.19	0.42
74:O8:3:ARG:NH1	74:O8:52:TYR:HE1	3.52	0.42
59:N3:13:ILE:HD12	59:N3:85:TRP:CG	4.98	0.42
36:5:284:A:H4'	36:5:285:A:C2	2.55	0.42
1:6:1082:C:H2'	1:6:1083:G:O4'	2.20	0.42
36:1:2878:G:H5''	40:L3:5:LYS:HE2	2.00	0.42
47:M0:88:ARG:HG2	47:M0:90:ARG:HG2	2.95	0.42
35:SM:116:GLU:O	35:SM:119:ALA:N	2.47	0.42
6:S4:193:GLY:O	6:S4:210:ILE:HG23	2.19	0.42
36:5:1070:U:C4	36:5:1071:U:C4	3.07	0.42
9:S7:126:LEU:HD13	9:S7:173:TYR:CD2	3.00	0.42
9:S7:111:LYS:O	9:S7:112:ARG:HB2	2.19	0.42
1:6:1638:G:C2	1:6:1639:C:H1'	2.54	0.42
2:S0:22:THR:HG22	2:S0:169:SER:OG	2.37	0.42
63:N7:97:SER:OG	63:N7:98:THR:N	2.97	0.42
1:2:694:U:H5	9:S7:96:ARG:O	2.02	0.42
26:D4:52:LYS:O	26:D4:54:ALA:N	2.57	0.42
36:1:1485:G:N2	70:O4:4:ARG:HD2	2.34	0.42
54:M8:178:ARG:HA	54:M8:178:ARG:HD3	1.80	0.42
49:M3:191:ALA:C	49:M3:193:ALA:H	2.23	0.42
1:2:872:G:H2'	1:2:873:U:O4'	2.20	0.42
8:S6:119:GLN:HG3	8:S6:120:GLU:N	2.35	0.42
55:M9:10:LEU:HD12	55:M9:10:LEU:HA	1.82	0.42
36:1:1373:A:H2'	36:1:1374:G:C8	2.55	0.42
34:SR:106:HIS:ND1	34:SR:128:ASP:OD2	2.86	0.42
1:2:809:A:C6	1:2:810:G:C6	3.07	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:603:U:H2'	1:2:604:A:C8	2.54	0.42
36:1:3193:C:H2'	36:1:3194:C:O4'	2.20	0.42
42:L5:21:ARG:HA	42:L5:24:ARG:NH2	2.35	0.42
41:L4:285:ASP:OD2	41:L4:288:ARG:HB2	2.19	0.42
36:5:1500:G:H2'	36:5:1501:U:H6	1.84	0.42
1:6:312:A:C2	1:6:314:C:H2'	2.54	0.42
38:8:4:C:H2'	38:8:5:U:H6	1.83	0.42
36:1:2686:A:OP2	86:1:3903:OHX:N2	2.52	0.42
36:5:123:A:C6	36:5:150:A:C5	3.08	0.42
36:1:126:U:OP1	51:M5:144:ARG:NH1	2.47	0.42
1:6:602:U:H2'	1:6:603:U:C6	2.54	0.42
36:5:2390:A:H2'	36:5:2391:G:O4'	2.20	0.42
36:1:601:U:H2'	36:1:602:A:O4'	2.18	0.42
31:D9:26:SER:OG	31:D9:27:HIS:N	2.89	0.42
40:L3:43:LEU:HD22	40:L3:203:VAL:HG11	2.02	0.42
40:L3:114:VAL:O	40:L3:117:ARG:HB3	2.20	0.42
3:S1:223:PHE:O	3:S1:224:ASP:HB3	2.67	0.42
36:1:908:G:H4'	36:1:909:G:O5'	2.19	0.42
7:S5:44:ASN:HD22	7:S5:44:ASN:H	3.75	0.42
53:M7:30:ARG:HD3	53:M7:30:ARG:C	2.46	0.42
1:2:1756:A:H8	1:2:1756:A:OP2	2.02	0.42
9:S7:166:LEU:HA	9:S7:166:LEU:HD12	2.09	0.42
36:1:1162:U:H4'	68:O2:57:TYR:CE1	2.55	0.42
1:2:545:A:H4'	1:2:546:U:OP1	2.20	0.42
17:C5:99:GLY:O	1:6:1211:A:H1'	375.84	0.42
36:1:1668:G:C6	36:1:1669:C:C4	3.08	0.42
47:M0:63:GLU:H	47:M0:63:GLU:HG2	1.35	0.42
25:D3:23:ARG:HD3	25:D3:26:GLU:OE1	3.96	0.42
74:O8:2:ALA:HB3	36:5:1613:A:OP1	140.02	0.42
56:N0:139:TYR:CD2	56:N0:140:VAL:HG23	2.72	0.42
41:L4:338:LYS:C	41:L4:340:GLY:H	2.17	0.42
57:N1:68:THR:OG1	36:5:2737:C:H4'	223.14	0.42
1:2:538:A:C8	1:2:543:C:C4	3.07	0.42
1:6:1253:U:H2'	1:6:1254:U:O4'	2.19	0.42
37:3:28:C:H1'	37:3:55:A:H61	1.83	0.42
7:S5:112:ARG:NH1	18:C6:43:ILE:HD11	2.33	0.42
45:L8:189:LEU:O	45:L8:190:VAL:HG23	3.91	0.42
1:2:149:C:H2'	1:2:150:U:C6	2.55	0.42
58:N2:17:VAL:HA	58:N2:103:TYR:O	2.20	0.42
49:M3:70:ARG:HD2	49:M3:71:ALA:O	2.54	0.42
46:L9:95:ALA:HA	76:Q0:78:ILE:HG22	7.76	0.42
26:D4:27:VAL:HG21	26:D4:40:LEU:HD11	2.01	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:S2:115:ILE:HD13	4:S2:208:GLU:OE1	2.36	0.42
56:N0:1:MET:HE3	56:N0:2:ALA:HB3	2.00	0.42
86:5:4023:OHX:N2	86:5:4215:OHX:N5	2.67	0.42
1:2:707:A:O2'	1:2:731:C:N4	2.53	0.42
26:D4:62:THR:HB	26:D4:69:SER:OG	2.19	0.42
22:D0:57:ARG:HD2	22:D0:89:ARG:HD3	2.02	0.42
36:1:612:U:H2'	36:1:613:G:H8	1.84	0.42
6:S4:181:VAL:HG21	6:S4:195:ILE:HD11	2.86	0.42
6:S4:93:ASP:C	6:S4:95:THR:H	4.36	0.42
1:6:902:G:H2'	1:6:903:U:C6	2.54	0.42
36:1:437:G:H2'	36:1:438:A:O4'	2.19	0.42
46:L9:124:ARG:HD3	46:L9:164:ILE:O	2.19	0.42
5:S3:29:LEU:HB2	5:S3:34:TYR:HB2	2.01	0.42
1:6:1752:U:H2'	1:6:1753:A:C8	2.54	0.42
11:S9:149:ARG:H	11:S9:149:ARG:HD3	1.85	0.42
1:6:1388:A:H4'	1:6:1389:C:O5'	2.20	0.42
42:L5:196:ARG:HH11	42:L5:196:ARG:HB3	1.85	0.42
36:5:702:C:O2	36:5:788:C:H4'	2.20	0.42
3:S1:115:ARG:HG3	3:S1:116:LYS:N	2.34	0.42
1:2:1511:U:H2'	1:2:1512:G:H8	1.85	0.42
58:N2:99:LYS:HE3	58:N2:102:GLU:HB2	2.01	0.42
45:L8:72:PRO:HA	45:L8:73:PRO:HD3	1.87	0.42
3:S1:106:THR:HA	16:C4:116:GLU:OE1	2.88	0.42
24:D2:122:SER:OG	24:D2:123:GLY:N	2.53	0.42
1:6:926:A:H1'	1:6:988:A:C2	2.55	0.42
1:6:704:C:H2'	1:6:705:U:O4'	2.20	0.42
17:C5:74:ALA:HA	17:C5:75:PRO:HD3	2.04	0.42
37:3:64:A:H3'	47:M0:204:GLY:O	2.18	0.42
58:N2:35:LYS:O	58:N2:38:ILE:HB	2.19	0.42
2:S0:126:PRO:HB2	2:S0:152:PRO:HG2	2.01	0.42
13:C1:29:LYS:O	13:C1:31:THR:N	2.46	0.42
59:N3:90:GLY:O	60:N4:16:GLY:HA2	2.19	0.42
36:1:1074:U:O2'	36:1:1075:A:H2'	2.19	0.42
42:L5:224:LYS:HB2	42:L5:224:LYS:HE3	2.40	0.42
42:L5:188:GLU:HG3	42:L5:188:GLU:O	2.20	0.42
1:6:187:G:H8	1:6:187:G:O5'	2.01	0.42
60:N4:55:PHE:CE2	60:N4:59:HIS:CE1	3.07	0.42
49:M3:82:ALA:C	49:M3:84:GLY:H	2.33	0.42
36:5:1786:G:H2'	36:5:1787:A:C8	2.54	0.42
73:O7:12:HIS:O	36:5:1491:A:H5'	137.68	0.42
50:M4:53:VAL:HA	50:M4:54:PRO:HD3	1.82	0.42
2:S0:52:LYS:HG2	2:S0:52:LYS:H	1.35	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
72:O6:28:TYR:OH	36:5:315:C:OP2	98.23	0.42
33:E1:121:CYS:HB2	33:E1:132:LEU:HD21	2.28	0.42
36:1:2988:C:O2	40:L3:266:ARG:NH1	2.52	0.42
7:S5:185:ARG:NH1	1:6:1471:A:OP1	333.96	0.42
74:O8:62:ALA:C	74:O8:64:LYS:H	3.11	0.42
47:M0:45:GLU:O	47:M0:141:LYS:HE3	3.04	0.42
15:C3:65:VAL:HG23	15:C3:66:ILE:CG2	6.08	0.42
3:S1:159:SER:OG	1:6:874:C:OP1	319.44	0.42
51:M5:174:ILE:HG22	51:M5:174:ILE:O	2.84	0.42
14:C2:62:LEU:HB3	14:C2:120:VAL:HG13	2.37	0.42
54:M8:19:PRO:HD3	54:M8:30:VAL:HG21	2.45	0.42
45:L8:50:VAL:HG11	61:N5:27:ARG:HG3	2.00	0.42
1:6:1590:G:H2'	1:6:1591:C:H6	1.85	0.42
42:L5:148:ILE:HD13	42:L5:148:ILE:HG21	1.73	0.42
49:M3:174:ARG:CZ	72:O6:9:ILE:HD13	2.50	0.42
40:L3:211:GLN:NE2	40:L3:284:ARG:HA	2.34	0.42
36:5:1817:G:O2'	36:5:1818:U:OP2	2.32	0.42
22:D0:60:THR:HG22	1:6:1382:A:H5''	438.47	0.42
6:S4:163:ASP:HB3	6:S4:167:GLY:O	4.95	0.42
38:8:62:C:H4'	38:8:63:G:O5'	2.20	0.42
15:C3:64:ARG:HG3	15:C3:70:LYS:HD2	5.50	0.42
6:S4:95:THR:O	6:S4:97:GLU:HG3	2.20	0.42
86:5:4034:OHX:N1	86:5:4117:OHX:N3	2.68	0.42
54:M8:182:LYS:HA	54:M8:182:LYS:HD3	2.47	0.42
9:S7:35:LYS:HG2	9:S7:36:ALA:H	1.84	0.42
63:N7:22:LYS:HE3	63:N7:134:LEU:HB2	2.58	0.42
49:M3:35:ARG:NH1	36:5:685:G:P	82.97	0.42
1:2:558:U:HO2'	1:2:559:C:P	2.42	0.42
34:SR:117:LYS:H	34:SR:117:LYS:HE2	1.84	0.42
36:1:2414:G:H2'	36:1:2415:C:O4'	2.19	0.42
36:1:916:G:N1	39:L2:207:VAL:HG11	2.35	0.42
51:M5:135:VAL:CG1	51:M5:142:ILE:HG12	2.50	0.42
40:L3:244:ARG:HG2	40:L3:244:ARG:HH11	1.84	0.42
6:S4:132:GLY:O	1:6:252:U:H4'	326.16	0.42
1:2:1317:C:H2'	1:2:1318:G:O4'	2.20	0.42
1:2:624:G:OP2	86:2:2158:OHX:N2	2.53	0.42
5:S3:215:GLU:HA	5:S3:216:PRO:HD2	2.18	0.42
1:6:871:G:H2'	1:6:872:G:C8	2.55	0.42
36:1:3174:A:H2'	36:1:3175:U:H5'	2.01	0.42
36:5:177:U:OP2	86:5:4017:OHX:N6	2.52	0.42
25:D3:59:ILE:CD1	32:E0:4:VAL:HG13	2.49	0.42
58:N2:58:GLU:C	58:N2:60:GLY:H	2.21	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:S4:127:LYS:HG3	6:S4:142:HIS:HA	2.02	0.42
36:1:1638:A:N3	36:1:1709:C:H1'	2.34	0.42
1:2:1480:G:H3'	1:2:1481:C:C6	2.55	0.42
61:N5:77:GLU:HG3	61:N5:133:LEU:HG	2.02	0.42
6:S4:248:ILE:HG13	11:S9:71:PHE:CD2	4.20	0.42
52:M6:39:GLU:HG2	52:M6:40:GLU:HG2	2.01	0.42
34:SR:305:TYR:HH	34:SR:313:TRP:HH2	2.10	0.42
1:2:51:A:OP2	86:2:2073:OHX:N3	2.53	0.42
1:2:978:A:H2'	1:2:979:A:O4'	2.20	0.42
3:S1:67:GLU:OE2	3:S1:83:LYS:HE3	2.19	0.42
21:C9:126:GLU:CD	21:C9:126:GLU:H	2.23	0.42
36:1:1081:U:H2'	36:1:1081:U:H6	1.58	0.42
1:2:814:A:OP1	55:M9:170:ARG:NH2	2.48	0.42
36:5:2611:U:H2'	36:5:2612:U:C6	2.55	0.42
34:SR:49:GLY:O	34:SR:51:ASP:N	2.44	0.42
50:M4:48:GLY:N	50:M4:49:PRO:HD3	2.89	0.42
78:Q2:72:LEU:O	78:Q2:80:ARG:HA	2.19	0.42
11:S9:110:GLN:HE21	11:S9:110:GLN:HA	3.11	0.42
56:N0:91:TYR:OH	56:N0:93:GLU:OE2	2.23	0.42
25:D3:102:VAL:CG1	25:D3:127:VAL:HG12	2.44	0.42
86:5:3973:OHX:N1	86:5:4241:OHX:N5	2.68	0.42
36:1:26:A:C4	36:1:330:G:C8	3.08	0.42
36:5:2970:C:H4'	36:5:2971:A:C2	2.55	0.42
8:S6:63:MET:HA	8:S6:98:ARG:O	2.20	0.42
56:N0:115:ARG:NH2	36:5:1320:C:O2	289.41	0.42
76:Q0:78:ILE:HG21	76:Q0:78:ILE:HD13	2.74	0.42
42:L5:64:ILE:HD13	42:L5:105:ILE:HD12	2.01	0.42
23:D1:64:GLU:HG3	29:D7:3:LEU:HG	2.01	0.42
5:S3:178:ARG:HE	5:S3:178:ARG:N	2.16	0.42
36:5:1879:A:H2'	36:5:1879:A:N3	2.35	0.42
52:M6:73:PHE:CD1	52:M6:78:ARG:HG2	3.15	0.42
1:6:825:U:O2'	1:6:826:U:H6	2.02	0.42
36:1:437:G:O2'	36:1:438:A:H5'	2.20	0.42
45:L8:195:SER:O	45:L8:195:SER:OG	2.49	0.42
69:O3:89:LEU:HA	69:O3:90:PRO:HD3	1.76	0.42
1:6:1634:C:O2	86:6:2156:OHX:N2	2.52	0.42
34:SR:307:ASP:O	34:SR:308:ASN:HB2	2.37	0.42
15:C3:15:ALA:H	29:D7:20:LYS:HZ3	1.68	0.42
58:N2:79:LEU:O	58:N2:82:LYS:HB3	2.20	0.42
86:1:3955:OHX:N4	86:1:4041:OHX:N6	2.68	0.42
1:6:93:A:C6	1:6:398:G:C6	3.08	0.42
40:L3:258:ALA:O	40:L3:259:HIS:CD2	2.98	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:8:145:U:H2'	38:8:146:U:O4'	2.20	0.42
62:N6:103:LYS:HA	62:N6:103:LYS:HD3	2.02	0.42
74:O8:10:GLN:HA	74:O8:13:GLU:OE1	2.19	0.42
36:1:848:A:H8	36:1:848:A:O5'	2.03	0.42
36:5:2921:U:H2'	36:5:2923:U:OP2	2.20	0.42
36:1:2186:U:H2'	36:1:2187:G:O4'	2.19	0.42
1:6:1175:U:H4'	1:6:1196:A:C6	2.54	0.42
62:N6:74:TYR:CZ	62:N6:77:LYS:HD2	5.14	0.42
1:2:1773:C:OP2	77:Q1:2:ARG:HD2	2.20	0.42
65:N9:9:ALA:O	65:N9:10:HIS:C	2.59	0.42
38:8:6:U:H2'	38:8:7:U:C6	2.54	0.42
39:L2:36:GLU:OE1	39:L2:163:ARG:NH1	2.85	0.42
17:C5:48:GLY:O	17:C5:52:LYS:HD3	2.19	0.42
64:N8:105:LEU:HB2	64:N8:148:ILE:HD11	2.01	0.42
36:1:1504:A:C5	36:1:1505:C:C5	3.08	0.42
1:6:1431:C:H1'	1:6:1437:U:O4	2.20	0.42
1:2:413:U:H2'	1:2:414:C:C6	2.54	0.42
36:1:1069:C:H2'	36:1:1070:U:H6	1.85	0.42
59:N3:104:ASN:HD21	59:N3:108:GLU:HB2	3.49	0.42
36:1:1293:U:O2'	36:1:1294:A:H5'	2.20	0.42
32:E0:56:MET:C	32:E0:58:PRO:HD3	2.40	0.42
36:5:231:G:O6	86:5:4132:OHX:N4	2.53	0.42
15:C3:114:ARG:HA	15:C3:114:ARG:HD3	1.47	0.42
86:5:4065:OHX:N2	86:5:4074:OHX:N1	2.67	0.42
86:5:4065:OHX:N4	86:5:4074:OHX:N1	2.67	0.42
36:1:2992:U:H1'	53:M7:69:ARG:NH2	2.35	0.42
40:L3:2:SER:N	36:5:2943:G:C8	236.02	0.42
1:6:470:A:C5'	1:6:470:A:C8	3.03	0.42
1:2:1153:G:H5'	28:D6:85:ARG:HD2	2.01	0.42
36:1:3186:A:O2'	46:L9:23:ARG:NH2	2.53	0.42
86:1:4136:OHX:N3	86:1:4194:OHX:N4	2.66	0.42
61:N5:67:ILE:HB	61:N5:83:VAL:HG12	2.17	0.42
36:5:300:G:O6	86:5:4189:OHX:N2	2.53	0.42
7:S5:37:GLN:NE2	18:C6:46:PHE:CE1	2.88	0.42
31:D9:19:ARG:CD	31:D9:32:ARG:HD2	2.50	0.42
45:L8:182:GLY:O	45:L8:186:LEU:HG	2.20	0.42
21:C9:100:ILE:H	21:C9:100:ILE:HG12	1.64	0.42
62:N6:3:LYS:HE2	62:N6:8:VAL:O	2.20	0.42
14:C2:67:THR:C	14:C2:69:ALA:H	2.24	0.42
1:2:927:C:H2'	1:2:928:U:C6	2.55	0.42
1:2:1657:U:N3	86:2:2090:OHX:N4	2.68	0.42
19:C7:34:LEU:O	19:C7:38:ILE:HD13	5.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:5:1111:U:O2'	36:5:1112:A:H5'	2.20	0.42
36:1:1636:U:H5''	63:N7:73:LYS:HZ1	1.83	0.42
12:C0:46:LEU:HA	12:C0:46:LEU:HD13	1.71	0.42
1:2:71:A:N1	1:2:72:A:C6	2.88	0.42
44:L7:175:LYS:HE2	44:L7:175:LYS:HB3	1.68	0.42
27:D5:93:SER:OG	27:D5:100:ILE:N	2.53	0.42
1:6:1082:C:C2'	1:6:1083:G:H5'	2.50	0.42
1:2:529:A:H2'	1:2:530:C:O4'	2.20	0.42
16:C4:41:ARG:O	16:C4:42:VAL:HG22	2.19	0.42
39:L2:245:LEU:HD23	39:L2:247:ARG:NH1	2.33	0.42
36:5:243:G:H2'	36:5:244:G:C8	2.55	0.42
61:N5:100:LYS:NZ	61:N5:106:ASP:OD2	2.37	0.42
65:N9:40:ARG:HB3	65:N9:40:ARG:HE	2.87	0.42
61:N5:92:LYS:HE2	61:N5:110:VAL:O	2.20	0.42
1:6:1080:U:H3	1:6:1091:A:H2	1.66	0.42
36:1:3254:G:O6	86:1:4059:OHX:N5	2.53	0.42
34:SR:307:ASP:OD2	34:SR:311:ARG:NH2	3.26	0.42
36:5:419:G:O3'	36:5:420:G:OP2	2.31	0.42
57:N1:104:GLU:HG2	36:5:989:A:O2'	258.24	0.42
36:1:1686:U:O2	36:1:1688:U:H1'	2.20	0.42
4:S2:40:LYS:HE3	4:S2:40:LYS:HB2	4.61	0.42
2:S0:102:PHE:CZ	2:S0:106:SER:HB2	2.55	0.42
36:1:111:C:O2'	36:1:112:U:H5'	2.19	0.42
36:1:191:U:H2'	36:1:192:C:H6	1.84	0.42
7:S5:20:PHE:CE1	7:S5:34:GLN:HB3	3.20	0.42
1:2:1039:A:N6	1:2:1091:A:C2	2.88	0.42
48:M1:150:ASN:C	48:M1:152:HIS:H	2.23	0.42
47:M0:191:LYS:NZ	47:M0:212:GLU:HG3	5.01	0.42
62:N6:103:LYS:NZ	36:5:221:A:H61	78.90	0.42
74:O8:32:ASN:ND2	74:O8:34:ALA:HB3	6.02	0.42
17:C5:109:PRO:O	17:C5:112:LEU:HG	2.20	0.42
39:L2:104:LEU:HB3	39:L2:146:THR:HG21	2.02	0.42
9:S7:185:ILE:HG22	9:S7:186:PRO:HD3	3.10	0.42
36:1:2425:G:H2'	36:1:2426:U:O4'	2.18	0.42
35:SM:37:VAL:HG12	35:SM:38:PRO:O	2.31	0.42
36:1:2921:U:H2'	36:1:2923:U:H5''	2.01	0.42
46:L9:7:GLU:CD	46:L9:54:LYS:HE3	2.40	0.42
45:L8:167:PRO:HB3	45:L8:177:TYR:CZ	2.90	0.42
5:S3:212:LYS:HE2	5:S3:212:LYS:HB2	1.53	0.42
1:2:867:G:OP2	15:C3:3:ARG:NH1	2.45	0.42
36:1:1114:U:H5''	64:N8:22:ILE:HD12	2.02	0.42
1:6:1144:U:H2'	1:6:1145:U:C6	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:1515:A:O2'	1:6:1517:U:OP2	2.31	0.42
61:N5:91:ASN:OD1	61:N5:94:GLN:HG3	2.20	0.42
36:1:2723:U:H2'	36:1:2724:U:C6	2.55	0.42
9:S7:91:ILE:HD11	9:S7:128:ASP:O	4.10	0.42
7:S5:27:THR:HA	7:S5:28:PRO:HD3	1.88	0.42
69:O3:10:LYS:O	69:O3:33:GLU:HB2	2.92	0.42
1:6:1731:A:H5'	1:6:1732:A:OP2	2.20	0.42
36:5:523:A:N6	36:5:570:A:C2	2.88	0.42
1:6:1740:A:H2'	1:6:1741:U:C6	2.55	0.42
44:L7:106:LEU:HD23	44:L7:106:LEU:HA	1.83	0.42
23:D1:48:GLY:O	23:D1:49:GLU:HB2	2.18	0.42
9:S7:31:SER:HB2	9:S7:32:PRO:HD3	2.01	0.42
39:L2:50:HIS:CD2	36:5:1795:U:H2'	198.71	0.42
78:Q2:14:GLY:O	78:Q2:17:CYS:O	4.56	0.42
36:1:663:C:H2'	36:1:664:U:C6	2.55	0.42
36:1:2943:G:H2'	36:1:2944:U:O4'	2.20	0.42
41:L4:329:PRO:HB2	41:L4:330:TYR:H	3.87	0.42
36:1:2896:A:C8	36:1:2896:A:H5'	2.55	0.42
41:L4:144:LYS:HD2	41:L4:145:ILE:HG22	7.19	0.42
1:6:646:C:H2'	1:6:647:G:C8	2.55	0.42
72:O6:25:LYS:HB3	72:O6:25:LYS:HE3	2.43	0.42
1:2:1291:G:N2	1:2:1324:G:H22	2.16	0.42
36:1:1741:A:C2	36:1:1742:U:C4	3.08	0.42
34:SR:192:PHE:HD1	34:SR:223:TRP:CE3	2.37	0.42
36:5:1566:A:H2'	36:5:1567:U:H5'	2.02	0.42
8:S6:71:THR:HG22	8:S6:72:ARG:N	4.68	0.42
34:SR:161:LYS:HB3	34:SR:161:LYS:HE3	4.68	0.42
33:E1:143:LYS:N	1:6:1253:U:H4'	450.39	0.42
51:M5:65:ARG:HD2	51:M5:129:TYR:CE1	2.55	0.42
64:N8:91:LEU:HD13	64:N8:91:LEU:HA	1.94	0.42
36:1:2899:C:C5	46:L9:171:ASP:HA	2.54	0.42
33:E1:113:LYS:HE3	33:E1:113:LYS:HB3	2.47	0.42
36:1:1724:U:OP2	55:M9:128:LYS:NZ	2.53	0.42
4:S2:41:LEU:HA	4:S2:41:LEU:HD23	2.38	0.42
36:5:3163:A:O2'	36:5:3164:C:H5'	2.20	0.42
36:5:1329:U:HO2'	36:5:1330:A:P	2.43	0.42
36:1:1507:G:N7	53:M7:129:THR:CG2	2.82	0.42
27:D5:61:SER:OG	27:D5:62:VAL:N	3.41	0.42
73:O7:3:LYS:HG2	36:5:2138:A:O2'	172.70	0.42
53:M7:36:ILE:CD1	53:M7:95:LEU:HD11	2.48	0.42
36:1:2105:G:H2'	36:1:2106:A:H5'	2.00	0.42
14:C2:33:ARG:HG2	14:C2:36:LEU:HD12	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:1628:U:H2'	1:2:1629:G:C8	2.55	0.42
54:M8:102:ALA:HB2	54:M8:122:ILE:HG22	2.02	0.42
1:2:980:G:H4'	1:2:1776:A:H4'	2.02	0.42
15:C3:72:MET:HE3	15:C3:81:ALA:HB1	2.02	0.42
71:O5:44:ILE:O	71:O5:47:VAL:HG12	2.19	0.42
36:1:2118:C:O5'	36:1:2118:C:H6	2.03	0.42
39:L2:181:LYS:HG3	39:L2:184:ARG:HG3	2.01	0.42
36:1:40:A:N7	64:N8:29:PRO:O	2.53	0.42
74:O8:11:PHE:O	74:O8:14:LEU:HB2	2.19	0.42
1:2:1063:U:OP1	29:D7:72:LYS:NZ	2.52	0.42
69:O3:14:LEU:HD11	69:O3:31:LYS:HB2	2.01	0.42
17:C5:77:ARG:NH1	1:6:1241:G:OP1	383.60	0.42
40:L3:86:VAL:HG22	40:L3:162:VAL:HG12	2.36	0.42
36:1:1767:C:C2'	36:1:1768:U:H5'	2.50	0.42
38:8:157:U:O2'	38:8:158:U:H5'	2.19	0.42
54:M8:157:PRO:CB	36:5:2729:U:H4'	191.31	0.42
1:2:1475:A:H2'	1:2:1476:C:O4'	2.19	0.42
39:L2:182:ALA:HB2	36:5:2148:U:O2'	211.98	0.42
49:M3:168:ARG:NH2	36:5:769:G:O2'	146.76	0.42
36:1:1316:C:O4'	52:M6:130:LYS:HD3	2.19	0.42
73:O7:45:ARG:HB3	73:O7:45:ARG:HE	1.60	0.42
45:L8:148:ALA:HA	45:L8:201:THR:HG22	2.02	0.42
9:S7:148:LYS:O	9:S7:149:ILE:HG13	2.19	0.42
51:M5:179:LYS:O	36:5:287:G:H5'	124.84	0.42
62:N6:97:ILE:HG22	62:N6:99:LEU:HG	2.54	0.42
1:2:1417:A:OP1	86:2:2072:OHX:N5	2.53	0.42
17:C5:87:PRO:HA	17:C5:90:ILE:HG13	2.01	0.42
42:L5:204:VAL:O	42:L5:208:MET:HG3	2.20	0.42
75:O9:7:PHE:HB3	38:8:113:U:H5''	108.26	0.42
36:5:2694:A:C6	36:5:2695:A:C6	3.08	0.42
35:SM:89:ARG:O	35:SM:89:ARG:HD2	2.20	0.42
18:C6:36:ILE:O	18:C6:36:ILE:HG12	2.20	0.42
38:4:148:G:H2'	38:4:149:A:C8	2.55	0.42
36:1:2775:U:H2'	36:1:2776:C:C6	2.55	0.42
36:5:2434:U:H4'	36:5:2435:G:H5''	2.00	0.42
34:SR:283:LYS:HG3	34:SR:284:ALA:N	4.90	0.42
36:1:913:A:H2	36:1:2134:G:N3	2.18	0.42
41:L4:57:GLY:HA3	41:L4:98:ARG:H	2.71	0.41
40:L3:291:GLU:O	40:L3:292:ALA:HB3	2.19	0.41
3:S1:179:SER:HB3	3:S1:183:GLN:HB2	2.01	0.41
86:5:4065:OHX:N6	86:5:4074:OHX:N5	2.68	0.41
53:M7:69:ARG:NH2	36:5:2991:A:C2	194.27	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:3:26:C:H5''	42:L5:56:THR:HB	2.02	0.41
36:1:92:G:O5'	78:Q2:46:LYS:NZ	2.53	0.41
36:1:1814:A:OP1	86:1:4094:OHX:N2	2.53	0.41
34:SR:182:ASN:ND2	34:SR:184:ASN:HD21	4.69	0.41
46:L9:106:LYS:HG3	46:L9:107:ASP:OD2	3.89	0.41
1:2:1102:G:OP1	24:D2:76:SER:HB2	2.19	0.41
54:M8:185:LYS:HD3	54:M8:186:VAL:HG23	2.01	0.41
13:C1:101:GLU:CD	25:D3:16:ARG:NH2	3.46	0.41
1:2:220:A:C6	1:2:221:A:N7	2.88	0.41
47:M0:216:TYR:CD2	47:M0:217:PHE:N	2.81	0.41
11:S9:109:LEU:HD22	11:S9:113:VAL:HG23	2.02	0.41
45:L8:134:TYR:CD2	45:L8:190:VAL:HG21	2.55	0.41
72:O6:9:ILE:HG12	72:O6:10:GLY:N	4.29	0.41
1:2:1250:U:O2'	33:E1:135:HIS:HD2	2.03	0.41
1:2:709:C:N4	1:2:710:U:H1'	2.35	0.41
42:L5:178:ASN:O	42:L5:179:ARG:HD3	2.20	0.41
11:S9:158:PHE:CD2	11:S9:164:PHE:HB3	2.55	0.41
1:2:434:G:N2	1:2:436:A:H3'	2.35	0.41
86:5:4212:OHX:N2	86:5:4222:OHX:N6	2.67	0.41
62:N6:120:GLN:HE22	62:N6:126:LEU:N	8.82	0.41
51:M5:93:LYS:HG3	36:5:289:A:H2	147.82	0.41
26:D4:53:ASP:CG	26:D4:96:LEU:HD21	2.40	0.41
14:C2:42:ALA:HB1	14:C2:47:GLU:HB3	2.90	0.41
15:C3:53:LEU:HA	15:C3:53:LEU:HD12	1.74	0.41
54:M8:122:ILE:HG21	54:M8:122:ILE:HD13	4.09	0.41
36:1:2947:G:H4'	36:1:2947:G:OP2	2.19	0.41
40:L3:227:GLU:HG3	40:L3:270:ARG:CB	5.00	0.41
36:1:1313:G:O6	86:1:4095:OHX:N3	2.53	0.41
69:O3:100:ILE:HD12	69:O3:100:ILE:N	2.96	0.41
1:6:1363:U:H3'	1:6:1364:G:H8	1.84	0.41
36:5:629:U:H2'	36:5:630:A:H8	1.81	0.41
86:1:3964:OHX:N2	86:1:4143:OHX:N6	2.68	0.41
37:7:79:A:C2	37:7:102:A:C4	3.08	0.41
18:C6:30:LYS:HD3	1:6:1366:U:OP1	426.44	0.41
36:5:1470:U:H2'	36:5:1471:U:H6	1.84	0.41
13:C1:86:ILE:HD11	13:C1:125:VAL:HG11	3.79	0.41
86:1:3980:OHX:N5	86:1:4158:OHX:N6	2.68	0.41
4:S2:242:ILE:HD12	4:S2:242:ILE:HA	1.85	0.41
2:S0:123:VAL:HG11	2:S0:133:ILE:HD11	2.02	0.41
11:S9:44:ARG:HG2	11:S9:45:ILE:HD13	2.76	0.41
14:C2:41:LEU:HD21	14:C2:123:VAL:HG22	2.02	0.41
55:M9:24:LEU:HD22	55:M9:50:ILE:HG12	5.73	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
44:L7:131:GLU:HG2	44:L7:230:GLY:HA2	2.47	0.41
36:5:1001:G:H5'	36:5:1002:A:O5'	2.20	0.41
1:6:733:A:H2'	1:6:734:A:O4'	2.20	0.41
1:6:1573:A:H4'	1:6:1574:G:H5'	2.02	0.41
67:O1:16:LEU:HD12	67:O1:16:LEU:HA	1.79	0.41
34:SR:286:GLU:HA	34:SR:287:PRO:HD3	1.66	0.41
63:N7:135:ARG:HH21	63:N7:135:ARG:CB	3.15	0.41
40:L3:3:HIS:ND1	40:L3:3:HIS:O	2.53	0.41
41:L4:302:ALA:HB2	54:M8:39:ARG:NH1	2.89	0.41
10:S8:36:THR:HA	10:S8:58:LEU:HA	2.00	0.41
41:L4:91:GLY:HA3	41:L4:93:MET:CE	2.48	0.41
18:C6:115:THR:HB	18:C6:118:ILE:O	2.20	0.41
1:6:647:G:N2	1:6:687:G:N2	2.52	0.41
1:2:542:A:O2'	1:2:543:C:P	2.77	0.41
7:S5:94:THR:O	7:S5:97:LEU:HB2	2.39	0.41
18:C6:5:PRO:HB3	18:C6:96:TYR:CE1	2.55	0.41
36:1:20:A:P	71:O5:90:ARG:HH11	2.42	0.41
51:M5:175:ASN:O	51:M5:184:LYS:HG3	2.20	0.41
16:C4:91:THR:O	16:C4:93:THR:N	3.15	0.41
36:5:2895:G:H5'	36:5:3107:U:O2'	2.20	0.41
1:2:196:G:O2'	1:2:197:A:P	2.78	0.41
1:6:194:U:H2'	1:6:194:U:O2	2.19	0.41
1:6:1541:G:C6	1:6:1542:G:N1	2.88	0.41
4:S2:116:LYS:HE3	4:S2:117:THR:O	3.10	0.41
39:L2:48:ILE:HG12	79:Q3:63:THR:CG2	2.87	0.41
39:L2:48:ILE:HD11	79:Q3:54:ILE:HG23	2.02	0.41
59:N3:10:LYS:HG2	59:N3:11:PHE:O	2.20	0.41
2:S0:56:LYS:HZ3	2:S0:158:VAL:HA	1.85	0.41
36:5:529:A:H2'	36:5:530:G:O4'	2.20	0.41
1:2:710:U:H2'	1:2:711:U:H5'	2.03	0.41
1:6:919:A:H2'	1:6:920:U:C6	2.55	0.41
21:C9:117:SER:HB2	21:C9:123:ARG:HB3	2.61	0.41
61:N5:103:TYR:O	61:N5:138:ARG:NH1	2.71	0.41
61:N5:103:TYR:HB3	61:N5:135:ILE:HD11	2.42	0.41
61:N5:82:LEU:HD21	61:N5:135:ILE:CG2	2.68	0.41
40:L3:313:HIS:O	40:L3:333:LYS:HD2	2.19	0.41
36:1:1100:U:OP2	44:L7:196:LYS:HE3	2.20	0.41
36:5:409:A:OP2	86:5:4102:OHX:N3	2.53	0.41
36:5:209:A:H4'	36:5:211:A:N7	2.34	0.41
69:O3:85:PHE:CZ	69:O3:89:LEU:HD11	2.70	0.41
63:N7:108:GLU:H	63:N7:108:GLU:HG2	1.47	0.41
62:N6:56:VAL:O	62:N6:67:GLU:HA	2.76	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:S5:145:ASP:CG	7:S5:146:THR:H	2.23	0.41
40:L3:261:MET:HE2	52:M6:64:PHE:CA	2.50	0.41
79:Q3:27:LYS:O	79:Q3:31:ILE:HD12	2.20	0.41
36:5:2529:A:H2'	36:5:2530:G:O4'	2.21	0.41
33:E1:98:VAL:HG13	33:E1:99:LYS:N	2.34	0.41
36:5:3219:G:H4'	36:5:3220:G:H5'	2.02	0.41
36:1:2320:A:C2	79:Q3:16:VAL:HG13	2.55	0.41
46:L9:7:GLU:OE1	46:L9:54:LYS:HE3	2.20	0.41
48:M1:89:TYR:O	48:M1:169:ALA:HB1	2.19	0.41
36:1:1522:U:H4'	36:1:1523:U:OP2	2.20	0.41
36:1:1168:U:OP1	44:L7:211:SER:O	2.38	0.41
37:7:112:G:OP2	86:7:221:OHX:N2	2.52	0.41
76:Q0:110:CYS:SG	76:Q0:112:LYS:HB2	2.60	0.41
3:S1:28:GLU:OE2	3:S1:94:LYS:NZ	2.44	0.41
36:1:67:A:OP1	86:1:3915:OHX:N6	2.53	0.41
45:L8:75:ILE:HG13	51:M5:18:VAL:HG23	2.23	0.41
36:1:402:A:C6	53:M7:21:TYR:CE2	3.08	0.41
7:S5:156:ARG:HA	7:S5:157:ARG:HH21	4.28	0.41
67:O1:64:VAL:HG13	36:5:1456:A:N1	161.88	0.41
36:5:3269:U:O2	36:5:3271:G:N1	2.53	0.41
36:5:3269:U:H5'	36:5:3271:G:O4'	2.20	0.41
36:5:1729:A:H4'	36:5:1730:G:OP2	2.19	0.41
42:L5:180:PHE:HB3	42:L5:195:LEU:HD13	2.01	0.41
48:M1:37:LEU:HD13	48:M1:69:VAL:HG12	2.53	0.41
64:N8:73:LEU:HD11	64:N8:78:LEU:HA	3.63	0.41
36:1:2964:G:N7	86:1:4068:OHX:N3	2.68	0.41
39:L2:221:LYS:NZ	36:5:2965:U:O2	213.33	0.41
40:L3:212:ASN:OD1	40:L3:354:VAL:HG22	2.20	0.41
1:6:114:C:H6	1:6:114:C:H5'	1.85	0.41
19:C7:119:LEU:H	19:C7:119:LEU:HD12	1.85	0.41
1:2:38:C:H2'	1:2:39:A:H5'	2.01	0.41
36:1:3181:C:H2'	36:1:3182:G:O4'	2.21	0.41
54:M8:170:ARG:HD2	64:N8:56:VAL:O	2.78	0.41
3:S1:130:SER:OG	3:S1:180:THR:HG22	5.50	0.41
71:O5:100:VAL:HG22	71:O5:104:GLN:HB3	2.03	0.41
10:S8:169:ILE:HD12	10:S8:179:CYS:SG	2.61	0.41
42:L5:40:HIS:HD2	42:L5:42:ALA:N	2.07	0.41
6:S4:87:MET:O	6:S4:122:LYS:HE3	2.21	0.41
7:S5:53:VAL:CG2	7:S5:59:VAL:HG22	2.50	0.41
28:D6:40:ALA:HB2	28:D6:71:LEU:HD21	2.01	0.41
22:D0:70:THR:HG23	1:6:1280:C:O2'	389.68	0.41
47:M0:24:ARG:CG	47:M0:24:ARG:HH11	2.26	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:3:19:C:H2'	37:3:20:A:C8	2.55	0.41
9:S7:12:ALA:HB3	9:S7:13:PRO:HD3	2.01	0.41
21:C9:89:ARG:HG3	21:C9:89:ARG:HH11	1.84	0.41
9:S7:70:PHE:O	9:S7:74:GLN:HB2	2.19	0.41
58:N2:97:SER:HB2	58:N2:103:TYR:CE1	2.85	0.41
36:5:599:C:H2'	36:5:600:G:O4'	2.20	0.41
45:L8:100:GLU:OE1	45:L8:108:ARG:NH1	2.50	0.41
5:S3:168:ILE:HA	5:S3:188:ILE:O	2.37	0.41
44:L7:244:ASN:C	44:L7:244:ASN:ND2	2.72	0.41
50:M4:37:GLU:HG2	56:N0:72:VAL:HG21	2.02	0.41
34:SR:45:TRP:CZ3	34:SR:57:PRO:HD3	3.34	0.41
36:1:2209:U:H2'	36:1:2209:U:H6	1.70	0.41
36:5:1481:A:O2'	36:5:1858:A:C2	2.65	0.41
53:M7:67:ILE:HD12	53:M7:82:ARG:NH1	2.42	0.41
51:M5:121:VAL:HG11	51:M5:131:GLU:HG3	3.29	0.41
36:5:2875:U:C2'	36:5:2876:C:O5'	2.68	0.41
6:S4:194:THR:O	6:S4:195:ILE:CB	2.68	0.41
63:N7:5:LEU:HD23	63:N7:25:ILE:CD1	3.40	0.41
36:1:2408:U:O2'	36:1:2409:G:H5'	2.20	0.41
56:N0:45:LEU:HD12	56:N0:49:HIS:HB2	2.01	0.41
67:O1:77:ARG:HA	67:O1:90:PHE:O	2.73	0.41
40:L3:152:LYS:HD3	40:L3:189:SER:HA	4.25	0.41
16:C4:19:ILE:HD11	16:C4:105:LEU:HD21	2.02	0.41
36:5:113:C:C2	36:5:319:A:C2	3.08	0.41
7:S5:188:LYS:HE2	7:S5:196:GLU:OE2	2.20	0.41
22:D0:36:ASN:HA	22:D0:39:SER:CB	4.38	0.41
36:5:2530:G:C2'	36:5:2531:C:H5'	2.50	0.41
55:M9:3:ASN:OD1	36:5:1471:U:H4'	113.92	0.41
74:O8:14:LEU:C	74:O8:16:ARG:H	2.37	0.41
1:6:1685:G:H1	1:6:1716:C:N4	2.18	0.41
9:S7:39:ARG:HH22	55:M9:185:LEU:HD22	2.78	0.41
42:L5:21:ARG:O	42:L5:25:GLU:HG3	2.37	0.41
86:2:2084:OHX:N3	86:2:2086:OHX:N1	2.67	0.41
67:O1:55:LEU:HB2	67:O1:95:PRO:HD3	2.01	0.41
44:L7:116:PHE:CZ	44:L7:144:ILE:HG12	2.55	0.41
53:M7:26:PHE:CE1	53:M7:120:ASN:HA	2.55	0.41
6:S4:21:ASP:OD1	6:S4:24:SER:OG	2.38	0.41
41:L4:3:ARG:HA	41:L4:4:PRO:HD3	2.16	0.41
48:M1:60:ARG:NH1	78:Q2:104:LEU:O	4.27	0.41
11:S9:182:GLU:OE1	11:S9:183:ALA:N	5.25	0.41
56:N0:44:PHE:CD1	57:N1:153:PRO:HG3	2.55	0.41
36:1:1769:G:O6	86:1:4172:OHX:N4	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
43:L6:152:THR:HA	43:L6:153:PRO:HD3	2.05	0.41
36:1:510:G:O6	86:1:4011:OHX:N1	2.53	0.41
36:1:2768:U:H2'	36:1:2769:A:C8	2.55	0.41
86:1:4144:OHX:N1	86:1:4187:OHX:N5	2.68	0.41
44:L7:37:ASN:HB3	36:5:597:G:OP1	249.75	0.41
36:5:1650:G:N7	86:5:4179:OHX:N3	2.67	0.41
39:L2:113:VAL:HG23	39:L2:134:VAL:HG22	2.12	0.41
1:6:1001:A:C6	1:6:1002:G:C6	3.09	0.41
47:M0:34:TYR:CD1	47:M0:34:TYR:N	2.89	0.41
55:M9:44:LEU:HA	55:M9:44:LEU:HD12	1.83	0.41
4:S2:35:TRP:CD1	4:S2:35:TRP:C	2.94	0.41
4:S2:44:LEU:HD23	4:S2:44:LEU:HA	1.86	0.41
38:4:143:U:H2'	38:4:144:G:O4'	2.20	0.41
36:5:3288:G:O2'	36:5:3289:G:P	2.78	0.41
1:6:1029:U:O2'	1:6:1030:A:H5'	2.21	0.41
36:1:2599:U:H2'	36:1:2600:C:C6	2.55	0.41
36:1:2183:A:P	39:L2:10:LYS:HZ2	2.42	0.41
40:L3:37:ARG:O	40:L3:186:GLY:HA3	4.13	0.41
42:L5:110:LEU:HD13	42:L5:171:LEU:HD23	2.01	0.41
18:C6:54:LEU:HD13	18:C6:54:LEU:HA	2.69	0.41
41:L4:145:ILE:HA	41:L4:146:PRO:HD3	2.69	0.41
61:N5:115:ARG:HH11	61:N5:115:ARG:CG	2.29	0.41
86:1:4084:OHX:N6	86:1:4153:OHX:N3	2.68	0.41
25:D3:96:VAL:HG12	25:D3:127:VAL:HG11	2.02	0.41
13:C1:98:ASN:ND2	24:D2:79:PHE:CD1	2.89	0.41
36:1:2356:A:O2'	53:M7:137:ASN:HB3	2.20	0.41
28:D6:4:LYS:HE2	28:D6:5:ARG:NH2	2.35	0.41
1:2:1500:C:OP1	21:C9:122:ARG:NH2	2.50	0.41
37:3:55:A:H2'	37:3:56:A:O4'	2.21	0.41
36:1:2261:G:O2'	36:1:2263:C:N4	2.53	0.41
36:5:29:C:H4'	36:5:62:A:H4'	2.02	0.41
36:1:1247:U:H2'	36:1:1268:G:O6	2.19	0.41
36:1:1246:G:N2	36:1:1264:G:HO2'	2.19	0.41
1:2:196:G:O2'	1:2:197:A:OP2	2.30	0.41
41:L4:274:TYR:CG	41:L4:275:THR:N	2.88	0.41
22:D0:63:LEU:HD22	31:D9:34:TYR:CE1	2.56	0.41
36:5:1646:G:N3	36:5:1808:G:C2	2.88	0.41
12:C0:33:GLU:O	12:C0:34:GLU:HB2	2.21	0.41
30:D8:11:LYS:O	30:D8:30:VAL:HA	2.49	0.41
22:D0:18:GLN:O	22:D0:96:PRO:HA	2.20	0.41
33:E1:93:HIS:HB3	33:E1:94:LYS:H	1.46	0.41
1:6:1274:C:N3	1:6:1427:A:C8	2.88	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
72:O6:62:ARG:O	72:O6:63:ASN:ND2	5.70	0.41
6:S4:114:ILE:HB	6:S4:118:GLU:OE2	2.20	0.41
36:1:1565:G:N2	36:1:1574:C:C2	2.89	0.41
6:S4:199:GLU:HB2	6:S4:207:LEU:HB2	2.03	0.41
1:6:1229:G:O2'	1:6:1230:A:OP2	2.36	0.41
40:L3:303:LYS:HZ1	40:L3:361:THR:HB	1.85	0.41
64:N8:47:LYS:O	64:N8:48:TYR:HB2	2.30	0.41
67:O1:41:LYS:HA	67:O1:46:THR:HG22	3.03	0.41
9:S7:35:LYS:NZ	9:S7:36:ALA:H	2.18	0.41
40:L3:124:LYS:HE3	40:L3:124:LYS:HB2	1.81	0.41
36:1:255:A:O2'	36:1:256:G:H5'	2.21	0.41
62:N6:59:VAL:O	62:N6:64:LYS:HD2	3.37	0.41
10:S8:117:TYR:O	10:S8:119:GLN:HG2	2.20	0.41
1:6:517:U:H2'	1:6:518:A:O4'	2.21	0.41
1:6:1248:C:H2'	1:6:1249:U:C6	2.55	0.41
38:4:141:C:O2'	38:4:142:C:H5'	2.19	0.41
9:S7:39:ARG:HH12	55:M9:188:ASP:HB2	1.85	0.41
7:S5:25:LEU:HB2	18:C6:27:GLY:O	2.25	0.41
76:Q0:113:ARG:NH1	36:5:1299:U:OP1	289.69	0.41
45:L8:84:ARG:NH1	45:L8:84:ARG:HB3	2.35	0.41
36:1:1211:U:H2'	36:1:1212:A:C8	2.55	0.41
34:SR:40:LYS:HG2	34:SR:66:HIS:O	2.20	0.41
41:L4:208:VAL:O	41:L4:251:THR:HG23	2.21	0.41
27:D5:49:ARG:HD2	27:D5:53:GLU:OE1	3.23	0.41
66:O0:20:SER:OG	66:O0:97:ASP:N	2.52	0.41
1:2:209:U:H2'	1:2:210:A:C8	2.56	0.41
36:5:1017:C:H42	36:5:2671:A:P	2.44	0.41
56:N0:7:TYR:CE1	56:N0:34:GLU:HG2	2.55	0.41
49:M3:55:ARG:O	49:M3:115:ARG:NH2	2.34	0.41
1:6:282:C:H2'	1:6:283:U:O4'	2.20	0.41
57:N1:115:LYS:HB2	57:N1:128:LEU:HD21	4.52	0.41
40:L3:246:LEU:HD12	40:L3:246:LEU:C	2.40	0.41
37:7:8:G:C6	37:7:9:C:C4	3.09	0.41
1:6:604:A:OP2	86:6:2151:OHX:N4	2.54	0.41
36:1:2137:U:C6	36:1:2141:U:C4	3.09	0.41
40:L3:159:ARG:HG2	40:L3:182:GLN:HA	2.02	0.41
25:D3:60:GLU:CD	32:E0:3:LYS:HB2	3.07	0.41
36:5:1143:A:H4'	36:5:1144:U:OP2	2.20	0.41
36:5:2403:G:N2	36:5:2404:A:C5	2.74	0.41
31:D9:14:TYR:OH	1:6:1553:G:O2'	403.63	0.41
7:S5:72:HIS:O	7:S5:73:THR:OG1	2.36	0.41
57:N1:68:THR:HG23	57:N1:69:LYS:N	2.36	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:S6:71:THR:OG1	8:S6:72:ARG:N	2.52	0.41
37:7:27:A:H2'	37:7:28:C:C6	2.55	0.41
25:D3:12:ALA:O	25:D3:16:ARG:HG3	2.20	0.41
36:1:439:C:C4	36:1:440:A:C6	3.08	0.41
52:M6:156:LEU:HB3	36:5:3243:A:C5	267.44	0.41
1:2:768:C:C6	11:S9:143:ILE:HD13	2.56	0.41
75:O9:21:ARG:HD3	75:O9:22:PRO:O	2.42	0.41
36:5:1817:G:O2'	36:5:1818:U:P	2.79	0.41
36:1:1048:A:H2'	47:M0:22:TYR:CZ	2.55	0.41
35:SM:102:THR:CG2	35:SM:105:LYS:H	2.32	0.41
40:L3:250:ALA:HB1	36:5:2947:G:C2	220.02	0.41
3:S1:89:ASP:OD1	3:S1:89:ASP:N	2.53	0.41
36:1:243:G:H2'	36:1:244:G:O4'	2.20	0.41
45:L8:121:SER:O	45:L8:123:GLN:N	3.22	0.41
8:S6:48:TYR:CD2	8:S6:117:GLY:HA3	2.73	0.41
51:M5:143:ARG:NH2	71:O5:92:LEU:HD23	2.34	0.41
40:L3:257:PRO:HG2	40:L3:261:MET:HE1	2.02	0.41
36:1:1349:G:N3	36:1:1349:G:H3'	2.35	0.41
8:S6:216:LEU:HD23	8:S6:216:LEU:HA	2.25	0.41
48:M1:152:HIS:O	48:M1:153:LYS:HB3	4.68	0.41
36:5:2518:C:C2	36:5:2590:A:C2	3.09	0.41
6:S4:180:LEU:HA	6:S4:180:LEU:HD23	1.74	0.41
36:5:578:A:H5''	36:5:579:G:O5'	2.21	0.41
1:6:994:G:C2'	1:6:995:A:H5'	2.51	0.41
7:S5:205:SER:O	7:S5:207:THR:HG23	2.20	0.41
42:L5:164:LYS:HG2	42:L5:180:PHE:CZ	2.55	0.41
36:5:3288:G:O2'	36:5:3289:G:OP2	2.33	0.41
43:L6:131:LYS:HD3	43:L6:132:ALA:N	5.52	0.41
6:S4:233:LYS:NZ	6:S4:235:TYR:HE2	8.06	0.41
4:S2:84:LYS:HA	4:S2:85:PRO:HD3	1.92	0.41
1:6:1095:U:O4	86:6:2180:OHX:N2	2.54	0.41
1:2:11:A:H4'	4:S2:87:GLN:HG3	2.03	0.41
37:7:91:G:H2'	37:7:92:A:C8	2.56	0.41
69:O3:13:HIS:HB3	69:O3:93:THR:O	2.21	0.41
36:1:1325:U:H2'	36:1:1326:A:O4'	2.20	0.41
36:5:908:G:H4'	36:5:909:G:O5'	2.21	0.41
36:1:147:U:O4	45:L8:157:VAL:HA	2.20	0.41
36:5:371:G:O6	86:5:4203:OHX:N5	2.52	0.41
36:5:2304:C:C5	36:5:2305:G:C6	3.08	0.41
36:1:1434:G:OP1	36:1:1437:C:N4	2.54	0.41
36:1:528:U:H2'	36:1:529:A:C8	2.55	0.41
36:5:3084:C:H2'	36:5:3085:G:O4'	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:S1:134:VAL:HB	3:S1:219:LYS:HB2	2.01	0.41
70:O4:100:ILE:H	70:O4:100:ILE:HG13	3.35	0.41
40:L3:183:LEU:HD12	40:L3:183:LEU:HA	2.16	0.41
36:5:217:U:O2'	36:5:218:G:OP1	2.36	0.41
72:O6:60:LEU:HA	72:O6:60:LEU:HD13	1.79	0.41
36:5:1864:A:H2'	36:5:1865:A:C8	2.55	0.41
66:O0:83:LYS:HG2	66:O0:85:PHE:CZ	3.19	0.41
12:C0:77:ARG:HA	12:C0:82:LEU:CD1	2.50	0.41
1:2:464:A:C2	1:2:465:G:C8	3.08	0.41
36:5:1393:A:C8	36:5:1418:A:C6	3.09	0.41
54:M8:170:ARG:HG3	54:M8:170:ARG:O	3.23	0.41
1:2:778:G:H22	26:D4:10:ARG:CZ	2.34	0.41
1:6:755:A:O2'	1:6:756:A:P	2.79	0.41
7:S5:73:THR:HG23	18:C6:114:ARG:HG3	2.01	0.41
41:L4:144:LYS:CG	41:L4:145:ILE:H	4.89	0.41
57:N1:92:ARG:NH1	36:5:2736:A:OP1	235.83	0.41
7:S5:43:PHE:HA	7:S5:68:ILE:O	2.20	0.41
35:SM:77:THR:C	35:SM:79:SER:H	2.98	0.41
2:S0:50:VAL:H	19:C7:109:LEU:HD21	1.86	0.41
1:2:927:C:H1'	16:C4:125:SER:HB2	2.01	0.41
6:S4:128:LYS:HA	6:S4:156:VAL:HG22	2.21	0.41
59:N3:119:GLY:HA2	59:N3:137:VAL:HG23	2.01	0.41
10:S8:21:PHE:HD1	10:S8:22:ARG:HG2	3.00	0.41
61:N5:25:LYS:HD3	61:N5:27:ARG:NH1	2.35	0.41
36:5:603:A:H2'	36:5:604:G:O4'	2.21	0.41
75:O9:27:ILE:HD13	38:8:52:A:N6	78.91	0.41
2:S0:185:ARG:H	23:D1:44:ARG:HA	1.85	0.41
64:N8:74:ASN:HB3	64:N8:115:LYS:HB2	2.01	0.41
21:C9:42:GLY:HA2	21:C9:84:LYS:HG3	2.89	0.41
40:L3:151:ILE:O	40:L3:155:ALA:HB3	2.38	0.41
25:D3:44:GLY:HA3	25:D3:78:LYS:HZ2	2.24	0.41
55:M9:7:GLN:HG2	55:M9:7:GLN:H	3.75	0.41
38:4:79:A:C6	38:4:80:A:C2	3.09	0.41
86:1:4065:OHX:N6	86:1:4177:OHX:N2	2.68	0.41
40:L3:305:ILE:H	40:L3:305:ILE:HG13	1.53	0.41
1:6:72:A:H2'	1:6:73:U:C1'	2.50	0.41
36:1:1560:G:C2	36:1:1561:G:N7	2.89	0.41
14:C2:52:LEU:HA	14:C2:85:LYS:HZ1	1.86	0.41
36:1:1947:G:H1	36:1:2101:C:N4	2.17	0.41
52:M6:126:VAL:HG23	52:M6:127:LEU:HD23	6.06	0.41
44:L7:158:LYS:CG	44:L7:159:GLN:N	2.81	0.41
54:M8:98:LYS:HB3	54:M8:99:THR:H	1.80	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:1310:G:N7	86:1:4031:OHX:N5	2.68	0.41
36:1:241:G:C6	36:1:242:C:C4	3.08	0.41
41:L4:23:PRO:O	41:L4:24:ALA:HB3	2.23	0.41
15:C3:47:PRO:HG3	15:C3:75:LEU:HD22	2.02	0.41
8:S6:4:ASN:HB3	8:S6:110:ALA:HA	2.36	0.41
1:2:1287:A:H4'	1:2:1288:G:OP1	2.21	0.41
13:C1:46:LYS:HE2	1:6:846:G:N2	311.00	0.41
1:6:1179:G:C6	1:6:1180:C:C4	3.08	0.41
36:5:2590:A:C6	36:5:2591:A:C5	3.09	0.41
4:S2:111:VAL:HG21	4:S2:218:ILE:HD13	2.03	0.41
38:4:9:A:H2'	38:4:10:A:C8	2.55	0.41
36:1:2611:U:H2'	36:1:2612:U:H6	1.86	0.41
1:6:1050:G:N2	1:6:1068:C:O2	2.54	0.41
36:5:1263:A:N3	36:5:1263:A:H2'	2.36	0.41
36:1:210:U:C2	36:1:230:U:H4'	2.56	0.41
49:M3:138:VAL:HB	71:O5:118:ILE:HB	2.02	0.41
43:L6:22:ARG:HD3	36:5:608:A:N6	242.23	0.41
6:S4:23:LEU:O	6:S4:24:SER:CB	3.09	0.41
36:1:1522:U:H3'	61:N5:113:LEU:HD22	2.02	0.41
36:1:362:U:OP1	73:O7:45:ARG:NH2	2.54	0.41
36:5:3287:U:H2'	36:5:3288:G:C5'	2.51	0.41
36:1:65:A:C4	36:1:110:G:N7	2.88	0.41
1:6:754:A:N6	1:6:793:A:N7	2.67	0.41
36:1:94:G:H2'	36:1:95:A:C8	2.56	0.41
36:1:508:U:H2'	36:1:509:U:C6	2.55	0.41
36:5:2587:U:O2'	36:5:2588:U:H5'	2.20	0.41
43:L6:7:PRO:HG2	43:L6:10:TYR:CZ	2.56	0.41
6:S4:35:PRO:HB3	6:S4:143:ASP:O	2.45	0.41
36:5:2872:A:OP2	86:5:4109:OHX:N5	2.54	0.41
63:N7:12:VAL:HB	63:N7:81:LEU:HB3	3.54	0.41
37:3:11:A:O2'	37:3:13:A:OP2	2.26	0.41
15:C3:46:THR:N	15:C3:49:GLN:OE1	2.46	0.41
36:1:2523:A:H2'	45:L8:49:TYR:O	2.21	0.41
86:5:4125:OHX:N6	86:5:4200:OHX:N2	2.69	0.41
12:C0:80:LEU:O	12:C0:81:ASN:ND2	2.47	0.41
36:5:698:U:H2'	36:5:699:A:O4'	2.20	0.41
69:O3:6:ARG:HG3	69:O3:8:TYR:CE1	2.61	0.41
38:4:157:U:H3'	38:4:158:U:C6	2.56	0.41
42:L5:59:ASP:OD1	42:L5:81:HIS:HD2	2.04	0.41
70:O4:52:GLN:HG2	36:5:1639:C:C5'	197.63	0.41
23:D1:74:GLN:OE1	23:D1:82:VAL:N	4.85	0.41
40:L3:139:GLN:HB2	40:L3:141:GLY:N	4.49	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:66:U:OP1	8:S6:136:LYS:NZ	2.34	0.41
42:L5:56:THR:C	42:L5:58:LYS:N	2.73	0.41
11:S9:41:GLU:OE1	11:S9:126:ARG:NH2	2.54	0.41
1:2:237:C:C5'	1:2:238:U:H5'	2.40	0.41
1:6:1793:G:H4'	86:6:2126:OHX:N5	2.36	0.41
36:5:1570:U:O2'	36:5:1571:A:O4'	2.37	0.41
41:L4:81:GLY:HA3	36:5:357:A:O4'	129.74	0.41
36:1:2514:U:C6	45:L8:68:ARG:HB3	2.56	0.41
51:M5:173:GLY:HA3	51:M5:183:THR:OG1	2.20	0.41
3:S1:72:ASP:OD2	28:D6:59:TYR:OH	2.24	0.41
40:L3:27:ALA:HB3	40:L3:218:ILE:HG22	2.01	0.41
1:2:832:U:H2'	1:2:833:U:H5''	2.03	0.41
47:M0:210:ILE:HG12	47:M0:217:PHE:CD2	3.10	0.41
61:N5:49:LYS:HE3	38:8:135:G:OP1	79.66	0.41
1:6:220:A:OP2	1:6:832:U:H5''	2.21	0.41
36:5:1481:A:H2'	36:5:1858:A:N3	2.35	0.41
36:5:3242:G:N2	36:5:3245:A:H5''	2.35	0.41
2:S0:202:TYR:HD2	2:S0:202:TYR:H	1.69	0.41
40:L3:4:ARG:O	40:L3:5:LYS:CB	2.68	0.41
24:D2:86:ILE:HG13	24:D2:87:GLU:H	1.83	0.41
16:C4:43:THR:OG1	16:C4:46:MET:HG3	2.95	0.41
32:E0:46:ASN:OD1	32:E0:47:VAL:N	2.59	0.41
40:L3:36:ASP:O	40:L3:38:SER:N	2.81	0.41
29:D7:61:THR:O	29:D7:62:ILE:HB	2.21	0.41
36:5:1797:A:H2'	36:5:1798:A:O4'	2.21	0.41
36:5:726:G:H8	36:5:726:G:H5'	1.85	0.41
36:1:685:G:OP2	49:M3:35:ARG:NH1	2.51	0.41
47:M0:202:LYS:HD3	37:7:64:A:C2	344.51	0.41
7:S5:189:THR:O	7:S5:193:THR:HG23	3.80	0.41
17:C5:128:HIS:O	17:C5:130:ARG:HG2	2.21	0.41
8:S6:147:LEU:O	8:S6:148:SER:OG	2.30	0.41
43:L6:56:LYS:HD2	43:L6:98:VAL:HG13	2.02	0.41
66:O0:81:VAL:HG11	66:O0:90:VAL:HG21	2.66	0.41
36:5:874:U:H5''	36:5:2950:G:OP1	2.20	0.41
4:S2:237:VAL:O	4:S2:238:SER:OG	5.16	0.41
60:N4:14:TYR:O	60:N4:17:ARG:HB3	2.20	0.41
40:L3:106:TRP:CH2	40:L3:161:LEU:HD13	2.77	0.41
36:5:618:C:H2'	36:5:619:A:C8	2.55	0.41
70:O4:67:LYS:O	70:O4:67:LYS:HG3	2.20	0.41
62:N6:16:ARG:HH21	38:8:23:U:P	88.85	0.41
9:S7:137:GLY:CA	9:S7:153:LEU:HB2	2.89	0.41
14:C2:41:LEU:HA	14:C2:41:LEU:HD23	1.75	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:S5:149:VAL:HG12	7:S5:156:ARG:O	3.51	0.41
9:S7:77:LEU:HD22	9:S7:81:LEU:HD11	2.03	0.41
4:S2:38:VAL:O	4:S2:39:THR:OG1	2.30	0.41
5:S3:207:THR:HB	19:C7:40:THR:OG1	2.20	0.41
1:6:805:U:C2'	1:6:806:A:H5'	2.50	0.41
30:D8:19:THR:HB	30:D8:20:GLY:H	2.19	0.41
66:O0:54:SER:OG	70:O4:94:LEU:HD13	2.66	0.41
1:6:817:A:H2'	1:6:818:C:C6	2.56	0.41
36:1:1720:U:C4	55:M9:124:TYR:CE2	3.08	0.41
36:5:748:U:H2'	36:5:749:C:C6	2.56	0.41
36:1:16:A:H2'	36:1:17:G:O4'	2.20	0.41
4:S2:162:CYS:SG	4:S2:212:LYS:HE2	2.85	0.41
50:M4:62:GLN:H	50:M4:62:GLN:HG2	3.94	0.41
39:L2:242:ARG:HG3	39:L2:242:ARG:HH11	2.26	0.41
64:N8:70:LYS:HB2	64:N8:70:LYS:HE3	3.44	0.41
74:O8:61:LYS:H	74:O8:61:LYS:HG2	3.04	0.41
12:C0:70:GLU:O	12:C0:73:VAL:HG22	4.80	0.41
20:C8:89:GLN:HA	20:C8:97:ASP:HA	2.52	0.41
36:1:795:G:O6	86:1:3898:OHX:N3	2.54	0.41
37:7:49:G:H4'	37:7:50:U:O5'	2.21	0.41
1:2:372:G:H1'	1:2:612:U:O2	2.21	0.41
40:L3:296:THR:HG21	40:L3:357:LYS:C	2.41	0.41
63:N7:17:ARG:HG3	36:5:1639:C:N4	198.47	0.41
3:S1:74:GLN:NE2	3:S1:189:ILE:HG21	2.54	0.41
27:D5:39:ALA:HB1	27:D5:71:ILE:C	2.41	0.41
1:2:1388:A:HO2'	1:2:1411:A:H2	1.65	0.41
72:O6:27:SER:O	72:O6:28:TYR:CB	2.67	0.41
47:M0:23:ASN:HB3	47:M0:24:ARG:H	1.70	0.41
14:C2:46:ARG:HG2	14:C2:50:LYS:HD3	5.48	0.41
33:E1:119:ARG:O	33:E1:132:LEU:HG	2.83	0.41
16:C4:13:VAL:HG23	16:C4:76:ILE:HA	4.09	0.41
41:L4:141:ARG:HH11	41:L4:141:ARG:HD3	1.67	0.41
37:3:28:C:O5'	37:3:28:C:H6	2.03	0.41
36:1:1355:A:H1'	36:1:1356:U:OP2	2.21	0.41
36:1:1262:G:C6	36:1:1278:A:N6	2.89	0.41
16:C4:121:VAL:HA	16:C4:122:PRO:HD3	2.33	0.41
41:L4:222:VAL:HG22	41:L4:225:VAL:HG23	2.60	0.41
1:2:1657:U:C5	36:1:2125:A:O3'	2.74	0.41
9:S7:41:LEU:HD13	9:S7:70:PHE:HD1	1.85	0.41
1:6:578:U:O2	86:6:2154:OHX:N3	2.54	0.41
25:D3:42:PRO:O	25:D3:79:ASN:ND2	2.53	0.41
39:L2:48:ILE:HG13	39:L2:48:ILE:O	2.22	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:D6:23:CYS:SG	28:D6:74:CYS:HB3	2.60	0.41
28:D6:74:CYS:O	28:D6:75:VAL:HB	2.21	0.41
47:M0:48:LEU:HD22	47:M0:49:CYS:N	2.82	0.41
69:O3:60:ARG:HB2	69:O3:60:ARG:CZ	2.49	0.41
21:C9:42:GLY:CA	21:C9:84:LYS:HB2	2.49	0.41
44:L7:96:PRO:HA	44:L7:97:PRO:HD3	1.94	0.41
5:S3:40:ARG:HE	22:D0:110:PRO:HG3	3.46	0.41
3:S1:103:MET:HG2	3:S1:104:ASP:N	2.36	0.41
53:M7:27:LYS:NZ	36:5:1447:G:OP2	161.07	0.41
1:2:1220:C:H5''	12:C0:52:LYS:HD2	2.03	0.41
13:C1:130:PRO:O	1:6:336:G:H5'	300.12	0.41
54:M8:102:ALA:CB	54:M8:122:ILE:HG22	2.51	0.41
46:L9:114:VAL:HB	46:L9:124:ARG:HB2	2.18	0.41
36:1:1576:G:C6	36:1:1577:G:C2	3.09	0.41
71:O5:21:LEU:CD2	71:O5:25:LYS:HE3	2.86	0.41
47:M0:208:ASN:O	47:M0:212:GLU:HB2	4.30	0.41
36:1:1486:G:N2	70:O4:6:THR:HG22	2.35	0.41
54:M8:40:THR:C	54:M8:42:ALA:H	2.24	0.41
68:O2:19:ARG:HD2	68:O2:28:VAL:HG13	2.71	0.41
36:5:873:C:H3'	36:5:874:U:H4'	2.01	0.41
31:D9:6:VAL:HG23	31:D9:7:TRP:CE3	2.59	0.41
68:O2:61:LYS:HD2	36:5:1340:G:OP2	191.54	0.41
36:5:2217:U:H2'	36:5:2218:G:C8	2.56	0.41
4:S2:54:GLU:H	4:S2:54:GLU:HG2	1.63	0.41
7:S5:205:SER:O	7:S5:207:THR:N	2.54	0.41
36:5:3288:G:O2'	36:5:3289:G:H8	2.03	0.41
36:5:2360:C:H5''	36:5:2361:A:P	2.61	0.41
36:5:2286:U:C4	36:5:2288:G:H1'	2.56	0.41
1:2:1116:A:P	77:Q1:17:ARG:HH21	2.44	0.41
36:1:1051:U:H4'	57:N1:19:PHE:CD2	2.55	0.41
15:C3:98:VAL:HG22	1:6:951:A:O2'	291.65	0.41
38:8:149:A:H2'	38:8:150:G:C8	2.55	0.41
36:5:2213:A:H2'	36:5:2214:A:C8	2.56	0.41
46:L9:141:LYS:HE2	46:L9:142:ASP:OD1	2.20	0.41
36:5:687:U:O2'	36:5:688:G:H5'	2.20	0.41
36:1:2597:U:H2'	36:1:2598:G:H8	1.86	0.41
1:2:275:C:N3	1:2:276:C:N4	2.67	0.41
32:E0:21:VAL:HG22	1:6:586:G:H4'	410.17	0.41
19:C7:87:GLU:O	19:C7:88:VAL:HG12	2.20	0.41
1:2:552:G:C6	1:2:553:G:C6	3.09	0.41
36:1:841:A:OP2	86:1:4178:OHX:N2	2.54	0.41
63:N7:17:ARG:C	63:N7:19:ALA:H	2.24	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
70:O4:74:ARG:HD3	70:O4:85:VAL:HG21	4.39	0.41
1:2:1340:U:C2	1:2:1378:U:H4'	2.55	0.41
36:1:1285:G:O2'	36:1:1286:A:OP2	2.30	0.41
1:6:1698:G:H1'	1:6:1699:G:OP1	2.20	0.41
3:S1:184:LEU:HA	3:S1:187:LYS:HB2	2.03	0.41
36:5:271:C:H2'	36:5:272:G:O4'	2.21	0.41
27:D5:39:ALA:O	27:D5:71:ILE:HA	2.21	0.41
27:D5:43:ASP:O	27:D5:44:GLN:HB3	3.54	0.41
22:D0:72:ASN:HD21	1:6:1429:G:H21	385.85	0.41
11:S9:138:LYS:HE2	26:D4:67:GLY:HA3	2.03	0.41
62:N6:115:ARG:HG3	62:N6:115:ARG:NH1	3.06	0.41
38:4:85:G:H3'	38:4:85:G:H8	1.86	0.41
11:S9:133:HIS:CD2	11:S9:162:SER:HB2	2.56	0.41
7:S5:35:GLN:HB3	7:S5:36:ALA:H	1.59	0.41
7:S5:36:ALA:HB3	7:S5:45:LYS:NZ	2.36	0.41
1:2:819:G:O6	1:2:853:G:C5	2.74	0.41
55:M9:106:LEU:HB3	55:M9:120:TYR:CE1	2.55	0.41
1:2:1759:C:H5''	1:2:1760:G:OP2	2.21	0.41
70:O4:103:LYS:HA	70:O4:103:LYS:HD3	2.32	0.41
36:5:2101:C:O2'	36:5:2102:U:P	2.78	0.41
62:N6:53:ASP:HB2	62:N6:110:HIS:CD2	2.56	0.41
6:S4:158:ASP:OD1	6:S4:158:ASP:N	2.52	0.41
1:2:196:G:HO2'	1:2:197:A:P	2.42	0.41
9:S7:133:THR:HG22	9:S7:157:LYS:O	3.72	0.41
10:S8:9:HIS:O	10:S8:10:LYS:CB	2.68	0.41
31:D9:40:ARG:NH2	1:6:1198:G:O3'	390.97	0.41
10:S8:8:ARG:NH2	10:S8:22:ARG:HH11	8.96	0.41
1:2:1402:G:H2'	1:2:1403:C:C6	2.56	0.41
1:2:1602:C:H2'	1:2:1603:U:O4'	2.21	0.41
34:SR:7:LEU:HD12	34:SR:7:LEU:H	1.86	0.41
45:L8:33:ASN:ND2	36:5:2549:G:C2	214.88	0.41
54:M8:64:VAL:HG11	54:M8:113:LYS:HD2	2.02	0.41
22:D0:106:ILE:O	22:D0:107:THR:OG1	2.32	0.41
64:N8:65:GLN:HA	64:N8:65:GLN:OE1	3.02	0.41
49:M3:64:LYS:HG3	64:N8:69:TRP:CD2	2.56	0.41
1:6:832:U:OP2	86:6:2202:OHX:N6	2.54	0.41
9:S7:55:LYS:HE2	9:S7:87:ASP:HA	3.31	0.41
26:D4:5:VAL:O	26:D4:6:THR:OG1	2.24	0.41
28:D6:66:LYS:HB2	28:D6:68:TYR:CE2	3.75	0.41
36:1:1015:U:O2'	36:1:1017:C:OP2	2.31	0.41
44:L7:175:LYS:HD3	44:L7:176:TYR:CZ	4.53	0.41
36:1:2536:A:H2'	36:1:2537:U:C5	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:2796:G:N7	78:Q2:63:LYS:NZ	2.67	0.41
2:S0:167:LYS:HD3	2:S0:168:HIS:CD2	2.56	0.41
36:5:1716:U:H3'	36:5:1716:U:P	2.61	0.41
39:L2:112:ILE:HD11	79:Q3:79:VAL:HG11	5.93	0.41
36:1:2138:A:C4	73:O7:3:LYS:HB3	2.55	0.41
86:5:4177:OHX:N4	86:5:4238:OHX:N1	2.69	0.41
1:2:525:A:C6	1:2:526:A:C6	3.08	0.41
2:S0:37:VAL:HG22	2:S0:149:LEU:HD13	4.32	0.41
24:D2:86:ILE:HD11	24:D2:117:ARG:HD3	2.02	0.41
36:5:3078:U:H4'	36:5:3079:U:O5'	2.21	0.41
64:N8:43:ILE:O	64:N8:46:ASP:O	2.42	0.41
67:O1:46:THR:HG21	67:O1:91:SER:OG	2.21	0.41
39:L2:15:ILE:HD11	36:5:904:A:H2	172.66	0.41
51:M5:73:ARG:NH1	51:M5:88:GLY:O	2.47	0.41
39:L2:227:ARG:HH21	36:5:2162:U:P	200.21	0.41
15:C3:48:SER:O	15:C3:52:VAL:HG23	2.99	0.41
15:C3:52:VAL:HG22	15:C3:55:ARG:NH2	2.36	0.41
50:M4:108:ARG:HA	50:M4:108:ARG:HD2	1.94	0.41
5:S3:25:PHE:HE1	5:S3:69:LEU:HD22	1.86	0.41
63:N7:97:SER:O	63:N7:100:THR:HB	2.21	0.41
1:6:1756:A:H2'	1:6:1757:G:H8	1.86	0.41
1:6:1645:G:OP2	86:6:2183:OHX:N3	2.54	0.41
36:1:789:A:H2'	36:1:790:U:H6	1.85	0.41
36:1:520:U:N3	41:L4:347:THR:O	2.54	0.41
34:SR:275:ARG:HA	34:SR:276:PRO:HD2	1.96	0.41
1:2:1274:C:N4	35:SM:95:SER:HA	2.36	0.41
36:1:2635:A:H4'	36:1:2636:A:O5'	2.21	0.41
51:M5:120:TRP:CE3	36:5:269:G:H5'	133.19	0.41
1:2:1546:G:H21	20:C8:87:ASN:HB2	1.86	0.41
1:2:683:C:H2'	1:2:684:A:C8	2.56	0.41
8:S6:214:LYS:HA	8:S6:217:SER:OG	2.21	0.41
13:C1:77:SER:HB3	13:C1:85:VAL:HB	2.25	0.41
51:M5:101:THR:O	51:M5:105:ARG:HG2	2.72	0.41
1:2:491:C:H42	1:2:496:G:H1	1.68	0.41
1:2:1170:G:C2	1:2:1171:A:C8	3.09	0.41
1:6:491:C:H42	1:6:497:G:H21	1.69	0.41
36:5:1632:A:H2'	36:5:1633:C:C6	2.56	0.41
42:L5:140:ARG:HD3	36:5:1080:A:OP1	227.40	0.41
36:5:1012:G:H2'	36:5:1013:G:O4'	2.21	0.41
1:6:682:C:H2'	1:6:683:C:C6	2.56	0.41
36:1:1927:G:P	79:Q3:6:LYS:H	2.43	0.41
17:C5:77:ARG:HB3	17:C5:102:PHE:CD1	3.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:S2:59:HIS:CD2	4:S2:238:SER:HA	2.55	0.41
40:L3:49:TYR:O	40:L3:80:ASP:N	2.53	0.41
36:1:2158:A:O4'	36:1:2160:G:C8	2.74	0.41
35:SM:51:ARG:CZ	35:SM:52:PRO:HD2	6.36	0.41
34:SR:167:VAL:HG12	34:SR:183:LEU:HB2	2.03	0.41
86:2:2084:OHX:N4	86:2:2086:OHX:N1	2.69	0.41
57:N1:88:ARG:H	57:N1:88:ARG:HG2	2.59	0.41
66:O0:53:LYS:NZ	36:5:2552:C:H5	243.29	0.41
36:5:279:U:H2'	36:5:280:U:H6	1.86	0.41
43:L6:55:LEU:HD12	43:L6:64:LEU:HD13	2.54	0.41
36:1:1081:U:H4'	36:1:1081:U:OP2	2.21	0.41
40:L3:83:PRO:O	40:L3:165:GLN:HG3	2.21	0.41
23:D1:85:TYR:CD1	29:D7:6:ASP:HB2	3.16	0.41
1:2:763:G:C6	1:2:764:U:C4	3.09	0.41
36:5:278:U:O5'	36:5:278:U:H6	2.04	0.41
2:S0:110:TYR:HA	2:S0:115:PHE:CE1	2.56	0.41
36:1:1844:C:O2	73:O7:9:GLY:HA2	2.20	0.41
1:6:1357:A:H2'	1:6:1358:G:C8	2.55	0.41
43:L6:23:LYS:HE3	36:5:611:A:O4'	234.39	0.41
36:5:34:A:C4	36:5:51:A:C2	3.09	0.41
5:S3:219:ALA:HA	5:S3:220:PRO:HD2	2.27	0.41
36:1:3251:U:H2'	36:1:3252:G:C8	2.56	0.41
36:5:277:G:H2'	36:5:278:U:C6	2.56	0.41
36:5:3136:G:OP2	86:5:4106:OHX:N3	2.54	0.41
58:N2:90:ARG:O	58:N2:91:ASP:HB2	2.20	0.41
1:2:1623:C:H2'	1:2:1624:C:C6	2.56	0.41
66:O0:28:LYS:HD3	36:5:1713:G:O6	237.29	0.41
1:6:325:G:C2	1:6:344:A:C2	3.09	0.41
36:1:1424:C:H2'	36:1:1425:U:O4'	2.21	0.41
20:C8:7:GLU:HB3	20:C8:10:SER:OG	3.11	0.41
36:1:1194:G:OP1	86:1:3967:OHX:N1	2.54	0.41
36:1:2842:U:OP1	36:1:2844:C:N4	2.53	0.41
59:N3:69:LEU:HD12	59:N3:69:LEU:HA	1.96	0.41
36:5:3284:G:OP2	36:5:3284:G:H8	2.03	0.41
39:L2:92:LYS:HA	39:L2:103:PRO:CD	2.79	0.41
70:O4:74:ARG:NH2	70:O4:82:ALA:HB2	2.36	0.41
10:S8:76:THR:HB	10:S8:105:ASP:CB	2.51	0.41
6:S4:50:ASN:O	6:S4:53:LYS:NZ	2.92	0.41
36:1:3343:G:N2	36:1:3362:A:H2	1.93	0.41
19:C7:44:LYS:HG3	19:C7:47:ARG:NH1	3.29	0.41
17:C5:126:VAL:HG22	17:C5:127:ARG:N	2.66	0.41
7:S5:73:THR:CG2	18:C6:114:ARG:HE	5.46	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
63:N7:47:GLU:OE2	63:N7:69:LYS:HE2	2.21	0.41
1:2:1433:G:N2	31:D9:45:GLU:OE1	2.51	0.41
24:D2:77:PRO:HD2	24:D2:79:PHE:CE2	2.56	0.41
1:2:1793:G:O2'	28:D6:5:ARG:NH2	2.54	0.41
28:D6:38:ARG:HH21	28:D6:83:ILE:CG1	2.33	0.41
6:S4:43:PRO:HA	6:S4:82:TYR:O	2.32	0.41
86:5:4093:OHX:N3	86:5:4199:OHX:N1	2.69	0.41
41:L4:205:PRO:HB3	41:L4:247:PHE:CD2	2.56	0.41
51:M5:183:THR:HA	51:M5:187:ARG:HB2	2.03	0.41
59:N3:48:ARG:NH1	59:N3:48:ARG:HG3	2.36	0.41
15:C3:16:ILE:HD12	15:C3:16:ILE:HA	4.28	0.41
54:M8:19:PRO:HB3	54:M8:53:PHE:HA	2.02	0.41
38:4:1:A:H2'	38:4:2:A:O5'	2.21	0.41
1:2:639:U:OP2	1:2:639:U:H4'	2.21	0.41
36:5:3285:C:H3'	36:5:3286:G:H5''	2.02	0.41
70:O4:8:ARG:NH1	70:O4:8:ARG:HG2	2.36	0.41
1:6:523:G:O2'	1:6:529:A:N6	2.50	0.41
20:C8:61:LEU:HA	20:C8:65:GLU:OE1	2.54	0.41
9:S7:55:LYS:HB3	9:S7:55:LYS:HE2	2.35	0.41
1:2:71:A:H2'	1:2:72:A:O4'	2.20	0.41
5:S3:194:LYS:O	5:S3:196:ARG:N	2.54	0.41
33:E1:82:LYS:HE2	33:E1:82:LYS:HB3	1.82	0.41
67:O1:79:ARG:H	67:O1:79:ARG:HE	1.69	0.41
16:C4:16:VAL:O	16:C4:30:VAL:HA	2.28	0.41
16:C4:30:VAL:HG13	16:C4:39:ILE:O	2.21	0.41
86:1:4088:OHX:N2	86:1:4157:OHX:N1	2.69	0.41
34:SR:255:ALA:N	34:SR:292:LEU:HD11	3.60	0.41
72:O6:95:ALA:O	72:O6:99:ARG:HB2	2.20	0.41
3:S1:101:HIS:HA	3:S1:217:LEU:HD22	2.03	0.41
61:N5:105:VAL:CG1	61:N5:126:LEU:HD22	2.54	0.41
1:2:199:G:O2'	1:2:200:A:H8	2.04	0.41
51:M5:73:ARG:HB2	51:M5:92:LEU:HD23	2.17	0.41
67:O1:72:ARG:O	67:O1:96:VAL:HG13	2.21	0.41
56:N0:49:HIS:HB3	56:N0:51:VAL:HG23	3.51	0.41
55:M9:21:LYS:HE3	55:M9:55:VAL:HA	2.03	0.41
24:D2:103:ILE:HD13	24:D2:126:LEU:HB2	2.05	0.41
18:C6:123:ARG:HB2	18:C6:123:ARG:HE	1.51	0.41
36:5:2770:G:H2'	36:5:2771:U:H5'	2.03	0.41
1:2:288:A:H2'	1:2:289:U:O4'	2.20	0.41
15:C3:47:PRO:HG2	15:C3:72:MET:HG3	4.79	0.41
24:D2:38:LEU:HD23	24:D2:41:MET:CE	3.08	0.41
36:1:916:G:H1	39:L2:207:VAL:HG11	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:S9:37:LYS:HB3	32:E0:33:ARG:HB2	2.03	0.41
12:C0:23:ALA:CB	12:C0:64:TYR:HB2	3.86	0.41
17:C5:128:HIS:HA	1:6:1180:C:O2'	335.03	0.41
48:M1:7:ASN:H	48:M1:8:PRO:HD3	2.13	0.41
1:2:1636:C:C2	1:2:1638:G:C5	3.09	0.41
42:L5:258:LYS:O	42:L5:259:LYS:HG2	2.21	0.41
42:L5:259:LYS:H	42:L5:259:LYS:HG2	4.06	0.41
3:S1:120:LEU:CD2	3:S1:122:GLU:HG3	2.59	0.41
36:1:1610:G:H2'	36:1:1611:G:O4'	2.20	0.41
50:M4:8:LYS:O	50:M4:9:ALA:HB2	2.21	0.41
1:6:703:G:H2'	1:6:704:C:C6	2.56	0.41
1:6:1130:G:OP2	86:6:2113:OHX:N1	2.54	0.41
42:L5:143:LYS:HG3	42:L5:172:TYR:HD2	2.13	0.41
5:S3:137:VAL:HG22	5:S3:151:LYS:HG3	2.01	0.41
1:6:1395:G:O6	86:6:2089:OHX:N3	2.54	0.41
36:5:2924:U:O4	86:5:4059:OHX:N2	2.54	0.41
3:S1:190:PRO:C	3:S1:191:GLU:HG2	2.42	0.41
46:L9:116:ASN:O	46:L9:119:GLY:N	2.53	0.41
1:2:88:U:H4'	1:2:171:A:O4'	2.21	0.41
29:D7:33:LEU:HD13	29:D7:73:LEU:HD21	3.24	0.41
1:2:964:U:H5''	15:C3:128:TYR:CE1	2.56	0.41
36:1:2369:G:H2'	36:1:2370:G:C8	2.56	0.41
65:N9:17:HIS:O	86:N9:101:OHX:N6	2.53	0.41
57:N1:120:LYS:HB2	57:N1:120:LYS:HE3	1.92	0.41
46:L9:38:LEU:HA	46:L9:38:LEU:HD23	1.91	0.41
45:L8:70:LYS:HD2	45:L8:70:LYS:HA	1.90	0.41
16:C4:110:LEU:HA	16:C4:110:LEU:HD23	2.17	0.41
1:6:1359:C:O5'	1:6:1359:C:H6	2.04	0.41
57:N1:41:ASP:OD1	57:N1:99:SER:HB2	2.21	0.41
36:5:2358:A:H2'	36:5:2359:C:O4'	2.20	0.41
36:1:1571:A:H2'	36:1:1572:U:O4'	2.20	0.41
36:1:979:U:H1'	36:1:980:A:N7	2.29	0.40
47:M0:174:THR:HG23	47:M0:176:LEU:N	2.10	0.40
48:M1:94:ARG:HB2	48:M1:95:ASN:H	1.81	0.40
1:2:702:G:N2	1:2:703:G:H1'	2.36	0.40
28:D6:38:ARG:O	28:D6:71:LEU:N	2.51	0.40
1:6:1281:G:C2	1:6:1282:U:C2	3.09	0.40
40:L3:169:THR:CG2	40:L3:171:LEU:HG	2.94	0.40
33:E1:143:LYS:CA	1:6:1253:U:H4'	451.04	0.40
36:1:2392:C:O2	36:1:2987:A:N1	2.54	0.40
40:L3:21:ARG:HD3	40:L3:269:GLN:OE1	3.28	0.40
51:M5:186:GLY:O	51:M5:190:THR:HG22	2.21	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
39:L2:222:ALA:HB1	39:L2:224:THR:HG22	5.82	0.40
45:L8:180:VAL:HG11	45:L8:186:LEU:HD21	2.96	0.40
6:S4:105:VAL:HG13	6:S4:243:GLY:HA2	2.33	0.40
56:N0:155:ARG:NH1	36:5:3206:C:O2	310.65	0.40
1:6:329:G:H2'	1:6:330:G:C8	2.56	0.40
70:O4:20:ILE:HD11	70:O4:34:HIS:NE2	2.73	0.40
42:L5:78:ALA:HB3	42:L5:105:ILE:HG12	2.03	0.40
46:L9:86:TYR:CE1	46:L9:151:VAL:HG13	2.56	0.40
36:1:2554:A:H5''	39:L2:85:GLY:O	2.20	0.40
36:1:1307:G:C2	36:1:1308:A:C2	3.08	0.40
36:5:1025:A:H5'	36:5:1026:A:OP2	2.20	0.40
36:5:1027:A:N7	36:5:1029:G:C2	2.89	0.40
2:S0:189:VAL:HG22	2:S0:190:ASP:H	1.85	0.40
49:M3:135:ALA:O	49:M3:136:GLU:HB3	2.20	0.40
72:O6:98:ARG:HD2	72:O6:98:ARG:H	1.86	0.40
41:L4:138:ARG:HG3	41:L4:244:LEU:O	2.21	0.40
45:L8:113:ALA:C	45:L8:115:ALA:H	3.83	0.40
67:O1:44:MET:HE3	67:O1:44:MET:HB3	4.23	0.40
29:D7:49:HIS:CD2	1:6:958:U:H5'	343.83	0.40
42:L5:119:TYR:OH	42:L5:141:PRO:HD3	2.30	0.40
61:N5:79:GLY:O	61:N5:81:ILE:HG13	2.20	0.40
9:S7:43:PHE:CE1	9:S7:46:ILE:HG13	2.57	0.40
39:L2:2:GLY:HA2	39:L2:207:VAL:HG12	2.30	0.40
36:1:2333:C:H2'	36:1:2334:U:C1'	2.50	0.40
36:5:428:A:H2'	36:5:429:U:C6	2.56	0.40
49:M3:47:ALA:HB1	49:M3:48:PRO:CD	2.51	0.40
86:D9:102:OHX:N3	86:6:2128:OHX:N5	406.42	0.40
11:S9:28:LEU:HD11	32:E0:39:LEU:HB3	2.22	0.40
36:5:1507:G:N3	36:5:1507:G:H2'	2.36	0.40
70:O4:37:LYS:NZ	36:5:1591:G:OP1	160.63	0.40
1:2:1474:G:H2'	1:2:1475:A:C8	2.56	0.40
6:S4:233:LYS:H	6:S4:233:LYS:HD2	1.85	0.40
34:SR:21:THR:O	34:SR:291:SER:HB3	2.21	0.40
36:1:2328:U:H2'	36:1:2329:C:C6	2.56	0.40
53:M7:50:GLN:OE1	53:M7:56:ARG:HD3	2.21	0.40
36:1:1207:G:N7	86:1:4066:OHX:N2	2.70	0.40
36:1:1528:G:N3	36:1:1588:A:H2	2.19	0.40
1:6:90:C:O2'	1:6:91:G:H5'	2.21	0.40
39:L2:140:ASN:OD1	39:L2:142:ASP:HB3	4.86	0.40
11:S9:48:GLN:O	11:S9:52:ILE:HG13	2.74	0.40
11:S9:49:LEU:HD23	11:S9:104:PHE:CE2	2.56	0.40
55:M9:42:ARG:HH22	36:5:1601:U:P	103.14	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
55:M9:121:HIS:HE1	36:5:1719:G:N7	241.04	0.40
1:6:615:A:N3	1:6:1107:G:C2	2.89	0.40
64:N8:2:PRO:HG2	64:N8:5:PHE:CD2	2.56	0.40
1:2:685:A:O2'	1:2:686:C:H5'	2.21	0.40
57:N1:36:VAL:HA	57:N1:64:VAL:HG12	2.74	0.40
36:5:3232:G:H2'	36:5:3233:C:O4'	2.22	0.40
36:1:2677:G:H2'	36:1:2679:A:H2	1.86	0.40
1:2:941:A:O2'	1:2:977:A:H5'	2.21	0.40
40:L3:59:ASP:OD1	40:L3:71:GLU:HG2	2.39	0.40
59:N3:45:ARG:O	59:N3:46:LEU:C	2.66	0.40
17:C5:35:LYS:HE2	17:C5:35:LYS:HB3	4.11	0.40
52:M6:129:LEU:HD12	52:M6:129:LEU:HA	1.87	0.40
16:C4:129:LYS:HB2	16:C4:129:LYS:HE3	1.84	0.40
70:O4:19:LYS:HE2	70:O4:19:LYS:HB3	2.59	0.40
1:2:268:C:N4	8:S6:186:ARG:HD2	2.36	0.40
5:S3:90:ARG:HB3	5:S3:91:VAL:H	2.81	0.40
36:5:879:U:O2	36:5:2357:A:H1'	2.21	0.40
55:M9:168:ALA:O	55:M9:172:ARG:HD2	2.21	0.40
36:1:661:G:N7	64:N8:19:LYS:HE3	2.36	0.40
1:2:448:C:OP1	6:S4:29:PRO:HD3	2.20	0.40
49:M3:46:ILE:HG23	49:M3:46:ILE:HD12	2.93	0.40
36:5:1096:U:H4'	36:5:1097:G:O5'	2.21	0.40
41:L4:319:LYS:O	41:L4:320:ASN:CB	2.82	0.40
86:5:4065:OHX:N2	86:5:4074:OHX:N5	2.69	0.40
37:3:27:A:OP2	42:L5:57:ASN:HB2	2.21	0.40
27:D5:44:GLN:HA	27:D5:47:TYR:HB3	3.08	0.40
72:O6:28:TYR:HE1	36:5:315:C:H5	102.52	0.40
1:6:1098:U:C6	1:6:1098:U:H5''	2.57	0.40
28:D6:35:ALA:O	28:D6:36:ILE:HG22	2.21	0.40
37:3:22:A:C6	37:3:23:A:C6	3.09	0.40
1:2:512:A:H5''	11:S9:163:PRO:HG3	2.02	0.40
5:S3:113:LEU:HD13	5:S3:113:LEU:HA	4.07	0.40
1:2:821:U:C5	1:2:853:G:N2	2.89	0.40
1:2:1544:U:OP1	20:C8:136:GLN:NE2	2.55	0.40
21:C9:28:LEU:HD23	21:C9:55:TYR:CE1	2.55	0.40
36:1:1913:A:N3	36:1:2120:A:H2'	2.36	0.40
36:5:3163:A:C5	36:5:3164:C:N4	2.89	0.40
79:Q3:50:GLY:O	79:Q3:51:ALA:CB	2.69	0.40
36:5:437:G:H1	36:5:622:A:N6	2.19	0.40
47:M0:74:LYS:HA	47:M0:74:LYS:HD3	3.01	0.40
1:6:1157:A:OP2	86:6:2142:OHX:N1	2.53	0.40
1:2:325:G:H4'	13:C1:83:THR:HG21	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:722:G:O2'	1:6:723:G:H5''	2.21	0.40
36:1:1593:A:N3	36:1:1615:C:O2'	2.50	0.40
1:6:1671:A:H2'	1:6:1672:G:O4'	2.22	0.40
10:S8:146:ARG:O	10:S8:147:ALA:HB3	2.21	0.40
36:1:2941:A:N7	40:L3:255:TRP:CE2	2.89	0.40
14:C2:125:ASN:HB2	35:SM:169:ALA:HB3	6.17	0.40
36:1:3094:A:H2'	36:1:3095:U:C6	2.56	0.40
36:1:1818:U:H2'	36:1:1819:U:O4'	2.21	0.40
36:1:2408:U:C2'	36:1:2409:G:H5'	2.50	0.40
67:O1:12:TYR:O	67:O1:72:ARG:HD2	2.20	0.40
36:1:2741:C:O2'	78:Q2:20:HIS:ND1	2.33	0.40
41:L4:26:PHE:HA	41:L4:127:ALA:HA	2.02	0.40
12:C0:16:PHE:CD1	12:C0:76:LEU:HD12	8.50	0.40
40:L3:243:HIS:C	40:L3:244:ARG:HG3	2.42	0.40
8:S6:214:LYS:C	8:S6:216:LEU:H	3.36	0.40
1:2:1039:A:O2'	1:2:1040:G:P	2.78	0.40
34:SR:114:ASP:OD1	34:SR:115:ILE:N	2.67	0.40
70:O4:58:ARG:CG	70:O4:58:ARG:NH1	2.84	0.40
36:5:2822:U:H2'	36:5:2823:G:O4'	2.21	0.40
74:O8:32:ASN:C	74:O8:32:ASN:HD22	2.24	0.40
39:L2:109:GLU:HA	39:L2:136:ILE:HG22	2.16	0.40
40:L3:358:TRP:CZ2	40:L3:360:ASP:HA	2.56	0.40
36:5:238:A:H2'	36:5:239:G:O4'	2.21	0.40
4:S2:242:ILE:HG22	4:S2:243:TYR:CD2	2.55	0.40
34:SR:112:SER:CB	34:SR:153:GLN:HA	2.51	0.40
36:5:619:A:OP2	36:5:619:A:H8	2.04	0.40
39:L2:44:ILE:HD13	39:L2:46:LYS:HD2	3.49	0.40
42:L5:208:MET:HG2	42:L5:223:PHE:CZ	2.56	0.40
1:2:553:G:C6	1:2:554:C:N3	2.88	0.40
51:M5:149:ASN:OD1	86:M5:304:OHX:N2	2.54	0.40
25:D3:48:HIS:CD2	25:D3:105:ALA:HB2	2.56	0.40
9:S7:21:ALA:O	9:S7:24:PHE:HB2	2.22	0.40
36:1:2608:G:O2'	36:1:2609:A:H5'	2.21	0.40
36:1:1301:A:H4'	36:1:1302:A:O5'	2.21	0.40
36:1:2162:U:OP1	39:L2:234:LYS:NZ	2.50	0.40
3:S1:32:ILE:HD11	3:S1:46:THR:HG23	2.03	0.40
1:2:953:G:H2'	1:2:954:G:C8	2.56	0.40
1:2:1260:U:C2	1:2:1261:G:C8	3.10	0.40
44:L7:25:GLN:O	44:L7:28:ALA:HB3	3.75	0.40
50:M4:46:ILE:HD13	50:M4:58:ILE:HG21	2.04	0.40
45:L8:43:LYS:HD3	45:L8:43:LYS:HA	1.82	0.40
36:1:2314:U:H2'	36:1:2314:U:H6	1.46	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:1196:A:H3'	1:2:1196:A:OP2	2.22	0.40
36:1:1282:G:C6	36:1:1283:C:C4	3.09	0.40
36:1:2862:U:H2'	36:1:2863:G:O4'	2.20	0.40
52:M6:149:TYR:OH	36:5:3006:A:OP1	252.62	0.40
36:5:2144:A:H1'	36:5:2281:A:N6	2.37	0.40
8:S6:173:PRO:HB2	8:S6:174:LYS:H	1.47	0.40
3:S1:77:GLU:C	3:S1:79:HIS:N	2.74	0.40
27:D5:47:TYR:CE1	27:D5:51:LEU:HD11	3.76	0.40
18:C6:109:PHE:O	18:C6:113:ASP:N	2.55	0.40
86:5:4187:OHX:N3	86:5:4189:OHX:N6	2.69	0.40
64:N8:79:TRP:CH2	64:N8:121:VAL:HG11	2.56	0.40
64:N8:77:LYS:NZ	36:5:785:G:N7	138.34	0.40
25:D3:31:LYS:HA	25:D3:31:LYS:HD3	2.16	0.40
36:5:2572:C:O2'	36:5:2573:G:OP2	2.38	0.40
15:C3:36:GLN:NE2	15:C3:39:LYS:HD2	7.42	0.40
15:C3:62:GLN:HB2	15:C3:65:VAL:HG23	2.02	0.40
14:C2:67:THR:O	14:C2:68:GLU:HB2	2.34	0.40
16:C4:126:THR:O	16:C4:127:ARG:C	2.59	0.40
10:S8:138:ASN:O	10:S8:142:LYS:HG3	2.21	0.40
1:2:220:A:H5''	1:2:832:U:H1'	2.04	0.40
36:1:200:C:P	62:N6:60:ARG:NH1	2.95	0.40
20:C8:14:ILE:HA	20:C8:22:VAL:O	2.21	0.40
1:6:484:C:N4	1:6:503:G:H22	2.18	0.40
74:O8:4:GLU:OE1	36:5:1746:U:O2'	155.78	0.40
5:S3:196:ARG:HB3	5:S3:197:THR:H	2.58	0.40
36:1:3393:U:O2'	36:1:3394:U:H5'	2.21	0.40
48:M1:16:LYS:HG2	48:M1:130:VAL:CG1	2.51	0.40
27:D5:59:TYR:CE2	27:D5:100:ILE:HG12	2.56	0.40
39:L2:133:TYR:CD2	39:L2:168:VAL:HG12	2.56	0.40
67:O1:100:SER:OG	67:O1:102:LYS:HB3	2.22	0.40
53:M7:36:ILE:HD13	53:M7:36:ILE:HG21	1.58	0.40
17:C5:22:LEU:HD13	17:C5:26:LEU:HD11	2.03	0.40
64:N8:46:ASP:O	64:N8:47:LYS:O	2.47	0.40
29:D7:75:GLU:HB3	29:D7:76:GLY:H	2.37	0.40
36:5:726:G:C8	36:5:726:G:C5'	3.04	0.40
36:5:3357:U:O2'	36:5:3358:U:OP1	2.32	0.40
7:S5:172:ILE:O	7:S5:176:THR:HG23	2.47	0.40
38:4:15:G:C6	38:4:16:G:N1	2.89	0.40
51:M5:200:TRP:CZ3	36:5:683:U:H5''	101.06	0.40
45:L8:67:ILE:HA	45:L8:67:ILE:HD13	4.48	0.40
15:C3:119:GLU:O	15:C3:123:HIS:ND1	3.09	0.40
36:5:627:U:H4'	36:5:1399:A:O2'	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:S1:128:LYS:HE3	3:S1:132:ASP:OD1	2.22	0.40
36:5:1340:G:H2'	36:5:1341:U:C6	2.56	0.40
5:S3:11:LEU:HD12	22:D0:86:ILE:HG12	2.02	0.40
1:2:1261:G:H2'	1:2:1262:U:C6	2.56	0.40
1:2:848:C:H2'	1:2:849:C:H6	1.87	0.40
1:2:1530:C:OP2	27:D5:95:HIS:CD2	2.74	0.40
36:5:349:A:O4'	38:8:24:G:H1'	2.20	0.40
78:Q2:69:VAL:HG22	78:Q2:84:THR:HB	2.03	0.40
36:5:734:C:H2'	36:5:735:A:O4'	2.21	0.40
51:M5:165:THR:O	51:M5:169:LYS:HG3	2.22	0.40
1:2:1231:U:O5'	1:2:1259:U:H1'	2.22	0.40
1:2:540:G:H2'	1:2:540:G:OP2	2.21	0.40
36:1:1573:G:H2'	36:1:1573:G:N3	2.36	0.40
40:L3:252:ILE:HD12	40:L3:252:ILE:HA	2.08	0.40
11:S9:6:ARG:HD3	11:S9:6:ARG:HA	1.87	0.40
71:O5:114:ARG:HD2	71:O5:114:ARG:HA	2.06	0.40
88:5:4251:3H3:C3	88:5:4251:3H3:C9	2.99	0.40
55:M9:92:GLN:O	55:M9:92:GLN:HG2	2.22	0.40
36:1:1653:G:H2'	36:1:1654:A:O4'	2.21	0.40
36:5:792:G:H2'	36:5:793:C:C6	2.56	0.40
36:5:3182:G:H2'	36:5:3183:A:O4'	2.20	0.40
1:2:778:G:N2	1:2:780:A:C6	2.90	0.40
27:D5:38:HIS:HB3	27:D5:39:ALA:H	4.26	0.40
1:2:1409:G:N2	1:2:1411:A:H3'	2.37	0.40
36:5:2211:U:H5	36:5:2234:G:C6	2.39	0.40
1:2:1291:G:H1	1:2:1324:G:H22	1.69	0.40
51:M5:67:ARG:O	51:M5:68:ARG:HB3	4.73	0.40
64:N8:121:VAL:HA	64:N8:122:PRO:HD3	1.94	0.40
36:1:3375:A:H5''	36:1:3378:C:H5	1.85	0.40
54:M8:147:ARG:H	54:M8:147:ARG:HG2	4.22	0.40
36:1:1230:G:OP2	86:1:4089:OHX:N2	2.55	0.40
19:C7:82:ASP:O	19:C7:83:GLN:HB2	2.21	0.40
1:6:198:A:C2'	1:6:199:G:H5'	2.51	0.40
6:S4:106:LYS:NZ	1:6:788:A:OP1	398.61	0.40
1:2:1199:G:O6	31:D9:31:ILE:HD11	2.21	0.40
11:S9:113:VAL:HG21	11:S9:134:ILE:HG21	2.64	0.40
30:D8:22:ARG:HD2	1:6:1619:C:O2	343.17	0.40
26:D4:40:LEU:O	26:D4:44:LEU:HB2	2.22	0.40
36:5:715:A:H4'	36:5:716:A:OP1	2.21	0.40
36:1:3271:G:OP1	53:M7:171:ARG:HG2	2.22	0.40
4:S2:235:LEU:HD11	23:D1:54:ALA:HB2	2.02	0.40
4:S2:61:LEU:HA	4:S2:62:PRO:HD2	1.97	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
45:L8:156:ASP:OD1	45:L8:183:LYS:HG2	2.65	0.40
48:M1:108:GLU:HA	48:M1:122:ILE:CG2	2.73	0.40
39:L2:77:ILE:HD13	39:L2:128:ARG:HB3	2.03	0.40
20:C8:31:ALA:CB	20:C8:58:ALA:HB2	2.60	0.40
14:C2:81:ASP:HA	14:C2:82:PRO:HD2	2.62	0.40
2:S0:35:PRO:HG3	23:D1:87:ARG:NH2	2.37	0.40
4:S2:98:PHE:CD2	4:S2:121:VAL:HG23	3.77	0.40
4:S2:121:VAL:O	4:S2:125:ILE:HG13	2.21	0.40
4:S2:170:ILE:HA	4:S2:171:PRO:HD3	1.86	0.40
40:L3:255:TRP:O	40:L3:255:TRP:HD1	2.04	0.40
20:C8:135:GLY:HA3	1:6:1559:A:H5''	366.51	0.40
64:N8:44:ASN:O	64:N8:47:LYS:O	2.40	0.40
44:L7:158:LYS:CE	44:L7:159:GLN:H	2.34	0.40
36:5:2772:C:H1'	36:5:2773:C:OP2	2.22	0.40
36:1:2656:A:C8	36:1:2658:G:C8	3.10	0.40
36:1:671:U:O2'	54:M8:20:LYS:HD3	2.21	0.40
10:S8:136:SER:HB3	10:S8:139:ALA:CB	2.52	0.40
6:S4:85:GLY:N	6:S4:88:ASP:OD2	2.53	0.40
36:1:2777:G:H5''	36:1:2778:G:OP1	2.21	0.40
1:6:607:G:H5'	1:6:613:G:N2	2.37	0.40
5:S3:157:LEU:HD23	5:S3:189:MET:HB2	3.07	0.40
36:5:1313:G:H2'	36:5:1314:C:C6	2.57	0.40
1:2:548:G:H2'	1:2:549:G:O4'	2.21	0.40
36:1:377:A:O2'	36:1:391:A:N1	2.50	0.40
39:L2:180:LEU:HD23	39:L2:180:LEU:HA	1.90	0.40
15:C3:54:LEU:HB3	15:C3:60:VAL:HG11	2.70	0.40
23:D1:5:LYS:O	23:D1:7:GLN:N	2.54	0.40
70:O4:94:LEU:HA	70:O4:94:LEU:HD23	2.00	0.40
52:M6:181:ALA:O	52:M6:183:ALA:N	2.54	0.40
49:M3:149:GLN:HA	49:M3:150:PRO:HD3	1.90	0.40
36:1:3366:G:H2'	36:1:3367:C:C6	2.56	0.40
53:M7:65:SER:O	53:M7:66:SER:HB2	2.23	0.40
1:6:1146:G:C6	1:6:1147:A:C6	3.09	0.40
1:2:113:U:H4'	1:2:115:G:OP1	2.22	0.40
36:1:2257:C:H2'	36:1:2258:U:O4'	2.21	0.40
36:5:260:C:H2'	36:5:261:U:C6	2.57	0.40
1:6:1614:A:C6	1:6:1615:C:N4	2.89	0.40
1:6:1102:G:H2'	1:6:1103:U:O4'	2.21	0.40
46:L9:94:TYR:CD2	46:L9:98:PRO:HA	2.84	0.40
36:1:2567:C:C2'	36:1:2568:C:H5'	2.52	0.40
40:L3:240:ARG:HG2	40:L3:240:ARG:O	2.20	0.40
59:N3:128:ARG:CZ	59:N3:128:ARG:HB3	3.35	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:5:2623:G:H2'	36:5:2624:G:O4'	2.21	0.40
36:1:1106:G:H2'	36:1:1107:C:O4'	2.22	0.40
6:S4:29:PRO:O	1:6:449:C:OP1	363.32	0.40
50:M4:47:ASP:C	50:M4:49:PRO:HD3	3.12	0.40
10:S8:61:GLU:OE2	10:S8:77:ARG:NH1	8.29	0.40
42:L5:111:GLN:O	42:L5:113:LEU:N	2.55	0.40
25:D3:7:ARG:HH11	25:D3:7:ARG:CG	2.34	0.40
28:D6:37:LYS:HD3	28:D6:70:LYS:NZ	2.36	0.40
8:S6:31:ARG:HE	8:S6:68:LEU:CD1	2.34	0.40
64:N8:119:PRO:O	64:N8:121:VAL:N	3.21	0.40
7:S5:39:GLU:HB3	7:S5:40:ILE:H	1.68	0.40
12:C0:29:GLN:O	12:C0:30:ALA:HB3	2.21	0.40
51:M5:163:GLY:CA	51:M5:168:GLY:HA3	2.90	0.40
1:2:119:A:H1'	1:2:397:A:C5	2.56	0.40
9:S7:157:LYS:HB2	9:S7:157:LYS:HE3	3.91	0.40
36:1:1765:U:H2'	36:1:1766:G:C8	2.57	0.40
22:D0:63:LEU:O	22:D0:83:GLU:HA	2.21	0.40
36:1:38:U:H2'	36:1:39:A:O4'	2.21	0.40
36:5:119:U:H4'	36:5:120:G:H3'	2.04	0.40
24:D2:21:GLY:O	29:D7:3:LEU:HD22	2.39	0.40
5:S3:30:ALA:C	5:S3:32:GLU:H	2.24	0.40
6:S4:66:MET:HB3	1:6:454:U:C4	376.57	0.40
1:2:260:U:HO2'	1:2:261:U:P	2.45	0.40
46:L9:84:LYS:NZ	46:L9:191:LEU:HD13	2.36	0.40
22:D0:99:ILE:H	22:D0:99:ILE:HG12	4.44	0.40
1:6:1208:A:H5''	1:6:1209:C:OP2	2.22	0.40
2:S0:202:TYR:O	2:S0:203:PHE:CG	2.74	0.40
86:1:4065:OHX:N4	86:1:4177:OHX:N1	2.70	0.40
16:C4:42:VAL:HA	16:C4:46:MET:SD	2.62	0.40
14:C2:57:ALA:O	14:C2:85:LYS:HE3	3.51	0.40
14:C2:131:ASP:OD1	14:C2:132:GLU:N	2.49	0.40
36:5:2770:G:C2'	36:5:2771:U:H5'	2.51	0.40
42:L5:114:GLY:O	42:L5:116:ASP:N	2.47	0.40
71:O5:21:LEU:HD21	71:O5:51:ILE:HG23	2.03	0.40
29:D7:36:LYS:HB3	29:D7:43:ILE:HG23	2.03	0.40
36:1:2655:U:H2'	78:Q2:3:ASN:O	2.21	0.40
11:S9:149:ARG:CZ	1:6:765:G:N7	428.55	0.40
55:M9:130:ASN:C	55:M9:132:PHE:N	2.75	0.40
36:5:1221:A:H4'	36:5:1222:G:OP2	2.22	0.40
58:N2:21:SER:HA	58:N2:24:GLU:OE2	2.22	0.40
1:6:922:G:H2'	1:6:923:A:C8	2.57	0.40
57:N1:88:ARG:NH2	65:N9:33:LYS:O	2.34	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:1:3006:A:OP2	52:M6:148:LYS:NZ	2.41	0.40
36:5:2767:U:H2'	36:5:2768:U:C6	2.57	0.40
45:L8:167:PRO:HB3	45:L8:177:TYR:CE1	3.00	0.40
45:L8:149:LYS:O	45:L8:176:PRO:HG2	2.22	0.40
1:2:180:A:H2'	1:2:181:A:O4'	2.21	0.40
48:M1:60:ARG:NH1	48:M1:60:ARG:HB2	2.36	0.40
27:D5:49:ARG:O	27:D5:53:GLU:HB2	2.51	0.40
63:N7:81:LEU:HA	63:N7:81:LEU:HD22	2.14	0.40
1:2:1:U:O4	11:S9:54:ARG:HD3	2.21	0.40
1:6:481:A:C2	1:6:508:U:C2	3.09	0.40
36:1:128:G:H2'	36:1:129:U:O4'	2.22	0.40
1:2:1369:U:OP2	21:C9:69:LYS:HE3	2.22	0.40
1:2:976:G:C6	1:2:1023:A:C4	3.10	0.40
1:6:1344:A:O2'	1:6:1345:A:OP1	2.36	0.40
54:M8:70:ALA:HB1	54:M8:138:LEU:HD11	2.03	0.40
29:D7:30:SER:HB2	29:D7:48:SER:OG	2.53	0.40
1:6:634:G:H2'	1:6:635:A:OP2	2.22	0.40
1:6:548:G:H2'	1:6:549:G:O4'	2.22	0.40
22:D0:29:THR:OG1	22:D0:30:LYS:HE2	2.21	0.40
20:C8:8:GLN:HB2	20:C8:9:GLY:H	1.51	0.40
54:M8:58:ASN:HB3	54:M8:144:ARG:NH2	2.52	0.40
36:1:1083:G:C6	36:1:1084:A:C6	3.09	0.40
11:S9:150:LEU:HA	11:S9:150:LEU:HD12	2.23	0.40
56:N0:38:LYS:HB2	56:N0:38:LYS:HE3	2.13	0.40
6:S4:48:LEU:HD12	6:S4:48:LEU:HA	1.80	0.40
27:D5:83:LEU:HD23	27:D5:83:LEU:HA	1.81	0.40
36:1:1549:U:H2'	36:1:1550:C:C6	2.56	0.40
56:N0:81:TYR:CE1	56:N0:88:HIS:HB2	2.56	0.40
36:1:1569:U:H5'	36:1:1570:U:H5''	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	1	1
2	s0	204/251 (81%)	161 (79%)	27 (13%)	16 (8%)	1	3
3	S1	212/254 (84%)	152 (72%)	31 (15%)	29 (14%)	0	1
3	s1	214/254 (84%)	179 (84%)	23 (11%)	12 (6%)	3	7
4	S2	215/253 (85%)	181 (84%)	25 (12%)	9 (4%)	4	13
4	s2	215/253 (85%)	187 (87%)	16 (7%)	12 (6%)	3	7
5	S3	221/239 (92%)	198 (90%)	14 (6%)	9 (4%)	4	14
5	s3	221/239 (92%)	193 (87%)	15 (7%)	13 (6%)	2	6
6	S4	258/260 (99%)	219 (85%)	27 (10%)	12 (5%)	4	11
6	s4	258/260 (99%)	223 (86%)	23 (9%)	12 (5%)	4	11
7	S5	204/224 (91%)	162 (79%)	21 (10%)	21 (10%)	1	1
7	s5	204/224 (91%)	164 (80%)	23 (11%)	17 (8%)	1	3
8	S6	224/236 (95%)	195 (87%)	21 (9%)	8 (4%)	5	17
8	s6	216/236 (92%)	194 (90%)	14 (6%)	8 (4%)	5	16
9	S7	182/189 (96%)	143 (79%)	21 (12%)	18 (10%)	1	2
9	s7	184/189 (97%)	148 (80%)	22 (12%)	14 (8%)	2	3
10	S8	184/200 (92%)	159 (86%)	12 (6%)	13 (7%)	2	4
10	s8	184/200 (92%)	164 (89%)	11 (6%)	9 (5%)	3	10
11	S9	183/196 (93%)	159 (87%)	15 (8%)	9 (5%)	3	10
11	s9	183/196 (93%)	148 (81%)	23 (13%)	12 (7%)	2	5
12	C0	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	2	5
12	c0	92/105 (88%)	63 (68%)	16 (17%)	13 (14%)	0	1
13	C1	153/155 (99%)	125 (82%)	18 (12%)	10 (6%)	2	5
13	c1	144/155 (93%)	117 (81%)	18 (12%)	9 (6%)	2	5
14	C2	122/142 (86%)	70 (57%)	26 (21%)	26 (21%)	0	0
14	c2	122/142 (86%)	71 (58%)	29 (24%)	22 (18%)	0	0
15	C3	148/150 (99%)	132 (89%)	13 (9%)	3 (2%)	11	35
15	c3	148/150 (99%)	123 (83%)	16 (11%)	9 (6%)	2	6
16	C4	125/136 (92%)	97 (78%)	16 (13%)	12 (10%)	1	2
16	c4	126/136 (93%)	101 (80%)	15 (12%)	10 (8%)	1	3
17	C5	122/141 (86%)	95 (78%)	16 (13%)	11 (9%)	1	2
17	c5	133/141 (94%)	97 (73%)	16 (12%)	20 (15%)	0	1

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	121 (87%)	13 (9%)	5 (4%)	5	17
18	c6	140/142 (99%)	121 (86%)	11 (8%)	8 (6%)	3	7
19	C7	116/136 (85%)	87 (75%)	22 (19%)	7 (6%)	2	6
19	c7	113/136 (83%)	96 (85%)	11 (10%)	6 (5%)	3	9
20	C8	143/145 (99%)	121 (85%)	11 (8%)	11 (8%)	1	3
20	c8	143/145 (99%)	115 (80%)	21 (15%)	7 (5%)	3	10
21	C9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	6	18
21	c9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	6	18
22	D0	105/120 (88%)	88 (84%)	15 (14%)	2 (2%)	12	37
22	d0	108/120 (90%)	85 (79%)	15 (14%)	8 (7%)	2	3
23	D1	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	2	4
23	d1	85/87 (98%)	75 (88%)	5 (6%)	5 (6%)	2	6
24	D2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	27	65
24	d2	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	27	65
25	D3	142/144 (99%)	117 (82%)	14 (10%)	11 (8%)	1	3
25	d3	142/144 (99%)	131 (92%)	10 (7%)	1 (1%)	30	69
26	D4	132/134 (98%)	110 (83%)	14 (11%)	8 (6%)	2	6
26	d4	132/134 (98%)	106 (80%)	15 (11%)	11 (8%)	1	3
27	D5	68/107 (64%)	51 (75%)	9 (13%)	8 (12%)	1	1
27	d5	67/107 (63%)	48 (72%)	13 (19%)	6 (9%)	1	2
28	D6	95/97 (98%)	69 (73%)	12 (13%)	14 (15%)	0	1
28	d6	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	1	3
29	D7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	2	5
29	d7	79/81 (98%)	60 (76%)	10 (13%)	9 (11%)	1	1
30	D8	61/66 (92%)	51 (84%)	7 (12%)	3 (5%)	3	10
30	d8	61/66 (92%)	46 (75%)	10 (16%)	5 (8%)	1	3
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	2	6
31	d9	51/55 (93%)	42 (82%)	5 (10%)	4 (8%)	1	3
32	E0	58/60 (97%)	45 (78%)	12 (21%)	1 (2%)	14	42
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	274 (87%)	29 (9%)	13 (4%)	4	14
34	sR	316/318 (99%)	268 (85%)	40 (13%)	8 (2%)	9	28
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	1
39	L2	250/253 (99%)	226 (90%)	20 (8%)	4 (2%)	14	44
39	l2	250/253 (99%)	214 (86%)	27 (11%)	9 (4%)	5	17
40	L3	384/386 (100%)	340 (88%)	31 (8%)	13 (3%)	6	19
40	l3	384/386 (100%)	350 (91%)	25 (6%)	9 (2%)	10	31
41	L4	359/361 (99%)	315 (88%)	23 (6%)	21 (6%)	3	7
41	l4	359/361 (99%)	308 (86%)	38 (11%)	13 (4%)	5	17
42	L5	294/296 (99%)	253 (86%)	23 (8%)	18 (6%)	2	6
42	l5	292/296 (99%)	262 (90%)	21 (7%)	9 (3%)	7	21
43	L6	152/175 (87%)	141 (93%)	8 (5%)	3 (2%)	11	35
43	l6	153/175 (87%)	132 (86%)	17 (11%)	4 (3%)	8	26
44	L7	220/243 (90%)	205 (93%)	6 (3%)	9 (4%)	4	14
44	l7	221/243 (91%)	203 (92%)	15 (7%)	3 (1%)	16	49
45	L8	231/255 (91%)	193 (84%)	30 (13%)	8 (4%)	6	18
45	l8	229/255 (90%)	184 (80%)	25 (11%)	20 (9%)	1	2
46	L9	189/191 (99%)	170 (90%)	14 (7%)	5 (3%)	8	26
46	l9	189/191 (99%)	173 (92%)	10 (5%)	6 (3%)	6	20
47	M0	207/220 (94%)	185 (89%)	17 (8%)	5 (2%)	9	29
47	m0	209/220 (95%)	181 (87%)	20 (10%)	8 (4%)	5	15
48	M1	167/173 (96%)	133 (80%)	20 (12%)	14 (8%)	1	3
48	m1	167/173 (96%)	146 (87%)	11 (7%)	10 (6%)	2	6
49	M3	191/198 (96%)	164 (86%)	19 (10%)	8 (4%)	4	13
49	m3	192/198 (97%)	164 (85%)	17 (9%)	11 (6%)	3	7
50	M4	134/137 (98%)	118 (88%)	11 (8%)	5 (4%)	5	16
50	m4	135/137 (98%)	127 (94%)	6 (4%)	2 (2%)	15	46
51	M5	201/203 (99%)	188 (94%)	7 (4%)	6 (3%)	7	22
51	m5	201/203 (99%)	180 (90%)	14 (7%)	7 (4%)	6	18
52	M6	195/198 (98%)	185 (95%)	6 (3%)	4 (2%)	11	33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	m6	195/198 (98%)	185 (95%)	8 (4%)	2 (1%)	22	60
53	M7	181/183 (99%)	159 (88%)	16 (9%)	6 (3%)	6	19
53	m7	153/183 (84%)	140 (92%)	10 (6%)	3 (2%)	11	35
54	M8	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	10	32
54	m8	183/185 (99%)	165 (90%)	11 (6%)	7 (4%)	5	15
55	M9	186/188 (99%)	173 (93%)	12 (6%)	1 (0%)	38	76
55	m9	186/188 (99%)	175 (94%)	8 (4%)	3 (2%)	14	44
56	N0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	19	54
56	n0	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	13	39
57	N1	157/159 (99%)	138 (88%)	14 (9%)	5 (3%)	6	20
57	n1	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	9	28
58	N2	98/120 (82%)	79 (81%)	15 (15%)	4 (4%)	4	14
58	n2	96/120 (80%)	84 (88%)	9 (9%)	3 (3%)	7	21
59	N3	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	30	69
59	n3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	30	69
60	N4	96/155 (62%)	77 (80%)	14 (15%)	5 (5%)	3	9
60	n4	133/155 (86%)	113 (85%)	12 (9%)	8 (6%)	2	6
61	N5	119/141 (84%)	110 (92%)	8 (7%)	1 (1%)	27	65
61	n5	118/141 (84%)	100 (85%)	13 (11%)	5 (4%)	4	13
62	N6	124/126 (98%)	114 (92%)	6 (5%)	4 (3%)	6	20
62	n6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	5	14
63	N7	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	2	3
63	n7	133/135 (98%)	111 (84%)	14 (10%)	8 (6%)	2	6
64	N8	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	3	8
64	n8	146/148 (99%)	126 (86%)	16 (11%)	4 (3%)	8	25
65	N9	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	5	17
65	n9	56/58 (97%)	43 (77%)	9 (16%)	4 (7%)	2	4
66	O0	95/104 (91%)	87 (92%)	6 (6%)	2 (2%)	11	33
66	o0	98/104 (94%)	89 (91%)	7 (7%)	2 (2%)	11	35
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	4	11
67	o1	107/112 (96%)	98 (92%)	5 (5%)	4 (4%)	5	16

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	O2	125/129 (97%)	116 (93%)	8 (6%)	1 (1%)	27	65
68	o2	125/129 (97%)	111 (89%)	11 (9%)	3 (2%)	9	29
69	O3	104/106 (98%)	101 (97%)	2 (2%)	1 (1%)	22	60
69	o3	104/106 (98%)	92 (88%)	7 (7%)	5 (5%)	4	10
70	O4	110/119 (92%)	103 (94%)	4 (4%)	3 (3%)	8	25
70	o4	110/119 (92%)	100 (91%)	8 (7%)	2 (2%)	13	39
71	O5	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	6	19
71	o5	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	14	42
72	O6	97/99 (98%)	78 (80%)	11 (11%)	8 (8%)	1	3
72	o6	97/99 (98%)	81 (84%)	9 (9%)	7 (7%)	2	4
73	O7	85/87 (98%)	76 (89%)	6 (7%)	3 (4%)	6	18
73	o7	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	6	18
74	O8	75/77 (97%)	62 (83%)	10 (13%)	3 (4%)	5	14
74	o8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	5	14
75	O9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	11	33
76	Q0	50/52 (96%)	48 (96%)	0	2 (4%)	5	14
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	11	35
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%)	7	23
78	q2	103/105 (98%)	92 (89%)	8 (8%)	3 (3%)	7	23
79	Q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	10	32
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	21	57
80	e0	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	2	5
82	p0	139/311 (45%)	117 (84%)	19 (14%)	3 (2%)	10	32
All	All	22333/24141 (92%)	19119 (86%)	2092 (9%)	1122 (5%)	3	10

All (1122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	66	ALA

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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%)	2	7
2	s0	165/209 (79%)	131 (79%)	34 (21%)	2	5
3	S1	191/223 (86%)	162 (85%)	29 (15%)	4	12
3	s1	192/223 (86%)	162 (84%)	30 (16%)	4	11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	S2	176/204 (86%)	137 (78%)	39 (22%)	1	4
4	s2	176/204 (86%)	139 (79%)	37 (21%)	1	5
5	S3	182/194 (94%)	149 (82%)	33 (18%)	2	7
5	s3	182/194 (94%)	149 (82%)	33 (18%)	2	7
6	S4	221/221 (100%)	182 (82%)	39 (18%)	3	8
6	s4	221/221 (100%)	187 (85%)	34 (15%)	4	12
7	S5	173/190 (91%)	140 (81%)	33 (19%)	2	6
7	s5	173/190 (91%)	138 (80%)	35 (20%)	2	5
8	S6	188/201 (94%)	155 (82%)	33 (18%)	3	8
8	s6	187/201 (93%)	152 (81%)	35 (19%)	2	7
9	S7	165/169 (98%)	140 (85%)	25 (15%)	4	12
9	s7	165/169 (98%)	134 (81%)	31 (19%)	2	7
10	S8	150/161 (93%)	128 (85%)	22 (15%)	4	13
10	s8	150/161 (93%)	129 (86%)	21 (14%)	5	15
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	4
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	6
12	C0	77/98 (79%)	58 (75%)	19 (25%)	1	2
12	c0	73/98 (74%)	61 (84%)	12 (16%)	3	10
13	C1	129/136 (95%)	104 (81%)	25 (19%)	2	6
13	c1	129/136 (95%)	107 (83%)	22 (17%)	3	8
14	C2	88/118 (75%)	68 (77%)	20 (23%)	1	3
14	c2	88/118 (75%)	65 (74%)	23 (26%)	1	2
15	C3	127/127 (100%)	101 (80%)	26 (20%)	2	5
15	c3	127/127 (100%)	105 (83%)	22 (17%)	3	8
16	C4	81/104 (78%)	61 (75%)	20 (25%)	1	2
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	3
17	C5	101/117 (86%)	86 (85%)	15 (15%)	4	12
17	c5	103/117 (88%)	83 (81%)	20 (19%)	2	6
18	C6	117/118 (99%)	94 (80%)	23 (20%)	2	6
18	c6	118/118 (100%)	98 (83%)	20 (17%)	3	9
19	C7	94/124 (76%)	70 (74%)	24 (26%)	1	2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	c7	92/124 (74%)	76 (83%)	16 (17%)	3	8
20	C8	128/128 (100%)	102 (80%)	26 (20%)	2	5
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	4
21	C9	115/115 (100%)	93 (81%)	22 (19%)	2	6
21	c9	115/115 (100%)	95 (83%)	20 (17%)	3	8
22	D0	100/113 (88%)	74 (74%)	26 (26%)	1	2
22	d0	103/113 (91%)	80 (78%)	23 (22%)	1	4
23	D1	74/74 (100%)	60 (81%)	14 (19%)	2	7
23	d1	74/74 (100%)	57 (77%)	17 (23%)	1	3
24	D2	110/110 (100%)	94 (86%)	16 (14%)	5	13
24	d2	110/110 (100%)	96 (87%)	14 (13%)	6	19
25	D3	119/119 (100%)	97 (82%)	22 (18%)	2	7
25	d3	119/119 (100%)	104 (87%)	15 (13%)	7	19
26	D4	112/112 (100%)	93 (83%)	19 (17%)	3	9
26	d4	112/112 (100%)	99 (88%)	13 (12%)	8	23
27	D5	61/88 (69%)	43 (70%)	18 (30%)	0	1
27	d5	61/88 (69%)	54 (88%)	7 (12%)	8	23
28	D6	83/83 (100%)	66 (80%)	17 (20%)	2	5
28	d6	83/83 (100%)	69 (83%)	14 (17%)	3	9
29	D7	70/70 (100%)	57 (81%)	13 (19%)	2	7
29	d7	70/70 (100%)	59 (84%)	11 (16%)	4	11
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	4
30	d8	56/59 (95%)	48 (86%)	8 (14%)	5	14
31	D9	47/48 (98%)	38 (81%)	9 (19%)	2	6
31	d9	47/48 (98%)	39 (83%)	8 (17%)	3	9
32	E0	51/51 (100%)	41 (80%)	10 (20%)	2	6
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	3
33	e1	66/66 (100%)	48 (73%)	18 (27%)	0	2
34	SR	260/261 (100%)	237 (91%)	23 (9%)	14	38
34	sR	260/261 (100%)	232 (89%)	28 (11%)	9	26
35	SM	97/228 (42%)	79 (81%)	18 (19%)	2	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	sM	54/228 (24%)	47 (87%)	7 (13%)	6	17
39	L2	193/195 (99%)	157 (81%)	36 (19%)	2	7
39	l2	192/195 (98%)	155 (81%)	37 (19%)	2	6
40	L3	321/322 (100%)	258 (80%)	63 (20%)	2	6
40	l3	320/322 (99%)	255 (80%)	65 (20%)	2	5
41	L4	288/288 (100%)	239 (83%)	49 (17%)	3	9
41	l4	288/288 (100%)	235 (82%)	53 (18%)	2	7
42	L5	244/244 (100%)	194 (80%)	50 (20%)	2	5
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	5
43	L6	134/152 (88%)	115 (86%)	19 (14%)	5	14
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	8
44	L7	186/204 (91%)	162 (87%)	24 (13%)	6	18
44	l7	187/204 (92%)	159 (85%)	28 (15%)	4	12
45	L8	187/207 (90%)	154 (82%)	33 (18%)	3	8
45	l8	177/207 (86%)	143 (81%)	34 (19%)	2	6
46	L9	171/171 (100%)	139 (81%)	32 (19%)	2	7
46	l9	171/171 (100%)	137 (80%)	34 (20%)	2	6
47	M0	177/186 (95%)	144 (81%)	33 (19%)	2	7
47	m0	179/186 (96%)	142 (79%)	37 (21%)	2	5
48	M1	147/150 (98%)	119 (81%)	28 (19%)	2	6
48	m1	147/150 (98%)	125 (85%)	22 (15%)	4	12
49	M3	154/158 (98%)	126 (82%)	28 (18%)	2	7
49	m3	154/158 (98%)	130 (84%)	24 (16%)	4	11
50	M4	107/108 (99%)	86 (80%)	21 (20%)	2	6
50	m4	108/108 (100%)	90 (83%)	18 (17%)	3	9
51	M5	175/175 (100%)	146 (83%)	29 (17%)	3	9
51	m5	175/175 (100%)	148 (85%)	27 (15%)	4	12
52	M6	160/161 (99%)	137 (86%)	23 (14%)	5	13
52	m6	160/161 (99%)	132 (82%)	28 (18%)	3	8
53	M7	140/145 (97%)	113 (81%)	27 (19%)	2	6
53	m7	125/145 (86%)	108 (86%)	17 (14%)	5	16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	M8	150/150 (100%)	125 (83%)	25 (17%)	3	9
54	m8	150/150 (100%)	122 (81%)	28 (19%)	2	7
55	M9	153/153 (100%)	133 (87%)	20 (13%)	6	17
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	4
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	7
56	n0	156/156 (100%)	132 (85%)	24 (15%)	4	12
57	N1	136/136 (100%)	108 (79%)	28 (21%)	2	5
57	n1	136/136 (100%)	116 (85%)	20 (15%)	4	13
58	N2	87/106 (82%)	76 (87%)	11 (13%)	7	19
58	n2	85/106 (80%)	73 (86%)	12 (14%)	5	14
59	N3	104/104 (100%)	90 (86%)	14 (14%)	6	16
59	n3	104/104 (100%)	95 (91%)	9 (9%)	15	39
60	N4	57/129 (44%)	52 (91%)	5 (9%)	14	38
60	n4	100/129 (78%)	88 (88%)	12 (12%)	7	21
61	N5	104/117 (89%)	79 (76%)	25 (24%)	1	3
61	n5	104/117 (89%)	80 (77%)	24 (23%)	1	3
62	N6	109/109 (100%)	88 (81%)	21 (19%)	2	6
62	n6	109/109 (100%)	84 (77%)	25 (23%)	1	3
63	N7	115/115 (100%)	91 (79%)	24 (21%)	1	5
63	n7	115/115 (100%)	92 (80%)	23 (20%)	2	6
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	8
64	n8	118/118 (100%)	95 (80%)	23 (20%)	2	6
65	N9	46/46 (100%)	38 (83%)	8 (17%)	3	8
65	n9	46/46 (100%)	35 (76%)	11 (24%)	1	3
66	O0	81/87 (93%)	66 (82%)	15 (18%)	2	7
66	o0	84/87 (97%)	68 (81%)	16 (19%)	2	6
67	O1	92/96 (96%)	72 (78%)	20 (22%)	1	4
67	o1	94/96 (98%)	77 (82%)	17 (18%)	2	7
68	O2	109/110 (99%)	94 (86%)	15 (14%)	5	15
68	o2	109/110 (99%)	92 (84%)	17 (16%)	4	11
69	O3	90/90 (100%)	76 (84%)	14 (16%)	4	11

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	o3	90/90 (100%)	82 (91%)	8 (9%)	14	38
70	O4	95/101 (94%)	78 (82%)	17 (18%)	2	7
70	o4	95/101 (94%)	81 (85%)	14 (15%)	4	13
71	O5	104/104 (100%)	83 (80%)	21 (20%)	2	5
71	o5	103/104 (99%)	76 (74%)	27 (26%)	1	2
72	O6	81/81 (100%)	60 (74%)	21 (26%)	1	2
72	o6	80/81 (99%)	52 (65%)	28 (35%)	0	0
73	O7	70/70 (100%)	58 (83%)	12 (17%)	3	8
73	o7	70/70 (100%)	59 (84%)	11 (16%)	4	11
74	O8	68/68 (100%)	55 (81%)	13 (19%)	2	6
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	7
75	O9	45/45 (100%)	36 (80%)	9 (20%)	2	6
75	o9	45/45 (100%)	35 (78%)	10 (22%)	1	4
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	4	12
76	q0	47/47 (100%)	40 (85%)	7 (15%)	4	12
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%)	4	11
78	q2	90/90 (100%)	73 (81%)	17 (19%)	2	7
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	5	14
79	q3	71/71 (100%)	58 (82%)	13 (18%)	2	7
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	3
82	p0	105/253 (42%)	84 (80%)	21 (20%)	2	6
All	All	18729/20239 (92%)	15348 (82%)	3381 (18%)	2	7

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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
39	l2	157	VAL
39	l2	158	ILE
39	l2	165	VAL
39	l2	179	LEU
39	l2	180	LEU
39	l2	181	LYS
39	l2	193	ARG
39	l2	194	ASN
39	l2	202	VAL
39	l2	207	VAL
39	l2	215	ASN
39	l2	224	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
39	l2	225	ILE
39	l2	230	VAL
39	l2	241	ARG
39	l2	246	LEU
39	l2	249	SER
40	l3	3	HIS
40	l3	4	ARG
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	21	ARG
40	l3	30	LYS
40	l3	39	LYS
40	l3	47	LEU
40	l3	50	LYS
40	l3	56	ILE
40	l3	77	THR
40	l3	79	VAL
40	l3	81	THR
40	l3	84	VAL
40	l3	103	THR
40	l3	114	VAL
40	l3	120	LYS
40	l3	124	LYS
40	l3	134	SER
40	l3	145	GLU
40	l3	146	ARG
40	l3	148	LEU
40	l3	150	ARG
40	l3	157	VAL
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
41	l4	25	VAL
41	l4	52	VAL
41	l4	60	THR
41	l4	67	THR
41	l4	93	MET
41	l4	112	LYS
41	l4	120	TYR
41	l4	122	THR
41	l4	143	GLU
41	l4	144	LYS
41	l4	145	ILE
41	l4	150	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
41	l4	156	LEU
41	l4	160	GLN
41	l4	161	LYS
41	l4	172	VAL
41	l4	176	SER
41	l4	179	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	188	ARG
41	l4	191	LYS
41	l4	198	ARG
41	l4	200	THR
41	l4	203	ARG
41	l4	206	LEU
41	l4	217	LYS
41	l4	220	ARG
41	l4	222	VAL
41	l4	226	GLU
41	l4	229	ASN
41	l4	230	VAL
41	l4	246	ARG
41	l4	258	LEU
41	l4	267	VAL
41	l4	283	THR
41	l4	284	SER
41	l4	287	THR
41	l4	295	ILE
41	l4	300	ARG
41	l4	306	THR
41	l4	307	GLN
41	l4	313	LEU
41	l4	319	LYS
41	l4	323	VAL
41	l4	327	LEU
41	l4	342	LYS
41	l4	345	GLU
41	l4	358	THR
41	l4	359	LEU
41	l4	360	LYS
42	l5	4	GLN
42	l5	5	LYS
42	l5	15	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
46	19	120	ASP
46	19	130	ASP
46	19	133	THR
46	19	151	VAL
46	19	157	ASN
46	19	161	LEU
46	19	162	GLN
46	19	168	ARG
46	19	169	ASN
46	19	177	ASP
46	19	179	ILE
46	19	191	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	0/1800	-	-
1	6	0/1800	-	-
36	1	0/3396	-	-
36	5	0/3396	-	-
37	3	0/121	-	-
37	7	0/121	-	-
38	4	0/158	-	-
38	8	0/158	-	-
All	All	0/10950	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 carbohydrates 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	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	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	-	0,15,15	0.00	-
86	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3H3	1	4216	-	34,34,34	1.01	3 (8%)	45,45,45	1.77	8 (17%)
86	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2032	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2147	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3942	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4232	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3H3	5	4251	-	34,34,34	1.13	2 (5%)	45,45,45	1.38	5 (11%)
86	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	3803	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o4	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	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
86	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3869	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3909	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3951	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3993	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4035	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4077	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4119	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4161	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4203	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
88	3H3	1	4216	-	-	0/39/51/51	0/1/2/2
86	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2032	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2094	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2136	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	3	215	-	-	0/0/0/0	0/0/0/0
86	OHX	3	216	-	-	0/0/0/0	0/0/0/0
86	OHX	3	217	-	-	0/0/0/0	0/0/0/0
86	OHX	3	218	-	-	0/0/0/0	0/0/0/0
86	OHX	3	219	-	-	0/0/0/0	0/0/0/0
86	OHX	3	220	-	-	0/0/0/0	0/0/0/0
86	OHX	3	221	-	-	0/0/0/0	0/0/0/0
86	OHX	3	222	-	-	0/0/0/0	0/0/0/0
86	OHX	3	223	-	-	0/0/0/0	0/0/0/0
86	OHX	3	224	-	-	0/0/0/0	0/0/0/0
86	OHX	3	225	-	-	0/0/0/0	0/0/0/0
86	OHX	3	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	222	-	-	0/0/0/0	0/0/0/0
86	OHX	4	223	-	-	0/0/0/0	0/0/0/0
86	OHX	4	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	227	-	-	0/0/0/0	0/0/0/0
86	OHX	4	228	-	-	0/0/0/0	0/0/0/0
86	OHX	4	229	-	-	0/0/0/0	0/0/0/0
86	OHX	4	230	-	-	0/0/0/0	0/0/0/0
86	OHX	4	231	-	-	0/0/0/0	0/0/0/0
86	OHX	4	232	-	-	0/0/0/0	0/0/0/0
86	OHX	4	233	-	-	0/0/0/0	0/0/0/0
86	OHX	4	234	-	-	0/0/0/0	0/0/0/0
86	OHX	4	235	-	-	0/0/0/0	0/0/0/0
86	OHX	4	236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3909	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3942	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3951	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3993	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4035	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4077	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4119	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4161	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4203	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	86	-	0/0/0/0	0/0/0/0
86	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4245	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
88	3H3	5	4251	-	-	0/39/51/51	0/1/2/2
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2124	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
86	OHX	7	216	-	-	0/0/0/0	0/0/0/0
86	OHX	7	217	-	-	0/0/0/0	0/0/0/0
86	OHX	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	214	-	-	0/0/0/0	0/0/0/0
86	OHX	8	215	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	229	-	-	0/0/0/0	0/0/0/0
86	OHX	C1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	M6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	208	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O2	201	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
86	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c1	202	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	3803	-	-	0/0/0/0	0/0/0/0
86	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	o4	203	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s9	201	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4251	3H3	C14-C16	5.04	1.56	1.52
88	1	4216	3H3	C3-C2	3.25	1.47	1.33
88	5	4251	3H3	C15-C14	-2.47	1.50	1.53
88	1	4216	3H3	C15-C14	-2.47	1.50	1.53
88	1	4216	3H3	C14-C16	2.45	1.54	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4216	3H3	C-C1-C11	5.41	119.56	111.11
88	1	4216	3H3	C1-C11-C12	4.79	122.64	113.80
88	5	4251	3H3	C15-C14-C16	4.11	116.50	109.83
88	1	4216	3H3	C15-C14-C16	4.07	116.44	109.83
88	1	4216	3H3	C11-C1-C2	4.04	118.12	110.54
88	5	4251	3H3	C11-C1-C2	3.73	117.55	110.54
88	5	4251	3H3	C1-C11-C12	3.72	120.67	113.80
88	1	4216	3H3	C-C1-C2	-3.32	102.02	110.05
88	1	4216	3H3	O1-C11-C12	-2.65	103.55	109.28
88	1	4216	3H3	C6-C7-C8	-2.16	106.97	112.88
88	1	4216	3H3	C8-C9-C10	-2.05	117.49	122.55
88	5	4251	3H3	O2-C16-C17	2.04	124.38	121.37
88	5	4251	3H3	C6-C7-C8	-2.03	107.32	112.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	2	1750/1800 (97%)	0.52	92 (5%) 25 26	40, 69, 136, 230	0
1	6	1795/1800 (99%)	0.50	82 (4%) 31 31	30, 58, 149, 237	0
2	S0	206/251 (82%)	1.13	44 (21%) 1 1	73, 88, 101, 127	0
2	s0	206/251 (82%)	0.67	22 (10%) 6 6	54, 71, 86, 92	0
3	S1	214/254 (84%)	2.28	87 (40%) 1 0	79, 109, 140, 148	0
3	s1	216/254 (85%)	1.00	39 (18%) 2 2	53, 65, 88, 95	0
4	S2	217/253 (85%)	1.76	92 (42%) 1 0	54, 68, 83, 96	0
4	s2	217/253 (85%)	1.58	72 (33%) 1 1	42, 56, 69, 78	0
5	S3	223/239 (93%)	2.60	125 (56%) 0 0	59, 72, 92, 108	0
5	s3	223/239 (93%)	2.23	108 (48%) 1 0	55, 76, 98, 104	0
6	S4	260/260 (100%)	1.02	46 (17%) 2 2	47, 69, 80, 108	0
6	s4	260/260 (100%)	0.67	18 (6%) 17 15	37, 58, 69, 100	0
7	S5	206/224 (91%)	1.56	67 (32%) 1 1	73, 92, 107, 120	0
7	s5	206/224 (91%)	1.21	47 (22%) 1 1	56, 77, 101, 113	0
8	S6	226/236 (95%)	1.02	44 (19%) 2 1	49, 82, 98, 126	0
8	s6	218/236 (92%)	0.61	17 (7%) 13 11	38, 66, 87, 107	0
9	S7	184/189 (97%)	0.74	20 (10%) 6 5	65, 92, 123, 131	0
9	s7	186/189 (98%)	1.25	30 (16%) 2 2	49, 78, 112, 122	0
10	S8	188/200 (94%)	0.96	34 (18%) 2 2	40, 55, 89, 104	0
10	s8	188/200 (94%)	1.05	32 (17%) 2 2	33, 52, 95, 111	0
11	S9	185/196 (94%)	2.38	94 (50%) 0 0	64, 77, 113, 146	0
11	s9	185/196 (94%)	0.69	14 (7%) 14 12	49, 62, 99, 125	0
12	C0	96/105 (91%)	2.77	57 (59%) 0 0	63, 83, 110, 128	0
12	c0	96/105 (91%)	3.57	66 (68%) 0 0	69, 99, 122, 140	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	C1	155/155 (100%)	2.23	59 (38%)	1	0	43, 53, 103, 117	0
13	c1	146/155 (94%)	1.48	30 (20%)	1	1	34, 48, 76, 96	0
14	C2	124/142 (87%)	3.56	77 (62%)	0	0	105, 118, 138, 151	0
14	c2	124/142 (87%)	5.19	99 (79%)	0	0	139, 159, 175, 184	0
15	C3	150/150 (100%)	0.64	12 (8%)	12	11	50, 67, 80, 86	0
15	c3	150/150 (100%)	0.58	9 (6%)	21	21	40, 55, 71, 85	0
16	C4	127/136 (93%)	2.47	64 (50%)	0	0	54, 113, 128, 131	0
16	c4	128/136 (94%)	1.68	43 (33%)	1	1	38, 71, 80, 83	0
17	C5	124/141 (87%)	1.28	30 (24%)	1	1	58, 72, 108, 128	0
17	c5	135/141 (95%)	1.11	24 (17%)	2	2	58, 74, 98, 120	0
18	C6	141/142 (99%)	1.06	26 (18%)	2	2	62, 82, 87, 89	0
18	c6	142/142 (100%)	0.86	25 (17%)	2	2	50, 71, 84, 105	0
19	C7	120/136 (88%)	0.50	13 (10%)	6	5	68, 85, 111, 113	0
19	c7	117/136 (86%)	0.65	14 (11%)	5	4	59, 72, 98, 109	0
20	C8	145/145 (100%)	0.56	16 (11%)	6	5	58, 80, 105, 114	0
20	c8	145/145 (100%)	0.09	5 (3%)	43	44	55, 65, 90, 103	0
21	C9	143/143 (100%)	0.16	4 (2%)	50	52	66, 80, 94, 105	0
21	c9	143/143 (100%)	0.27	6 (4%)	35	35	51, 64, 82, 98	0
22	D0	107/120 (89%)	2.01	42 (39%)	1	0	56, 87, 118, 129	0
22	d0	110/120 (91%)	3.45	51 (46%)	1	0	50, 82, 120, 132	0
23	D1	87/87 (100%)	1.29	24 (27%)	1	1	69, 75, 92, 99	0
23	d1	87/87 (100%)	0.75	8 (9%)	9	7	53, 59, 77, 88	0
24	D2	129/129 (100%)	1.78	53 (41%)	1	0	52, 62, 68, 78	0
24	d2	129/129 (100%)	0.68	6 (4%)	30	30	37, 47, 53, 61	0
25	D3	144/144 (100%)	1.78	52 (36%)	1	1	43, 49, 59, 73	0
25	d3	144/144 (100%)	1.03	18 (12%)	5	4	33, 38, 52, 65	0
26	D4	134/134 (100%)	0.86	23 (17%)	2	2	59, 82, 97, 105	0
26	d4	134/134 (100%)	0.20	5 (3%)	39	39	46, 66, 81, 100	0
27	D5	70/107 (65%)	1.42	18 (25%)	1	1	87, 103, 115, 121	0
27	d5	69/107 (64%)	1.14	18 (26%)	1	1	66, 87, 99, 101	0
28	D6	97/97 (100%)	3.25	64 (65%)	0	0	59, 74, 129, 133	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	d6	97/97 (100%)	1.77	33 (34%) 1 1	43, 55, 84, 93	0
29	D7	81/81 (100%)	0.75	8 (9%) 8 6	64, 79, 113, 123	0
29	d7	81/81 (100%)	1.09	11 (13%) 4 3	49, 66, 106, 109	0
30	D8	63/66 (95%)	3.90	45 (71%) 0 0	89, 104, 118, 130	0
30	d8	63/66 (95%)	2.42	37 (58%) 0 0	74, 89, 103, 112	0
31	D9	53/55 (96%)	0.83	6 (11%) 6 5	56, 60, 80, 89	0
31	d9	53/55 (96%)	1.08	12 (22%) 1 1	52, 58, 95, 109	0
32	E0	60/60 (100%)	4.86	45 (75%) 0 0	47, 79, 115, 121	0
33	E1	71/76 (93%)	1.84	27 (38%) 1 0	91, 102, 113, 115	0
33	e1	76/76 (100%)	2.10	30 (39%) 1 0	117, 130, 148, 153	0
34	SR	318/318 (100%)	0.47	30 (9%) 9 7	55, 87, 106, 129	0
34	sR	318/318 (100%)	1.34	93 (29%) 1 1	73, 91, 107, 124	0
35	SM	159/273 (58%)	2.69	83 (52%) 0 0	51, 73, 118, 120	0
35	sM	104/273 (38%)	1.62	32 (30%) 1 1	40, 75, 155, 158	0
36	1	3149/3396 (92%)	0.48	89 (2%) 50 52	17, 37, 108, 219	0
36	5	3150/3396 (92%)	0.48	91 (2%) 49 50	17, 36, 101, 220	0
37	3	121/121 (100%)	0.21	1 (0%) 83 83	28, 53, 70, 75	0
37	7	121/121 (100%)	0.29	0 100 100	24, 40, 51, 59	0
38	4	158/158 (100%)	0.62	6 (3%) 38 38	22, 40, 74, 105	0
38	8	158/158 (100%)	0.72	8 (5%) 27 27	27, 46, 80, 102	0
39	L2	252/253 (99%)	0.95	34 (13%) 4 3	20, 35, 50, 58	0
39	l2	252/253 (99%)	0.69	18 (7%) 16 14	21, 37, 55, 62	0
40	L3	386/386 (100%)	0.36	13 (3%) 43 44	23, 41, 54, 87	0
40	l3	386/386 (100%)	0.17	4 (1%) 79 79	17, 30, 42, 73	0
41	L4	361/361 (100%)	0.06	7 (1%) 64 64	19, 33, 49, 57	0
41	l4	361/361 (100%)	0.37	24 (6%) 18 16	21, 38, 55, 62	0
42	L5	296/296 (100%)	0.10	7 (2%) 56 57	37, 59, 77, 103	0
42	l5	294/296 (99%)	0.01	3 (1%) 79 79	29, 43, 66, 101	0
43	L6	156/175 (89%)	-0.08	1 (0%) 86 88	28, 35, 53, 69	0
43	l6	157/175 (89%)	-0.00	5 (3%) 45 46	30, 38, 56, 68	0
44	L7	222/243 (91%)	0.02	1 (0%) 88 90	21, 29, 54, 92	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	l7	223/243 (91%)	0.06	4 (1%) 65 66	20, 28, 65, 105	0
45	L8	233/255 (91%)	0.79	33 (14%) 3 3	42, 54, 88, 105	0
45	l8	231/255 (90%)	1.13	47 (20%) 1 1	51, 63, 88, 93	0
46	L9	191/191 (100%)	0.25	5 (2%) 53 54	37, 48, 60, 76	0
46	l9	191/191 (100%)	0.15	3 (1%) 68 69	27, 35, 54, 75	0
47	M0	211/220 (95%)	0.32	10 (4%) 30 30	24, 38, 72, 91	0
47	m0	213/220 (96%)	0.59	13 (6%) 21 20	25, 41, 64, 83	0
48	M1	169/173 (97%)	0.22	7 (4%) 35 36	45, 63, 76, 84	0
48	m1	169/173 (97%)	0.11	2 (1%) 75 76	32, 48, 60, 71	0
49	M3	193/198 (97%)	0.54	11 (5%) 23 23	21, 39, 73, 98	0
49	m3	194/198 (97%)	0.66	21 (10%) 6 5	27, 47, 80, 102	0
50	M4	136/137 (99%)	-0.01	4 (2%) 49 50	31, 38, 51, 59	0
50	m4	137/137 (100%)	-0.06	3 (2%) 59 60	28, 33, 51, 62	0
51	M5	203/203 (100%)	0.51	6 (2%) 48 49	20, 34, 42, 49	0
51	m5	203/203 (100%)	0.59	5 (2%) 54 55	25, 41, 51, 56	0
52	M6	197/198 (99%)	0.13	2 (1%) 79 79	22, 29, 48, 54	0
52	m6	197/198 (99%)	0.09	4 (2%) 62 63	18, 23, 47, 53	0
53	M7	183/183 (100%)	0.83	17 (9%) 9 7	25, 32, 82, 114	0
53	m7	155/183 (84%)	0.45	3 (1%) 64 64	21, 28, 40, 64	0
54	M8	185/185 (100%)	0.02	0 100 100	22, 31, 44, 56	0
54	m8	185/185 (100%)	0.30	0 100 100	26, 37, 46, 52	0
55	M9	188/188 (100%)	0.90	32 (17%) 2 2	38, 51, 127, 140	0
55	m9	188/188 (100%)	0.71	25 (13%) 4 3	34, 45, 105, 122	0
56	N0	172/172 (100%)	0.28	4 (2%) 57 58	29, 36, 48, 54	0
56	n0	172/172 (100%)	0.09	3 (1%) 67 68	23, 30, 40, 48	0
57	N1	159/159 (100%)	0.18	5 (3%) 47 47	25, 35, 71, 78	0
57	n1	159/159 (100%)	0.19	4 (2%) 54 55	25, 31, 64, 70	0
58	N2	100/120 (83%)	0.38	11 (11%) 6 5	67, 81, 92, 101	0
58	n2	98/120 (81%)	1.00	20 (20%) 1 1	58, 70, 80, 81	0
59	N3	136/136 (100%)	0.64	13 (9%) 8 7	27, 37, 50, 57	0
59	n3	136/136 (100%)	0.86	11 (8%) 12 10	19, 28, 42, 45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
60	N4	98/155 (63%)	2.88	34 (34%)	1 1	37, 48, 127, 130	0
60	n4	135/155 (87%)	0.99	13 (9%)	8 7	28, 74, 108, 124	0
61	N5	121/141 (85%)	1.04	20 (16%)	2 2	34, 46, 61, 83	0
61	n5	120/141 (85%)	1.25	30 (25%)	1 1	36, 49, 67, 72	0
62	N6	126/126 (100%)	0.66	11 (8%)	10 9	27, 42, 53, 61	0
62	n6	126/126 (100%)	1.70	42 (33%)	1 1	32, 45, 60, 65	0
63	N7	135/135 (100%)	0.24	4 (2%)	48 49	53, 66, 80, 88	0
63	n7	135/135 (100%)	0.35	11 (8%)	12 10	57, 72, 91, 99	0
64	N8	148/148 (100%)	0.36	5 (3%)	43 44	18, 32, 54, 63	0
64	n8	148/148 (100%)	0.43	2 (1%)	72 72	19, 39, 56, 58	0
65	N9	58/58 (100%)	0.27	4 (6%)	17 15	19, 39, 79, 90	0
65	n9	58/58 (100%)	0.16	1 (1%)	67 68	19, 40, 59, 70	0
66	O0	97/104 (93%)	0.39	6 (6%)	20 19	51, 60, 81, 85	0
66	o0	100/104 (96%)	1.09	20 (20%)	2 1	54, 63, 88, 100	0
67	O1	109/112 (97%)	0.54	9 (8%)	11 10	35, 48, 77, 91	0
67	o1	109/112 (97%)	0.31	5 (4%)	31 31	28, 39, 72, 90	0
68	O2	127/129 (98%)	0.24	3 (2%)	56 57	18, 30, 40, 56	0
68	o2	127/129 (98%)	0.70	6 (4%)	30 30	19, 34, 46, 65	0
69	O3	106/106 (100%)	-0.11	0 100 100		23, 28, 47, 56	0
69	o3	106/106 (100%)	0.10	1 (0%)	81 81	20, 27, 51, 60	0
70	O4	112/119 (94%)	0.97	24 (21%)	1 1	34, 49, 87, 100	0
70	o4	112/119 (94%)	0.42	6 (5%)	25 25	34, 49, 85, 93	0
71	O5	119/119 (100%)	1.32	26 (21%)	1 1	32, 49, 55, 58	0
71	o5	119/119 (100%)	1.45	28 (23%)	1 1	40, 54, 62, 68	0
72	O6	99/99 (100%)	0.60	7 (7%)	16 14	36, 45, 72, 86	0
72	o6	99/99 (100%)	0.58	9 (9%)	9 8	45, 55, 74, 90	0
73	O7	87/87 (100%)	1.40	20 (22%)	1 1	23, 28, 50, 71	0
73	o7	87/87 (100%)	1.69	24 (27%)	1 1	24, 30, 60, 95	0
74	O8	77/77 (100%)	1.45	18 (23%)	1 1	57, 69, 90, 98	0
74	o8	77/77 (100%)	1.13	22 (28%)	1 1	57, 69, 87, 91	0
75	O9	50/50 (100%)	1.56	12 (24%)	1 1	32, 35, 44, 49	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
75	o9	50/50 (100%)	2.02	20 (40%) 1 0	35, 38, 48, 52	0
76	Q0	52/52 (100%)	0.09	1 (1%) 64 64	33, 38, 53, 64	0
76	q0	52/52 (100%)	0.03	2 (3%) 38 38	23, 26, 38, 44	0
77	Q1	25/25 (100%)	1.58	9 (36%) 1 1	41, 43, 47, 52	0
77	q1	25/25 (100%)	0.70	2 (8%) 12 11	31, 35, 44, 50	0
78	Q2	105/105 (100%)	0.40	5 (4%) 29 30	22, 38, 56, 82	0
78	q2	105/105 (100%)	0.61	8 (7%) 14 12	26, 38, 51, 78	0
79	Q3	91/91 (100%)	0.74	6 (6%) 18 16	28, 38, 53, 66	0
79	q3	91/91 (100%)	0.59	5 (5%) 24 24	27, 38, 51, 59	0
80	e0	62/62 (100%)	2.38	24 (38%) 1 0	46, 64, 97, 99	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	0.74	15 (10%) 7 6	72, 90, 159, 170	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35344 (93%)	0.78	3939 (11%) 5 4	17, 52, 109, 237	0

All (3939) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	c2	20	ALA	41.0
60	N4	76	VAL	34.4
12	c0	98	THR	26.5
32	E0	53	LYS	21.3
32	E0	54	ARG	20.3
13	c1	3	THR	18.9
22	d0	18	GLN	18.5
22	d0	98	GLN	18.4
22	d0	121	ASN	18.4
60	n4	68	ALA	18.4
60	N4	75	THR	18.3
22	d0	97	VAL	17.7
35	SM	87	THR	17.6
60	N4	86	SER	17.3
7	S5	152	GLY	16.7
9	s7	2	SER	16.5
14	C2	112	ALA	16.3
11	S9	181	ALA	16.1
7	s5	151	GLY	16.1

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
16	C4	15	GLY	15.7
1	6	662	U	15.5
35	SM	88	ARG	15.4
32	E0	49	LEU	15.4
35	SM	85	SER	15.1
14	c2	131	ASP	14.5
68	o2	128	LEU	14.5
80	e0	62	VAL	14.4
13	C1	147	ALA	14.4
1	2	491	C	14.3
53	M7	161	ALA	14.3
60	N4	69	LYS	14.2
14	C2	108	ARG	14.1
14	c2	21	GLU	14.0
3	S1	55	LYS	14.0
14	c2	126	TRP	13.9
35	SM	84	LYS	13.9
14	C2	111	ASN	13.9
13	C1	146	ALA	13.7
80	e0	63	GLN	13.5
60	N4	88	ASP	13.5
32	E0	48	THR	13.2
47	m0	111	LEU	13.2
60	n4	67	VAL	13.1
13	c1	5	LEU	13.1
5	S3	87	TYR	13.1
22	d0	17	GLN	13.0
3	S1	54	LEU	13.0
14	c2	128	ALA	13.0
13	C1	156	PHE	13.0
30	D8	7	VAL	12.9
14	C2	110	GLY	12.9
3	S1	20	VAL	12.8
71	o5	120	ALA	12.7
17	c5	4	ALA	12.6
80	e0	49	LEU	12.5
1	6	494	U	12.5
1	2	488	G	12.3
22	d0	99	ILE	12.3
1	6	664	U	12.3
32	E0	61	SER	12.3
9	s7	3	ALA	12.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	d0	100	VAL	12.1
28	D6	62	TYR	12.1
17	c5	5	VAL	12.0
33	E1	85	TYR	11.9
12	c0	97	PRO	11.9
32	E0	52	GLY	11.6
35	SM	89	ARG	11.4
73	o7	87	SER	11.4
14	c2	123	VAL	11.4
13	C1	145	ALA	11.3
14	c2	24	ILE	11.3
11	S9	182	GLU	11.3
5	s3	42	THR	11.3
36	1	1568	U	11.2
73	o7	88	ALA	11.1
14	c2	30	VAL	11.1
12	c0	64	TYR	11.1
36	1	1569	U	11.0
47	m0	103	LEU	10.9
47	m0	221	ALA	10.9
60	n4	69	LYS	10.9
1	6	663	U	10.7
13	C1	2	SER	10.6
13	C1	148	LYS	10.6
35	SM	151	LEU	10.6
12	C0	93	GLN	10.5
14	C2	20	ALA	10.5
60	N4	78	ALA	10.4
60	N4	87	LEU	10.3
33	e1	80	ARG	10.3
60	N4	77	LYS	10.3
60	n4	66	GLU	10.2
12	c0	95	ARG	10.2
3	S1	45	LYS	10.1
14	c2	22	VAL	10.1
14	c2	132	GLU	10.1
5	S3	88	ALA	10.1
12	C0	92	ILE	10.0
30	D8	44	VAL	10.0
35	SM	175	ASP	10.0
13	C1	152	GLN	10.0
8	S6	226	ILE	9.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	c2	28	LEU	9.9
14	c2	56	GLU	9.8
7	S5	36	ALA	9.8
11	S9	180	LYS	9.8
1	6	493	U	9.8
30	D8	15	VAL	9.8
22	d0	119	ALA	9.7
1	2	506	A	9.7
13	c1	2	SER	9.5
22	d0	104	THR	9.5
17	c5	134	THR	9.5
22	d0	95	ALA	9.4
22	d0	14	GLN	9.4
3	S1	96	LEU	9.4
71	O5	120	ALA	9.4
7	s5	152	GLY	9.4
22	d0	105	GLN	9.3
1	6	495	C	9.2
22	d0	107	THR	9.2
3	S1	47	LEU	9.2
14	c2	106	ILE	9.2
3	S1	46	THR	9.2
16	C4	41	ARG	9.2
9	s7	52	ALA	9.1
30	D8	16	LEU	9.1
14	c2	23	THR	9.1
36	1	1572	U	9.1
80	e0	50	VAL	9.1
14	c2	124	LYS	9.1
14	C2	109	GLU	9.0
28	d6	98	PRO	9.0
9	s7	187	SER	9.0
32	E0	55	ARG	9.0
22	d0	120	SER	9.0
1	2	238	U	9.0
14	c2	63	VAL	9.0
36	1	2539	C	9.0
16	C4	14	PHE	9.0
22	d0	102	ARG	8.9
14	C2	85	LYS	8.9
30	D8	43	ASN	8.9
60	N4	90	ILE	8.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
38	8	81	U	8.8
3	S1	94	LYS	8.8
5	S3	179	GLN	8.8
35	sM	119	ALA	8.8
1	6	658	C	8.7
27	D5	88	ILE	8.7
60	n4	65	GLU	8.7
33	e1	85	TYR	8.7
16	C4	40	ALA	8.7
60	N4	89	LEU	8.7
5	s3	44	THR	8.7
13	c1	146	ALA	8.7
14	c2	25	GLU	8.7
1	2	495	C	8.6
14	C2	130	THR	8.6
13	c1	4	GLU	8.6
14	C2	138	GLU	8.6
7	S5	37	GLN	8.6
3	S1	95	ASN	8.6
60	n4	70	LYS	8.6
12	c0	94	GLU	8.5
28	D6	61	GLU	8.5
11	S9	35	GLY	8.5
34	sR	121	MET	8.5
60	N4	67	VAL	8.5
1	6	490	C	8.5
12	c0	79	TYR	8.4
1	2	714	G	8.4
71	o5	2	ALA	8.4
36	1	1952	G	8.4
32	E0	46	ASN	8.3
18	C6	143	ARG	8.3
35	sM	83	LYS	8.3
3	S1	31	ASP	8.3
14	c2	85	LYS	8.3
33	e1	90	LYS	8.3
32	E0	51	ASN	8.3
14	c2	29	LYS	8.2
59	n3	2	SER	8.2
14	C2	126	TRP	8.2
60	N4	68	ALA	8.2
13	C1	3	THR	8.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	S3	148	LYS	8.2
68	o2	127	ALA	8.2
16	C4	79	VAL	8.2
14	C2	141	SER	8.1
32	E0	42	ARG	8.1
14	c2	136	ILE	8.1
16	c4	60	ALA	8.1
12	C0	94	GLU	8.1
1	6	659	C	8.1
75	O9	2	ALA	8.0
1	6	506	A	8.0
5	S3	45	LYS	8.0
46	l9	191	LEU	8.0
3	S1	229	MET	8.0
12	C0	96	ASN	8.0
5	s3	145	ALA	8.0
1	2	490	C	8.0
11	S9	186	GLU	8.0
31	d9	4	GLU	8.0
82	p0	209	LEU	8.0
16	C4	96	PRO	8.0
36	1	1571	A	7.9
8	s6	169	TYR	7.9
11	S9	101	VAL	7.9
16	C4	16	VAL	7.9
7	s5	37	GLN	7.9
1	2	913	G	7.9
35	sM	84	LYS	7.9
14	C2	62	LEU	7.9
36	5	2871	G	7.8
28	D6	53	LEU	7.8
36	5	2874	G	7.8
17	c5	133	ALA	7.8
36	5	2873	U	7.8
22	D0	98	GLN	7.7
30	D8	5	THR	7.7
35	SM	86	ASN	7.7
3	S1	32	ILE	7.7
14	c2	115	VAL	7.7
5	s3	43	PRO	7.7
30	D8	60	GLU	7.6
3	S1	60	ALA	7.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
12	c0	20	VAL	7.6
1	6	1800	A	7.6
14	c2	100	TRP	7.6
35	sM	168	GLU	7.6
14	c2	133	LEU	7.6
5	S3	37	VAL	7.5
30	D8	65	ARG	7.5
14	C2	143	GLN	7.5
14	C2	107	ASP	7.5
33	E1	86	THR	7.5
82	p0	192	ASP	7.5
60	N4	73	ARG	7.5
1	6	660	G	7.5
35	SM	176	ALA	7.5
12	c0	93	GLN	7.5
28	D6	47	ALA	7.5
25	D3	137	LYS	7.5
29	D7	38	PRO	7.5
5	S3	178	ARG	7.5
14	C2	91	VAL	7.4
22	d0	20	ILE	7.4
7	s5	154	ALA	7.4
14	c2	112	ALA	7.4
32	E0	2	ALA	7.4
1	2	493	U	7.4
22	D0	93	LEU	7.4
35	SM	83	LYS	7.4
14	c2	36	LEU	7.4
1	6	489	C	7.4
14	C2	106	ILE	7.4
12	c0	65	TYR	7.4
18	c6	143	ARG	7.4
36	1	2205	U	7.3
53	M7	157	VAL	7.3
62	n6	127	GLU	7.3
73	O7	87	SER	7.3
12	c0	66	TYR	7.3
18	c6	142	TYR	7.3
22	D0	104	THR	7.3
14	c2	105	LYS	7.3
11	S9	29	LYS	7.3
36	5	1352	A	7.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	E0	50	VAL	7.3
5	s3	144	ALA	7.3
14	C2	128	ALA	7.3
1	6	668	C	7.3
17	C5	131	ALA	7.3
4	s2	90	THR	7.3
22	D0	97	VAL	7.3
14	c2	60	VAL	7.2
1	2	486	G	7.2
13	C1	150	ASN	7.2
12	C0	19	GLY	7.2
5	s3	83	THR	7.2
7	s5	155	ALA	7.2
53	M7	162	GLU	7.2
4	s2	84	LYS	7.2
13	C1	155	LYS	7.2
1	6	665	U	7.2
17	c5	7	ALA	7.1
22	D0	19	ILE	7.1
30	D8	66	LEU	7.1
22	d0	96	PRO	7.1
17	c5	11	VAL	7.1
58	n2	52	ASN	7.1
5	s3	3	ALA	7.1
33	E1	87	THR	7.1
14	c2	86	VAL	7.1
42	L5	293	LEU	7.1
4	s2	97	ARG	7.1
11	S9	32	GLY	7.1
3	S1	56	SER	7.1
28	D6	85	ARG	7.1
16	C4	29	HIS	7.0
7	S5	151	GLY	7.0
33	e1	77	GLY	7.0
71	O5	2	ALA	7.0
1	6	491	C	7.0
22	D0	99	ILE	7.0
28	d6	97	PRO	7.0
20	C8	2	SER	6.9
28	D6	50	VAL	6.9
5	S3	44	THR	6.9
30	D8	67	ARG	6.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	sM	122	GLU	6.9
30	D8	27	GLN	6.9
66	o0	6	SER	6.9
14	c2	96	GLN	6.9
18	C6	57	LEU	6.9
14	c2	125	ASN	6.9
14	C2	88	LEU	6.9
60	N4	74	LYS	6.9
28	D6	60	PRO	6.8
1	2	494	U	6.8
36	1	1762	C	6.8
32	E0	38	LEU	6.8
10	s8	200	LYS	6.8
1	2	719	U	6.8
1	2	718	U	6.8
14	c2	127	GLY	6.8
66	O0	105	ALA	6.8
4	s2	98	PHE	6.8
1	6	666	U	6.8
14	c2	59	LEU	6.7
36	5	2539	C	6.7
34	sR	118	LYS	6.7
4	s2	86	VAL	6.7
36	1	1955	U	6.7
36	1	1581	C	6.7
1	6	487	G	6.7
35	SM	110	TRP	6.7
28	D6	42	ARG	6.7
35	SM	174	LEU	6.7
40	L3	387	LEU	6.7
32	E0	26	LYS	6.7
32	E0	40	TYR	6.7
22	d0	103	ILE	6.7
1	2	489	C	6.6
3	S1	93	GLY	6.6
3	S1	29	TRP	6.6
82	p0	217	VAL	6.6
28	d6	80	HIS	6.6
12	c0	92	ILE	6.6
22	D0	100	VAL	6.6
28	D6	69	ASN	6.6
1	2	492	A	6.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	d0	21	LYS	6.6
35	sM	85	SER	6.6
32	E0	45	VAL	6.6
36	1	1566	A	6.5
28	D6	63	ALA	6.5
5	S3	43	PRO	6.5
14	c2	113	ARG	6.5
68	O2	128	LEU	6.5
13	C1	151	LYS	6.5
22	D0	121	ASN	6.5
5	s3	215	GLU	6.5
75	o9	51	ILE	6.5
5	S3	70	THR	6.5
7	S5	222	LYS	6.5
14	c2	92	ALA	6.5
7	S5	154	ALA	6.5
53	M7	160	ALA	6.5
5	S3	54	ARG	6.5
14	c2	34	THR	6.5
14	c2	74	LEU	6.5
28	D6	41	ILE	6.5
3	S1	92	GLN	6.4
12	c0	78	GLU	6.4
1	2	658	C	6.4
9	s7	93	LEU	6.4
14	C2	28	LEU	6.4
17	C5	50	THR	6.4
36	1	2402	A	6.4
3	S1	25	THR	6.4
14	c2	75	VAL	6.4
14	c2	121	VAL	6.4
55	M9	187	GLU	6.4
32	E0	60	PRO	6.4
1	2	502	U	6.4
35	sM	120	GLU	6.4
61	N5	22	LYS	6.4
36	1	1951	C	6.4
56	n0	1	MET	6.4
7	S5	161	ASP	6.4
14	C2	50	LYS	6.4
14	C2	68	GLU	6.4
56	N0	1	MET	6.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	S3	142	LEU	6.4
36	1	1565	G	6.4
14	c2	37	VAL	6.4
14	c2	40	GLY	6.4
14	c2	104	GLY	6.4
33	e1	81	LYS	6.4
60	N4	92	GLU	6.3
36	1	1570	U	6.3
36	5	1569	U	6.3
35	sM	82	THR	6.3
35	SM	16	ASP	6.3
30	D8	40	ILE	6.3
24	D2	37	PHE	6.3
5	s3	128	GLU	6.3
14	C2	105	LYS	6.3
60	N4	84	GLY	6.3
80	e0	51	ASN	6.3
5	S3	124	ARG	6.3
16	C4	137	LEU	6.3
5	s3	175	VAL	6.2
22	d0	106	ILE	6.2
14	C2	32	LEU	6.2
12	c0	37	THR	6.2
16	C4	67	VAL	6.2
36	1	1352	A	6.2
3	S1	28	GLU	6.2
25	d3	145	SER	6.2
16	C4	42	VAL	6.2
1	6	661	A	6.2
14	c2	82	PRO	6.2
11	S9	36	LEU	6.2
14	c2	142	GLN	6.2
32	E0	57	ASN	6.2
5	S3	50	ILE	6.2
36	1	1567	U	6.2
1	2	239	C	6.2
76	Q0	77	ILE	6.2
53	M7	159	LYS	6.2
34	sR	186	PHE	6.1
1	6	718	U	6.1
11	S9	113	VAL	6.1
12	C0	87	VAL	6.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	D8	9	LEU	6.1
36	1	2403	G	6.1
2	s0	24	LEU	6.1
12	c0	23	ALA	6.1
14	c2	26	ASP	6.1
22	d0	19	ILE	6.1
27	D5	36	ALA	6.1
1	2	505	A	6.1
1	2	507	U	6.1
7	s5	156	ARG	6.0
12	C0	95	ARG	6.0
55	m9	184	LEU	6.0
36	5	439	C	6.0
29	d7	38	PRO	6.0
53	M7	163	LYS	6.0
36	1	3155	U	6.0
45	l8	254	ASP	6.0
4	s2	82	ASN	6.0
24	D2	129	VAL	6.0
22	d0	93	LEU	6.0
14	c2	80	ASN	6.0
2	S0	166	GLY	6.0
14	c2	57	ALA	6.0
45	l8	252	ASN	6.0
28	D6	48	ALA	6.0
29	D7	41	LEU	6.0
16	C4	39	ILE	5.9
34	sR	167	VAL	5.9
6	s4	261	LEU	5.9
33	E1	145	HIS	5.9
66	o0	105	ALA	5.9
16	C4	94	PRO	5.9
11	S9	47	PHE	5.9
33	e1	78	LYS	5.9
6	S4	123	LEU	5.9
18	C6	3	ALA	5.9
77	Q1	1	MET	5.9
30	D8	25	VAL	5.9
33	e1	89	LYS	5.9
12	c0	77	ARG	5.9
14	c2	130	THR	5.9
39	l2	252	THR	5.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
26	D4	100	VAL	5.9
13	C1	4	GLU	5.9
10	s8	117	TYR	5.8
59	n3	3	GLY	5.8
16	c4	62	LEU	5.8
5	s3	118	ALA	5.8
22	d0	101	LYS	5.8
5	S3	149	ALA	5.8
34	sR	120	SER	5.8
18	C6	20	ALA	5.8
32	E0	58	PRO	5.8
14	c2	62	LEU	5.8
10	S8	21	PHE	5.8
35	SM	19	VAL	5.8
22	D0	105	GLN	5.8
60	N4	81	PRO	5.8
10	S8	200	LYS	5.8
80	e0	59	GLY	5.8
5	s3	152	PHE	5.8
3	S1	91	VAL	5.8
53	M7	184	ALA	5.8
80	e0	48	THR	5.7
34	sR	102	ARG	5.7
3	S1	97	LEU	5.7
62	N6	127	GLU	5.7
12	c0	96	ASN	5.7
80	e0	53	LYS	5.7
60	N4	85	ALA	5.7
82	p0	100	ILE	5.7
14	C2	140	PHE	5.7
5	S3	66	ILE	5.7
14	c2	140	PHE	5.7
72	o6	2	THR	5.7
5	S3	89	GLU	5.7
70	O4	110	GLU	5.7
33	E1	83	LYS	5.7
2	S0	28	ASN	5.7
12	c0	76	LEU	5.7
7	s5	153	GLY	5.7
3	S1	42	ASN	5.7
14	C2	41	LEU	5.7
56	n0	2	ALA	5.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
60	N4	93	ARG	5.7
46	l9	190	ASP	5.7
36	1	2401	A	5.7
16	c4	48	VAL	5.6
11	S9	5	PRO	5.6
36	5	1566	A	5.6
30	d8	9	LEU	5.6
3	S1	232	HIS	5.6
1	2	496	G	5.6
7	s5	36	ALA	5.6
28	D6	98	PRO	5.6
28	d6	45	VAL	5.6
32	E0	44	PHE	5.6
36	5	2503	G	5.6
11	S9	31	ALA	5.6
4	S2	218	ILE	5.6
3	S1	100	PHE	5.6
8	s6	162	VAL	5.6
5	S3	217	ILE	5.6
12	C0	30	ALA	5.6
14	c2	116	VAL	5.6
17	C5	55	GLY	5.6
14	c2	79	ALA	5.6
28	d6	53	LEU	5.6
26	d4	99	LYS	5.6
3	S1	84	ILE	5.5
17	c5	10	ARG	5.5
61	n5	142	ILE	5.5
12	C0	86	ILE	5.5
30	d8	66	LEU	5.5
11	S9	138	LYS	5.5
17	c5	6	ASN	5.5
1	6	719	U	5.5
4	S2	154	LEU	5.5
13	C1	149	ALA	5.5
8	s6	166	GLU	5.5
6	s4	260	GLY	5.5
32	E0	56	MET	5.5
1	6	492	A	5.5
23	D1	10	GLU	5.5
28	D6	35	ALA	5.5
38	8	80	A	5.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	S1	225	VAL	5.5
4	S2	224	PHE	5.5
5	s3	110	LEU	5.5
4	S2	155	ALA	5.5
4	s2	118	ALA	5.5
11	S9	95	TYR	5.5
17	c5	135	THR	5.5
38	8	79	A	5.5
4	S2	145	GLY	5.5
16	c4	58	TYR	5.5
14	c2	84	ASN	5.4
1	2	715	U	5.4
14	c2	33	ARG	5.4
14	c2	76	GLU	5.4
3	S1	43	VAL	5.4
14	C2	67	THR	5.4
7	S5	153	GLY	5.4
36	1	1351	U	5.4
5	S3	41	VAL	5.4
22	d0	108	ILE	5.4
36	5	2403	G	5.4
30	d8	43	ASN	5.4
80	e0	2	ALA	5.4
1	6	678	A	5.4
12	c0	17	GLN	5.4
16	c4	28	VAL	5.4
34	sR	157	VAL	5.4
33	e1	145	HIS	5.4
62	n6	92	GLY	5.4
1	6	1491	U	5.4
5	s3	148	LYS	5.4
5	S3	65	ARG	5.4
7	s5	148	ARG	5.4
31	D9	4	GLU	5.4
18	c6	89	LEU	5.4
30	D8	26	THR	5.4
12	c0	16	PHE	5.4
28	D6	46	GLU	5.4
1	6	1712	A	5.4
5	S3	40	ARG	5.4
5	s3	176	LEU	5.4
16	C4	102	LEU	5.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	S3	90	ARG	5.4
35	SM	128	ALA	5.3
22	D0	103	ILE	5.3
3	S1	59	ASP	5.3
10	S8	195	ARG	5.3
30	d8	5	THR	5.3
11	S9	106	GLU	5.3
1	6	579	A	5.3
7	s5	150	GLY	5.3
28	D6	51	ARG	5.3
36	1	2871	G	5.3
1	2	500	C	5.3
32	E0	29	LYS	5.3
35	sM	123	ALA	5.3
12	c0	22	VAL	5.3
30	D8	57	MET	5.3
72	o6	100	HIS	5.3
35	sM	136	ALA	5.3
36	1	2404	A	5.2
4	s2	64	LYS	5.2
25	D3	114	LYS	5.2
22	D0	96	PRO	5.2
7	S5	150	GLY	5.2
30	d8	24	GLY	5.2
5	s3	109	LEU	5.2
5	S3	143	ARG	5.2
34	sR	165	ASP	5.2
12	C0	90	THR	5.2
35	sM	121	LYS	5.2
36	1	1350	A	5.2
30	D8	28	VAL	5.2
22	D0	107	THR	5.2
5	S3	69	LEU	5.2
5	s3	151	LYS	5.2
36	1	2874	G	5.2
30	D8	8	THR	5.2
33	E1	106	TYR	5.2
1	6	488	G	5.2
3	S1	44	GLY	5.2
35	SM	106	VAL	5.2
32	E0	27	PRO	5.2
16	C4	80	HIS	5.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
22	d0	113	ASP	5.2
73	o7	2	GLY	5.2
35	sM	155	LEU	5.2
5	s3	79	TYR	5.2
12	c0	57	THR	5.2
28	D6	79	ILE	5.2
30	d8	13	ILE	5.2
2	S0	139	VAL	5.2
35	SM	137	GLU	5.2
14	c2	43	ARG	5.2
4	S2	101	VAL	5.1
28	D6	44	ILE	5.1
13	c1	144	ALA	5.1
27	D5	69	LEU	5.1
30	D8	54	LEU	5.1
36	1	1576	G	5.1
22	d0	115	GLU	5.1
14	c2	111	ASN	5.1
5	S3	39	VAL	5.1
5	S3	25	PHE	5.1
14	c2	64	SER	5.1
17	c5	136	SER	5.1
22	d0	16	GLN	5.1
28	d6	49	ALA	5.1
14	C2	137	MET	5.1
16	C4	75	GLY	5.1
36	1	1349	G	5.1
14	c2	35	ALA	5.1
35	SM	96	ARG	5.1
35	SM	98	GLY	5.1
36	5	2401	A	5.1
5	s3	92	GLN	5.1
5	s3	182	LEU	5.1
14	C2	21	GLU	5.1
22	d0	114	VAL	5.1
1	2	487	G	5.1
14	c2	55	GLY	5.1
12	c0	25	LYS	5.1
1	2	713	A	5.1
11	S9	102	GLU	5.1
4	s2	96	THR	5.1
22	D0	110	PRO	5.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
16	C4	27	PHE	5.0
5	s3	41	VAL	5.0
13	c1	147	ALA	5.0
34	SR	284	ALA	5.0
35	SM	140	ASP	5.0
25	D3	72	VAL	5.0
4	S2	164	SER	5.0
49	m3	133	PRO	5.0
35	SM	61	ILE	5.0
9	s7	58	LEU	5.0
11	S9	105	LEU	5.0
48	m1	174	LYS	5.0
16	c4	98	GLY	5.0
36	5	1349	G	5.0
3	S1	41	ARG	5.0
27	d5	89	ILE	5.0
23	D1	69	LEU	5.0
34	sR	183	LEU	5.0
33	E1	116	LYS	5.0
34	sR	136	ILE	5.0
16	C4	95	GLY	5.0
19	c7	88	VAL	5.0
23	D1	51	VAL	5.0
45	L8	116	VAL	5.0
8	S6	12	SER	5.0
2	S0	170	ILE	5.0
12	C0	66	TYR	5.0
4	S2	134	LEU	5.0
9	S7	126	LEU	5.0
7	s5	48	PHE	5.0
35	SM	105	LYS	5.0
60	n4	76	VAL	5.0
1	6	676	G	5.0
22	D0	20	ILE	5.0
4	s2	126	ARG	5.0
5	S3	106	LYS	5.0
14	c2	114	LYS	5.0
11	S9	87	SER	4.9
14	c2	41	LEU	4.9
35	SM	97	THR	4.9
53	M7	158	ALA	4.9
14	C2	33	ARG	4.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	C1	154	ALA	4.9
35	SM	127	ALA	4.9
2	S0	97	PRO	4.9
14	C2	127	GLY	4.9
7	S5	24	VAL	4.9
11	S9	117	GLY	4.9
80	e0	52	GLY	4.9
3	S1	30	PHE	4.9
36	1	2873	U	4.9
12	c0	71	GLU	4.9
22	d0	94	GLU	4.9
1	2	656	G	4.9
3	S1	230	ALA	4.9
5	s3	153	ALA	4.9
13	c1	145	ALA	4.9
27	D5	82	HIS	4.9
45	l8	253	SER	4.9
61	N5	23	ALA	4.9
3	S1	26	ARG	4.9
28	D6	82	ARG	4.9
4	S2	63	VAL	4.9
39	L2	250	GLN	4.9
36	5	1350	A	4.9
1	6	1711	C	4.9
12	c0	67	THR	4.9
28	D6	52	ASP	4.9
33	e1	134	ASN	4.9
25	D3	144	ARG	4.9
30	d8	32	PHE	4.9
82	p0	212	HIS	4.9
18	c6	141	SER	4.9
1	2	794	U	4.9
4	S2	85	PRO	4.9
14	C2	129	GLU	4.8
4	S2	86	VAL	4.8
10	S8	104	ILE	4.8
78	Q2	106	PHE	4.8
16	c4	59	ALA	4.8
30	D8	59	SER	4.8
3	S1	23	PRO	4.8
14	C2	113	ARG	4.8
12	C0	5	LYS	4.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	S3	84	ILE	4.8
38	8	83	C	4.8
28	D6	24	VAL	4.8
14	C2	40	GLY	4.8
11	S9	118	LEU	4.8
28	D6	71	LEU	4.8
58	n2	56	VAL	4.8
9	S7	52	ALA	4.8
5	S3	182	LEU	4.8
7	s5	68	ILE	4.8
30	d8	44	VAL	4.8
66	o0	100	ILE	4.8
14	c2	107	ASP	4.8
67	O1	82	GLU	4.8
36	1	2207	A	4.8
12	c0	44	LYS	4.8
45	l8	211	LEU	4.8
75	O9	46	ARG	4.7
12	c0	91	TYR	4.7
21	c9	17	ALA	4.7
59	N3	2	SER	4.7
4	s2	85	PRO	4.7
36	1	3154	C	4.7
11	S9	45	ILE	4.7
16	c4	67	VAL	4.7
67	o1	82	GLU	4.7
1	2	541	A	4.7
49	m3	131	LYS	4.7
24	D2	70	ASN	4.7
5	s3	143	ARG	4.7
5	S3	176	LEU	4.7
5	s3	73	VAL	4.7
27	d5	86	GLU	4.7
36	5	1016	C	4.7
5	S3	51	ARG	4.7
60	N4	95	SER	4.7
12	c0	43	ILE	4.7
13	c1	30	ARG	4.7
32	E0	35	TYR	4.7
12	C0	40	LEU	4.7
5	S3	147	ALA	4.7
14	C2	26	ASP	4.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	e1	79	LYS	4.7
9	S7	38	LEU	4.7
50	M4	138	ALA	4.7
3	S1	35	PRO	4.7
33	e1	102	VAL	4.7
75	o9	11	GLN	4.7
8	S6	1	MET	4.6
7	S5	54	LYS	4.6
74	O8	5	ILE	4.6
12	c0	70	GLU	4.6
5	s3	186	VAL	4.6
34	sR	72	THR	4.6
3	S1	140	ILE	4.6
5	S3	49	ILE	4.6
14	C2	142	GLN	4.6
53	M7	2	ALA	4.6
35	sM	174	LEU	4.6
5	S3	46	THR	4.6
3	S1	233	GLY	4.6
5	S3	107	PHE	4.6
82	p0	197	PHE	4.6
5	s3	196	ARG	4.6
30	D8	6	PRO	4.6
34	sR	104	VAL	4.6
12	C0	24	LYS	4.6
74	O8	21	LYS	4.6
14	c2	102	GLY	4.6
16	C4	44	GLY	4.6
49	M3	135	ALA	4.6
4	s2	80	VAL	4.6
35	SM	152	GLN	4.6
62	n6	114	ASP	4.6
55	M9	131	ALA	4.6
3	S1	231	LEU	4.6
4	S2	169	LEU	4.6
14	C2	22	VAL	4.6
14	C2	61	VAL	4.6
62	n6	118	LEU	4.6
66	o0	104	LEU	4.6
4	s2	83	ILE	4.5
28	d6	44	ILE	4.5
25	D3	102	VAL	4.5

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	S4	259	GLN	4.5
16	C4	71	CYS	4.5
25	D3	107	PHE	4.5
10	S8	199	LYS	4.5
32	E0	25	GLU	4.5
74	O8	69	LEU	4.5
14	C2	86	VAL	4.5
28	D6	86	VAL	4.5
30	D8	30	VAL	4.5
14	c2	110	GLY	4.5
28	D6	73	TYR	4.5
12	C0	67	THR	4.5
16	c4	61	MET	4.5
35	SM	162	GLN	4.5
39	L2	253	GLN	4.5
33	e1	111	GLU	4.5
63	n7	2	ALA	4.5
5	s3	136	VAL	4.5
14	c2	61	VAL	4.5
32	E0	4	VAL	4.5
12	C0	12	HIS	4.5
3	S1	98	THR	4.5
5	s3	113	LEU	4.5
5	S3	58	VAL	4.5
11	S9	85	VAL	4.5
4	S2	93	GLY	4.5
45	l8	106	LYS	4.5
11	S9	86	LEU	4.5
16	C4	93	THR	4.5
28	D6	49	ALA	4.5
55	m9	183	ALA	4.5
75	o9	16	ALA	4.5
3	S1	114	VAL	4.5
16	C4	13	VAL	4.5
34	sR	107	LYS	4.5
24	D2	130	TYR	4.5
1	6	484	C	4.5
5	S3	52	ALA	4.5
12	C0	13	GLN	4.5
28	D6	40	ALA	4.5
35	SM	135	ALA	4.5
28	D6	80	HIS	4.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	S3	71	LEU	4.5
12	C0	76	LEU	4.5
17	c5	50	THR	4.5
68	o2	2	ALA	4.5
1	6	234	G	4.4
12	c0	36	ASP	4.4
36	5	2538	U	4.4
38	4	81	U	4.4
27	D5	38	HIS	4.4
22	d0	15	GLN	4.4
36	5	2402	A	4.4
7	s5	157	ARG	4.4
9	S7	32	PRO	4.4
28	D6	8	ASN	4.4
35	SM	108	GLN	4.4
75	o9	9	ILE	4.4
2	s0	41	ARG	4.4
33	E1	129	GLY	4.4
59	N3	3	GLY	4.4
49	m3	132	ALA	4.4
79	q3	2	ALA	4.4
5	s3	65	ARG	4.4
11	S9	89	ASP	4.4
6	S4	159	THR	4.4
80	e0	3	LYS	4.4
58	N2	9	GLN	4.4
25	D3	45	GLY	4.4
29	D7	39	GLY	4.4
7	s5	43	PHE	4.4
5	s3	69	LEU	4.4
5	s3	82	GLY	4.4
53	M7	164	LYS	4.4
59	N3	4	ASN	4.4
36	1	1579	C	4.4
5	S3	85	VAL	4.4
13	c1	117	VAL	4.4
14	C2	63	VAL	4.4
14	c2	122	VAL	4.4
23	d1	42	GLU	4.4
28	D6	45	VAL	4.4
14	C2	52	LEU	4.4
41	l4	67	THR	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	S5	137	ILE	4.4
55	M9	186	LYS	4.4
5	s3	87	TYR	4.4
5	S3	47	GLU	4.4
2	S0	113	ARG	4.4
5	S3	177	MET	4.4
28	D6	92	ARG	4.4
30	D8	48	VAL	4.4
35	SM	163	PHE	4.4
60	N4	70	LYS	4.4
5	S3	95	GLY	4.4
14	c2	39	ASP	4.4
30	d8	59	SER	4.4
35	SM	90	ALA	4.4
71	O5	13	SER	4.4
1	6	194	U	4.4
14	c2	38	HIS	4.4
36	1	252	U	4.4
14	C2	89	ILE	4.3
11	S9	141	VAL	4.3
5	S3	119	ALA	4.3
7	S5	25	LEU	4.3
9	s7	32	PRO	4.3
28	d6	81	ALA	4.3
34	sR	279	ALA	4.3
67	O1	79	ARG	4.3
62	n6	120	GLN	4.3
8	S6	148	SER	4.3
32	E0	39	LEU	4.3
9	S7	145	GLY	4.3
62	n6	113	LYS	4.3
5	S3	111	ASN	4.3
4	S2	144	TRP	4.3
19	c7	62	GLN	4.3
34	SR	52	GLN	4.3
5	S3	38	GLU	4.3
5	S3	86	LEU	4.3
5	s3	85	VAL	4.3
14	C2	73	LYS	4.3
30	d8	29	ARG	4.3
12	c0	9	ASN	4.3
24	D2	85	ASP	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	S6	33	GLY	4.3
25	D3	27	ASN	4.3
40	l3	140	ASP	4.3
60	n4	64	THR	4.3
66	O0	104	LEU	4.3
11	S9	178	ALA	4.3
30	D8	63	ALA	4.3
16	c4	83	ILE	4.3
5	S3	74	GLN	4.3
4	s2	121	VAL	4.3
72	O6	97	SER	4.3
35	sM	75	ASP	4.3
34	SR	115	ILE	4.3
70	O4	113	LYS	4.3
16	C4	99	GLN	4.3
27	D5	58	ARG	4.3
4	S2	190	LEU	4.2
11	S9	28	LEU	4.2
30	D8	35	ASP	4.2
44	L7	23	ALA	4.2
5	S3	64	ARG	4.2
7	S5	58	LEU	4.2
25	D3	34	LEU	4.2
35	SM	103	LYS	4.2
30	d8	63	ALA	4.2
73	O7	84	SER	4.2
72	O6	56	ARG	4.2
5	s3	112	GLY	4.2
35	SM	134	ASP	4.2
7	S5	209	TYR	4.2
24	D2	102	VAL	4.2
28	d6	89	ARG	4.2
30	d8	61	ARG	4.2
8	S6	18	ILE	4.2
35	SM	170	LYS	4.2
3	s1	89	ASP	4.2
28	D6	55	GLU	4.2
58	N2	89	LEU	4.2
17	C5	10	ARG	4.2
72	O6	98	ARG	4.2
5	S3	56	GLN	4.2
26	d4	134	ALA	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	e1	83	LYS	4.2
61	n5	23	ALA	4.2
82	p0	211	SER	4.2
35	sM	167	PRO	4.2
10	s8	118	GLY	4.2
36	5	1581	C	4.2
12	C0	20	VAL	4.2
14	c2	135	MET	4.2
58	n2	34	ALA	4.2
2	S0	44	GLY	4.2
14	c2	109	GLU	4.2
16	C4	103	ARG	4.2
32	E0	43	ARG	4.2
13	C1	118	GLN	4.2
25	D3	96	VAL	4.2
66	o0	42	ILE	4.2
45	l8	91	PHE	4.2
12	C0	80	LEU	4.2
12	c0	46	LEU	4.2
14	C2	58	LEU	4.2
62	n6	126	LEU	4.2
1	2	503	G	4.2
1	6	667	U	4.2
11	S9	90	LYS	4.2
35	SM	121	LYS	4.2
36	5	244	G	4.2
19	C7	69	ILE	4.2
28	D6	83	ILE	4.2
34	SR	310	ILE	4.2
24	D2	73	GLY	4.2
4	S2	141	ARG	4.2
55	M9	178	ALA	4.2
11	S9	60	LEU	4.2
11	S9	111	THR	4.2
62	n6	104	LEU	4.2
4	s2	99	LYS	4.1
7	S5	155	ALA	4.1
74	o8	37	PRO	4.1
2	S0	110	TYR	4.1
12	c0	24	LYS	4.1
23	D1	75	ASN	4.1
34	SR	261	LYS	4.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
72	O6	99	ARG	4.1
11	s9	184	SER	4.1
3	s1	218	LEU	4.1
3	S1	52	THR	4.1
36	5	1356	U	4.1
5	S3	75	LYS	4.1
71	o5	83	LYS	4.1
4	S2	35	TRP	4.1
3	s1	232	HIS	4.1
13	C1	144	ALA	4.1
55	m9	187	GLU	4.1
6	S4	134	LYS	4.1
9	s7	108	GLN	4.1
17	C5	52	LYS	4.1
16	C4	81	VAL	4.1
30	d8	25	VAL	4.1
82	p0	87	VAL	4.1
2	S0	40	ALA	4.1
8	s6	217	SER	4.1
22	D0	101	LYS	4.1
35	SM	165	LYS	4.1
7	S5	86	GLN	4.1
3	s1	150	VAL	4.1
36	5	1573	G	4.1
3	S1	110	LEU	4.1
3	s1	184	LEU	4.1
5	s3	45	LYS	4.1
6	S4	261	LEU	4.1
22	d0	48	HIS	4.1
33	E1	124	PRO	4.1
60	N4	64	THR	4.1
18	c6	140	LYS	4.1
12	C0	68	LEU	4.1
30	D8	38	ARG	4.1
34	sR	214	ALA	4.1
7	s5	23	VAL	4.1
5	S3	59	LEU	4.1
5	S3	79	TYR	4.1
36	5	1103	A	4.1
16	C4	22	SER	4.1
16	c4	97	GLY	4.1
4	s2	101	VAL	4.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	S3	48	VAL	4.1
33	E1	84	VAL	4.1
5	s3	25	PHE	4.1
25	D3	57	LEU	4.1
35	SM	164	ASN	4.1
4	S2	84	LYS	4.1
26	D4	2	SER	4.1
71	o5	115	LYS	4.1
10	S8	198	ALA	4.1
11	S9	67	PRO	4.1
26	D4	132	ARG	4.0
30	D8	42	ARG	4.0
35	SM	53	ARG	4.0
7	S5	149	VAL	4.0
36	1	1573	G	4.0
24	D2	41	MET	4.0
11	S9	13	SER	4.0
61	N5	47	ALA	4.0
4	s2	94	GLN	4.0
12	c0	10	LYS	4.0
44	l7	26	VAL	4.0
5	s3	135	GLU	4.0
39	l2	249	SER	4.0
1	2	135	A	4.0
7	S5	20	PHE	4.0
24	D2	128	PHE	4.0
12	C0	41	TYR	4.0
15	C3	40	TYR	4.0
5	S3	27	ARG	4.0
11	S9	53	ARG	4.0
11	S9	185	GLY	4.0
30	D8	45	LYS	4.0
1	6	496	G	4.0
11	S9	49	LEU	4.0
24	D2	27	ILE	4.0
25	D3	33	LEU	4.0
26	D4	125	LEU	4.0
9	s7	48	GLU	4.0
17	C5	76	VAL	4.0
6	S4	168	LYS	4.0
33	e1	113	LYS	4.0
74	O8	29	LYS	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	S5	179	ALA	4.0
8	S6	224	ALA	4.0
12	C0	89	ALA	4.0
14	c2	143	GLN	4.0
20	C8	17	LEU	4.0
36	1	1763	U	4.0
78	q2	106	PHE	4.0
2	S0	124	THR	4.0
28	D6	2	PRO	4.0
2	S0	102	PHE	4.0
25	D3	127	VAL	4.0
80	e0	54	ARG	4.0
34	sR	177	MET	4.0
71	O5	3	GLY	4.0
36	5	1580	A	4.0
5	S3	29	LEU	4.0
2	S0	107	PHE	4.0
6	S4	114	ILE	4.0
7	s5	149	VAL	4.0
13	C1	117	VAL	4.0
22	D0	51	VAL	4.0
14	c2	44	GLY	4.0
3	s1	234	GLU	4.0
14	c2	141	SER	4.0
17	C5	14	THR	4.0
71	O5	11	THR	4.0
5	s3	4	LEU	4.0
5	s3	178	ARG	4.0
16	C4	110	LEU	4.0
8	S6	162	VAL	3.9
9	s7	51	VAL	3.9
8	S6	214	LYS	3.9
10	s8	199	LYS	3.9
45	l8	92	LYS	3.9
5	s3	46	THR	3.9
6	s4	256	ARG	3.9
19	C7	71	PHE	3.9
47	M0	217	PHE	3.9
14	c2	31	VAL	3.9
36	1	2206	G	3.9
13	C1	78	THR	3.9
17	C5	51	SER	3.9

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	C2	36	LEU	3.9
6	S4	236	ILE	3.9
8	s6	167	LYS	3.9
36	5	1351	U	3.9
36	1	1240	A	3.9
4	s2	92	ALA	3.9
66	o0	14	LEU	3.9
28	D6	93	LYS	3.9
29	D7	75	GLU	3.9
30	D8	29	ARG	3.9
1	2	793	A	3.9
3	s1	217	LEU	3.9
16	C4	92	LYS	3.9
58	N2	10	LYS	3.9
62	n6	35	LEU	3.9
71	o5	119	LYS	3.9
3	s1	100	PHE	3.9
34	sR	180	ALA	3.9
71	o5	11	THR	3.9
18	C6	141	SER	3.9
33	e1	110	ALA	3.9
35	sM	169	ALA	3.9
57	N1	121	ALA	3.9
5	s3	5	ILE	3.9
11	S9	3	ARG	3.9
15	c3	150	VAL	3.9
22	d0	44	ASN	3.9
35	sM	156	ASN	3.9
36	1	1239	C	3.9
2	S0	155	PHE	3.9
34	sR	313	TRP	3.9
14	C2	136	ILE	3.9
17	C5	54	ALA	3.9
31	d9	38	ILE	3.9
66	O0	100	ILE	3.9
22	D0	92	ASP	3.9
60	N4	65	GLU	3.9
34	sR	210	LEU	3.9
5	s3	84	ILE	3.9
6	S4	162	ILE	3.9
34	sR	244	ALA	3.9
35	SM	52	PRO	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	C0	73	VAL	3.9
5	S3	62	ASN	3.8
11	S9	30	LEU	3.8
16	c4	47	LYS	3.8
17	C5	49	MET	3.8
24	D2	101	TYR	3.8
16	C4	17	ALA	3.8
28	D6	23	CYS	3.8
12	c0	21	VAL	3.8
52	m6	184	THR	3.8
17	c5	13	LYS	3.8
20	C8	3	LEU	3.8
34	sR	141	LEU	3.8
11	S9	104	PHE	3.8
35	sM	158	GLN	3.8
24	D2	65	LEU	3.8
24	D2	69	LEU	3.8
1	2	497	G	3.8
16	C4	113	GLY	3.8
27	d5	87	GLY	3.8
75	o9	37	TYR	3.8
1	2	754	A	3.8
1	6	673	A	3.8
13	C1	9	SER	3.8
19	c7	69	ILE	3.8
8	s6	173	PRO	3.8
34	sR	134	TRP	3.8
71	o5	5	LYS	3.8
5	s3	142	LEU	3.8
12	c0	14	TYR	3.8
18	C6	92	TYR	3.8
64	n8	85	ASP	3.8
80	e0	9	ALA	3.8
5	S3	181	VAL	3.8
24	D2	74	VAL	3.8
68	o2	126	LEU	3.8
30	d8	26	THR	3.8
36	5	1567	U	3.8
16	c4	27	PHE	3.8
39	l2	119	LYS	3.8
5	S3	18	TYR	3.8
5	s3	149	ALA	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
47	M0	2	ALA	3.8
7	S5	160	VAL	3.8
17	c5	27	GLU	3.8
25	D3	132	LEU	3.8
1	2	232	U	3.8
1	6	1710	U	3.8
22	D0	111	GLY	3.8
23	d1	75	ASN	3.8
39	L2	252	THR	3.8
4	S2	143	TYR	3.8
30	d8	65	ARG	3.8
33	e1	106	TYR	3.8
7	S5	55	ASP	3.8
9	S7	7	LYS	3.8
28	D6	84	VAL	3.8
49	M3	131	LYS	3.8
70	O4	21	LYS	3.8
1	2	558	U	3.8
1	2	1151	A	3.8
4	S2	90	THR	3.8
5	s3	111	ASN	3.8
2	s0	110	TYR	3.8
39	L2	225	ILE	3.8
5	S3	3	ALA	3.8
3	S1	142	PHE	3.8
16	C4	114	ARG	3.8
23	D1	22	ARG	3.8
55	M9	181	ARG	3.8
16	C4	31	THR	3.8
16	C4	25	ASP	3.7
38	4	79	A	3.7
1	2	730	G	3.7
4	S2	45	VAL	3.7
4	S2	184	VAL	3.7
34	sR	252	LEU	3.7
71	o5	21	LEU	3.7
16	C4	90	ARG	3.7
11	S9	38	ASN	3.7
16	C4	24	ASN	3.7
82	p0	218	SER	3.7
4	S2	249	ALA	3.7
5	s3	71	LEU	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	s7	16	LEU	3.7
16	C4	97	GLY	3.7
30	D8	55	VAL	3.7
30	d8	67	ARG	3.7
35	SM	21	PRO	3.7
79	Q3	71	VAL	3.7
1	6	239	C	3.7
10	s8	67	TRP	3.7
8	S6	78	THR	3.7
12	c0	90	THR	3.7
18	c6	114	ARG	3.7
14	c2	88	LEU	3.7
9	S7	33	GLU	3.7
1	2	194	U	3.7
1	6	794	U	3.7
38	4	82	U	3.7
14	c2	71	ILE	3.7
58	n2	11	ILE	3.7
3	S1	207	LEU	3.7
32	E0	20	LYS	3.7
34	sR	55	GLY	3.7
45	L8	152	LEU	3.7
16	c4	112	ILE	3.7
3	s1	53	GLY	3.7
16	c4	102	LEU	3.7
34	sR	172	ALA	3.7
71	o5	82	ALA	3.7
42	L5	185	PHE	3.7
1	6	721	U	3.7
5	S3	200	LYS	3.7
30	d8	64	ARG	3.7
72	o6	68	ARG	3.7
2	S0	98	ILE	3.7
5	S3	184	ILE	3.7
10	s8	183	ILE	3.7
11	S9	52	ILE	3.7
18	C6	29	ILE	3.7
4	s2	93	GLY	3.7
14	C2	59	LEU	3.7
6	S4	166	SER	3.7
58	n2	55	THR	3.7
74	O8	13	GLU	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
11	s9	148	VAL	3.7
63	n7	11	ALA	3.7
1	2	716	C	3.7
7	S5	41	LYS	3.7
14	c2	108	ARG	3.7
11	S9	103	ASP	3.7
36	5	1572	U	3.7
45	L8	254	ASP	3.7
49	m3	93	ILE	3.7
5	s3	47	GLU	3.7
7	s5	35	GLN	3.7
16	C4	37	GLU	3.7
58	n2	33	TYR	3.7
1	2	485	A	3.7
4	S2	57	PHE	3.7
4	S2	78	ASP	3.7
27	D5	48	ASP	3.7
3	S1	135	LEU	3.7
10	S8	193	LEU	3.7
12	C0	91	TYR	3.7
12	c0	63	TYR	3.7
20	C8	22	VAL	3.6
34	sR	253	ALA	3.6
27	d5	88	ILE	3.6
31	d9	5	ASN	3.6
39	l2	253	GLN	3.6
55	m9	151	ARG	3.6
4	S2	162	CYS	3.6
44	l7	23	ALA	3.6
2	s0	186	GLY	3.6
36	1	2872	A	3.6
77	q1	6	ARG	3.6
27	d5	101	TYR	3.6
82	p0	221	ALA	3.6
3	s1	152	ARG	3.6
9	s7	104	ARG	3.6
25	D3	133	LEU	3.6
30	D8	64	ARG	3.6
12	C0	79	TYR	3.6
16	C4	23	PHE	3.6
17	C5	12	PHE	3.6
61	n5	46	TYR	3.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
60	N4	72	SER	3.6
11	S9	18	PRO	3.6
28	d6	96	ALA	3.6
3	S1	102	GLY	3.6
4	s2	87	GLN	3.6
24	D2	100	GLY	3.6
61	n5	119	THR	3.6
71	O5	46	THR	3.6
28	D6	5	ARG	3.6
34	sR	116	ASP	3.6
6	s4	218	PHE	3.6
71	o5	7	TYR	3.6
10	S8	167	ALA	3.6
71	o5	39	PRO	3.6
8	S6	196	ARG	3.6
47	m0	112	GLN	3.6
12	C0	46	LEU	3.6
34	sR	292	LEU	3.6
45	l8	36	ILE	3.6
14	c2	129	GLU	3.6
45	l8	122	LYS	3.6
16	c4	46	MET	3.6
17	c5	12	PHE	3.6
24	D2	46	TYR	3.6
10	s8	195	ARG	3.6
10	s8	198	ALA	3.6
47	m0	2	ALA	3.6
29	d7	57	GLU	3.6
41	L4	2	SER	3.6
16	c4	50	ALA	3.6
3	s1	54	LEU	3.6
4	s2	208	GLU	3.6
14	c2	52	LEU	3.6
39	l2	19	HIS	3.6
7	s5	224	ASN	3.6
36	5	3275	U	3.6
38	4	158	U	3.6
36	1	1562	C	3.6
5	S3	141	LYS	3.6
16	c4	87	GLY	3.6
34	sR	315	VAL	3.6
49	M3	160	GLN	3.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	s1	96	LEU	3.6
24	D2	117	ARG	3.5
28	D6	25	ASN	3.5
26	D4	129	VAL	3.5
31	d9	23	VAL	3.5
80	e0	47	VAL	3.5
34	SR	254	ALA	3.5
39	L2	235	ALA	3.5
17	C5	13	LYS	3.5
70	O4	109	THR	3.5
74	o8	29	LYS	3.5
14	c2	119	SER	3.5
45	L8	121	SER	3.5
9	s7	12	ALA	3.5
14	C2	27	ALA	3.5
39	L2	71	LEU	3.5
5	S3	208	ILE	3.5
12	c0	11	ILE	3.5
27	D5	89	ILE	3.5
58	N2	11	ILE	3.5
73	o7	12	HIS	3.5
5	S3	213	GLU	3.5
47	m0	102	MET	3.5
5	s3	125	TYR	3.5
7	S5	23	VAL	3.5
48	M1	167	TYR	3.5
16	c4	52	ARG	3.5
24	D2	68	ARG	3.5
34	sR	32	LEU	3.5
28	D6	56	ALA	3.5
28	D6	78	ALA	3.5
70	O4	16	ARG	3.5
75	O9	45	ARG	3.5
68	o2	9	ILE	3.5
34	sR	125	GLY	3.5
41	l4	65	TRP	3.5
49	m3	152	THR	3.5
58	n2	98	THR	3.5
59	n3	4	ASN	3.5
5	s3	51	ARG	3.5
18	C6	142	TYR	3.5
22	D0	120	SER	3.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	D8	41	VAL	3.5
28	D6	20	PRO	3.5
45	l8	237	ILE	3.5
73	O7	86	ALA	3.5
27	D5	37	GLN	3.5
60	N4	79	GLN	3.5
12	c0	19	GLY	3.5
22	D0	54	GLY	3.5
1	6	1059	U	3.5
3	S1	113	MET	3.5
1	6	677	G	3.5
2	s0	185	ARG	3.5
34	sR	25	THR	3.5
3	S1	120	LEU	3.5
11	s9	83	VAL	3.5
24	D2	14	ILE	3.5
34	SR	78	ALA	3.5
49	M3	124	ILE	3.5
6	S4	112	HIS	3.5
50	m4	8	LYS	3.5
62	n6	116	LYS	3.5
15	c3	149	LEU	3.5
11	S9	12	TYR	3.5
35	SM	172	VAL	3.5
22	D0	109	GLU	3.5
1	2	729	G	3.5
25	D3	77	ILE	3.5
5	S3	36	GLY	3.5
25	D3	92	CYS	3.5
28	d6	42	ARG	3.5
41	l4	69	ARG	3.5
36	5	2505	U	3.5
3	S1	90	GLU	3.5
18	c6	90	VAL	3.5
58	n2	14	THR	3.5
71	o5	8	GLU	3.5
11	S9	19	TYR	3.5
25	d3	40	SER	3.5
28	d6	76	SER	3.5
7	S5	210	ALA	3.5
1	2	484	C	3.5
14	C2	55	GLY	3.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
30	D8	32	PHE	3.5
80	e0	55	ARG	3.5
36	1	2522	G	3.5
22	d0	13	GLU	3.4
24	d2	26	LEU	3.4
75	o9	23	LEU	3.4
71	O5	7	TYR	3.4
3	s1	233	GLY	3.4
30	D8	17	GLY	3.4
36	5	2542	U	3.4
2	S0	144	ILE	3.4
3	S1	130	SER	3.4
12	C0	17	GLN	3.4
14	C2	43	ARG	3.4
14	C2	64	SER	3.4
33	E1	115	THR	3.4
73	O7	71	SER	3.4
5	S3	183	GLY	3.4
13	C1	13	PHE	3.4
68	O2	127	ALA	3.4
22	D0	21	LYS	3.4
14	c2	58	LEU	3.4
26	D4	17	LEU	3.4
1	6	232	U	3.4
12	C0	42	VAL	3.4
28	D6	89	ARG	3.4
28	d6	84	VAL	3.4
75	O9	36	ARG	3.4
50	m4	2	SER	3.4
11	S9	100	LYS	3.4
35	SM	141	ALA	3.4
1	6	754	A	3.4
11	S9	171	ARG	3.4
71	O5	48	ARG	3.4
36	1	3156	U	3.4
5	S3	137	VAL	3.4
8	S6	114	VAL	3.4
19	C7	74	GLN	3.4
73	O7	70	VAL	3.4
12	c0	54	TYR	3.4
24	D2	110	ILE	3.4
35	SM	95	SER	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
82	p0	220	ILE	3.4
74	o8	11	PHE	3.4
3	S1	163	ALA	3.4
20	C8	146	ALA	3.4
29	d7	80	ARG	3.4
34	SR	23	LEU	3.4
18	C6	62	ASN	3.4
36	5	1353	U	3.4
55	m9	186	LYS	3.4
12	C0	75	TYR	3.4
19	C7	70	SER	3.4
62	n6	43	TYR	3.4
36	5	1574	C	3.4
75	o9	2	ALA	3.4
62	n6	52	ARG	3.4
33	e1	100	LEU	3.4
35	SM	99	LYS	3.4
10	s8	61	GLU	3.4
14	C2	81	ASP	3.4
61	n5	58	ASP	3.4
36	1	2445	A	3.4
45	l8	234	GLY	3.4
7	S5	225	ARG	3.4
26	D4	127	LYS	3.4
29	d7	33	LEU	3.4
20	C8	5	VAL	3.4
22	d0	22	ILE	3.4
24	D2	103	ILE	3.4
33	e1	114	VAL	3.4
29	D7	37	CYS	3.4
13	c1	116	ARG	3.4
73	o7	36	SER	3.4
1	6	669	G	3.4
12	c0	45	ALA	3.4
3	S1	73	LEU	3.4
61	n5	40	LEU	3.4
14	c2	99	GLU	3.4
17	C5	104	GLN	3.4
45	l8	107	GLU	3.4
6	S4	124	GLY	3.4
15	C3	138	ASN	3.4
34	SR	308	ASN	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	s2	139	ILE	3.4
22	D0	106	ILE	3.4
55	M9	177	VAL	3.4
57	n1	124	VAL	3.4
2	S0	24	LEU	3.3
35	SM	120	GLU	3.3
38	4	80	A	3.3
47	m0	195	ALA	3.3
80	e0	5	HIS	3.3
13	C1	6	THR	3.3
33	e1	112	GLY	3.3
32	E0	47	VAL	3.3
3	S1	24	PHE	3.3
7	S5	43	PHE	3.3
72	o6	58	ILE	3.3
16	C4	20	TYR	3.3
2	S0	146	LEU	3.3
13	C1	5	LEU	3.3
3	s1	52	THR	3.3
5	S3	42	THR	3.3
8	s6	168	THR	3.3
36	1	2397	A	3.3
2	S0	160	ILE	3.3
16	C4	76	ILE	3.3
25	D3	86	PHE	3.3
4	S2	231	ALA	3.3
7	S5	66	GLN	3.3
17	c5	9	LYS	3.3
18	C6	5	PRO	3.3
45	L8	232	HIS	3.3
47	M0	221	ALA	3.3
60	N4	71	ARG	3.3
62	n6	115	ARG	3.3
14	c2	93	ASP	3.3
1	6	679	U	3.3
4	s2	38	VAL	3.3
6	S4	129	VAL	3.3
8	s6	218	GLU	3.3
31	d9	31	ILE	3.3
34	sR	94	VAL	3.3
25	D3	145	SER	3.3
45	L8	245	LYS	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	S5	158	GLN	3.3
10	s8	165	LEU	3.3
11	S9	80	LEU	3.3
45	l8	121	SER	3.3
73	O7	46	SER	3.3
13	C1	30	ARG	3.3
16	C4	101	ALA	3.3
19	C7	86	PRO	3.3
28	D6	95	ARG	3.3
4	s2	78	ASP	3.3
16	C4	38	THR	3.3
12	C0	3	MET	3.3
14	c2	137	MET	3.3
9	s7	109	VAL	3.3
14	C2	37	VAL	3.3
31	D9	23	VAL	3.3
74	O8	43	PHE	3.3
4	S2	140	ARG	3.3
11	S9	97	LEU	3.3
74	o8	31	LEU	3.3
14	C2	94	ALA	3.3
40	L3	94	GLU	3.3
1	2	559	C	3.3
61	N5	142	ILE	3.3
62	n6	45	ILE	3.3
1	6	229	U	3.3
7	s5	42	LEU	3.3
8	S6	77	LEU	3.3
18	C6	66	ARG	3.3
21	c9	28	LEU	3.3
25	d3	63	GLN	3.3
2	S0	126	PRO	3.3
4	S2	222	TYR	3.3
5	s3	35	SER	3.3
6	s4	124	GLY	3.3
73	o7	86	ALA	3.3
5	s3	208	ILE	3.3
26	D4	133	ASN	3.3
34	sR	123	ILE	3.3
3	S1	48	VAL	3.3
55	M9	5	ARG	3.3
1	2	557	G	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	s1	73	LEU	3.3
7	S5	198	LEU	3.3
8	S6	124	LEU	3.3
61	N5	24	LEU	3.3
3	S1	33	LYS	3.3
5	S3	120	TYR	3.3
5	s3	120	TYR	3.3
8	s6	164	LYS	3.3
23	D1	57	GLY	3.3
73	o7	57	HIS	3.3
39	L2	158	ILE	3.3
1	6	501	U	3.3
3	s1	110	LEU	3.3
25	D3	139	LYS	3.3
74	o8	74	LYS	3.3
8	S6	165	GLY	3.3
13	C1	38	ALA	3.2
35	SM	15	ALA	3.2
39	l2	48	ILE	3.2
63	n7	4	PHE	3.2
71	o5	68	GLN	3.2
5	S3	83	THR	3.2
22	D0	67	THR	3.2
31	D9	5	ASN	3.2
71	O5	43	LYS	3.2
5	S3	68	GLU	3.2
11	S9	27	GLU	3.2
62	n6	111	LEU	3.2
5	S3	139	SER	3.2
19	C7	125	SER	3.2
24	d2	55	ASP	3.2
61	N5	116	PRO	3.2
14	C2	57	ALA	3.2
53	m7	126	ARG	3.2
55	M9	183	ALA	3.2
70	O4	32	ALA	3.2
25	d3	39	LYS	3.2
34	sR	61	PHE	3.2
71	o5	25	LYS	3.2
73	o7	54	LYS	3.2
2	S0	120	LEU	3.2
7	S5	162	VAL	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	S8	196	LEU	3.2
1	2	579	A	3.2
15	C3	61	THR	3.2
34	sR	135	THR	3.2
35	SM	82	THR	3.2
1	6	240	U	3.2
36	1	1764	U	3.2
45	l8	182	GLY	3.2
8	S6	217	SER	3.2
20	C8	13	HIS	3.2
12	c0	84	GLU	3.2
27	d5	37	GLN	3.2
3	S1	184	LEU	3.2
7	s5	165	LEU	3.2
75	o9	49	MET	3.2
13	c1	21	ASN	3.2
1	2	504	U	3.2
36	5	249	U	3.2
5	s3	124	ARG	3.2
23	D1	18	SER	3.2
3	S1	104	ASP	3.2
8	S6	73	ILE	3.2
9	s7	49	ILE	3.2
3	S1	228	LEU	3.2
5	s3	86	LEU	3.2
11	s9	93	LEU	3.2
30	D8	61	ARG	3.2
55	M9	104	ARG	3.2
75	o9	12	LYS	3.2
77	Q1	15	ARG	3.2
1	2	501	U	3.2
5	S3	197	THR	3.2
34	sR	205	SER	3.2
33	E1	148	TYR	3.2
61	n5	60	TYR	3.2
3	s1	24	PHE	3.2
18	c6	29	ILE	3.2
27	d5	71	ILE	3.2
8	s6	216	LEU	3.2
5	S3	116	ARG	3.2
55	M9	170	ARG	3.2
34	sR	51	ASP	3.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	S8	65	PHE	3.2
14	C2	100	TRP	3.2
1	6	1371	A	3.2
5	S3	109	LEU	3.2
5	s3	49	ILE	3.2
14	C2	24	ILE	3.2
4	S2	75	GLY	3.2
4	S2	123	GLY	3.2
14	c2	32	LEU	3.2
30	D8	56	LEU	3.2
36	1	1580	A	3.2
36	1	2208	A	3.2
39	l2	238	ILE	3.2
55	M9	185	LEU	3.2
60	N4	94	ARG	3.2
78	Q2	104	LEU	3.2
5	S3	122	VAL	3.2
33	E1	130	VAL	3.2
22	d0	36	ASN	3.2
28	d6	69	ASN	3.2
5	S3	53	THR	3.2
27	D5	56	THR	3.2
34	sR	168	THR	3.2
35	SM	102	THR	3.2
35	sM	162	GLN	3.2
3	S1	128	LYS	3.2
6	S4	175	PHE	3.2
34	sR	79	TYR	3.2
47	m0	217	PHE	3.2
18	c6	44	LEU	3.2
27	D5	83	LEU	3.2
34	SR	122	ILE	3.2
61	N5	124	VAL	3.2
5	S3	28	GLU	3.2
11	s9	186	GLU	3.2
12	C0	28	ASN	3.2
36	5	2404	A	3.2
3	s1	33	LYS	3.2
34	sR	53	LYS	3.2
35	SM	124	GLN	3.2
36	1	2418	G	3.2
7	s5	161	ASP	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
21	C9	5	SER	3.2
33	E1	104	SER	3.2
71	O5	40	SER	3.2
5	S3	24	PHE	3.2
5	S3	173	ARG	3.2
77	Q1	17	ARG	3.2
5	S3	110	LEU	3.2
6	S4	207	LEU	3.2
20	C8	66	LEU	3.2
27	D5	65	LEU	3.2
55	M9	142	ILE	3.2
59	N3	69	LEU	3.2
77	Q1	5	TRP	3.2
58	n2	54	VAL	3.1
22	d0	30	LYS	3.1
26	D4	128	LYS	3.1
35	sM	170	LYS	3.1
4	S2	250	GLN	3.1
11	S9	123	HIS	3.1
15	c3	106	ARG	3.1
35	SM	14	ASP	3.1
55	m9	181	ARG	3.1
13	C1	153	PHE	3.1
13	c1	60	PHE	3.1
80	e0	58	PRO	3.1
5	S3	61	GLU	3.1
10	S8	79	ALA	3.1
11	s9	4	ALA	3.1
13	C1	91	LEU	3.1
14	c2	78	LEU	3.1
16	C4	83	ILE	3.1
35	SM	169	ALA	3.1
13	C1	111	VAL	3.1
24	D2	6	VAL	3.1
7	s5	145	ASP	3.1
5	s3	61	GLU	3.1
34	sR	48	THR	3.1
36	5	1025	A	3.1
2	s0	40	ALA	3.1
5	s3	114	ALA	3.1
40	L3	102	LEU	3.1
74	o8	69	LEU	3.1

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
59	n3	66	LYS	3.1
4	s2	104	VAL	3.1
5	S3	138	VAL	3.1
14	C2	96	GLN	3.1
35	SM	107	ASN	3.1
75	o9	45	ARG	3.1
45	l8	222	PHE	3.1
5	S3	78	LYS	3.1
33	e1	92	LYS	3.1
34	SR	33	LEU	3.1
34	sR	49	GLY	3.1
34	sR	137	LYS	3.1
73	o7	26	SER	3.1
55	M9	164	LEU	3.1
4	S2	115	ILE	3.1
14	C2	23	THR	3.1
72	o6	94	ILE	3.1
3	S1	215	VAL	3.1
23	D1	36	VAL	3.1
40	l3	146	ARG	3.1
44	l7	25	GLN	3.1
55	m9	139	VAL	3.1
5	s3	78	LYS	3.1
30	D8	34	GLU	3.1
39	l2	186	PHE	3.1
5	S3	96	LEU	3.1
5	s3	59	LEU	3.1
45	L8	93	LEU	3.1
18	c6	63	ILE	3.1
79	Q3	37	TYR	3.1
4	s2	89	GLN	3.1
22	d0	12	GLN	3.1
22	d0	118	VAL	3.1
12	c0	61	TRP	3.1
3	S1	53	GLY	3.1
11	S9	34	PHE	3.1
1	6	1634	C	3.1
16	c4	135	ARG	3.1
14	C2	49	THR	3.1
15	c3	15	ALA	3.1
36	1	1577	G	3.1
16	C4	89	THR	3.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
45	l8	210	ALA	3.1
28	D6	18	VAL	3.1
63	n7	12	VAL	3.1
71	O5	14	LYS	3.1
71	O5	35	LYS	3.1
9	s7	184	GLU	3.1
14	C2	125	ASN	3.1
1	2	369	A	3.1
17	C5	56	PHE	3.1
23	d1	11	LEU	3.1
38	8	158	U	3.1
8	S6	208	TYR	3.1
14	c2	89	ILE	3.1
34	sR	30	PRO	3.1
55	m9	109	TYR	3.1
71	O5	12	LYS	3.1
11	S9	20	GLU	3.1
13	c1	6	THR	3.1
28	D6	75	VAL	3.1
30	d8	48	VAL	3.1
35	SM	166	VAL	3.1
45	l8	197	VAL	3.1
55	M9	139	VAL	3.1
24	D2	21	GLY	3.1
5	S3	21	LEU	3.1
11	S9	116	LEU	3.1
35	sM	49	LYS	3.1
36	5	182	U	3.1
71	o5	28	LEU	3.1
25	D3	59	ILE	3.1
71	O5	39	PRO	3.1
3	s1	65	VAL	3.1
4	S2	206	THR	3.1
18	c6	19	VAL	3.1
22	D0	31	VAL	3.1
22	d0	116	VAL	3.1
82	p0	205	THR	3.1
25	d3	44	GLY	3.0
35	SM	78	ASP	3.1
16	C4	136	ARG	3.0
35	SM	104	LYS	3.0
1	2	1795	U	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	6	656	G	3.0
4	S2	232	GLU	3.0
9	S7	108	GLN	3.0
55	m9	142	ILE	3.0
56	N0	17	GLU	3.0
7	S5	159	ALA	3.0
34	SR	180	ALA	3.0
36	1	2502	A	3.0
36	5	440	A	3.0
45	L8	198	ALA	3.0
9	S7	20	VAL	3.0
5	S3	180	GLY	3.0
5	s3	185	LYS	3.0
55	M9	167	ARG	3.0
4	s2	215	PHE	3.0
28	D6	43	ASN	3.0
45	l8	200	LEU	3.0
49	m3	139	LEU	3.0
1	2	717	C	3.0
17	C5	27	GLU	3.0
36	1	1950	U	3.0
36	5	2506	U	3.0
14	c2	134	SER	3.0
28	D6	54	SER	3.0
1	2	498	G	3.0
5	S3	73	VAL	3.0
5	s3	40	ARG	3.0
8	S6	149	LYS	3.0
26	D4	90	ARG	3.0
70	O4	106	LYS	3.0
71	O5	45	LYS	3.0
1	6	1217	A	3.0
2	s0	25	GLY	3.0
3	S1	21	VAL	3.0
16	c4	15	GLY	3.0
36	5	2256	A	3.0
4	S2	188	LEU	3.0
9	S7	34	LEU	3.0
12	C0	16	PHE	3.0
25	d3	36	THR	3.0
12	c0	74	GLU	3.0
30	D8	62	GLU	3.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
55	M9	179	GLU	3.0
74	o8	14	LEU	3.0
7	S5	208	SER	3.0
11	S9	134	ILE	3.0
16	C4	19	ILE	3.0
22	d0	41	ILE	3.0
5	S3	76	ARG	3.0
36	5	2098	C	3.0
10	S8	106	ALA	3.0
11	S9	125	ALA	3.0
16	c4	63	ALA	3.0
10	S8	2	GLY	3.0
79	Q3	90	VAL	3.0
5	S3	31	GLU	3.0
7	S5	140	THR	3.0
35	SM	81	THR	3.0
36	1	1954	G	3.0
36	1	1103	A	3.0
36	5	2536	A	3.0
61	n5	113	LEU	3.0
5	s3	187	LYS	3.0
28	D6	36	ILE	3.0
35	SM	131	ILE	3.0
46	l9	106	LYS	3.0
16	c4	96	PRO	3.0
4	S2	121	VAL	3.0
4	S2	167	VAL	3.0
6	S4	260	GLY	3.0
12	c0	42	VAL	3.0
18	C6	11	GLY	3.0
35	sM	166	VAL	3.0
45	L8	132	VAL	3.0
19	c7	57	LEU	3.0
45	L8	91	PHE	3.0
45	l8	246	MET	3.0
27	d5	102	THR	3.0
75	O9	40	LYS	3.0
1	2	720	G	3.0
5	s3	76	ARG	3.0
11	S9	46	SER	3.0
9	s7	53	GLY	3.0
43	l6	11	PRO	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
62	n6	88	GLU	3.0
13	C1	89	ALA	3.0
4	S2	111	VAL	3.0
55	m9	177	VAL	3.0
7	s5	82	PHE	3.0
24	D2	71	LYS	3.0
73	o7	18	LEU	3.0
36	1	2548	C	3.0
36	5	1579	C	3.0
3	S1	213	ARG	3.0
4	s2	201	ASN	3.0
7	S5	94	THR	3.0
18	C6	36	ILE	3.0
24	d2	27	ILE	3.0
45	L8	67	ILE	3.0
1	2	657	U	3.0
41	l4	61	SER	3.0
9	S7	146	GLY	3.0
32	E0	32	GLY	3.0
1	6	651	G	3.0
35	SM	138	ALA	3.0
73	O7	10	LYS	3.0
74	o8	30	LYS	3.0
3	s1	68	VAL	3.0
16	C4	28	VAL	3.0
34	sR	13	LEU	3.0
34	sR	103	PHE	3.0
45	l8	180	VAL	3.0
16	C4	105	LEU	3.0
35	SM	158	GLN	3.0
22	D0	40	ASN	3.0
3	s1	32	ILE	3.0
4	s2	59	HIS	3.0
5	S3	115	ILE	3.0
7	S5	172	ILE	3.0
16	C4	115	ILE	3.0
36	1	1563	C	3.0
5	s3	195	SER	3.0
34	sR	294	TRP	3.0
50	m4	9	ALA	3.0
7	S5	143	ARG	3.0
8	S6	68	LEU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
17	C5	108	ARG	3.0
22	d0	50	LEU	3.0
34	sR	33	LEU	3.0
42	L5	297	GLN	3.0
45	l8	238	LEU	3.0
52	M6	80	PHE	3.0
14	c2	83	GLU	3.0
30	D8	31	GLU	3.0
67	o1	111	GLU	3.0
75	o9	50	ASN	3.0
18	C6	26	LYS	3.0
22	D0	86	ILE	3.0
75	O9	51	ILE	3.0
1	2	230	C	2.9
3	S1	38	PHE	2.9
28	d6	56	ALA	2.9
39	l2	247	ARG	2.9
53	m7	156	ALA	2.9
62	n6	83	ASP	2.9
70	o4	16	ARG	2.9
4	s2	120	GLU	2.9
5	s3	177	MET	2.9
3	S1	83	LYS	2.9
4	S2	203	LYS	2.9
2	s0	173	ILE	2.9
4	s2	69	ILE	2.9
13	C1	122	ILE	2.9
23	D1	29	HIS	2.9
58	n2	38	ILE	2.9
9	s7	54	GLY	2.9
39	L2	226	SER	2.9
74	O8	16	ARG	2.9
1	6	1399	C	2.9
5	s3	137	VAL	2.9
6	S4	225	VAL	2.9
8	S6	41	VAL	2.9
20	C8	18	LEU	2.9
23	D1	37	ALA	2.9
28	d6	18	VAL	2.9
28	d6	71	LEU	2.9
8	S6	21	GLU	2.9
70	o4	113	LYS	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	2	483	A	2.9
12	C0	35	ILE	2.9
27	d5	50	ILE	2.9
31	D9	38	ILE	2.9
32	E0	24	THR	2.9
35	SM	93	ARG	2.9
39	L2	247	ARG	2.9
62	n6	51	ARG	2.9
30	D8	21	SER	2.9
32	E0	30	PRO	2.9
34	SR	79	TYR	2.9
34	SR	81	LEU	2.9
40	l3	387	LEU	2.9
62	n6	69	LYS	2.9
70	o4	106	LYS	2.9
24	D2	63	VAL	2.9
56	N0	2	ALA	2.9
1	2	233	C	2.9
17	C5	89	MET	2.9
43	l6	9	TRP	2.9
3	s1	204	ILE	2.9
14	C2	84	ASN	2.9
19	C7	38	ILE	2.9
39	l2	7	ASN	2.9
41	L4	69	ARG	2.9
42	L5	231	ILE	2.9
2	S0	128	SER	2.9
7	S5	207	THR	2.9
17	c5	8	LYS	2.9
29	d7	5	GLN	2.9
4	s2	103	VAL	2.9
5	s3	138	VAL	2.9
11	S9	122	VAL	2.9
55	M9	78	TYR	2.9
14	C2	104	GLY	2.9
36	1	1953	G	2.9
27	D5	50	ILE	2.9
32	E0	28	LYS	2.9
33	E1	107	LYS	2.9
36	5	3154	C	2.9
74	o8	32	ASN	2.9
1	2	132	U	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	6	192	U	2.9
30	d8	35	ASP	2.9
36	5	2504	U	2.9
39	L2	224	THR	2.9
80	e0	27	PRO	2.9
34	sR	303	ALA	2.9
75	o9	39	ALA	2.9
5	s3	54	ARG	2.9
76	q0	128	LYS	2.9
3	S1	164	ILE	2.9
31	d9	50	ILE	2.9
35	sM	139	GLU	2.9
74	O8	57	ASN	2.9
3	s1	38	PHE	2.9
30	d8	56	LEU	2.9
39	l2	16	PHE	2.9
67	o1	4	LEU	2.9
78	Q2	35	LEU	2.9
4	S2	64	LYS	2.9
7	s5	202	ALA	2.9
9	S7	142	TYR	2.9
18	C6	39	VAL	2.9
28	D6	68	TYR	2.9
35	SM	125	ALA	2.9
65	n9	25	LYS	2.9
1	6	485	A	2.9
14	C2	135	MET	2.9
17	C5	28	MET	2.9
11	s9	33	GLU	2.9
4	S2	189	GLN	2.9
19	C7	123	ASN	2.9
57	N1	159	PHE	2.9
61	n5	57	LEU	2.9
62	N6	83	ASP	2.9
71	o5	9	LEU	2.9
4	S2	166	THR	2.9
4	s2	91	ARG	2.9
4	s2	133	LYS	2.9
10	S8	194	ARG	2.9
14	c2	95	LYS	2.9
22	D0	30	LYS	2.9
27	d5	85	LYS	2.9

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
38	4	86	U	2.9
74	O8	33	LYS	2.9
1	6	720	G	2.9
6	S4	208	VAL	2.9
36	5	1562	C	2.9
34	SR	285	ALA	2.9
36	5	1953	G	2.9
61	n5	64	GLU	2.9
18	c6	93	HIS	2.9
3	S1	70	LEU	2.9
5	S3	72	LEU	2.9
12	c0	68	LEU	2.9
14	C2	90	LYS	2.9
14	c2	103	LEU	2.9
15	c3	53	LEU	2.9
35	SM	114	LYS	2.9
73	o7	32	LYS	2.9
1	2	681	U	2.9
36	1	1815	U	2.9
17	C5	11	VAL	2.8
5	s3	80	ALA	2.8
10	S8	78	ILE	2.8
12	c0	35	ILE	2.8
22	D0	91	ILE	2.8
23	D1	21	ASN	2.8
25	D3	126	LYS	2.8
32	E0	36	LYS	2.8
5	S3	190	ARG	2.8
7	S5	167	ARG	2.8
39	l2	246	LEU	2.8
77	Q1	6	ARG	2.8
25	D3	46	SER	2.8
22	D0	117	VAL	2.8
24	D2	72	CYS	2.8
53	M7	165	VAL	2.8
2	S0	138	TYR	2.8
5	S3	125	TYR	2.8
7	S5	125	THR	2.8
45	l8	198	ALA	2.8
4	S2	88	LYS	2.8
34	sR	46	LYS	2.8
34	sR	187	GLN	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
45	l8	248	LYS	2.8
74	O8	36	LYS	2.8
2	S0	111	ILE	2.8
4	S2	130	ILE	2.8
53	M7	136	ILE	2.8
2	s0	9	LEU	2.8
35	SM	122	GLU	2.8
61	n5	104	GLU	2.8
33	E1	102	VAL	2.8
36	5	235	A	2.8
52	m6	180	SER	2.8
6	S4	167	GLY	2.8
41	l4	52	VAL	2.8
74	o8	71	PRO	2.8
7	s5	86	GLN	2.8
16	c4	26	THR	2.8
74	o8	72	THR	2.8
2	S0	32	HIS	2.8
4	S2	225	LEU	2.8
1	6	1192	C	2.8
5	s3	154	ASP	2.8
8	S6	156	PHE	2.8
24	D2	89	TRP	2.8
25	D3	24	TRP	2.8
29	d7	82	LYS	2.8
2	S0	29	VAL	2.8
2	S0	143	VAL	2.8
16	C4	30	VAL	2.8
22	d0	51	VAL	2.8
70	O4	5	VAL	2.8
1	6	1694	A	2.8
4	S2	126	ARG	2.8
5	s3	56	GLN	2.8
10	s8	159	GLN	2.8
12	C0	23	ALA	2.8
75	o9	19	GLN	2.8
11	S9	156	ILE	2.8
13	c1	94	ILE	2.8
5	s3	141	LYS	2.8
6	s4	226	PHE	2.8
12	C0	39	ASN	2.8
35	SM	117	LEU	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
22	d0	92	ASP	2.8
34	sR	50	ASP	2.8
71	O5	72	GLY	2.8
1	6	674	C	2.8
29	d7	54	VAL	2.8
36	1	1761	C	2.8
36	5	132	C	2.8
13	C1	86	ILE	2.8
43	l6	129	GLU	2.8
25	D3	39	LYS	2.8
36	5	2971	A	2.8
6	S4	176	ASP	2.8
12	C0	9	ASN	2.8
13	C1	52	SER	2.8
23	d1	87	ARG	2.8
12	C0	45	ALA	2.8
12	c0	34	GLU	2.8
10	s8	60	ILE	2.8
14	c2	90	LYS	2.8
22	D0	94	GLU	2.8
33	E1	105	TYR	2.8
35	SM	168	GLU	2.8
23	D1	23	ILE	2.8
24	D2	83	ILE	2.8
60	N4	91	LYS	2.8
4	S2	76	LEU	2.8
7	s5	198	LEU	2.8
9	S7	87	ASP	2.8
11	s9	104	PHE	2.8
12	c0	59	PHE	2.8
13	c1	42	PHE	2.8
35	SM	94	HIS	2.8
62	n6	110	HIS	2.8
4	S2	163	GLY	2.8
4	s2	34	GLY	2.8
6	s4	111	VAL	2.8
19	C7	14	LYS	2.8
33	e1	147	VAL	2.8
41	l4	54	GLU	2.8
45	l8	120	LYS	2.8
59	n3	137	VAL	2.8
60	N4	98	PRO	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	s0	20	ALA	2.8
24	D2	34	ILE	2.8
28	d6	35	ALA	2.8
35	SM	154	TYR	2.8
39	L2	239	ALA	2.8
27	d5	83	LEU	2.8
45	l8	152	LEU	2.8
67	O1	97	LEU	2.8
4	S2	156	THR	2.8
12	C0	57	THR	2.8
36	1	1574	C	2.8
36	5	1582	C	2.8
12	C0	77	ARG	2.8
4	s2	77	GLN	2.8
10	S8	103	GLN	2.8
16	c4	99	GLN	2.8
1	6	1702	A	2.8
36	5	2872	A	2.8
30	d8	28	VAL	2.8
55	m9	22	VAL	2.8
62	n6	105	VAL	2.8
2	S0	54	TRP	2.8
7	s5	164	PRO	2.8
10	s8	143	TRP	2.8
16	C4	50	ALA	2.8
62	n6	39	LEU	2.8
32	E0	5	HIS	2.7
61	n5	106	ASP	2.7
55	M9	133	LYS	2.7
41	L4	54	GLU	2.7
71	O5	8	GLU	2.7
1	2	134	U	2.7
16	c4	55	SER	2.7
49	M3	46	ILE	2.7
5	s3	94	ARG	2.7
10	s8	8	ARG	2.7
5	S3	166	ASP	2.7
11	S9	146	PHE	2.7
43	L6	8	LYS	2.7
60	n4	74	LYS	2.7
61	n5	88	MET	2.7
78	q2	61	LYS	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
78	q2	91	PHE	2.7
12	C0	34	GLU	2.7
35	sM	124	GLN	2.7
71	o5	85	THR	2.7
5	s3	37	VAL	2.7
6	s4	183	VAL	2.7
34	sR	166	SER	2.7
36	1	545	U	2.7
36	1	1564	U	2.7
59	N3	137	VAL	2.7
4	S2	139	ILE	2.7
11	s9	3	ARG	2.7
29	D7	33	LEU	2.7
55	M9	189	ALA	2.7
1	6	483	A	2.7
12	C0	27	PHE	2.7
11	s9	151	ASP	2.7
24	D2	87	GLU	2.7
28	d6	52	ASP	2.7
35	sM	78	ASP	2.7
62	N6	88	GLU	2.7
8	S6	163	THR	2.7
75	O9	34	THR	2.7
4	s2	95	ARG	2.7
6	S4	245	LYS	2.7
6	s4	225	VAL	2.7
13	C1	56	LYS	2.7
16	c4	92	LYS	2.7
22	D0	102	ARG	2.7
59	N3	135	VAL	2.7
70	O4	66	SER	2.7
13	C1	63	LEU	2.7
23	D1	55	LEU	2.7
30	D8	33	LEU	2.7
51	M5	10	LEU	2.7
62	n6	70	ILE	2.7
5	s3	19	ALA	2.7
13	C1	60	PHE	2.7
16	C4	87	GLY	2.7
39	l2	235	ALA	2.7
61	n5	103	TYR	2.7
7	s5	127	GLN	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	C8	55	HIS	2.7
22	d0	47	GLN	2.7
62	N6	120	GLN	2.7
1	6	1693	A	2.7
5	s3	64	ARG	2.7
55	M9	151	ARG	2.7
71	o5	114	ARG	2.7
32	E0	7	SER	2.7
39	L2	113	VAL	2.7
45	L8	197	VAL	2.7
14	c2	97	LEU	2.7
15	c3	16	ILE	2.7
17	C5	65	LEU	2.7
35	sM	52	PRO	2.7
39	L2	238	ILE	2.7
62	n6	76	LEU	2.7
74	o8	73	LEU	2.7
5	s3	36	GLY	2.7
6	s4	165	ALA	2.7
18	C6	96	TYR	2.7
20	c8	146	ALA	2.7
36	1	2095	G	2.7
36	5	1565	G	2.7
1	6	654	C	2.7
5	s3	74	GLN	2.7
9	S7	74	GLN	2.7
62	n6	53	ASP	2.7
2	S0	23	HIS	2.7
30	D8	14	LYS	2.7
33	E1	82	LYS	2.7
5	S3	67	ASN	2.7
28	d6	82	ARG	2.7
33	e1	123	ASN	2.7
49	m3	129	ASN	2.7
55	M9	85	ARG	2.7
34	sR	74	THR	2.7
70	O4	64	THR	2.7
12	C0	33	GLU	2.7
14	C2	31	VAL	2.7
25	D3	93	LEU	2.7
33	E1	100	LEU	2.7
39	L2	202	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
14	c2	87	PRO	2.7
22	D0	41	ILE	2.7
22	D0	65	ILE	2.7
6	S4	25	GLY	2.7
32	E0	59	GLY	2.7
49	M3	133	PRO	2.7
12	c0	75	TYR	2.7
23	D1	25	LYS	2.7
27	D5	67	ASP	2.7
34	sR	314	GLN	2.7
75	o9	7	PHE	2.7
11	S9	62	ARG	2.7
34	sR	150	TRP	2.7
39	l2	190	ARG	2.7
36	5	243	G	2.7
7	S5	49	GLU	2.7
80	e0	24	THR	2.7
55	M9	138	LEU	2.7
82	p0	210	VAL	2.7
2	S0	141	ILE	2.7
10	s8	80	GLY	2.7
34	sR	131	ILE	2.7
35	SM	111	GLY	2.7
36	1	1269	U	2.7
61	n5	97	LYS	2.7
8	S6	43	ASP	2.7
8	S6	152	ASP	2.7
11	S9	6	ARG	2.7
11	S9	54	ARG	2.7
14	c2	94	ALA	2.7
25	D3	113	ALA	2.7
4	s2	81	MET	2.7
25	D3	71	CYS	2.7
3	s1	98	THR	2.7
36	5	1354	G	2.7
36	5	1492	G	2.7
7	s5	29	ILE	2.7
10	s8	43	ILE	2.7
16	C4	11	SER	2.7
18	C6	63	ILE	2.7
18	c6	88	GLY	2.7
24	D2	47	ILE	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
34	sR	28	GLY	2.7
52	m6	178	VAL	2.7
66	o0	67	VAL	2.7
80	e0	6	GLY	2.7
11	s9	5	PRO	2.7
13	C1	113	PRO	2.7
16	C4	69	ALA	2.7
47	M0	72	ALA	2.7
35	SM	173	GLU	2.7
62	n6	108	LYS	2.6
4	s2	211	LEU	2.6
6	S4	180	LEU	2.6
16	c4	33	LEU	2.6
34	SR	32	LEU	2.6
70	O4	81	CYS	2.6
8	S6	42	GLY	2.6
30	D8	19	THR	2.6
34	sR	317	THR	2.6
36	5	1017	C	2.6
62	n6	121	ARG	2.6
1	2	912	U	2.6
61	n5	52	PRO	2.6
62	n6	54	ASP	2.6
14	C2	51	ALA	2.6
55	m9	54	ALA	2.6
62	n6	93	ALA	2.6
2	S0	198	MET	2.6
17	c5	25	LEU	2.6
25	d3	34	LEU	2.6
51	M5	7	LEU	2.6
7	S5	33	VAL	2.6
15	c3	104	ARG	2.6
11	S9	77	ILE	2.6
48	M1	79	ILE	2.6
13	C1	27	THR	2.6
12	C0	18	GLU	2.6
49	m3	136	GLU	2.6
1	2	237	C	2.6
41	l4	101	ALA	2.6
58	N2	83	TYR	2.6
36	1	547	G	2.6
36	1	2503	G	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	2	1797	A	2.6
18	C6	28	LEU	2.6
26	d4	18	LEU	2.6
30	d8	42	ARG	2.6
26	d4	106	GLN	2.6
36	5	2441	A	2.6
66	o0	16	LEU	2.6
5	s3	50	ILE	2.6
10	s8	152	ILE	2.6
25	D3	101	GLU	2.6
41	l4	42	VAL	2.6
74	o8	27	ILE	2.6
24	D2	19	LYS	2.6
28	D6	29	SER	2.6
35	SM	75	ASP	2.6
36	1	3351	U	2.6
73	O7	58	THR	2.6
4	s2	124	ALA	2.6
25	d3	67	ALA	2.6
63	n7	7	ALA	2.6
27	d5	58	ARG	2.6
3	S1	86	LEU	2.6
4	S2	89	GLN	2.6
6	S4	101	LEU	2.6
10	s8	121	LEU	2.6
19	C7	73	LEU	2.6
28	d6	11	ASN	2.6
59	N3	5	GLY	2.6
61	N5	82	LEU	2.6
4	S2	38	VAL	2.6
4	S2	178	ILE	2.6
11	S9	120	LYS	2.6
13	C1	26	LYS	2.6
4	s2	63	VAL	2.6
5	s3	12	VAL	2.6
1	2	217	A	2.6
7	S5	48	PHE	2.6
33	e1	91	ILE	2.6
45	l8	52	TRP	2.6
10	s8	170	SER	2.6
1	2	725	U	2.6
13	c1	113	PRO	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
36	5	1764	U	2.6
6	S4	100	ARG	2.6
18	C6	114	ARG	2.6
24	D2	111	MET	2.6
28	d6	10	ARG	2.6
28	d6	48	ALA	2.6
5	s3	21	LEU	2.6
28	d6	46	GLU	2.6
29	d7	7	LEU	2.6
22	d0	49	ASN	2.6
34	sR	62	LYS	2.6
12	C0	43	ILE	2.6
45	l8	203	VAL	2.6
76	q0	77	ILE	2.6
55	M9	188	ASP	2.6
1	2	550	A	2.6
1	2	904	G	2.6
1	2	1635	A	2.6
1	6	675	U	2.6
4	S2	151	PRO	2.6
5	s3	90	ARG	2.6
7	S5	21	THR	2.6
48	M1	55	ARG	2.6
4	S2	118	ALA	2.6
10	s8	57	ALA	2.6
11	S9	119	ALA	2.6
22	d0	45	ALA	2.6
24	d2	22	LYS	2.6
30	d8	10	ALA	2.6
40	L3	51	ALA	2.6
49	M3	2	ALA	2.6
59	N3	113	ALA	2.6
78	q2	59	HIS	2.6
79	q3	7	LYS	2.6
4	s2	154	LEU	2.6
28	D6	64	LEU	2.6
31	D9	20	GLN	2.6
34	sR	185	GLN	2.6
35	SM	155	LEU	2.6
66	o0	56	LEU	2.6
71	o5	30	GLU	2.6
73	o7	48	ASN	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	s2	111	VAL	2.6
5	s3	181	VAL	2.6
9	s7	61	PHE	2.6
12	c0	55	VAL	2.6
20	C8	28	ILE	2.6
34	sR	54	PHE	2.6
60	N4	82	ILE	2.6
63	n7	92	PHE	2.6
70	O4	23	VAL	2.6
1	6	230	C	2.6
35	SM	153	ASP	2.6
5	s3	146	ARG	2.6
7	s5	225	ARG	2.6
3	s1	86	LEU	2.6
4	S2	233	GLN	2.6
22	D0	48	HIS	2.6
23	D1	12	TYR	2.6
4	s2	188	LEU	2.6
7	S5	175	LEU	2.6
17	C5	26	LEU	2.6
20	c8	17	LEU	2.6
22	d0	26	LEU	2.6
55	M9	155	LEU	2.6
61	n5	108	LEU	2.6
25	D3	65	ASN	2.6
21	c9	37	VAL	2.6
28	d6	79	ILE	2.6
58	n2	15	PHE	2.6
62	n6	90	VAL	2.6
5	s3	10	LYS	2.6
5	s3	221	SER	2.6
7	S5	164	PRO	2.6
36	1	2101	C	2.6
36	5	252	U	2.6
61	n5	101	GLU	2.6
71	O5	64	GLU	2.6
80	e0	60	PRO	2.6
11	S9	98	ALA	2.6
8	S6	76	LEU	2.6
13	C1	110	HIS	2.6
16	C4	98	GLY	2.6
33	e1	86	THR	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
52	m6	181	ALA	2.6
18	c6	52	LEU	2.6
23	D1	8	LEU	2.6
64	N8	33	GLY	2.6
71	o5	24	LEU	2.6
10	S8	8	ARG	2.6
11	S9	42	ILE	2.6
11	S9	179	ARG	2.6
45	l8	67	ILE	2.6
25	D3	124	VAL	2.6
40	L3	89	VAL	2.6
11	S9	25	ASP	2.5
11	S9	66	ASP	2.5
32	E0	22	GLU	2.5
34	sR	163	ASP	2.5
36	1	1243	G	2.5
34	sR	26	SER	2.5
12	c0	47	GLN	2.5
17	C5	75	PRO	2.5
13	C1	68	GLY	2.5
16	c4	45	GLY	2.5
62	N6	26	GLN	2.5
4	S2	73	LEU	2.5
11	S9	43	TYR	2.5
22	D0	84	MET	2.5
26	D4	4	ALA	2.5
62	n6	109	LEU	2.5
75	O9	39	ALA	2.5
23	d1	15	ARG	2.5
24	D2	88	LYS	2.5
25	D3	110	LYS	2.5
45	l8	213	LYS	2.5
72	o6	99	ARG	2.5
74	o8	26	LYS	2.5
4	S2	82	ASN	2.5
4	S2	125	ILE	2.5
5	S3	77	PHE	2.5
10	S8	152	ILE	2.5
24	D2	125	ILE	2.5
28	d6	41	ILE	2.5
58	N2	41	ILE	2.5
70	O4	20	ILE	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	c0	73	VAL	2.5
13	C1	107	VAL	2.5
24	D2	33	VAL	2.5
35	SM	112	ASP	2.5
71	o5	54	VAL	2.5
50	M4	5	SER	2.5
1	2	133	U	2.5
1	2	1059	U	2.5
7	S5	22	PRO	2.5
18	c6	94	GLN	2.5
36	5	1950	U	2.5
14	C2	92	ALA	2.5
36	5	1493	G	2.5
65	N9	2	ALA	2.5
11	S9	174	ARG	2.5
16	C4	119	THR	2.5
28	D6	87	ARG	2.5
73	o7	58	THR	2.5
4	s2	170	ILE	2.5
6	s4	162	ILE	2.5
7	S5	29	ILE	2.5
10	S8	187	GLU	2.5
45	L8	179	ILE	2.5
55	m9	179	GLU	2.5
43	l6	15	VAL	2.5
49	M3	153	ASP	2.5
74	o8	25	VAL	2.5
2	S0	131	GLN	2.5
9	S7	101	LYS	2.5
13	C1	16	GLN	2.5
13	C1	79	LYS	2.5
25	D3	50	LYS	2.5
28	D6	9	GLY	2.5
33	E1	143	LYS	2.5
36	5	2100	A	2.5
1	2	240	U	2.5
1	2	721	U	2.5
9	s7	63	PRO	2.5
65	N9	24	PRO	2.5
27	d5	68	ARG	2.5
4	s2	247	ALA	2.5
62	n6	18	ALA	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
73	O7	66	TYR	2.5
2	S0	108	THR	2.5
4	s2	166	THR	2.5
22	d0	109	GLU	2.5
25	d3	98	GLU	2.5
70	o4	93	PHE	2.5
14	c2	72	ILE	2.5
3	S1	72	ASP	2.5
3	S1	132	ASP	2.5
11	S9	94	ASP	2.5
4	S2	186	LYS	2.5
61	N5	45	LYS	2.5
49	M3	130	GLY	2.5
60	n4	72	SER	2.5
9	S7	81	LEU	2.5
25	d3	6	PRO	2.5
41	l4	219	LEU	2.5
1	2	1766	A	2.5
4	S2	230	TRP	2.5
5	s3	105	MET	2.5
5	s3	150	MET	2.5
36	1	2540	A	2.5
39	L2	196	TRP	2.5
48	m1	116	TYR	2.5
2	S0	203	PHE	2.5
12	c0	27	PHE	2.5
15	C3	66	ILE	2.5
18	c6	37	THR	2.5
61	n5	84	PHE	2.5
28	D6	66	LYS	2.5
43	l6	8	LYS	2.5
55	m9	153	LYS	2.5
9	S7	144	VAL	2.5
45	l8	132	VAL	2.5
1	6	235	G	2.5
19	C7	80	ARG	2.5
35	sM	53	ARG	2.5
12	c0	48	SER	2.5
23	D1	65	SER	2.5
1	2	1637	C	2.5
24	D2	126	LEU	2.5
4	s2	79	GLU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	s3	81	PRO	2.5
28	d6	90	GLU	2.5
26	D4	126	ALA	2.5
39	L2	125	ALA	2.5
80	e0	56	MET	2.5
18	C6	60	PHE	2.5
7	s5	90	ILE	2.5
12	C0	11	ILE	2.5
36	5	1571	A	2.5
39	l2	15	ILE	2.5
58	N2	80	THR	2.5
75	O9	43	ASN	2.5
4	s2	184	VAL	2.5
6	S4	130	GLN	2.5
30	d8	55	VAL	2.5
78	Q2	105	GLN	2.5
39	L2	236	GLY	2.5
2	s0	184	LEU	2.5
35	sM	79	SER	2.5
47	M0	215	GLU	2.5
55	M9	59	SER	2.5
16	c4	94	PRO	2.5
32	E0	31	LYS	2.5
1	2	724	C	2.5
6	S4	99	PHE	2.5
10	s8	109	PHE	2.5
23	D1	26	ALA	2.5
36	5	1762	C	2.5
13	c1	54	ILE	2.5
7	S5	35	GLN	2.5
7	s5	158	GLN	2.5
8	s6	215	ARG	2.5
71	O5	76	GLN	2.5
5	S3	140	GLY	2.5
6	S4	219	VAL	2.5
13	c1	123	VAL	2.5
31	d9	6	VAL	2.5
34	sR	312	VAL	2.5
36	5	1575	A	2.5
79	Q3	79	VAL	2.5
11	S9	33	GLU	2.5
45	L8	161	GLU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
60	N4	66	GLU	2.5
6	s4	246	LEU	2.5
14	C2	78	LEU	2.5
25	D3	123	LYS	2.5
45	l8	109	LEU	2.5
55	M9	4	LEU	2.5
8	S6	16	PHE	2.5
31	d9	47	ALA	2.5
4	S2	174	ARG	2.5
35	SM	72	ARG	2.5
62	n6	74	TYR	2.5
55	m9	143	ILE	2.5
13	C1	121	ASP	2.5
3	s1	127	VAL	2.5
5	S3	151	LYS	2.5
8	s6	71	THR	2.5
25	D3	125	VAL	2.5
26	D4	117	LYS	2.5
33	e1	149	LYS	2.5
34	SR	99	THR	2.5
8	S6	3	LEU	2.5
8	S6	109	LEU	2.5
13	c1	143	SER	2.5
24	D2	76	SER	2.5
71	O5	50	SER	2.5
7	s5	30	PRO	2.4
3	s1	223	PHE	2.4
6	S4	256	ARG	2.4
22	D0	87	HIS	2.4
8	S6	221	ALA	2.4
55	m9	162	ARG	2.4
4	S2	53	ILE	2.4
20	C8	71	GLN	2.4
23	d1	12	TYR	2.4
46	L9	10	ILE	2.4
74	o8	8	ILE	2.4
11	S9	37	LYS	2.4
27	D5	52	LYS	2.4
34	SR	49	GLY	2.4
45	l8	63	LYS	2.4
4	S2	102	VAL	2.4
7	s5	38	THR	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	s6	163	THR	2.4
10	s8	58	LEU	2.4
11	S9	14	THR	2.4
24	D2	40	VAL	2.4
41	L4	106	TRP	2.4
59	n3	135	VAL	2.4
67	O1	33	VAL	2.4
75	o9	44	TRP	2.4
12	C0	2	LEU	2.4
28	d6	64	LEU	2.4
30	d8	54	LEU	2.4
34	sR	222	LEU	2.4
31	d9	13	ARG	2.4
35	SM	62	ARG	2.4
31	D9	43	PHE	2.4
34	sR	106	HIS	2.4
36	1	1353	U	2.4
46	L9	45	PHE	2.4
10	s8	100	ALA	2.4
16	C4	82	LYS	2.4
35	SM	136	ALA	2.4
41	l4	55	LYS	2.4
55	m9	152	GLU	2.4
58	N2	108	TYR	2.4
61	N5	41	ALA	2.4
7	S5	68	ILE	2.4
7	s5	190	ILE	2.4
33	E1	137	ASP	2.4
35	SM	101	ASP	2.4
71	O5	44	ILE	2.4
3	s1	88	VAL	2.4
61	n5	86	VAL	2.4
16	c4	110	LEU	2.4
20	C8	101	LEU	2.4
66	o0	93	LEU	2.4
25	D3	69	ARG	2.4
31	d9	44	ARG	2.4
59	N3	32	ARG	2.4
2	s0	4	PRO	2.4
3	S1	67	GLU	2.4
17	C5	59	LYS	2.4
25	D3	42	PRO	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
27	D5	94	LYS	2.4
28	D6	3	LYS	2.4
36	5	3155	U	2.4
38	8	82	U	2.4
70	O4	7	PHE	2.4
11	S9	48	GLN	2.4
66	o0	12	GLN	2.4
7	S5	221	ALA	2.4
9	s7	50	ASP	2.4
18	c6	85	ILE	2.4
41	l4	62	ALA	2.4
39	L2	228	GLY	2.4
45	l8	97	TYR	2.4
2	s0	59	LEU	2.4
4	s2	61	LEU	2.4
7	S5	134	VAL	2.4
15	C3	151	ASN	2.4
16	C4	74	VAL	2.4
18	C6	52	LEU	2.4
20	C8	32	LEU	2.4
39	L2	79	ASN	2.4
58	n2	66	VAL	2.4
59	n3	17	LEU	2.4
80	e0	4	VAL	2.4
3	s1	45	LYS	2.4
16	C4	91	THR	2.4
64	N8	98	THR	2.4
4	s2	62	PRO	2.4
7	s5	129	PRO	2.4
36	1	1578	C	2.4
7	S5	56	ALA	2.4
34	sR	78	ALA	2.4
34	sR	105	GLY	2.4
35	sM	132	ALA	2.4
41	L4	68	GLY	2.4
39	L2	189	TYR	2.4
45	L8	156	ASP	2.4
49	m3	108	ILE	2.4
62	N6	92	GLY	2.4
14	C2	39	ASP	2.4
3	S1	62	LYS	2.4
5	S3	117	ARG	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	s8	102	VAL	2.4
17	C5	72	LYS	2.4
20	c8	116	LEU	2.4
24	D2	93	LEU	2.4
30	d8	49	ARG	2.4
39	L2	104	LEU	2.4
62	n6	91	ASN	2.4
71	O5	36	LEU	2.4
77	Q1	18	ARG	2.4
12	C0	61	TRP	2.4
36	1	2571	U	2.4
39	L2	210	PRO	2.4
49	m3	48	PRO	2.4
4	s2	183	ALA	2.4
5	S3	93	ASP	2.4
27	d5	92	ILE	2.4
34	sR	170	ILE	2.4
34	sR	212	ALA	2.4
45	l8	199	ALA	2.4
48	M1	122	ILE	2.4
12	C0	38	LYS	2.4
13	C1	29	LYS	2.4
21	c9	134	ARG	2.4
24	D2	32	LYS	2.4
27	D5	57	TYR	2.4
70	O4	19	LYS	2.4
73	O7	47	TYR	2.4
4	S2	104	VAL	2.4
4	S2	187	LEU	2.4
6	S4	56	LEU	2.4
21	C9	71	VAL	2.4
34	SR	319	ASN	2.4
58	n2	65	VAL	2.4
75	O9	50	ASN	2.4
36	1	2256	A	2.4
38	8	111	A	2.4
6	S4	172	PHE	2.4
6	S4	258	GLN	2.4
12	c0	50	THR	2.4
13	c1	83	THR	2.4
16	c4	91	THR	2.4
66	o0	7	GLN	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	s3	180	GLY	2.4
45	l8	174	GLY	2.4
51	m5	2	GLY	2.4
11	S9	51	LYS	2.4
47	m0	101	LYS	2.4
45	l8	250	ALA	2.4
75	o9	3	ALA	2.4
75	o9	46	ARG	2.4
6	S4	138	TYR	2.4
7	S5	61	TYR	2.4
10	S8	166	TYR	2.4
13	C1	71	LEU	2.4
15	c3	54	LEU	2.4
20	c8	15	LEU	2.4
26	D4	44	LEU	2.4
13	c1	7	VAL	2.4
13	c1	142	VAL	2.4
25	d3	125	VAL	2.4
71	o5	57	VAL	2.4
1	2	1634	C	2.4
1	2	1796	C	2.4
36	5	131	C	2.4
1	6	541	A	2.4
2	S0	116	LYS	2.4
11	s9	185	GLY	2.4
13	C1	141	LYS	2.4
73	o7	74	PHE	2.4
73	o7	78	PHE	2.4
33	E1	93	HIS	2.4
36	5	2439	A	2.4
2	S0	127	ARG	2.4
6	S4	191	ARG	2.4
7	s5	92	ARG	2.4
10	s8	77	ARG	2.4
11	S9	2	PRO	2.4
28	d6	85	ARG	2.4
36	5	3156	U	2.4
75	O9	24	PRO	2.4
3	S1	131	ASP	2.4
7	s5	130	ILE	2.4
74	O8	27	ILE	2.4
9	s7	57	ALA	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
25	D3	85	ALA	2.4
47	m0	186	GLU	2.4
24	D2	104	LEU	2.4
47	M0	181	TYR	2.4
55	m9	105	LEU	2.4
62	N6	111	LEU	2.4
3	S1	88	VAL	2.4
6	S4	89	VAL	2.4
7	S5	139	ASN	2.4
14	c2	120	VAL	2.4
39	L2	62	VAL	2.4
39	L2	230	VAL	2.4
41	l4	18	ASN	2.4
2	s0	162	CYS	2.4
16	c4	49	LYS	2.4
17	C5	8	LYS	2.4
66	O0	12	GLN	2.4
37	3	73	C	2.4
41	l4	68	GLY	2.4
45	L8	66	SER	2.4
77	q1	18	ARG	2.4
5	s3	26	THR	2.4
6	S4	78	THR	2.4
10	s8	112	TRP	2.4
13	C1	72	THR	2.4
74	O8	72	THR	2.4
34	sR	316	MET	2.4
36	1	1095	U	2.4
36	5	2097	U	2.4
3	s1	228	LEU	2.3
7	s5	175	LEU	2.3
10	S8	144	ALA	2.4
36	5	2398	A	2.4
14	C2	133	LEU	2.3
22	d0	34	LEU	2.3
70	O4	112	ALA	2.4
51	m5	129	TYR	2.3
36	1	1242	G	2.3
39	L2	46	LYS	2.3
62	n6	73	VAL	2.3
70	O4	33	GLN	2.3
18	c6	46	PHE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	S1	51	SER	2.3
9	s7	103	SER	2.3
30	d8	34	GLU	2.3
45	L8	107	GLU	2.3
72	O6	66	GLU	2.3
4	s2	130	ILE	2.3
19	c7	25	THR	2.3
23	D1	34	ILE	2.3
35	SM	91	THR	2.3
36	1	1556	C	2.3
45	L8	158	ASP	2.3
66	o0	44	ILE	2.3
4	s2	217	ALA	2.3
5	s3	11	LEU	2.3
11	S9	109	LEU	2.3
21	C9	108	LEU	2.3
29	D7	50	ALA	2.3
40	L3	22	ALA	2.3
40	L3	47	LEU	2.3
52	M6	155	LYS	2.3
67	O1	73	LEU	2.3
71	o5	73	LYS	2.3
73	o7	14	LYS	2.3
71	o5	116	TYR	2.3
7	s5	168	VAL	2.3
14	C2	116	VAL	2.3
49	m3	80	VAL	2.3
6	S4	187	ARG	2.3
11	S9	57	ARG	2.3
34	sR	31	ASN	2.3
45	L8	240	ASN	2.3
73	O7	55	ARG	2.3
73	o7	73	ARG	2.3
75	o9	8	ARG	2.3
4	S2	66	PHE	2.3
7	S5	181	GLU	2.3
25	D3	38	PHE	2.3
35	sM	173	GLU	2.3
55	m9	113	GLY	2.3
1	6	655	G	2.3
4	S2	110	HIS	2.3
2	S0	207	PRO	2.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	6	558	U	2.3
1	6	1398	U	2.3
4	S2	158	THR	2.3
4	s2	115	ILE	2.3
4	s2	125	ILE	2.3
12	C0	25	LYS	2.3
12	c0	12	HIS	2.3
45	L8	255	SER	2.3
59	N3	112	SER	2.3
15	C3	131	THR	2.3
34	sR	158	PRO	2.3
57	N1	148	PRO	2.3
60	n4	63	ILE	2.3
66	o0	22	LYS	2.3
36	1	2538	U	2.3
46	L9	191	LEU	2.3
61	N5	102	LEU	2.3
79	q3	63	THR	2.3
15	C3	7	ALA	2.3
36	5	1951	C	2.3
7	s5	61	TYR	2.3
12	c0	41	TYR	2.3
13	C1	90	TYR	2.3
2	s0	58	VAL	2.3
5	s3	222	VAL	2.3
40	l3	139	GLN	2.3
42	l5	296	GLN	2.3
47	M0	89	VAL	2.3
61	N5	105	VAL	2.3
75	o9	28	ARG	2.3
3	S1	209	ASN	2.3
2	S0	105	GLY	2.3
4	S2	55	GLU	2.3
24	D2	15	ASN	2.3
4	S2	98	PHE	2.3
58	n2	13	LYS	2.3
4	S2	83	ILE	2.3
35	SM	113	ASP	2.3
55	M9	182	ASP	2.3
11	S9	93	LEU	2.3
31	d9	36	LEU	2.3
33	E1	103	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
48	M1	159	THR	2.3
61	N5	40	LEU	2.3
71	o5	88	LEU	2.3
1	2	1362	U	2.3
36	1	240	U	2.3
26	D4	22	GLN	2.3
28	D6	10	ARG	2.3
33	E1	152	ALA	2.3
36	5	442	G	2.3
8	S6	84	TYR	2.3
22	D0	16	GLN	2.3
79	q3	65	ALA	2.3
78	q2	43	TYR	2.3
3	s1	202	LYS	2.3
32	E0	23	LYS	2.3
47	M0	213	PHE	2.3
55	M9	43	LYS	2.3
73	O7	50	GLY	2.3
2	S0	152	PRO	2.3
2	S0	201	LEU	2.3
6	s4	222	LEU	2.3
7	S5	211	ILE	2.3
11	S9	184	SER	2.3
36	5	2208	A	2.3
25	d3	18	HIS	2.3
29	d7	49	HIS	2.3
7	S5	217	LEU	2.3
34	sR	310	ILE	2.3
12	c0	83	PRO	2.3
14	c2	46	ARG	2.3
47	m0	185	ARG	2.3
72	o6	11	LEU	2.3
4	s2	249	ALA	2.3
18	c6	20	ALA	2.3
50	M4	9	ALA	2.3
60	N4	83	THR	2.3
5	S3	185	LYS	2.3
5	s3	126	VAL	2.3
12	C0	65	TYR	2.3
26	D4	5	VAL	2.3
45	L8	120	LYS	2.3
41	l4	13	GLY	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	S3	17	PHE	2.3
11	S9	164	PHE	2.3
61	n5	117	ASN	2.3
36	1	546	C	2.3
36	5	1023	C	2.3
4	S2	61	LEU	2.3
9	s7	126	LEU	2.3
25	D3	66	SER	2.3
29	d7	24	LEU	2.3
63	n7	72	ILE	2.3
1	2	1425	A	2.3
36	1	1025	A	2.3
25	d3	31	LYS	2.3
34	SR	53	LYS	2.3
39	l2	250	GLN	2.3
45	L8	246	MET	2.3
62	n6	87	LYS	2.3
63	n7	56	LYS	2.3
10	s8	79	ALA	2.3
13	C1	48	ALA	2.3
25	D3	134	ALA	2.3
33	e1	87	THR	2.3
79	Q3	11	THR	2.3
4	S2	112	GLY	2.3
5	S3	175	VAL	2.3
6	S4	182	TYR	2.3
11	S9	8	TYR	2.3
14	C2	60	VAL	2.3
25	d3	96	VAL	2.3
61	N5	118	GLY	2.3
25	D3	122	PHE	2.3
3	s1	115	ARG	2.3
1	6	722	G	2.3
2	s0	169	SER	2.3
4	S2	119	LYS	2.3
4	s2	190	LEU	2.3
10	S8	96	LEU	2.3
11	S9	124	HIS	2.3
17	c5	32	ASP	2.3
14	C2	25	GLU	2.3
12	c0	62	GLN	2.3
22	d0	43	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
36	5	2507	C	2.3
49	m3	17	HIS	2.3
49	m3	23	LYS	2.3
49	m3	134	GLU	2.3
62	n6	106	ILE	2.3
68	O2	26	HIS	2.3
74	O8	63	LYS	2.3
74	o8	66	ILE	2.3
55	M9	175	GLN	2.3
12	c0	69	THR	2.3
14	C2	101	ALA	2.3
23	D1	20	THR	2.3
27	d5	105	THR	2.3
34	SR	77	GLY	2.3
42	L5	294	ALA	2.3
62	N6	2	ALA	2.3
66	O0	95	ALA	2.3
9	S7	61	PHE	2.3
61	N5	84	PHE	2.3
8	S6	80	ASN	2.3
25	D3	99	ASN	2.3
45	l8	57	ARG	2.3
60	n4	73	ARG	2.3
73	o7	24	ARG	2.3
77	Q1	2	ARG	2.3
45	L8	231	LYS	2.3
23	D1	4	ASP	2.3
35	SM	20	LEU	2.3
67	o1	112	ASP	2.3
3	s1	101	HIS	2.3
11	S9	112	GLN	2.3
12	C0	85	HIS	2.3
12	c0	58	GLN	2.3
28	D6	27	SER	2.3
11	s9	2	PRO	2.3
36	1	1555	U	2.3
57	n1	123	GLY	2.3
73	O7	51	ALA	2.3
4	s2	165	VAL	2.3
6	s4	208	VAL	2.3
4	S2	97	ARG	2.3
18	c6	10	PHE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
57	N1	141	VAL	2.3
63	N7	65	ARG	2.3
35	SM	171	LYS	2.2
5	S3	32	GLU	2.2
8	s6	35	GLU	2.2
14	C2	56	GLU	2.2
2	S0	76	ILE	2.2
11	S9	63	ASP	2.2
12	c0	13	GLN	2.2
14	C2	71	ILE	2.2
46	L9	9	GLN	2.2
63	N7	46	ILE	2.2
74	O8	37	PRO	2.2
1	2	241	U	2.2
1	2	261	U	2.2
1	2	499	U	2.2
13	C1	80	MET	2.2
3	S1	57	ALA	2.2
3	S1	156	ALA	2.2
7	s5	41	LYS	2.2
8	S6	223	LYS	2.2
12	C0	44	LYS	2.2
16	c4	101	ALA	2.2
36	1	2996	U	2.2
36	5	620	U	2.2
25	D3	120	VAL	2.2
31	d9	22	ARG	2.2
39	L2	155	LYS	2.2
59	n3	52	ALA	2.2
1	2	696	C	2.2
21	C9	6	VAL	2.2
51	m5	59	PHE	2.2
53	M7	166	VAL	2.2
73	o7	72	ARG	2.2
3	S1	106	THR	2.2
74	o8	15	THR	2.2
82	p0	86	PHE	2.2
7	S5	144	GLU	2.2
8	S6	118	GLU	2.2
36	1	3286	G	2.2
62	N6	91	ASN	2.2
5	s3	169	ASP	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
36	1	1252	A	2.2
60	n4	87	LEU	2.2
6	S4	169	ILE	2.2
13	C1	54	ILE	2.2
2	S0	151	SER	2.2
13	C1	77	SER	2.2
3	S1	75	GLY	2.2
3	S1	226	GLY	2.2
10	S8	22	ARG	2.2
55	M9	52	LYS	2.2
4	s2	66	PHE	2.2
5	S3	145	ALA	2.2
5	S3	34	TYR	2.2
13	C1	25	VAL	2.2
26	d4	100	VAL	2.2
27	d5	60	VAL	2.2
34	SR	186	PHE	2.2
61	n5	32	PHE	2.2
71	O5	30	GLU	2.2
2	S0	6	THR	2.2
3	s1	42	ASN	2.2
34	sR	300	THR	2.2
45	l8	194	THR	2.2
61	N5	68	THR	2.2
4	s2	58	LEU	2.2
39	L2	179	LEU	2.2
55	m9	106	LEU	2.2
62	N6	109	LEU	2.2
8	S6	175	ILE	2.2
9	s7	181	ILE	2.2
22	D0	108	ILE	2.2
1	2	707	A	2.2
3	S1	179	SER	2.2
5	s3	139	SER	2.2
18	c6	102	LYS	2.2
36	1	1270	A	2.2
45	L8	57	ARG	2.2
51	m5	41	ARG	2.2
58	n2	97	SER	2.2
73	o7	25	ARG	2.2
73	o7	65	ARG	2.2
79	Q3	58	SER	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
15	c3	83	GLU	2.2
25	D3	143	PRO	2.2
25	d3	60	GLU	2.2
45	l8	89	GLU	2.2
49	m3	150	PRO	2.2
69	o3	90	PRO	2.2
36	5	181	U	2.2
4	S2	165	VAL	2.2
5	S3	186	VAL	2.2
33	e1	84	VAL	2.2
34	sR	309	VAL	2.2
71	O5	47	VAL	2.2
78	q2	57	VAL	2.2
7	s5	58	LEU	2.2
10	s8	90	LEU	2.2
26	D4	107	GLN	2.2
45	L8	189	LEU	2.2
49	M3	51	LEU	2.2
63	n7	5	LEU	2.2
73	O7	17	THR	2.2
13	c1	43	LYS	2.2
74	o8	63	LYS	2.2
7	S5	157	ARG	2.2
7	s5	137	ILE	2.2
9	S7	125	ILE	2.2
30	d8	38	ARG	2.2
40	L3	146	ARG	2.2
5	S3	63	GLY	2.2
25	D3	44	GLY	2.2
49	M3	136	GLU	2.2
33	E1	88	PRO	2.2
5	S3	152	PHE	2.2
13	c1	139	VAL	2.2
28	D6	21	VAL	2.2
30	d8	30	VAL	2.2
62	N6	85	VAL	2.2
66	O0	50	VAL	2.2
5	S3	101	GLN	2.2
10	S8	20	GLN	2.2
61	n5	85	GLN	2.2
63	N7	60	LYS	2.2
77	Q1	14	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	S0	84	ARG	2.2
4	S2	168	ARG	2.2
13	c1	31	THR	2.2
49	m3	37	ASN	2.2
70	o4	90	ILE	2.2
5	S3	128	GLU	2.2
30	d8	31	GLU	2.2
35	SM	116	GLU	2.2
41	l4	14	GLU	2.2
59	n3	68	GLU	2.2
6	S4	24	SER	2.2
1	6	1082	C	2.2
5	s3	77	PHE	2.2
5	s3	127	MET	2.2
17	C5	73	PRO	2.2
10	S8	37	LYS	2.2
10	S8	191	PHE	2.2
7	S5	71	ALA	2.2
30	D8	10	ALA	2.2
49	m3	44	ALA	2.2
64	N8	35	ALA	2.2
67	O1	67	VAL	2.2
73	o7	10	LYS	2.2
74	o8	36	LYS	2.2
77	Q1	3	ALA	2.2
1	2	706	A	2.2
1	2	898	A	2.2
12	C0	54	TYR	2.2
18	C6	105	LEU	2.2
19	c7	113	LEU	2.2
30	D8	18	ARG	2.2
36	1	2100	A	2.2
48	M1	112	LEU	2.2
53	M7	130	TYR	2.2
53	M7	128	ARG	2.2
16	c4	51	ASP	2.2
45	L8	24	ASN	2.2
4	s2	129	ILE	2.2
10	S8	186	GLY	2.2
28	D6	30	ILE	2.2
35	sM	77	THR	2.2
45	l8	75	ILE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
61	N5	67	ILE	2.2
61	n5	63	ILE	2.2
16	c4	125	SER	2.2
34	sR	129	LYS	2.2
12	c0	1	MET	2.2
19	c7	65	PRO	2.2
25	d3	38	PHE	2.2
1	6	320	U	2.2
3	s1	192	VAL	2.2
4	S2	205	ARG	2.2
6	S4	2	ALA	2.2
6	s4	187	ARG	2.2
10	s8	111	GLN	2.2
12	C0	22	VAL	2.2
16	c4	79	VAL	2.2
24	D2	81	VAL	2.2
46	L9	25	VAL	2.2
61	n5	107	VAL	2.2
10	S8	192	TYR	2.2
15	C3	80	LEU	2.2
34	sR	73	LEU	2.2
45	l8	130	TYR	2.2
2	s0	49	ASN	2.2
28	d6	94	ASN	2.2
33	e1	137	ASP	2.2
34	sR	196	ASN	2.2
39	l2	194	ASN	2.2
58	N2	52	ASN	2.2
4	s2	56	ILE	2.2
4	s2	68	ILE	2.2
4	s2	218	ILE	2.2
36	5	1026	A	2.2
7	S5	146	THR	2.2
16	c4	93	THR	2.2
18	C6	128	LYS	2.2
42	l5	120	LYS	2.2
61	n5	109	LYS	2.2
73	O7	69	HIS	2.2
3	s1	51	SER	2.2
34	SR	3	SER	2.2
34	sR	213	SER	2.2
36	5	2095	G	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
41	l4	85	SER	2.2
8	S6	45	PHE	2.2
74	o8	38	PHE	2.2
35	SM	157	GLN	2.2
2	S0	3	LEU	2.2
3	S1	218	LEU	2.2
4	S2	120	GLU	2.2
5	S3	135	GLU	2.2
8	S6	75	LEU	2.2
9	s7	153	LEU	2.2
11	S9	177	ALA	2.2
16	C4	78	ALA	2.2
36	1	1765	U	2.2
51	M5	104	GLU	2.2
58	N2	43	VAL	2.2
58	n2	69	ALA	2.2
59	n3	118	VAL	2.2
28	D6	59	TYR	2.2
66	o0	23	TYR	2.2
4	s2	53	ILE	2.2
4	s2	131	ILE	2.2
17	C5	48	GLY	2.2
20	C8	72	ILE	2.2
41	l4	79	GLY	2.2
51	M5	36	ILE	2.2
55	M9	53	LYS	2.2
57	n1	160	ILE	2.2
66	o0	32	LYS	2.2
74	O8	30	LYS	2.2
7	s5	21	THR	2.2
22	D0	29	THR	2.2
1	2	1427	A	2.1
25	D3	136	TRP	2.1
34	sR	92	TRP	2.1
40	L3	194	TRP	2.1
57	n1	159	PHE	2.1
64	N8	79	TRP	2.1
12	c0	29	GLN	2.1
13	c1	118	GLN	2.1
5	S3	214	GLU	2.1
10	S8	61	GLU	2.1
4	S2	207	LEU	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
19	c7	66	VAL	2.1
26	D4	79	VAL	2.1
27	d5	104	ALA	2.1
28	D6	81	ALA	2.1
36	5	1851	G	2.1
36	5	1952	G	2.1
36	5	2537	U	2.1
42	L5	2	ALA	2.1
49	m3	10	LEU	2.1
57	N1	126	VAL	2.1
63	N7	13	VAL	2.1
73	O7	67	LEU	2.1
3	s1	31	ASP	2.1
4	S2	161	LYS	2.1
11	S9	115	LYS	2.1
34	SR	76	ASP	2.1
40	L3	154	TYR	2.1
45	L8	63	LYS	2.1
61	N5	60	TYR	2.1
65	N9	22	LYS	2.1
71	O5	5	LYS	2.1
71	o5	72	GLY	2.1
4	S2	170	ILE	2.1
6	S4	173	ILE	2.1
42	l5	290	ILE	2.1
55	m9	115	ILE	2.1
16	C4	18	ARG	2.1
17	C5	78	THR	2.1
23	D1	62	ARG	2.1
28	D6	26	CYS	2.1
34	sR	10	ARG	2.1
72	o6	62	ARG	2.1
3	S1	36	SER	2.1
5	S3	156	PHE	2.1
18	C6	138	PHE	2.1
30	d8	58	GLU	2.1
62	n6	9	SER	2.1
72	O6	79	SER	2.1
78	q2	105	GLN	2.1
4	s2	35	TRP	2.1
73	O7	14	LYS	2.1
1	6	1058	U	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	S1	68	VAL	2.1
4	S2	113	LEU	2.1
6	S4	65	LEU	2.1
16	c4	137	LEU	2.1
21	c9	132	LEU	2.1
23	D1	32	VAL	2.1
61	n5	124	VAL	2.1
61	n5	126	LEU	2.1
2	s0	95	ALA	2.1
16	c4	40	ALA	2.1
64	n8	125	VAL	2.1
4	s2	222	TYR	2.1
5	S3	154	ASP	2.1
5	s3	15	GLY	2.1
6	s4	138	TYR	2.1
8	S6	66	GLY	2.1
5	s3	217	ILE	2.1
23	d1	24	ILE	2.1
80	e0	43	ARG	2.1
7	S5	147	THR	2.1
8	S6	225	GLU	2.1
25	D3	31	LYS	2.1
25	D3	36	THR	2.1
39	L2	119	LYS	2.1
53	m7	125	GLN	2.1
62	n6	55	GLU	2.1
9	s7	30	SER	2.1
33	E1	99	LYS	2.1
70	O4	6	THR	2.1
73	o7	85	LYS	2.1
6	s4	101	LEU	2.1
10	S8	165	LEU	2.1
15	C3	149	LEU	2.1
17	c5	26	LEU	2.1
33	e1	117	LEU	2.1
34	SR	144	LEU	2.1
39	L2	61	VAL	2.1
41	l4	286	VAL	2.1
42	L5	131	LEU	2.1
47	M0	87	LEU	2.1
50	M4	135	LEU	2.1
55	m9	119	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
74	O8	70	PRO	2.1
1	2	260	U	2.1
36	1	1820	U	2.1
39	L2	4	VAL	2.1
1	6	1707	A	2.1
5	s3	30	ALA	2.1
8	S6	213	ALA	2.1
14	c2	27	ALA	2.1
17	c5	131	ALA	2.1
40	L3	386	ASP	2.1
41	l4	78	GLY	2.1
45	l8	247	ASP	2.1
60	N4	16	GLY	2.1
20	C8	69	ILE	2.1
40	L3	328	ILE	2.1
58	N2	93	ILE	2.1
66	o0	58	TYR	2.1
59	n3	28	ASN	2.1
70	O4	60	ARG	2.1
12	C0	52	LYS	2.1
17	c5	52	LYS	2.1
39	L2	73	GLU	2.1
12	C0	62	GLN	2.1
1	6	1228	G	2.1
5	S3	55	THR	2.1
29	d7	58	SER	2.1
30	d8	36	THR	2.1
15	C3	53	LEU	2.1
17	c5	28	MET	2.1
24	D2	11	LEU	2.1
28	d6	39	MET	2.1
30	d8	6	PRO	2.1
34	sR	301	LEU	2.1
4	S2	103	VAL	2.1
15	C3	2	GLY	2.1
25	D3	108	GLY	2.1
34	sR	181	TRP	2.1
58	n2	92	TRP	2.1
70	O4	22	VAL	2.1
75	o9	26	TRP	2.1
7	S5	145	ASP	2.1
22	D0	45	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
45	L8	199	ALA	2.1
45	l8	117	ALA	2.1
51	M5	102	ALA	2.1
72	O6	48	ALA	2.1
73	O7	24	ARG	2.1
74	O8	62	ALA	2.1
1	6	900	A	2.1
4	S2	208	GLU	2.1
4	s2	119	LYS	2.1
25	d3	52	ILE	2.1
26	D4	116	LYS	2.1
26	D4	123	LYS	2.1
78	q2	29	LYS	2.1
14	C2	80	ASN	2.1
26	D4	15	ASN	2.1
2	s0	46	HIS	2.1
10	s8	20	GLN	2.1
70	o4	33	GLN	2.1
24	d2	50	PHE	2.1
24	D2	105	THR	2.1
34	sR	47	LEU	2.1
45	l8	90	THR	2.1
74	O8	22	THR	2.1
4	s2	236	PRO	2.1
2	s0	54	TRP	2.1
4	S2	91	ARG	2.1
8	s6	157	VAL	2.1
13	c1	75	VAL	2.1
18	c6	7	VAL	2.1
39	l2	113	VAL	2.1
61	N5	51	VAL	2.1
10	S8	17	LYS	2.1
10	S8	40	ALA	2.1
11	S9	4	ALA	2.1
19	c7	103	ASP	2.1
26	D4	3	ASP	2.1
32	E0	34	ALA	2.1
68	o2	16	LYS	2.1
24	D2	75	ILE	2.1
62	n6	119	ILE	2.1
75	O9	27	ILE	2.1
71	o5	16	GLN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	2	1794	A	2.1
36	1	2971	A	2.1
36	5	1842	A	2.1
70	O4	93	PHE	2.1
10	S8	189	LEU	2.1
11	S9	99	LEU	2.1
58	n2	76	LEU	2.1
70	O4	51	LEU	2.1
71	O5	41	LEU	2.1
5	S3	132	LYS	2.1
5	s3	7	LYS	2.1
18	C6	56	GLY	2.1
19	c7	67	ARG	2.1
23	d1	5	LYS	2.1
24	D2	67	GLY	2.1
32	E0	3	LYS	2.1
34	SR	25	THR	2.1
41	L4	103	THR	2.1
7	S5	53	VAL	2.1
7	s5	51	VAL	2.1
13	C1	125	VAL	2.1
39	L2	157	VAL	2.1
67	O1	23	VAL	2.1
67	o1	81	GLU	2.1
5	S3	98	ALA	2.1
16	C4	100	ALA	2.1
28	d6	40	ALA	2.1
34	sR	85	TRP	2.1
41	l4	106	TRP	2.1
45	L8	114	ALA	2.1
70	O4	111	ALA	2.1
71	o5	6	ALA	2.1
78	Q2	30	ALA	2.1
5	s3	34	TYR	2.1
16	c4	20	TYR	2.1
24	D2	39	GLN	2.1
28	d6	68	TYR	2.1
36	5	2440	G	2.1
5	S3	174	HIS	2.1
5	s3	134	CYS	2.1
5	S3	218	LEU	2.1
9	s7	34	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
11	S9	128	LEU	2.1
18	c6	117	LEU	2.1
24	D2	82	LYS	2.1
25	d3	144	ARG	2.1
32	E0	8	LEU	2.1
67	O1	20	LEU	2.1
72	o6	36	ARG	2.1
73	O7	26	SER	2.1
74	o8	39	ARG	2.1
1	6	1193	A	2.1
1	6	1756	A	2.1
36	5	2540	A	2.1
44	l7	24	GLU	2.1
5	S3	123	VAL	2.1
8	S6	81	VAL	2.1
33	e1	108	VAL	2.1
45	L8	90	THR	2.1
58	n2	27	VAL	2.1
1	2	320	U	2.1
24	D2	86	ILE	2.1
24	d2	108	ALA	2.1
36	5	1570	U	2.1
36	5	1763	U	2.1
4	S2	77	GLN	2.1
6	S4	228	ILE	2.1
16	C4	12	GLN	2.1
47	M0	216	TYR	2.1
70	O4	62	TYR	2.1
9	s7	56	LYS	2.1
9	s7	131	PHE	2.1
13	C1	46	LYS	2.1
62	n6	98	ASN	2.1
4	S2	41	LEU	2.1
7	S5	93	LEU	2.1
41	l4	252	GLU	2.1
55	m9	164	LEU	2.1
18	c6	61	SER	2.1
13	C1	108	PRO	2.0
23	D1	14	PRO	2.0
30	d8	15	VAL	2.0
30	d8	41	VAL	2.0
34	SR	51	ASP	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
41	l4	103	THR	2.0
73	o7	29	VAL	2.0
79	q3	64	VAL	2.0
5	S3	92	GLN	2.0
17	c5	107	ILE	2.0
36	5	441	U	2.0
48	M1	174	LYS	2.0
17	C5	33	PHE	2.0
25	D3	121	ARG	2.0
29	D7	42	ASN	2.0
5	s3	174	HIS	2.0
12	c0	18	GLU	2.0
27	d5	38	HIS	2.0
73	O7	57	HIS	2.0
9	S7	77	LEU	2.0
32	E0	6	GLY	2.0
34	sR	23	LEU	2.0
39	L2	248	GLY	2.0
45	l8	186	LEU	2.0
66	o0	34	LEU	2.0
4	S2	136	VAL	2.0
5	S3	136	VAL	2.0
15	C3	60	VAL	2.0
17	C5	53	PRO	2.0
20	c8	5	VAL	2.0
28	D6	39	MET	2.0
36	5	3285	C	2.0
38	8	84	C	2.0
45	L8	157	VAL	2.0
62	n6	11	ASP	2.0
63	n7	10	VAL	2.0
1	2	1243	G	2.0
5	s3	170	THR	2.0
30	d8	27	GLN	2.0
65	N9	25	LYS	2.0
36	1	2505	U	2.0
36	5	134	U	2.0
36	5	1555	U	2.0
40	L3	151	ILE	2.0
45	L8	196	ALA	2.0
64	N8	94	ALA	2.0
16	C4	133	ARG	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
55	m9	85	ARG	2.0
6	S4	54	TYR	2.0
19	c7	71	PHE	2.0
19	c7	87	GLU	2.0
41	l4	63	GLU	2.0
45	L8	94	PHE	2.0
51	m5	150	TRP	2.0
55	m9	140	GLU	2.0
56	n0	17	GLU	2.0
66	o0	59	TYR	2.0
25	D3	79	ASN	2.0
6	S4	190	GLY	2.0
19	c7	26	LEU	2.0
24	D2	38	LEU	2.0
59	N3	8	GLY	2.0
11	s9	87	SER	2.0
13	c1	77	SER	2.0
18	C6	140	LYS	2.0
33	E1	122	SER	2.0
34	sR	22	SER	2.0
3	s1	114	VAL	2.0
4	s2	45	VAL	2.0
6	s4	150	PRO	2.0
8	S6	9	VAL	2.0
8	s6	34	GLN	2.0
16	c4	57	PRO	2.0
22	d0	117	VAL	2.0
24	D2	121	VAL	2.0
28	D6	31	PRO	2.0
30	d8	47	PRO	2.0
34	SR	307	ASP	2.0
41	l4	8	VAL	2.0
47	m0	148	VAL	2.0
53	M7	96	GLN	2.0
63	n7	13	VAL	2.0
1	2	590	C	2.0
1	2	708	C	2.0
1	6	321	C	2.0
1	6	1426	C	2.0
3	S1	129	THR	2.0
10	S8	197	THR	2.0
19	C7	41	ILE	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
21	c9	113	ILE	2.0
22	D0	24	ILE	2.0
26	D4	130	ALA	2.0
35	sM	129	ALA	2.0
45	l8	102	ALA	2.0
45	l8	154	ALA	2.0
49	m3	3	ILE	2.0
49	m3	151	ALA	2.0
59	N3	51	ALA	2.0
7	s5	20	PHE	2.0
16	c4	23	PHE	2.0
19	C7	53	TYR	2.0
2	s0	21	ASN	2.0
2	s0	23	HIS	2.0
3	s1	226	GLY	2.0
60	N4	39	LEU	2.0
34	sR	161	LYS	2.0
39	L2	176	ASP	2.0
56	N0	18	SER	2.0
5	S3	94	ARG	2.0
5	s3	48	VAL	2.0
5	s3	179	GLN	2.0
7	S5	156	ARG	2.0
13	C1	59	PRO	2.0
13	c1	76	VAL	2.0
19	c7	58	MET	2.0
47	m0	79	VAL	2.0
49	m3	57	VAL	2.0
55	M9	94	VAL	2.0
58	n2	30	PRO	2.0
61	N5	44	PRO	2.0
61	n5	62	VAL	2.0
10	s8	72	ILE	2.0
18	c6	36	ILE	2.0
34	sR	122	ILE	2.0
61	n5	95	ILE	2.0
66	o0	76	GLU	2.0
3	S1	143	THR	2.0
27	D5	105	THR	2.0
34	SR	2	ALA	2.0
41	L4	67	THR	2.0
53	M7	129	THR	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	S2	215	PHE	2.0
10	s8	191	PHE	2.0
34	sR	241	PHE	2.0
8	s6	10	ASN	2.0
17	c5	132	GLY	2.0
34	SR	283	LYS	2.0
35	SM	109	GLY	2.0
36	5	247	C	2.0
51	M5	88	GLY	2.0
59	N3	33	ASN	2.0
67	O1	37	LYS	2.0
82	p0	184	GLY	2.0
13	C1	92	HIS	2.0
13	C1	104	HIS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3624	1/1	0.49	657.00	69,69,69,69	0
85	MG	1	3865	1/1	0.45	617.00	67,67,67,67	0
85	MG	6	1945	1/1	0.43	288.00	43,43,43,43	0
85	MG	6	1933	1/1	0.32	281.00	53,53,53,53	0
85	MG	6	2020	1/1	0.51	261.92	40,40,40,40	0
85	MG	2	1989	1/1	0.23	151.00	65,65,65,65	0
85	MG	5	3655	1/1	0.30	144.00	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3481	1/1	0.38	143.67	57,57,57,57	0
85	MG	2	1983	1/1	0.28	122.00	62,62,62,62	0
85	MG	4	211	1/1	0.28	115.00	52,52,52,52	0
85	MG	1	3419	1/1	0.36	108.00	74,74,74,74	0
85	MG	1	3827	1/1	0.44	107.40	33,33,33,33	0
85	MG	5	3707	1/1	0.40	104.60	75,75,75,75	0
85	MG	1	3761	1/1	0.26	102.00	42,42,42,42	0
85	MG	1	3861	1/1	0.96	97.00	65,65,65,65	0
85	MG	1	3634	1/1	0.33	87.28	60,60,60,60	0
85	MG	2	2003	1/1	0.52	80.56	96,96,96,96	0
85	MG	1	3548	1/1	0.30	80.50	42,42,42,42	0
85	MG	8	213	1/1	0.36	77.80	31,31,31,31	0
85	MG	6	1944	1/1	0.46	73.44	50,50,50,50	0
85	MG	2	1959	1/1	0.41	71.75	66,66,66,66	0
85	MG	1	3687	1/1	0.19	71.00	69,69,69,69	0
86	OHX	5	4236	7/7	0.32	70.89	125,125,125,125	0
85	MG	6	2019	1/1	0.26	59.67	48,48,48,48	0
85	MG	1	3590	1/1	0.40	54.53	34,34,34,34	0
85	MG	1	3583	1/1	0.26	54.50	31,31,31,31	0
85	MG	2	2017	1/1	0.39	54.11	58,58,58,58	0
85	MG	1	3789	1/1	0.56	53.27	26,26,26,26	0
85	MG	1	3529	1/1	0.39	52.23	29,29,29,29	0
85	MG	2	1946	1/1	0.38	52.20	64,64,64,64	0
86	OHX	1	4144	7/7	0.41	50.47	112,112,112,112	0
85	MG	1	3409	1/1	0.35	49.93	30,30,30,30	0
85	MG	5	3661	1/1	0.43	49.82	59,59,59,59	0
85	MG	5	3756	1/1	0.28	49.50	36,36,36,36	0
85	MG	3	204	1/1	0.58	49.10	51,51,51,51	0
86	OHX	5	4227	7/7	0.38	47.91	96,96,96,96	0
85	MG	5	3466	1/1	0.56	46.89	88,88,88,88	0
85	MG	6	1918	1/1	0.44	45.55	57,57,57,57	0
85	MG	5	3594	1/1	0.45	44.51	26,26,26,26	0
85	MG	6	1983	1/1	0.51	44.50	38,38,38,38	0
85	MG	1	3546	1/1	0.39	44.49	52,52,52,52	0
86	OHX	5	4212	7/7	0.42	42.31	98,98,98,98	0
85	MG	5	3573	1/1	0.29	41.52	26,26,26,26	0
85	MG	5	3856	1/1	0.47	40.50	68,68,68,68	0
85	MG	6	2029	1/1	0.55	40.11	68,68,68,68	0
85	MG	1	3579	1/1	0.47	39.16	33,33,33,33	0
85	MG	4	221	1/1	0.56	38.79	45,45,45,45	0
85	MG	N3	201	1/1	0.30	38.58	25,25,25,25	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3575	1/1	0.36	38.16	33,33,33,33	0
85	MG	5	3872	1/1	0.29	37.68	34,34,34,34	0
85	MG	2	1913	1/1	0.49	37.63	64,64,64,64	0
85	MG	2	2020	1/1	0.35	37.60	59,59,59,59	0
85	MG	6	1959	1/1	0.41	37.33	52,52,52,52	0
85	MG	1	3444	1/1	0.36	37.00	49,49,49,49	0
85	MG	2	1904	1/1	0.49	36.56	62,62,62,62	0
85	MG	6	2040	1/1	0.50	35.97	82,82,82,82	0
85	MG	1	3493	1/1	0.30	34.54	69,69,69,69	0
85	MG	1	3573	1/1	0.47	34.23	32,32,32,32	0
85	MG	5	3630	1/1	0.47	34.10	75,75,75,75	0
85	MG	5	3874	1/1	0.51	33.21	41,41,41,41	0
85	MG	2	1967	1/1	0.40	32.87	70,70,70,70	0
85	MG	1	3552	1/1	0.43	32.35	32,32,32,32	0
85	MG	5	3540	1/1	0.38	31.75	28,28,28,28	0
85	MG	6	1961	1/1	0.38	31.63	60,60,60,60	0
85	MG	7	209	1/1	0.39	31.35	35,35,35,35	0
85	MG	1	3817	1/1	0.35	31.15	40,40,40,40	0
85	MG	7	204	1/1	0.43	31.13	61,61,61,61	0
85	MG	5	3673	1/1	0.34	31.00	37,37,37,37	0
85	MG	7	215	1/1	0.34	31.00	48,48,48,48	0
85	MG	5	3887	1/1	0.35	30.96	53,53,53,53	0
85	MG	2	1975	1/1	0.48	30.57	71,71,71,71	0
85	MG	6	2013	1/1	0.51	29.92	42,42,42,42	0
85	MG	1	3728	1/1	0.48	29.90	27,27,27,27	0
85	MG	2	1981	1/1	0.31	29.76	52,52,52,52	0
85	MG	5	3403	1/1	0.41	29.22	53,53,53,53	0
85	MG	5	3847	1/1	0.26	28.75	51,51,51,51	0
85	MG	1	3860	1/1	0.35	27.67	43,43,43,43	0
85	MG	1	3528	1/1	0.31	27.59	37,37,37,37	0
85	MG	1	3412	1/1	0.36	27.21	37,37,37,37	0
86	OHX	6	2181	7/7	0.40	27.19	113,113,113,113	0
85	MG	1	3809	1/1	0.78	27.18	162,162,162,162	0
85	MG	2	1984	1/1	0.34	26.87	60,60,60,60	0
85	MG	1	3463	1/1	0.32	26.82	19,19,19,19	0
85	MG	5	3477	1/1	0.32	26.69	59,59,59,59	0
85	MG	6	2046	1/1	0.47	26.12	66,66,66,66	0
85	MG	5	3683	1/1	0.28	25.78	51,51,51,51	0
85	MG	1	3646	1/1	0.22	25.78	30,30,30,30	0
85	MG	3	207	1/1	0.41	25.74	55,55,55,55	0
85	MG	5	3731	1/1	0.20	25.67	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3820	1/1	0.52	25.59	84,84,84,84	0
85	MG	1	3469	1/1	0.31	25.37	56,56,56,56	0
85	MG	1	3854	1/1	0.44	25.28	52,52,52,52	0
85	MG	1	3667	1/1	0.40	25.20	62,62,62,62	0
85	MG	1	3408	1/1	0.28	24.96	27,27,27,27	0
85	MG	1	3566	1/1	0.43	24.91	33,33,33,33	0
85	MG	5	3574	1/1	0.38	24.74	40,40,40,40	0
85	MG	5	3633	1/1	0.51	24.50	71,71,71,71	0
85	MG	1	3721	1/1	0.33	24.46	44,44,44,44	0
85	MG	5	3737	1/1	0.26	24.31	36,36,36,36	0
85	MG	5	3582	1/1	0.41	24.31	27,27,27,27	0
86	OHX	5	4151	7/7	0.33	23.98	92,92,92,92	0
85	MG	6	2027	1/1	0.31	23.91	61,61,61,61	0
85	MG	5	3511	1/1	0.38	23.89	45,45,45,45	0
85	MG	1	3537	1/1	0.47	23.87	25,25,25,25	0
85	MG	1	3591	1/1	0.34	23.68	34,34,34,34	0
85	MG	6	1946	1/1	0.39	23.64	52,52,52,52	0
85	MG	6	2039	1/1	0.42	23.50	67,67,67,67	0
85	MG	6	1956	1/1	0.43	23.39	38,38,38,38	0
85	MG	2	1960	1/1	0.45	22.91	87,87,87,87	0
85	MG	6	2011	1/1	0.34	22.86	54,54,54,54	0
85	MG	5	3646	1/1	0.25	22.65	35,35,35,35	0
85	MG	6	1943	1/1	0.38	22.56	32,32,32,32	0
85	MG	1	3405	1/1	0.70	22.25	95,95,95,95	0
86	OHX	1	4205	7/7	0.39	22.23	108,108,108,108	0
85	MG	6	1927	1/1	0.34	22.22	39,39,39,39	0
85	MG	5	3438	1/1	0.36	22.21	58,58,58,58	0
85	MG	2	1929	1/1	0.38	22.20	51,51,51,51	0
85	MG	5	3634	1/1	0.34	22.06	33,33,33,33	0
85	MG	5	3647	1/1	0.18	22.00	41,41,41,41	0
85	MG	1	3423	1/1	0.21	21.98	28,28,28,28	0
85	MG	5	3515	1/1	0.30	21.97	28,28,28,28	0
85	MG	1	3730	1/1	0.39	21.91	23,23,23,23	0
86	OHX	1	4142	7/7	0.40	21.56	89,89,89,89	0
85	MG	6	1951	1/1	0.39	21.34	55,55,55,55	0
86	OHX	5	4219	7/7	0.36	21.23	111,111,111,111	0
85	MG	5	3410	1/1	0.34	21.07	47,47,47,47	0
85	MG	2	2014	1/1	0.42	20.94	61,61,61,61	0
85	MG	2	1951	1/1	0.49	20.94	68,68,68,68	0
85	MG	1	3713	1/1	0.52	20.93	73,73,73,73	0
86	OHX	1	4179	7/7	0.43	20.82	101,101,101,101	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4180	7/7	0.31	20.82	120,120,120,120	0
85	MG	2	2010	1/1	0.39	20.77	62,62,62,62	0
85	MG	5	3821	1/1	0.42	20.58	32,32,32,32	0
85	MG	6	1955	1/1	0.46	20.54	32,32,32,32	0
85	MG	2	2018	1/1	0.34	20.47	62,62,62,62	0
85	MG	5	3535	1/1	0.38	20.43	32,32,32,32	0
85	MG	6	1935	1/1	0.34	20.38	46,46,46,46	0
85	MG	5	3618	1/1	0.24	20.25	37,37,37,37	0
86	OHX	1	4192	7/7	0.44	20.22	98,98,98,98	0
86	OHX	1	4071	7/7	0.24	20.21	99,99,99,99	0
86	OHX	5	4217	7/7	0.31	20.16	106,106,106,106	0
85	MG	5	3547	1/1	0.41	20.06	32,32,32,32	0
86	OHX	6	2147	7/7	0.31	20.05	90,90,90,90	0
86	OHX	1	4174	7/7	0.33	20.04	112,112,112,112	0
85	MG	2	1914	1/1	0.42	19.97	55,55,55,55	0
85	MG	5	3786	1/1	0.28	19.95	70,70,70,70	0
85	MG	n3	201	1/1	0.42	19.92	21,21,21,21	0
86	OHX	M9	202	7/7	0.24	19.89	130,130,130,130	0
85	MG	1	3540	1/1	0.34	19.70	48,48,48,48	0
86	OHX	6	2190	7/7	0.39	19.62	110,110,110,110	0
85	MG	1	3504	1/1	0.38	19.55	39,39,39,39	0
85	MG	5	3871	1/1	0.51	19.54	47,47,47,47	0
85	MG	3	201	1/1	0.46	19.28	59,59,59,59	0
85	MG	1	3858	1/1	0.33	19.12	36,36,36,36	0
85	MG	1	3684	1/1	0.24	19.00	41,41,41,41	0
86	OHX	5	4193	7/7	0.40	18.96	107,107,107,107	0
85	MG	2	2008	1/1	0.40	18.91	40,40,40,40	0
86	OHX	5	4184	7/7	0.28	18.88	98,98,98,98	0
85	MG	6	2028	1/1	0.39	18.83	56,56,56,56	0
85	MG	5	3453	1/1	0.34	18.81	34,34,34,34	0
86	OHX	6	2174	7/7	0.41	18.76	101,101,101,101	0
86	OHX	1	4208	7/7	0.46	18.68	100,100,100,100	0
85	MG	3	209	1/1	0.38	18.67	50,50,50,50	0
85	MG	1	3580	1/1	0.32	18.46	34,34,34,34	0
85	MG	1	3844	1/1	0.27	18.33	40,40,40,40	0
86	OHX	1	4191	7/7	0.31	18.29	104,104,104,104	0
85	MG	3	213	1/1	0.44	18.20	49,49,49,49	0
86	OHX	5	4173	7/7	0.32	18.20	110,110,110,110	0
86	OHX	5	4190	7/7	0.36	18.19	98,98,98,98	0
85	MG	1	3515	1/1	0.45	18.12	29,29,29,29	0
85	MG	2	1921	1/1	0.36	18.12	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3832	1/1	0.26	18.12	37,37,37,37	0
85	MG	6	1919	1/1	0.35	17.92	34,34,34,34	0
85	MG	5	3580	1/1	0.31	17.71	36,36,36,36	0
85	MG	5	3412	1/1	0.31	17.69	26,26,26,26	0
85	MG	2	1924	1/1	0.32	17.68	65,65,65,65	0
85	MG	6	1931	1/1	0.40	17.58	54,54,54,54	0
86	OHX	1	4166	7/7	0.20	17.57	130,130,130,130	0
86	OHX	2	2160	7/7	0.44	17.46	117,117,117,117	0
85	MG	5	3780	1/1	0.34	17.46	70,70,70,70	0
85	MG	1	3663	1/1	0.42	17.46	31,31,31,31	0
85	MG	1	3516	1/1	0.33	17.44	28,28,28,28	0
85	MG	5	3522	1/1	0.30	17.10	31,31,31,31	0
85	MG	1	3562	1/1	0.33	17.10	22,22,22,22	0
85	MG	6	2038	1/1	0.49	17.09	48,48,48,48	0
85	MG	5	3581	1/1	0.29	17.06	36,36,36,36	0
85	MG	5	3473	1/1	0.28	17.00	44,44,44,44	0
85	MG	3	214	1/1	0.33	16.94	50,50,50,50	0
85	MG	6	1907	1/1	0.35	16.90	53,53,53,53	0
85	MG	5	3570	1/1	0.34	16.89	30,30,30,30	0
86	OHX	5	4185	7/7	0.43	16.75	94,94,94,94	0
85	MG	1	3674	1/1	0.31	16.75	50,50,50,50	0
85	MG	1	3843	1/1	0.30	16.67	46,46,46,46	0
85	MG	1	3834	1/1	0.32	16.50	16,16,16,16	0
86	OHX	5	4149	7/7	0.27	16.47	96,96,96,96	0
85	MG	7	201	1/1	0.46	16.39	36,36,36,36	0
85	MG	8	201	1/1	0.38	16.27	31,31,31,31	0
85	MG	5	3783	1/1	0.31	16.25	50,50,50,50	0
85	MG	5	3793	1/1	0.46	16.25	36,36,36,36	0
85	MG	5	3755	1/1	0.25	16.19	47,47,47,47	0
85	MG	6	2021	1/1	0.29	16.18	93,93,93,93	0
86	OHX	6	2163	7/7	0.28	16.16	106,106,106,106	0
85	MG	6	1916	1/1	0.40	16.13	54,54,54,54	0
85	MG	6	1925	1/1	0.37	16.10	34,34,34,34	0
85	MG	5	3572	1/1	0.40	16.08	34,34,34,34	0
85	MG	6	1971	1/1	0.33	16.07	54,54,54,54	0
85	MG	1	3574	1/1	0.35	15.96	30,30,30,30	0
85	MG	7	205	1/1	0.30	15.81	23,23,23,23	0
85	MG	5	3566	1/1	0.35	15.80	24,24,24,24	0
85	MG	6	1934	1/1	0.39	15.77	62,62,62,62	0
85	MG	5	3644	1/1	0.30	15.69	29,29,29,29	0
85	MG	1	3456	1/1	0.38	15.69	50,50,50,50	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	6	1909	1/1	0.41	15.68	79,79,79,79	0
85	MG	1	3592	1/1	0.43	15.64	43,43,43,43	0
85	MG	6	1975	1/1	0.28	15.62	53,53,53,53	0
86	OHX	1	4195	7/7	0.28	15.62	116,116,116,116	0
85	MG	2	1965	1/1	0.35	15.60	74,74,74,74	0
85	MG	5	3578	1/1	0.29	15.58	28,28,28,28	0
85	MG	4	220	1/1	0.44	15.58	77,77,77,77	0
86	OHX	1	4165	7/7	0.35	15.54	123,123,123,123	0
85	MG	1	3526	1/1	0.27	15.34	21,21,21,21	0
85	MG	5	3517	1/1	0.32	15.25	18,18,18,18	0
85	MG	1	3585	1/1	0.41	15.19	40,40,40,40	0
85	MG	1	3509	1/1	0.28	15.15	34,34,34,34	0
86	OHX	5	4179	7/7	0.23	15.12	113,113,113,113	0
85	MG	2	1936	1/1	0.35	15.05	42,42,42,42	0
85	MG	5	3588	1/1	0.34	15.01	30,30,30,30	0
85	MG	2	2011	1/1	0.23	15.00	59,59,59,59	0
85	MG	6	1926	1/1	0.29	14.97	40,40,40,40	0
85	MG	1	3607	1/1	0.36	14.91	45,45,45,45	0
85	MG	5	3734	1/1	0.28	14.90	58,58,58,58	0
85	MG	5	3571	1/1	0.33	14.88	27,27,27,27	0
85	MG	2	1997	1/1	0.23	14.87	80,80,80,80	0
85	MG	5	3833	1/1	0.31	14.83	26,26,26,26	0
85	MG	1	3677	1/1	0.35	14.81	60,60,60,60	0
85	MG	5	3730	1/1	0.24	14.78	41,41,41,41	0
85	MG	6	1921	1/1	0.34	14.73	36,36,36,36	0
85	MG	n9	3802	1/1	0.48	14.72	31,31,31,31	0
85	MG	5	3521	1/1	0.37	14.63	34,34,34,34	0
85	MG	1	3475	1/1	0.24	14.60	64,64,64,64	0
85	MG	5	3593	1/1	0.39	14.57	34,34,34,34	0
86	OHX	5	4230	7/7	0.36	14.54	99,99,99,99	0
85	MG	8	206	1/1	0.74	14.53	44,44,44,44	0
85	MG	6	1960	1/1	0.34	14.50	38,38,38,38	0
85	MG	5	3751	1/1	0.30	14.44	49,49,49,49	0
85	MG	6	2015	1/1	0.56	14.27	104,104,104,104	0
85	MG	6	1914	1/1	0.30	14.24	29,29,29,29	0
85	MG	6	1928	1/1	0.30	14.19	54,54,54,54	0
85	MG	5	3880	1/1	0.33	14.18	45,45,45,45	0
85	MG	5	3652	1/1	0.28	13.95	55,55,55,55	0
85	MG	1	3859	1/1	0.47	13.95	54,54,54,54	0
85	MG	1	3799	1/1	0.40	13.87	21,21,21,21	0
86	OHX	1	4073	7/7	0.31	13.71	94,94,94,94	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3551	1/1	0.34	13.69	39,39,39,39	0
85	MG	5	3721	1/1	0.24	13.67	46,46,46,46	0
85	MG	5	3413	1/1	0.27	13.65	25,25,25,25	0
86	OHX	1	4187	7/7	0.45	13.63	105,105,105,105	0
86	OHX	5	4160	7/7	0.30	13.61	93,93,93,93	0
85	MG	5	3498	1/1	0.34	13.44	27,27,27,27	0
85	MG	5	3531	1/1	0.29	13.43	31,31,31,31	0
86	OHX	2	2144	7/7	0.33	13.40	105,105,105,105	0
86	OHX	2	2172	7/7	0.26	13.38	119,119,119,119	0
85	MG	5	3505	1/1	0.30	13.35	30,30,30,30	0
85	MG	6	1939	1/1	0.37	13.31	51,51,51,51	0
85	MG	5	3530	1/1	0.35	13.28	40,40,40,40	0
85	MG	1	3484	1/1	0.39	13.28	38,38,38,38	0
86	OHX	5	4159	7/7	0.22	13.28	101,101,101,101	0
85	MG	6	1958	1/1	0.35	13.27	46,46,46,46	0
85	MG	6	1911	1/1	0.24	13.25	38,38,38,38	0
85	MG	5	3595	1/1	0.33	13.19	27,27,27,27	0
85	MG	1	3614	1/1	0.26	13.17	29,29,29,29	0
85	MG	5	3738	1/1	0.38	13.15	61,61,61,61	0
85	MG	1	3510	1/1	0.32	13.14	25,25,25,25	0
85	MG	6	1903	1/1	0.27	13.12	36,36,36,36	0
85	MG	5	3606	1/1	0.30	13.10	18,18,18,18	0
85	MG	5	3562	1/1	0.32	13.08	24,24,24,24	0
85	MG	5	3884	1/1	0.41	13.05	55,55,55,55	0
85	MG	5	3548	1/1	0.39	13.00	44,44,44,44	0
85	MG	6	1947	1/1	0.45	12.90	50,50,50,50	0
85	MG	5	3560	1/1	0.35	12.88	25,25,25,25	0
85	MG	5	3881	1/1	0.49	12.88	81,81,81,81	0
85	MG	1	3587	1/1	0.38	12.77	26,26,26,26	0
86	OHX	6	2194	7/7	0.21	12.75	140,140,140,140	0
85	MG	3	206	1/1	0.35	12.74	29,29,29,29	0
86	OHX	2	2123	7/7	0.20	12.68	114,114,114,114	0
86	OHX	1	4145	7/7	0.27	12.65	110,110,110,110	0
85	MG	5	3770	1/1	0.29	12.53	70,70,70,70	0
86	OHX	1	4162	7/7	0.28	12.50	121,121,121,121	0
86	OHX	6	2168	7/7	0.29	12.50	97,97,97,97	0
85	MG	6	1904	1/1	0.40	12.48	56,56,56,56	0
85	MG	2	2013	1/1	0.19	12.43	44,44,44,44	0
85	MG	1	3543	1/1	0.31	12.35	29,29,29,29	0
85	MG	5	3841	1/1	0.28	12.33	37,37,37,37	0
85	MG	5	3727	1/1	0.22	12.23	85,85,85,85	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3766	1/1	0.41	12.22	32,32,32,32	0
85	MG	1	3853	1/1	0.22	12.20	35,35,35,35	0
85	MG	4	214	1/1	0.49	12.15	43,43,43,43	0
85	MG	5	3623	1/1	0.23	12.04	33,33,33,33	0
86	OHX	6	2183	7/7	0.46	11.94	118,118,118,118	0
85	MG	5	3523	1/1	0.31	11.92	23,23,23,23	0
86	OHX	8	227	7/7	0.31	11.86	108,108,108,108	0
85	MG	5	3869	1/1	0.26	11.86	28,28,28,28	0
85	MG	5	3858	1/1	0.21	11.86	70,70,70,70	0
85	MG	5	3643	1/1	0.35	11.81	37,37,37,37	0
85	MG	5	3596	1/1	0.36	11.79	25,25,25,25	0
85	MG	1	3749	1/1	0.23	11.76	43,43,43,43	0
85	MG	1	3506	1/1	0.31	11.70	37,37,37,37	0
85	MG	5	3569	1/1	0.32	11.66	20,20,20,20	0
85	MG	5	3896	1/1	0.23	11.60	82,82,82,82	0
85	MG	SM	301	1/1	0.23	11.51	38,38,38,38	0
85	MG	5	3467	1/1	0.28	11.48	31,31,31,31	0
85	MG	1	3410	1/1	0.27	11.47	36,36,36,36	0
85	MG	6	1937	1/1	0.34	11.47	36,36,36,36	0
86	OHX	14	403	7/7	0.37	11.45	111,111,111,111	0
85	MG	6	1917	1/1	0.34	11.44	44,44,44,44	0
85	MG	1	3485	1/1	0.27	11.43	35,35,35,35	0
85	MG	5	3431	1/1	0.34	11.30	37,37,37,37	0
85	MG	5	3748	1/1	0.28	11.29	29,29,29,29	0
85	MG	5	3426	1/1	0.30	11.28	37,37,37,37	0
86	OHX	5	4200	7/7	0.29	11.22	114,114,114,114	0
85	MG	6	1922	1/1	0.34	11.12	42,42,42,42	0
85	MG	1	3670	1/1	0.35	11.12	65,65,65,65	0
85	MG	5	3565	1/1	0.32	11.08	22,22,22,22	0
86	OHX	M7	207	7/7	0.43	11.01	83,83,83,83	0
85	MG	5	4254	1/1	0.60	11.00	19,19,19,19	0
85	MG	1	3623	1/1	0.19	10.97	42,42,42,42	0
85	MG	5	3518	1/1	0.40	10.97	32,32,32,32	0
85	MG	2	1915	1/1	0.40	10.96	53,53,53,53	0
85	MG	5	3508	1/1	0.34	10.96	24,24,24,24	0
85	MG	5	3579	1/1	0.29	10.95	28,28,28,28	0
86	OHX	3	225	7/7	0.27	10.94	103,103,103,103	0
85	MG	2	1995	1/1	0.30	10.93	75,75,75,75	0
85	MG	1	3716	1/1	0.44	10.92	39,39,39,39	0
85	MG	5	3520	1/1	0.27	10.90	24,24,24,24	0
85	MG	5	3855	1/1	0.28	10.83	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3544	1/1	0.36	10.77	41,41,41,41	0
85	MG	1	3556	1/1	0.34	10.76	30,30,30,30	0
86	OHX	2	2149	7/7	0.29	10.75	96,96,96,96	0
86	OHX	5	4214	7/7	0.38	10.74	110,110,110,110	0
85	MG	1	3401	1/1	0.34	10.73	33,33,33,33	0
85	MG	1	3575	1/1	0.32	10.71	22,22,22,22	0
86	OHX	5	4244	7/7	0.35	10.66	122,122,122,122	0
85	MG	5	3813	1/1	0.38	10.66	47,47,47,47	0
85	MG	1	3599	1/1	0.42	10.66	20,20,20,20	0
85	MG	1	3718	1/1	0.56	10.61	33,33,33,33	0
85	MG	5	3449	1/1	0.41	10.58	53,53,53,53	0
86	OHX	5	4234	7/7	0.34	10.58	111,111,111,111	0
85	MG	5	3559	1/1	0.28	10.52	21,21,21,21	0
85	MG	1	3522	1/1	0.34	10.50	27,27,27,27	0
85	MG	6	1940	1/1	0.58	10.49	70,70,70,70	0
86	OHX	1	4189	7/7	0.33	10.45	145,145,145,145	0
85	MG	1	3808	1/1	0.29	10.44	30,30,30,30	0
85	MG	5	3672	1/1	0.20	10.42	57,57,57,57	0
86	OHX	5	4164	7/7	0.27	10.39	111,111,111,111	0
85	MG	5	3502	1/1	0.33	10.38	28,28,28,28	0
86	OHX	1	4065	7/7	0.31	10.32	113,113,113,113	0
85	MG	1	3847	1/1	0.27	10.29	49,49,49,49	0
85	MG	2	1934	1/1	0.38	10.29	58,58,58,58	0
85	MG	2	1933	1/1	0.27	10.29	57,57,57,57	0
85	MG	1	3536	1/1	0.28	10.28	42,42,42,42	0
86	OHX	1	4049	7/7	0.23	10.27	87,87,87,87	0
85	MG	6	1929	1/1	0.25	10.21	49,49,49,49	0
85	MG	5	3561	1/1	0.47	10.19	31,31,31,31	0
85	MG	1	3796	1/1	0.74	10.15	31,31,31,31	0
85	MG	1	3742	1/1	0.34	10.14	53,53,53,53	0
86	OHX	5	4152	7/7	0.36	10.13	95,95,95,95	0
85	MG	5	3846	1/1	0.26	10.01	50,50,50,50	0
86	OHX	1	4116	7/7	0.34	10.00	91,91,91,91	0
85	MG	5	3598	1/1	0.27	9.96	30,30,30,30	0
85	MG	5	3499	1/1	0.27	9.96	24,24,24,24	0
85	MG	6	2043	1/1	0.25	9.88	39,39,39,39	0
85	MG	6	1980	1/1	0.28	9.88	60,60,60,60	0
85	MG	2	1907	1/1	0.37	9.87	46,46,46,46	0
85	MG	5	3576	1/1	0.38	9.87	36,36,36,36	0
85	MG	1	4219	1/1	0.30	9.85	24,24,24,24	0
86	OHX	5	4208	7/7	0.26	9.80	110,110,110,110	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3848	1/1	0.28	9.80	34,34,34,34	0
85	MG	6	1963	1/1	0.28	9.74	67,67,67,67	0
85	MG	1	3776	1/1	0.25	9.73	53,53,53,53	0
86	OHX	1	4123	7/7	0.32	9.71	94,94,94,94	0
85	MG	1	3479	1/1	0.34	9.67	70,70,70,70	0
85	MG	5	3796	1/1	0.24	9.64	27,27,27,27	0
86	OHX	1	4173	7/7	0.37	9.64	132,132,132,132	0
85	MG	5	3670	1/1	0.25	9.63	44,44,44,44	0
85	MG	1	3560	1/1	0.29	9.59	28,28,28,28	0
85	MG	1	3593	1/1	0.33	9.56	59,59,59,59	0
85	MG	5	3892	1/1	0.27	9.50	38,38,38,38	0
85	MG	7	206	1/1	0.20	9.50	36,36,36,36	0
85	MG	5	3558	1/1	0.26	9.49	24,24,24,24	0
86	OHX	5	4238	7/7	0.37	9.48	117,117,117,117	0
86	OHX	5	4140	7/7	0.27	9.42	101,101,101,101	0
85	MG	5	3807	1/1	0.24	9.41	29,29,29,29	0
85	MG	1	3709	1/1	0.25	9.36	28,28,28,28	0
86	OHX	8	228	7/7	0.30	9.33	101,101,101,101	0
85	MG	2	1926	1/1	0.39	9.33	77,77,77,77	0
86	OHX	1	4031	7/7	0.22	9.32	88,88,88,88	0
85	MG	1	3815	1/1	0.24	9.31	26,26,26,26	0
85	MG	5	3680	1/1	0.40	9.25	68,68,68,68	0
86	OHX	6	2186	7/7	0.35	9.25	113,113,113,113	0
86	OHX	6	2180	7/7	0.32	9.24	106,106,106,106	0
86	OHX	6	2165	7/7	0.26	9.23	119,119,119,119	0
85	MG	5	3519	1/1	0.24	9.20	35,35,35,35	0
85	MG	5	3875	1/1	0.28	9.19	30,30,30,30	0
85	MG	2	2019	1/1	0.36	9.16	61,61,61,61	0
86	OHX	1	4130	7/7	0.30	9.14	120,120,120,120	0
85	MG	1	3734	1/1	0.29	9.14	68,68,68,68	0
86	OHX	1	4185	7/7	0.25	9.10	111,111,111,111	0
85	MG	1	3527	1/1	0.34	9.10	27,27,27,27	0
85	MG	1	3402	1/1	0.33	9.02	51,51,51,51	0
85	MG	6	1991	1/1	0.29	9.02	56,56,56,56	0
85	MG	1	3561	1/1	0.27	9.01	30,30,30,30	0
85	MG	2	2012	1/1	0.20	9.00	57,57,57,57	0
85	MG	1	3679	1/1	0.23	8.97	38,38,38,38	0
86	OHX	1	4085	7/7	0.25	8.97	114,114,114,114	0
85	MG	1	3594	1/1	0.29	8.96	22,22,22,22	0
85	MG	6	1901	1/1	0.28	8.91	37,37,37,37	0
86	OHX	8	225	7/7	0.33	8.89	103,103,103,103	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4228	7/7	0.25	8.89	141,141,141,141	0
85	MG	6	1913	1/1	0.33	8.86	46,46,46,46	0
85	MG	1	3502	1/1	0.31	8.86	35,35,35,35	0
86	OHX	1	4140	7/7	0.27	8.85	100,100,100,100	0
86	OHX	5	4195	7/7	0.28	8.83	95,95,95,95	0
85	MG	6	1952	1/1	0.37	8.83	53,53,53,53	0
85	MG	5	3506	1/1	0.29	8.83	23,23,23,23	0
86	OHX	1	4199	7/7	0.28	8.80	107,107,107,107	0
85	MG	2	1958	1/1	0.23	8.78	62,62,62,62	0
85	MG	1	3637	1/1	0.32	8.73	41,41,41,41	0
85	MG	5	3462	1/1	0.29	8.73	27,27,27,27	0
85	MG	5	3746	1/1	0.25	8.72	51,51,51,51	0
86	OHX	2	2179	7/7	0.23	8.70	137,137,137,137	0
85	MG	2	1932	1/1	0.34	8.69	48,48,48,48	0
86	OHX	6	2187	7/7	0.32	8.66	136,136,136,136	0
85	MG	5	3537	1/1	0.22	8.65	33,33,33,33	0
86	OHX	4	236	7/7	0.32	8.60	105,105,105,105	0
86	OHX	1	4118	7/7	0.26	8.55	95,95,95,95	0
85	MG	5	3825	1/1	0.32	8.51	31,31,31,31	0
85	MG	1	3739	1/1	0.30	8.50	53,53,53,53	0
85	MG	5	3479	1/1	0.26	8.46	56,56,56,56	0
85	MG	2	2015	1/1	0.26	8.45	59,59,59,59	0
85	MG	1	3466	1/1	0.23	8.40	49,49,49,49	0
85	MG	7	203	1/1	0.28	8.39	43,43,43,43	0
85	MG	6	1954	1/1	0.32	8.39	33,33,33,33	0
85	MG	3	203	1/1	0.21	8.38	75,75,75,75	0
85	MG	5	3528	1/1	0.33	8.36	22,22,22,22	0
85	MG	5	3577	1/1	0.28	8.36	23,23,23,23	0
86	OHX	5	4089	7/7	0.24	8.35	84,84,84,84	0
86	OHX	2	2170	7/7	0.29	8.33	126,126,126,126	0
85	MG	1	3596	1/1	0.36	8.33	20,20,20,20	0
85	MG	1	3404	1/1	0.31	8.31	46,46,46,46	0
86	OHX	6	2171	7/7	0.30	8.30	90,90,90,90	0
86	OHX	1	4193	7/7	0.28	8.27	110,110,110,110	0
86	OHX	6	2160	7/7	0.45	8.26	103,103,103,103	0
85	MG	1	3451	1/1	0.30	8.26	34,34,34,34	0
86	OHX	5	4158	7/7	0.29	8.20	110,110,110,110	0
86	OHX	8	224	7/7	0.33	8.19	108,108,108,108	0
85	MG	1	3513	1/1	0.31	8.14	18,18,18,18	0
85	MG	6	2035	1/1	0.35	8.13	74,74,74,74	0
86	OHX	5	4176	7/7	0.40	8.11	86,86,86,86	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3583	1/1	0.39	8.09	27,27,27,27	0
85	MG	2	1943	1/1	0.25	8.08	55,55,55,55	0
85	MG	5	3693	1/1	0.24	8.08	59,59,59,59	0
86	OHX	2	2117	7/7	0.20	8.07	110,110,110,110	0
86	OHX	1	4178	7/7	0.29	8.04	126,126,126,126	0
85	MG	5	3546	1/1	0.30	8.02	39,39,39,39	0
85	MG	5	3463	1/1	0.31	8.01	44,44,44,44	0
85	MG	3	202	1/1	0.25	7.99	39,39,39,39	0
86	OHX	2	2137	7/7	0.32	7.97	104,104,104,104	0
85	MG	1	3848	1/1	0.21	7.95	45,45,45,45	0
85	MG	6	1964	1/1	0.24	7.89	44,44,44,44	0
85	MG	1	3532	1/1	0.32	7.88	34,34,34,34	0
85	MG	2	1969	1/1	0.24	7.88	79,79,79,79	0
85	MG	5	3823	1/1	0.30	7.88	51,51,51,51	0
86	OHX	2	2136	7/7	0.32	7.86	107,107,107,107	0
85	MG	1	3525	1/1	0.21	7.85	20,20,20,20	0
85	MG	1	3647	1/1	0.27	7.84	28,28,28,28	0
85	MG	1	3814	1/1	0.21	7.80	38,38,38,38	0
85	MG	5	3677	1/1	0.26	7.79	34,34,34,34	0
85	MG	1	3533	1/1	0.23	7.75	24,24,24,24	0
86	OHX	1	4128	7/7	0.27	7.74	96,96,96,96	0
85	MG	5	3529	1/1	0.31	7.73	25,25,25,25	0
85	MG	5	3415	1/1	0.25	7.73	19,19,19,19	0
85	MG	5	3648	1/1	0.23	7.71	72,72,72,72	0
85	MG	1	3542	1/1	0.34	7.69	27,27,27,27	0
85	MG	1	3512	1/1	0.29	7.69	22,22,22,22	0
85	MG	5	3458	1/1	0.24	7.67	54,54,54,54	0
86	OHX	1	4066	7/7	0.27	7.66	106,106,106,106	0
86	OHX	5	4248	7/7	0.24	7.66	126,126,126,126	0
85	MG	2	1928	1/1	0.32	7.66	69,69,69,69	0
85	MG	2	1957	1/1	0.29	7.64	47,47,47,47	0
85	MG	5	3586	1/1	0.47	7.62	52,52,52,52	0
85	MG	2	1917	1/1	0.36	7.60	46,46,46,46	0
86	OHX	5	3951	7/7	0.23	7.58	95,95,95,95	0
85	MG	5	3726	1/1	0.23	7.58	31,31,31,31	0
85	MG	n8	204	1/1	0.51	7.54	25,25,25,25	0
85	MG	1	3786	1/1	0.48	7.54	25,25,25,25	0
85	MG	6	1948	1/1	0.27	7.52	37,37,37,37	0
85	MG	1	3839	1/1	0.33	7.47	28,28,28,28	0
85	MG	2	1931	1/1	0.35	7.45	60,60,60,60	0
85	MG	5	3864	1/1	0.23	7.44	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4224	1/1	0.36	7.42	19,19,19,19	0
85	MG	1	3821	1/1	0.26	7.40	37,37,37,37	0
85	MG	2	1909	1/1	0.25	7.39	59,59,59,59	0
86	OHX	5	4136	7/7	0.27	7.32	103,103,103,103	0
85	MG	5	3638	1/1	0.24	7.27	29,29,29,29	0
86	OHX	4	232	7/7	0.29	7.26	93,93,93,93	0
85	MG	1	3773	1/1	0.25	7.25	37,37,37,37	0
85	MG	5	3766	1/1	0.24	7.25	35,35,35,35	0
86	OHX	5	4154	7/7	0.27	7.23	106,106,106,106	0
86	OHX	1	4201	7/7	0.24	7.23	100,100,100,100	0
85	MG	15	301	1/1	0.30	7.21	36,36,36,36	0
85	MG	7	213	1/1	0.28	7.20	44,44,44,44	0
85	MG	1	3774	1/1	0.21	7.20	45,45,45,45	0
85	MG	5	3563	1/1	0.25	7.20	17,17,17,17	0
85	MG	1	3653	1/1	0.20	7.19	49,49,49,49	0
85	MG	5	3503	1/1	0.27	7.18	45,45,45,45	0
85	MG	5	3475	1/1	0.27	7.12	25,25,25,25	0
85	MG	5	3422	1/1	0.24	7.12	47,47,47,47	0
86	OHX	1	4212	7/7	0.29	7.07	98,98,98,98	0
86	OHX	5	4112	7/7	0.26	7.06	79,79,79,79	0
85	MG	1	3551	1/1	0.30	7.04	25,25,25,25	0
86	OHX	2	2163	7/7	0.26	7.02	138,138,138,138	0
85	MG	5	3416	1/1	0.27	7.01	21,21,21,21	0
86	OHX	1	4209	7/7	0.33	7.00	104,104,104,104	0
86	OHX	1	4215	7/7	0.32	7.00	118,118,118,118	0
86	OHX	1	4169	7/7	0.27	6.99	90,90,90,90	0
86	OHX	5	4235	7/7	0.24	6.94	106,106,106,106	0
85	MG	6	1968	1/1	0.30	6.93	65,65,65,65	0
86	OHX	5	4147	7/7	0.28	6.91	104,104,104,104	0
86	OHX	2	2165	7/7	0.36	6.89	125,125,125,125	0
86	OHX	5	4177	7/7	0.28	6.88	110,110,110,110	0
85	MG	5	3409	1/1	0.31	6.84	39,39,39,39	0
85	MG	1	3418	1/1	0.25	6.84	41,41,41,41	0
85	MG	1	3417	1/1	0.27	6.83	34,34,34,34	0
85	MG	5	3443	1/1	0.28	6.83	20,20,20,20	0
86	OHX	1	4176	7/7	0.21	6.81	133,133,133,133	0
85	MG	5	3662	1/1	0.23	6.79	54,54,54,54	0
85	MG	5	3533	1/1	0.25	6.79	29,29,29,29	0
86	OHX	1	4148	7/7	0.22	6.70	118,118,118,118	0
86	OHX	1	4138	7/7	0.25	6.70	91,91,91,91	0
85	MG	5	3568	1/1	0.33	6.68	23,23,23,23	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3523	1/1	0.28	6.68	22,22,22,22	0
86	OHX	5	4134	7/7	0.28	6.68	99,99,99,99	0
85	MG	5	3706	1/1	0.24	6.66	42,42,42,42	0
85	MG	5	3764	1/1	0.25	6.65	30,30,30,30	0
85	MG	5	4255	1/1	0.40	6.63	23,23,23,23	0
85	MG	1	3494	1/1	0.24	6.63	30,30,30,30	0
85	MG	1	3450	1/1	0.25	6.63	35,35,35,35	0
86	OHX	1	4188	7/7	0.29	6.63	115,115,115,115	0
86	OHX	1	4067	7/7	0.24	6.60	100,100,100,100	0
85	MG	5	3470	1/1	0.28	6.56	25,25,25,25	0
85	MG	1	3569	1/1	0.32	6.56	21,21,21,21	0
85	MG	4	206	1/1	0.30	6.53	28,28,28,28	0
86	OHX	5	4233	7/7	0.36	6.52	118,118,118,118	0
85	MG	5	3894	1/1	0.25	6.49	45,45,45,45	0
85	MG	5	3584	1/1	0.38	6.49	19,19,19,19	0
86	OHX	1	4141	7/7	0.31	6.48	113,113,113,113	0
85	MG	6	2042	1/1	0.39	6.48	65,65,65,65	0
86	OHX	5	4216	7/7	0.23	6.46	113,113,113,113	0
86	OHX	5	4191	7/7	0.25	6.46	97,97,97,97	0
85	MG	5	3469	1/1	0.29	6.44	101,101,101,101	0
86	OHX	5	4220	7/7	0.29	6.43	133,133,133,133	0
85	MG	1	3460	1/1	0.26	6.41	26,26,26,26	0
85	MG	5	3785	1/1	0.23	6.40	31,31,31,31	0
85	MG	5	3619	1/1	0.23	6.38	34,34,34,34	0
86	OHX	2	2119	7/7	0.19	6.37	110,110,110,110	0
85	MG	5	3743	1/1	0.27	6.35	22,22,22,22	0
86	OHX	5	4181	7/7	0.28	6.34	107,107,107,107	0
86	OHX	6	2204	7/7	0.28	6.31	118,118,118,118	0
85	MG	1	3519	1/1	0.29	6.31	31,31,31,31	0
85	MG	2	1972	1/1	0.33	6.30	66,66,66,66	0
85	MG	5	3710	1/1	0.27	6.30	28,28,28,28	0
85	MG	6	1949	1/1	0.27	6.30	40,40,40,40	0
86	OHX	5	4142	7/7	0.19	6.29	96,96,96,96	0
85	MG	m1	201	1/1	0.24	6.26	51,51,51,51	0
85	MG	6	2000	1/1	0.58	6.26	42,42,42,42	0
85	MG	2	1901	1/1	0.48	6.24	57,57,57,57	0
86	OHX	1	4171	7/7	0.30	6.24	91,91,91,91	0
85	MG	1	3559	1/1	0.26	6.21	18,18,18,18	0
85	MG	1	3482	1/1	0.30	6.18	22,22,22,22	0
85	MG	1	3747	1/1	0.23	6.18	22,22,22,22	0
85	MG	6	1985	1/1	0.26	6.17	59,59,59,59	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4210	7/7	0.34	6.15	100,100,100,100	0
85	MG	5	3433	1/1	0.34	6.13	64,64,64,64	0
85	MG	5	3697	1/1	0.31	6.12	26,26,26,26	0
86	OHX	5	4137	7/7	0.31	6.12	101,101,101,101	0
86	OHX	1	4177	7/7	0.26	6.09	114,114,114,114	0
85	MG	2	1938	1/1	0.33	6.07	48,48,48,48	0
86	OHX	1	4172	7/7	0.24	6.05	123,123,123,123	0
85	MG	5	3507	1/1	0.27	6.03	33,33,33,33	0
86	OHX	6	2126	7/7	0.32	6.03	81,81,81,81	0
85	MG	5	3649	1/1	0.38	6.03	59,59,59,59	0
85	MG	6	1908	1/1	0.29	6.03	41,41,41,41	0
85	MG	5	3882	1/1	0.23	6.02	19,19,19,19	0
85	MG	5	3772	1/1	0.22	6.01	23,23,23,23	0
85	MG	5	3592	1/1	0.25	5.99	29,29,29,29	0
85	MG	2	1905	1/1	0.36	5.97	51,51,51,51	0
85	MG	6	2018	1/1	0.26	5.96	44,44,44,44	0
85	MG	2	1968	1/1	0.55	5.95	97,97,97,97	0
85	MG	5	3456	1/1	0.25	5.95	21,21,21,21	0
85	MG	1	3694	1/1	0.21	5.94	27,27,27,27	0
85	MG	5	3732	1/1	0.26	5.93	65,65,65,65	0
85	MG	3	212	1/1	0.21	5.93	63,63,63,63	0
85	MG	13	401	1/1	0.37	5.93	22,22,22,22	0
85	MG	5	3626	1/1	0.19	5.92	42,42,42,42	0
85	MG	6	1957	1/1	0.49	5.90	48,48,48,48	0
85	MG	6	2030	1/1	0.19	5.89	83,83,83,83	0
85	MG	2	1955	1/1	0.27	5.87	79,79,79,79	0
86	OHX	1	4125	7/7	0.23	5.86	85,85,85,85	0
86	OHX	4	233	7/7	0.29	5.84	121,121,121,121	0
85	MG	2	1944	1/1	0.22	5.81	53,53,53,53	0
85	MG	5	3439	1/1	0.20	5.81	24,24,24,24	0
86	OHX	5	4171	7/7	0.28	5.81	73,73,73,73	0
85	MG	6	2012	1/1	0.23	5.77	41,41,41,41	0
86	OHX	2	2138	7/7	0.21	5.77	132,132,132,132	0
85	MG	1	3454	1/1	0.26	5.76	30,30,30,30	0
85	MG	4	205	1/1	0.24	5.74	41,41,41,41	0
85	MG	6	1923	1/1	0.32	5.74	56,56,56,56	0
88	3H3	1	4216	33/33	0.40	5.73	26,26,26,26	0
86	OHX	5	4225	7/7	0.28	5.72	105,105,105,105	0
85	MG	o1	201	1/1	0.54	5.72	76,76,76,76	0
85	MG	1	3589	1/1	0.32	5.71	25,25,25,25	0
85	MG	1	3431	1/1	0.23	5.71	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4105	7/7	0.29	5.70	87,87,87,87	0
85	MG	1	3413	1/1	0.26	5.67	52,52,52,52	0
85	MG	5	3432	1/1	0.22	5.62	49,49,49,49	0
86	OHX	1	4111	7/7	0.27	5.61	110,110,110,110	0
85	MG	1	3610	1/1	0.21	5.60	34,34,34,34	0
86	OHX	6	2203	7/7	0.27	5.58	117,117,117,117	0
85	MG	1	3850	1/1	0.26	5.58	41,41,41,41	0
86	OHX	1	4214	7/7	0.29	5.57	103,103,103,103	0
86	OHX	2	2158	7/7	0.34	5.55	93,93,93,93	0
85	MG	1	3470	1/1	0.20	5.52	37,37,37,37	0
86	OHX	1	4146	7/7	0.32	5.51	94,94,94,94	0
85	MG	2	1923	1/1	0.26	5.50	53,53,53,53	0
85	MG	1	3733	1/1	0.28	5.46	46,46,46,46	0
85	MG	7	202	1/1	0.26	5.44	27,27,27,27	0
86	OHX	5	4157	7/7	0.22	5.44	87,87,87,87	0
86	OHX	6	2162	7/7	0.28	5.43	96,96,96,96	0
85	MG	1	3471	1/1	0.19	5.42	35,35,35,35	0
85	MG	5	3776	1/1	0.20	5.42	56,56,56,56	0
85	MG	1	3720	1/1	0.30	5.38	42,42,42,42	0
85	MG	5	3553	1/1	0.31	5.38	37,37,37,37	0
85	MG	8	207	1/1	0.21	5.37	53,53,53,53	0
85	MG	5	3468	1/1	0.20	5.37	29,29,29,29	0
86	OHX	1	4081	7/7	0.26	5.35	96,96,96,96	0
85	MG	5	3877	1/1	0.28	5.34	14,14,14,14	0
85	MG	1	3535	1/1	0.27	5.33	41,41,41,41	0
85	MG	4	203	1/1	0.32	5.33	44,44,44,44	0
85	MG	5	3671	1/1	0.34	5.30	21,21,21,21	0
85	MG	3	205	1/1	0.23	5.30	28,28,28,28	0
86	OHX	5	4246	7/7	0.34	5.27	122,122,122,122	0
86	OHX	6	2189	7/7	0.37	5.27	115,115,115,115	0
85	MG	5	3629	1/1	0.24	5.26	37,37,37,37	0
86	OHX	1	4203	7/7	0.26	5.26	108,108,108,108	0
86	OHX	2	2026	7/7	0.22	5.23	69,69,69,69	0
85	MG	1	3804	1/1	0.18	5.22	45,45,45,45	0
86	OHX	5	4175	7/7	0.22	5.21	105,105,105,105	0
85	MG	5	3516	1/1	0.39	5.21	20,20,20,20	0
85	MG	2	1971	1/1	0.28	5.20	56,56,56,56	0
85	MG	1	3538	1/1	0.20	5.18	31,31,31,31	0
86	OHX	1	4086	7/7	0.24	5.18	101,101,101,101	0
85	MG	1	3751	1/1	0.20	5.17	34,34,34,34	0
85	MG	1	3549	1/1	0.24	5.13	27,27,27,27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	5	3490	1/1	0.25	5.12	53,53,53,53	0
86	OHX	5	4163	7/7	0.24	5.12	145,145,145,145	0
85	MG	1	3630	1/1	0.19	5.11	21,21,21,21	0
85	MG	1	3743	1/1	0.21	5.11	36,36,36,36	0
85	MG	m4	201	1/1	0.23	5.11	46,46,46,46	0
85	MG	5	3542	1/1	0.26	5.08	53,53,53,53	0
85	MG	1	3572	1/1	0.26	5.08	24,24,24,24	0
85	MG	1	3652	1/1	0.42	5.08	84,84,84,84	0
86	OHX	1	4098	7/7	0.23	5.07	103,103,103,103	0
85	MG	6	1912	1/1	0.32	5.03	60,60,60,60	0
86	OHX	4	235	7/7	0.33	5.02	108,108,108,108	0
86	OHX	1	4076	7/7	0.31	5.00	81,81,81,81	0
85	MG	5	3605	1/1	0.24	4.98	46,46,46,46	0
85	MG	5	3427	1/1	0.25	4.95	23,23,23,23	0
86	OHX	1	4050	7/7	0.23	4.92	92,92,92,92	0
85	MG	2	1925	1/1	0.25	4.91	60,60,60,60	0
85	MG	6	1920	1/1	0.27	4.90	58,58,58,58	0
85	MG	5	3419	1/1	0.18	4.89	91,91,91,91	0
85	MG	5	4253	1/1	0.49	4.87	28,28,28,28	0
86	OHX	6	2176	7/7	0.23	4.87	87,87,87,87	0
85	MG	6	1966	1/1	0.34	4.86	73,73,73,73	0
85	MG	1	3631	1/1	0.33	4.85	62,62,62,62	0
86	OHX	5	4189	7/7	0.21	4.85	100,100,100,100	0
85	MG	5	3514	1/1	0.26	4.83	22,22,22,22	0
85	MG	1	3863	1/1	0.24	4.82	118,118,118,118	0
85	MG	1	3600	1/1	0.23	4.81	25,25,25,25	0
85	MG	5	3555	1/1	0.28	4.80	20,20,20,20	0
86	OHX	1	4061	7/7	0.23	4.77	97,97,97,97	0
85	MG	1	3576	1/1	0.28	4.76	21,21,21,21	0
85	MG	1	3856	1/1	0.21	4.75	22,22,22,22	0
85	MG	2	1990	1/1	0.20	4.74	51,51,51,51	0
85	MG	1	3474	1/1	0.24	4.73	20,20,20,20	0
86	OHX	5	3900	7/7	0.20	4.73	35,35,35,35	0
86	OHX	5	4245	7/7	0.24	4.73	119,119,119,119	0
86	OHX	1	4170	7/7	0.22	4.72	95,95,95,95	0
86	OHX	5	4210	7/7	0.21	4.70	109,109,109,109	0
86	OHX	2	2031	7/7	0.19	4.69	80,80,80,80	0
85	MG	5	3534	1/1	0.34	4.68	24,24,24,24	0
85	MG	1	3810	1/1	0.44	4.67	26,26,26,26	0
85	MG	5	3457	1/1	0.20	4.66	35,35,35,35	0
85	MG	1	3472	1/1	0.41	4.64	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3785	1/1	0.25	4.64	55,55,55,55	0
86	OHX	5	4239	7/7	0.30	4.64	149,149,149,149	0
85	MG	5	3828	1/1	0.25	4.63	50,50,50,50	0
85	MG	M7	201	1/1	0.41	4.62	52,52,52,52	0
85	MG	5	3564	1/1	0.36	4.61	38,38,38,38	0
85	MG	5	3790	1/1	0.24	4.61	41,41,41,41	0
86	OHX	5	4229	7/7	0.30	4.60	131,131,131,131	0
85	MG	1	3818	1/1	0.20	4.60	48,48,48,48	0
85	MG	1	3505	1/1	0.24	4.58	25,25,25,25	0
85	MG	5	3557	1/1	0.24	4.57	21,21,21,21	0
85	MG	2	1953	1/1	0.24	4.56	76,76,76,76	0
85	MG	1	3507	1/1	0.28	4.55	22,22,22,22	0
85	MG	2	1911	1/1	0.33	4.53	50,50,50,50	0
85	MG	5	3524	1/1	0.22	4.50	36,36,36,36	0
86	OHX	5	4148	7/7	0.32	4.49	119,119,119,119	0
85	MG	5	3441	1/1	0.32	4.49	26,26,26,26	0
86	OHX	5	4211	7/7	0.19	4.49	118,118,118,118	0
85	MG	5	3610	1/1	0.21	4.47	40,40,40,40	0
86	OHX	5	4125	7/7	0.20	4.47	113,113,113,113	0
85	MG	c7	201	1/1	0.34	4.46	63,63,63,63	0
85	MG	5	3585	1/1	0.24	4.43	20,20,20,20	0
86	OHX	5	3913	7/7	0.20	4.43	54,54,54,54	0
85	MG	1	3429	1/1	0.21	4.42	36,36,36,36	0
86	OHX	2	2180	7/7	0.24	4.42	116,116,116,116	0
85	MG	2	1937	1/1	0.29	4.41	46,46,46,46	0
85	MG	1	3707	1/1	0.20	4.40	46,46,46,46	0
85	MG	1	3748	1/1	0.21	4.39	28,28,28,28	0
85	MG	7	207	1/1	0.21	4.39	43,43,43,43	0
85	MG	2	1952	1/1	0.37	4.39	75,75,75,75	0
86	OHX	4	227	7/7	0.22	4.38	86,86,86,86	0
85	MG	5	3445	1/1	0.20	4.38	33,33,33,33	0
86	OHX	1	4124	7/7	0.21	4.37	104,104,104,104	0
85	MG	1	3518	1/1	0.30	4.37	19,19,19,19	0
85	MG	1	3702	1/1	0.18	4.36	39,39,39,39	0
86	OHX	6	2191	7/7	0.25	4.35	131,131,131,131	0
85	MG	1	3735	1/1	0.25	4.34	55,55,55,55	0
85	MG	1	3862	1/1	0.32	4.33	41,41,41,41	0
85	MG	6	1997	1/1	0.26	4.32	43,43,43,43	0
85	MG	5	3525	1/1	0.26	4.32	30,30,30,30	0
85	MG	2	1910	1/1	0.22	4.31	48,48,48,48	0
86	OHX	1	4202	7/7	0.24	4.29	110,110,110,110	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4135	7/7	0.25	4.28	95,95,95,95	0
86	OHX	5	4247	7/7	0.30	4.27	102,102,102,102	0
86	OHX	1	4184	7/7	0.26	4.27	86,86,86,86	0
85	MG	1	3625	1/1	0.21	4.25	27,27,27,27	0
86	OHX	6	2184	7/7	0.23	4.24	108,108,108,108	0
85	MG	3	210	1/1	0.24	4.22	50,50,50,50	0
86	OHX	5	4139	7/7	0.25	4.20	105,105,105,105	0
85	MG	5	3539	1/1	0.37	4.19	19,19,19,19	0
85	MG	1	3571	1/1	0.27	4.19	35,35,35,35	0
86	OHX	1	3982	7/7	0.28	4.17	69,69,69,69	0
86	OHX	5	4144	7/7	0.24	4.16	97,97,97,97	0
85	MG	5	3442	1/1	0.22	4.14	27,27,27,27	0
85	MG	5	3512	1/1	0.32	4.12	20,20,20,20	0
85	MG	1	3447	1/1	0.37	4.11	44,44,44,44	0
86	OHX	6	2127	7/7	0.25	4.10	98,98,98,98	0
85	MG	1	3813	1/1	0.26	4.09	26,26,26,26	0
85	MG	1	3604	1/1	0.20	4.05	27,27,27,27	0
85	MG	5	3474	1/1	0.28	4.05	64,64,64,64	0
86	OHX	6	2178	7/7	0.23	4.03	114,114,114,114	0
86	OHX	2	2164	7/7	0.22	4.02	140,140,140,140	0
85	MG	2	1962	1/1	0.25	3.99	44,44,44,44	0
85	MG	2	1978	1/1	0.21	3.99	80,80,80,80	0
86	OHX	2	2173	7/7	0.46	3.99	121,121,121,121	0
85	MG	5	3476	1/1	0.22	3.98	19,19,19,19	0
85	MG	1	3462	1/1	0.22	3.98	23,23,23,23	0
86	OHX	2	2099	7/7	0.21	3.97	94,94,94,94	0
85	MG	o4	202	1/1	0.29	3.96	50,50,50,50	0
85	MG	5	3465	1/1	0.20	3.94	48,48,48,48	0
85	MG	5	4257	1/1	0.35	3.93	22,22,22,22	0
86	OHX	6	2055	7/7	0.19	3.93	70,70,70,70	0
86	OHX	1	4197	7/7	0.21	3.92	117,117,117,117	0
86	OHX	1	4211	7/7	0.29	3.88	106,106,106,106	0
85	MG	2	2007	1/1	0.50	3.88	52,52,52,52	0
85	MG	1	3598	1/1	0.28	3.88	33,33,33,33	0
85	MG	1	3439	1/1	0.24	3.87	34,34,34,34	0
86	OHX	2	2146	7/7	0.30	3.86	115,115,115,115	0
86	OHX	6	2197	7/7	0.29	3.85	113,113,113,113	0
85	MG	1	3660	1/1	0.24	3.83	40,40,40,40	0
85	MG	1	3541	1/1	0.24	3.83	19,19,19,19	0
85	MG	1	3669	1/1	0.22	3.81	37,37,37,37	0
85	MG	5	3482	1/1	0.34	3.80	30,30,30,30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3545	1/1	0.22	3.77	37,37,37,37	0
85	MG	5	3844	1/1	0.23	3.76	22,22,22,22	0
85	MG	2	1974	1/1	0.30	3.74	59,59,59,59	0
86	OHX	5	4172	7/7	0.25	3.72	102,102,102,102	0
85	MG	5	3757	1/1	0.21	3.72	49,49,49,49	0
86	OHX	2	2134	7/7	0.21	3.72	127,127,127,127	0
86	OHX	1	4136	7/7	0.25	3.71	106,106,106,106	0
85	MG	17	301	1/1	0.24	3.71	32,32,32,32	0
85	MG	5	3612	1/1	0.20	3.70	26,26,26,26	0
85	MG	5	3424	1/1	0.20	3.68	34,34,34,34	0
85	MG	s1	301	1/1	0.32	3.65	62,62,62,62	0
86	OHX	2	2147	7/7	0.20	3.63	105,105,105,105	0
86	OHX	2	2177	7/7	0.24	3.58	113,113,113,113	0
86	OHX	7	227	7/7	0.22	3.58	127,127,127,127	0
85	MG	1	3517	1/1	0.28	3.58	22,22,22,22	0
86	OHX	1	3872	7/7	0.22	3.57	46,46,46,46	0
85	MG	1	3586	1/1	0.34	3.53	38,38,38,38	0
86	OHX	5	4202	7/7	0.25	3.53	112,112,112,112	0
85	MG	5	3667	1/1	0.20	3.52	31,31,31,31	0
85	MG	6	1906	1/1	0.25	3.50	43,43,43,43	0
86	OHX	1	4122	7/7	0.38	3.48	103,103,103,103	0
85	MG	1	3588	1/1	0.24	3.48	21,21,21,21	0
85	MG	5	3448	1/1	0.24	3.46	54,54,54,54	0
86	OHX	5	4150	7/7	0.25	3.46	113,113,113,113	0
85	MG	5	3763	1/1	0.26	3.46	26,26,26,26	0
85	MG	1	3826	1/1	0.18	3.45	59,59,59,59	0
86	OHX	5	4161	7/7	0.20	3.44	94,94,94,94	0
86	OHX	5	4127	7/7	0.20	3.44	100,100,100,100	0
86	OHX	2	2161	7/7	0.42	3.43	109,109,109,109	0
87	ZN	d7	101	1/1	0.42	3.43	119,119,119,119	0
85	MG	2	2023	1/1	0.22	3.43	101,101,101,101	0
85	MG	2	1961	1/1	0.22	3.42	54,54,54,54	0
86	OHX	1	4167	7/7	0.22	3.41	103,103,103,103	0
86	OHX	6	2053	7/7	0.18	3.41	61,61,61,61	0
86	OHX	1	4156	7/7	0.20	3.40	105,105,105,105	0
86	OHX	1	3874	7/7	0.20	3.40	48,48,48,48	0
86	OHX	6	2161	7/7	0.23	3.40	101,101,101,101	0
85	MG	5	3472	1/1	0.23	3.40	23,23,23,23	0
86	OHX	1	4157	7/7	0.26	3.39	105,105,105,105	0
85	MG	5	3639	1/1	0.27	3.39	40,40,40,40	0
86	OHX	1	4150	7/7	0.29	3.38	111,111,111,111	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3496	1/1	0.22	3.38	26,26,26,26	0
86	OHX	5	4108	7/7	0.25	3.38	95,95,95,95	0
85	MG	M3	202	1/1	0.38	3.37	34,34,34,34	0
86	OHX	5	3912	7/7	0.17	3.37	49,49,49,49	0
85	MG	2	1903	1/1	0.30	3.35	40,40,40,40	0
86	OHX	1	4204	7/7	0.31	3.33	109,109,109,109	0
85	MG	2	1998	1/1	0.20	3.33	60,60,60,60	0
85	MG	2	1918	1/1	0.30	3.33	46,46,46,46	0
86	OHX	5	3909	7/7	0.22	3.32	53,53,53,53	0
86	OHX	5	4114	7/7	0.27	3.32	95,95,95,95	0
85	MG	1	3806	1/1	0.23	3.31	48,48,48,48	0
85	MG	1	3458	1/1	0.20	3.30	30,30,30,30	0
86	OHX	5	4203	7/7	0.31	3.29	110,110,110,110	0
86	OHX	1	4160	7/7	0.22	3.28	114,114,114,114	0
86	OHX	2	2103	7/7	0.21	3.27	112,112,112,112	0
85	MG	o3	202	1/1	0.26	3.26	24,24,24,24	0
86	OHX	5	4027	7/7	0.20	3.26	83,83,83,83	0
86	OHX	6	2157	7/7	0.18	3.25	110,110,110,110	0
86	OHX	5	4145	7/7	0.23	3.23	93,93,93,93	0
85	MG	2	1986	1/1	0.30	3.23	50,50,50,50	0
85	MG	6	1950	1/1	0.22	3.22	35,35,35,35	0
86	OHX	6	2199	7/7	0.25	3.21	110,110,110,110	0
85	MG	5	3681	1/1	0.19	3.21	29,29,29,29	0
85	MG	2	1950	1/1	0.22	3.20	47,47,47,47	0
85	MG	8	203	1/1	0.24	3.19	37,37,37,37	0
85	MG	1	3700	1/1	0.21	3.19	31,31,31,31	0
86	OHX	1	4023	7/7	0.22	3.16	93,93,93,93	0
86	OHX	6	2177	7/7	0.22	3.16	97,97,97,97	0
85	MG	1	3550	1/1	0.25	3.15	31,31,31,31	0
86	OHX	5	4199	7/7	0.23	3.14	98,98,98,98	0
85	MG	n8	203	1/1	0.21	3.14	38,38,38,38	0
86	OHX	5	4110	7/7	0.19	3.13	103,103,103,103	0
85	MG	1	3726	1/1	0.21	3.11	33,33,33,33	0
85	MG	1	3530	1/1	0.25	3.10	52,52,52,52	0
85	MG	1	3618	1/1	0.27	3.08	48,48,48,48	0
86	OHX	5	4092	7/7	0.22	3.08	93,93,93,93	0
85	MG	1	3487	1/1	0.22	3.08	27,27,27,27	0
86	OHX	6	2048	7/7	0.19	3.08	60,60,60,60	0
85	MG	2	1977	1/1	0.27	3.07	73,73,73,73	0
85	MG	1	3769	1/1	0.23	3.02	53,53,53,53	0
86	OHX	6	2195	7/7	0.24	3.01	127,127,127,127	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3791	1/1	0.30	3.00	19,19,19,19	0
85	MG	1	3704	1/1	0.19	3.00	53,53,53,53	0
86	OHX	O9	101	7/7	0.45	2.99	88,88,88,88	0
85	MG	5	3695	1/1	0.19	2.99	46,46,46,46	0
86	OHX	5	4194	7/7	0.27	2.99	116,116,116,116	0
85	MG	1	3595	1/1	0.29	2.94	22,22,22,22	0
85	MG	1	3658	1/1	0.21	2.93	36,36,36,36	0
86	OHX	6	2144	7/7	0.25	2.91	105,105,105,105	0
85	MG	6	1998	1/1	0.25	2.90	49,49,49,49	0
86	OHX	5	4218	7/7	0.18	2.90	141,141,141,141	0
86	OHX	6	2198	7/7	0.28	2.87	117,117,117,117	0
85	MG	5	3827	1/1	0.21	2.86	20,20,20,20	0
85	MG	5	3867	1/1	0.52	2.85	31,31,31,31	0
85	MG	6	1977	1/1	0.26	2.85	40,40,40,40	0
86	OHX	2	2080	7/7	0.23	2.82	98,98,98,98	0
86	OHX	1	3891	7/7	0.18	2.81	65,65,65,65	0
86	OHX	2	2075	7/7	0.28	2.81	95,95,95,95	0
86	OHX	5	4188	7/7	0.20	2.80	111,111,111,111	0
85	MG	1	3762	1/1	0.20	2.80	24,24,24,24	0
85	MG	1	3521	1/1	0.27	2.75	60,60,60,60	0
85	MG	5	3541	1/1	0.22	2.73	22,22,22,22	0
86	OHX	5	4201	7/7	0.47	2.73	104,104,104,104	0
85	MG	1	3836	1/1	0.24	2.72	23,23,23,23	0
85	MG	6	2005	1/1	0.21	2.72	81,81,81,81	0
86	OHX	5	4221	7/7	0.27	2.71	113,113,113,113	0
86	OHX	7	225	7/7	0.18	2.71	118,118,118,118	0
86	OHX	1	4161	7/7	0.20	2.70	107,107,107,107	0
86	OHX	5	4183	7/7	0.22	2.69	100,100,100,100	0
85	MG	1	3805	1/1	0.40	2.68	49,49,49,49	0
85	MG	1	3757	1/1	0.21	2.65	35,35,35,35	0
86	OHX	1	3924	7/7	0.21	2.65	94,94,94,94	0
85	MG	5	3700	1/1	0.47	2.64	47,47,47,47	0
85	MG	2	2183	1/1	0.21	2.63	73,73,73,73	0
85	MG	2	1906	1/1	0.20	2.63	39,39,39,39	0
86	OHX	1	4114	7/7	0.25	2.62	87,87,87,87	0
86	OHX	2	2167	7/7	0.22	2.59	132,132,132,132	0
85	MG	1	3722	1/1	0.21	2.58	34,34,34,34	0
86	OHX	1	3915	7/7	0.20	2.55	73,73,73,73	0
85	MG	1	3615	1/1	0.22	2.55	31,31,31,31	0
86	OHX	1	4102	7/7	0.28	2.55	90,90,90,90	0
86	OHX	6	2188	7/7	0.19	2.54	120,120,120,120	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	c8	201	1/1	0.25	2.54	57,57,57,57	0
85	MG	5	3549	1/1	0.30	2.54	24,24,24,24	0
85	MG	6	1965	1/1	0.23	2.54	52,52,52,52	0
85	MG	5	3429	1/1	0.23	2.52	59,59,59,59	0
86	OHX	s9	201	7/7	0.31	2.52	102,102,102,102	0
86	OHX	3	223	7/7	0.23	2.52	96,96,96,96	0
85	MG	1	3481	1/1	0.23	2.51	31,31,31,31	0
85	MG	1	3708	1/1	0.18	2.50	34,34,34,34	0
85	MG	5	3446	1/1	0.19	2.50	30,30,30,30	0
85	MG	5	3717	1/1	0.18	2.48	58,58,58,58	0
85	MG	1	3539	1/1	0.25	2.48	17,17,17,17	0
85	MG	5	3567	1/1	0.24	2.48	26,26,26,26	0
86	OHX	m7	206	7/7	0.40	2.47	99,99,99,99	0
86	OHX	5	4039	7/7	0.28	2.46	67,67,67,67	0
85	MG	5	3665	1/1	0.21	2.45	19,19,19,19	0
85	MG	1	3752	1/1	0.22	2.45	48,48,48,48	0
85	MG	5	3659	1/1	0.24	2.43	22,22,22,22	0
85	MG	5	3423	1/1	0.24	2.42	36,36,36,36	0
86	OHX	8	229	7/7	0.25	2.41	108,108,108,108	0
86	OHX	5	4141	7/7	0.18	2.41	108,108,108,108	0
86	OHX	5	4156	7/7	0.20	2.40	107,107,107,107	0
85	MG	1	3622	1/1	0.20	2.40	42,42,42,42	0
86	OHX	5	3903	7/7	0.20	2.39	43,43,43,43	0
85	MG	5	3411	1/1	0.22	2.38	30,30,30,30	0
86	OHX	8	219	7/7	0.24	2.38	91,91,91,91	0
85	MG	1	3597	1/1	0.25	2.38	22,22,22,22	0
86	OHX	1	4113	7/7	0.21	2.37	106,106,106,106	0
86	OHX	2	2156	7/7	0.24	2.36	114,114,114,114	0
85	MG	1	3609	1/1	0.30	2.35	54,54,54,54	0
86	OHX	2	2174	7/7	0.22	2.35	115,115,115,115	0
85	MG	5	3853	1/1	0.33	2.35	34,34,34,34	0
86	OHX	1	4183	7/7	0.33	2.34	110,110,110,110	0
86	OHX	1	4155	7/7	0.21	2.34	115,115,115,115	0
85	MG	1	3629	1/1	0.21	2.34	30,30,30,30	0
85	MG	5	3538	1/1	0.28	2.34	19,19,19,19	0
85	MG	2	1935	1/1	0.28	2.31	60,60,60,60	0
86	OHX	2	2126	7/7	0.22	2.31	103,103,103,103	0
85	MG	1	3835	1/1	0.20	2.31	46,46,46,46	0
85	MG	2	2009	1/1	0.21	2.31	46,46,46,46	0
85	MG	2	1939	1/1	0.30	2.30	57,57,57,57	0
85	MG	5	3802	1/1	0.24	2.30	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3568	1/1	0.26	2.28	19,19,19,19	0
86	OHX	6	2200	7/7	0.23	2.28	115,115,115,115	0
86	OHX	2	2154	7/7	0.18	2.27	131,131,131,131	0
86	OHX	1	4129	7/7	0.18	2.27	118,118,118,118	0
86	OHX	5	4182	7/7	0.23	2.26	98,98,98,98	0
85	MG	5	3401	1/1	0.26	2.26	36,36,36,36	0
85	MG	2	1979	1/1	0.28	2.25	45,45,45,45	0
85	MG	5	3591	1/1	0.23	2.24	26,26,26,26	0
86	OHX	5	4099	7/7	0.20	2.23	94,94,94,94	0
86	OHX	6	2196	7/7	0.19	2.23	142,142,142,142	0
85	MG	1	3508	1/1	0.27	2.22	19,19,19,19	0
85	MG	5	3587	1/1	0.29	2.22	21,21,21,21	0
86	OHX	1	4206	7/7	0.20	2.22	106,106,106,106	0
85	MG	5	3815	1/1	0.22	2.21	36,36,36,36	0
85	MG	6	1942	1/1	0.22	2.21	30,30,30,30	0
86	OHX	2	2176	7/7	0.29	2.20	125,125,125,125	0
85	MG	2	1963	1/1	0.28	2.19	65,65,65,65	0
85	MG	1	3531	1/1	0.23	2.18	19,19,19,19	0
85	MG	d3	201	1/1	0.39	2.18	39,39,39,39	0
86	OHX	5	4126	7/7	0.19	2.17	103,103,103,103	0
85	MG	1	4217	1/1	0.21	2.17	19,19,19,19	0
85	MG	2	1930	1/1	0.23	2.16	53,53,53,53	0
86	OHX	5	4170	7/7	0.26	2.15	81,81,81,81	0
86	OHX	5	3899	7/7	0.19	2.15	34,34,34,34	0
85	MG	1	3578	1/1	0.27	2.14	20,20,20,20	0
85	MG	1	3801	1/1	0.25	2.13	41,41,41,41	0
85	MG	1	3655	1/1	0.26	2.13	25,25,25,25	0
85	MG	5	3526	1/1	0.30	2.13	42,42,42,42	0
85	MG	2	1919	1/1	0.37	2.12	62,62,62,62	0
86	OHX	5	4146	7/7	0.25	2.12	100,100,100,100	0
86	OHX	1	3868	7/7	0.20	2.10	35,35,35,35	0
85	MG	6	1910	1/1	0.22	2.08	54,54,54,54	0
85	MG	6	1987	1/1	0.18	2.08	54,54,54,54	0
86	OHX	6	2169	7/7	0.16	2.08	124,124,124,124	0
85	MG	5	3676	1/1	0.27	2.07	81,81,81,81	0
85	MG	5	3590	1/1	0.31	2.07	21,21,21,21	0
85	MG	1	3495	1/1	0.22	2.07	36,36,36,36	0
85	MG	5	3622	1/1	0.23	2.07	29,29,29,29	0
85	MG	1	3643	1/1	0.21	2.06	39,39,39,39	0
85	MG	5	3613	1/1	0.22	2.05	36,36,36,36	0
85	MG	6	1936	1/1	0.24	2.05	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4132	7/7	0.24	2.05	96,96,96,96	0
85	MG	5	3803	1/1	0.21	2.04	132,132,132,132	0
86	OHX	1	4149	7/7	0.20	2.04	105,105,105,105	0
86	OHX	5	4044	7/7	0.22	2.03	77,77,77,77	0
85	MG	1	3544	1/1	0.22	2.02	32,32,32,32	0
86	OHX	2	2155	7/7	0.19	2.02	114,114,114,114	0
85	MG	1	3685	1/1	0.20	2.02	45,45,45,45	0
86	OHX	1	4017	7/7	0.20	2.01	97,97,97,97	0
86	OHX	5	4093	7/7	0.22	2.00	97,97,97,97	0
86	OHX	4	231	7/7	0.23	1.99	115,115,115,115	0
86	OHX	5	3898	7/7	0.20	1.99	37,37,37,37	0
85	MG	1	3619	1/1	0.17	1.98	53,53,53,53	0
85	MG	1	3825	1/1	0.35	1.97	31,31,31,31	0
85	MG	1	3711	1/1	0.18	1.97	52,52,52,52	0
85	MG	1	3420	1/1	0.43	1.96	57,57,57,57	0
86	OHX	5	4186	7/7	0.31	1.96	120,120,120,120	0
86	OHX	5	4209	7/7	0.24	1.95	91,91,91,91	0
85	MG	q0	202	1/1	0.20	1.95	34,34,34,34	0
86	OHX	m4	202	7/7	0.19	1.95	190,190,190,190	0
85	MG	5	3625	1/1	0.17	1.93	53,53,53,53	0
85	MG	5	3608	1/1	0.22	1.93	29,29,29,29	0
86	OHX	2	2175	7/7	0.24	1.93	128,128,128,128	0
86	OHX	2	2109	7/7	0.17	1.93	123,123,123,123	0
86	OHX	1	3883	7/7	0.19	1.92	52,52,52,52	0
85	MG	s6	301	1/1	0.31	1.92	59,59,59,59	0
85	MG	5	3729	1/1	0.31	1.91	61,61,61,61	0
86	OHX	6	2151	7/7	0.20	1.90	92,92,92,92	0
85	MG	1	3436	1/1	0.21	1.90	35,35,35,35	0
86	OHX	1	3900	7/7	0.19	1.89	65,65,65,65	0
86	OHX	2	2153	7/7	0.20	1.87	118,118,118,118	0
85	MG	N0	201	1/1	0.26	1.87	42,42,42,42	0
86	OHX	m8	201	7/7	0.29	1.86	111,111,111,111	0
86	OHX	L6	202	7/7	0.29	1.85	112,112,112,112	0
85	MG	1	3644	1/1	0.19	1.84	50,50,50,50	0
86	OHX	1	4115	7/7	0.22	1.83	106,106,106,106	0
85	MG	6	2037	1/1	0.19	1.83	52,52,52,52	0
85	MG	1	3654	1/1	0.19	1.83	33,33,33,33	0
86	OHX	5	3907	7/7	0.18	1.83	44,44,44,44	0
85	MG	5	3607	1/1	0.21	1.83	20,20,20,20	0
85	MG	5	3814	1/1	0.17	1.82	53,53,53,53	0
85	MG	1	3680	1/1	0.19	1.81	30,30,30,30	0
85	MG	6	2022	1/1	0.20	1.80	71,71,71,71	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3798	1/1	0.18	1.80	39,39,39,39	0
85	MG	1	3784	1/1	0.29	1.78	29,29,29,29	0
85	MG	1	3790	1/1	0.20	1.78	33,33,33,33	0
86	OHX	5	4169	7/7	0.20	1.77	130,130,130,130	0
85	MG	1	3432	1/1	0.22	1.77	36,36,36,36	0
85	MG	1	3414	1/1	0.23	1.76	28,28,28,28	0
86	OHX	1	4133	7/7	0.21	1.76	121,121,121,121	0
85	MG	5	3640	1/1	0.21	1.75	32,32,32,32	0
85	MG	7	208	1/1	0.20	1.74	42,42,42,42	0
86	OHX	5	4062	7/7	0.21	1.74	99,99,99,99	0
85	MG	2	1949	1/1	0.26	1.73	68,68,68,68	0
86	OHX	6	2121	7/7	0.19	1.73	89,89,89,89	0
86	OHX	8	214	7/7	0.18	1.72	47,47,47,47	0
86	OHX	5	4115	7/7	0.16	1.70	118,118,118,118	0
86	OHX	5	4222	7/7	0.31	1.70	101,101,101,101	0
85	MG	L7	302	1/1	0.20	1.69	29,29,29,29	0
86	OHX	1	4132	7/7	0.17	1.69	129,129,129,129	0
86	OHX	6	2113	7/7	0.20	1.69	87,87,87,87	0
86	OHX	6	2175	7/7	0.28	1.68	122,122,122,122	0
86	OHX	4	226	7/7	0.28	1.68	91,91,91,91	0
85	MG	L5	301	1/1	0.38	1.67	50,50,50,50	0
88	3H3	5	4251	33/33	0.35	1.67	29,29,29,29	0
86	OHX	5	3938	7/7	0.18	1.65	71,71,71,71	0
86	OHX	6	2136	7/7	0.19	1.65	105,105,105,105	0
85	MG	2	1956	1/1	0.20	1.64	53,53,53,53	0
86	OHX	6	2193	7/7	0.28	1.64	142,142,142,142	0
86	OHX	1	4053	7/7	0.22	1.63	87,87,87,87	0
86	OHX	1	3877	7/7	0.18	1.63	46,46,46,46	0
85	MG	1	3514	1/1	0.19	1.62	29,29,29,29	0
85	MG	1	3673	1/1	0.33	1.61	56,56,56,56	0
85	MG	1	3849	1/1	0.23	1.60	33,33,33,33	0
85	MG	6	1938	1/1	0.23	1.59	35,35,35,35	0
85	MG	5	3627	1/1	0.22	1.57	52,52,52,52	0
86	OHX	2	2035	7/7	0.17	1.57	82,82,82,82	0
85	MG	2	1927	1/1	0.28	1.56	46,46,46,46	0
85	MG	1	3459	1/1	0.21	1.55	55,55,55,55	0
86	OHX	1	4103	7/7	0.22	1.55	98,98,98,98	0
86	OHX	o4	203	7/7	0.31	1.54	104,104,104,104	0
87	ZN	D7	101	1/1	0.34	1.54	133,133,133,133	0
85	MG	1	3648	1/1	0.18	1.52	35,35,35,35	0
85	MG	5	3532	1/1	0.17	1.51	39,39,39,39	0
86	OHX	2	2034	7/7	0.19	1.51	88,88,88,88	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3589	1/1	0.20	1.49	33,33,33,33	0
86	OHX	5	4243	7/7	0.26	1.49	109,109,109,109	0
85	MG	1	3767	1/1	0.19	1.48	50,50,50,50	0
86	OHX	1	4079	7/7	0.19	1.48	99,99,99,99	0
85	MG	6	2031	1/1	0.20	1.48	59,59,59,59	0
85	MG	6	1953	1/1	0.38	1.48	55,55,55,55	0
85	MG	5	3509	1/1	0.25	1.47	22,22,22,22	0
85	MG	5	3811	1/1	0.18	1.47	29,29,29,29	0
85	MG	5	3414	1/1	0.19	1.46	39,39,39,39	0
86	OHX	1	3876	7/7	0.17	1.46	50,50,50,50	0
86	OHX	5	3940	7/7	0.18	1.44	69,69,69,69	0
85	MG	1	3768	1/1	0.16	1.44	45,45,45,45	0
85	MG	3	211	1/1	0.22	1.44	62,62,62,62	0
85	MG	5	3709	1/1	0.22	1.44	74,74,74,74	0
85	MG	1	3661	1/1	0.25	1.43	30,30,30,30	0
86	OHX	6	2185	7/7	0.16	1.41	143,143,143,143	0
85	MG	2	1993	1/1	0.27	1.41	46,46,46,46	0
85	MG	1	3736	1/1	0.19	1.41	32,32,32,32	0
85	MG	6	2014	1/1	0.20	1.40	53,53,53,53	0
85	MG	5	3493	1/1	0.22	1.40	21,21,21,21	0
86	OHX	5	4207	7/7	0.42	1.39	89,89,89,89	0
85	MG	5	3762	1/1	0.17	1.39	34,34,34,34	0
85	MG	8	209	1/1	0.18	1.38	56,56,56,56	0
85	MG	5	3842	1/1	0.23	1.38	42,42,42,42	0
86	OHX	5	4204	7/7	0.42	1.38	111,111,111,111	0
85	MG	1	3553	1/1	0.21	1.37	46,46,46,46	0
86	OHX	1	4182	7/7	0.35	1.37	106,106,106,106	0
86	OHX	2	2087	7/7	0.22	1.36	93,93,93,93	0
86	OHX	1	4152	7/7	0.21	1.36	124,124,124,124	0
86	OHX	2	2166	7/7	0.14	1.35	144,144,144,144	0
86	OHX	15	306	7/7	0.24	1.34	114,114,114,114	0
85	MG	5	3713	1/1	0.18	1.33	41,41,41,41	0
86	OHX	1	4060	7/7	0.21	1.33	77,77,77,77	0
86	OHX	2	2113	7/7	0.26	1.32	108,108,108,108	0
85	MG	5	3405	1/1	0.19	1.32	18,18,18,18	0
85	MG	2	2004	1/1	0.17	1.32	67,67,67,67	0
85	MG	m7	204	1/1	0.22	1.32	36,36,36,36	0
86	OHX	6	2133	7/7	0.21	1.31	126,126,126,126	0
86	OHX	5	3999	7/7	0.17	1.31	91,91,91,91	0
85	MG	1	3612	1/1	0.16	1.30	37,37,37,37	0
85	MG	2	2001	1/1	0.18	1.30	63,63,63,63	0
86	OHX	5	4053	7/7	0.19	1.29	80,80,80,80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	M7	208	7/7	0.36	1.29	109,109,109,109	0
86	OHX	7	224	7/7	0.19	1.27	92,92,92,92	0
85	MG	2	1912	1/1	0.21	1.27	53,53,53,53	0
86	OHX	1	4190	7/7	0.22	1.26	115,115,115,115	0
85	MG	5	3868	1/1	0.66	1.26	32,32,32,32	0
86	OHX	1	4198	7/7	0.24	1.25	125,125,125,125	0
85	MG	1	3832	1/1	0.39	1.25	31,31,31,31	0
86	OHX	5	4205	7/7	0.26	1.24	113,113,113,113	0
85	MG	1	3555	1/1	0.30	1.23	25,25,25,25	0
86	OHX	1	4151	7/7	0.18	1.22	113,113,113,113	0
86	OHX	1	3894	7/7	0.18	1.20	64,64,64,64	0
85	MG	5	3478	1/1	0.28	1.19	50,50,50,50	0
86	OHX	5	4155	7/7	0.19	1.18	111,111,111,111	0
86	OHX	5	4082	7/7	0.19	1.17	85,85,85,85	0
85	MG	6	1996	1/1	0.24	1.17	62,62,62,62	0
86	OHX	1	4046	7/7	0.21	1.17	75,75,75,75	0
85	MG	1	3842	1/1	0.22	1.16	22,22,22,22	0
86	OHX	6	2059	7/7	0.16	1.16	81,81,81,81	0
86	OHX	1	3897	7/7	0.17	1.15	60,60,60,60	0
86	OHX	5	4250	7/7	0.19	1.14	128,128,128,128	0
86	OHX	2	2108	7/7	0.19	1.14	110,110,110,110	0
85	MG	1	3797	1/1	0.20	1.14	16,16,16,16	0
85	MG	5	3656	1/1	0.17	1.14	35,35,35,35	0
86	OHX	1	4131	7/7	0.17	1.13	102,102,102,102	0
86	OHX	1	3903	7/7	0.16	1.13	68,68,68,68	0
85	MG	C3	201	1/1	0.32	1.13	56,56,56,56	0
86	OHX	6	2156	7/7	0.31	1.12	119,119,119,119	0
86	OHX	1	4200	7/7	0.29	1.12	112,112,112,112	0
85	MG	2	1945	1/1	0.18	1.12	51,51,51,51	0
86	OHX	2	2116	7/7	0.26	1.12	111,111,111,111	0
86	OHX	1	4163	7/7	0.18	1.11	118,118,118,118	0
85	MG	2	1922	1/1	0.22	1.11	55,55,55,55	0
85	MG	L7	301	1/1	0.20	1.08	29,29,29,29	0
86	OHX	1	4104	7/7	0.16	1.08	119,119,119,119	0
85	MG	5	3434	1/1	0.21	1.07	24,24,24,24	0
85	MG	2	1987	1/1	0.24	1.07	91,91,91,91	0
86	OHX	1	4025	7/7	0.20	1.07	91,91,91,91	0
85	MG	5	3421	1/1	0.17	1.07	33,33,33,33	0
86	OHX	2	2092	7/7	0.21	1.05	103,103,103,103	0
85	MG	5	3805	1/1	0.19	1.05	87,87,87,87	0
86	OHX	1	3953	7/7	0.16	1.04	105,105,105,105	0
86	OHX	6	2173	7/7	0.22	1.02	116,116,116,116	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3699	1/1	0.21	1.02	31,31,31,31	0
85	MG	N5	201	1/1	0.21	1.00	61,61,61,61	0
85	MG	5	3545	1/1	0.21	1.00	42,42,42,42	0
85	MG	m1	202	1/1	0.18	1.00	49,49,49,49	0
86	OHX	6	2140	7/7	0.16	0.99	111,111,111,111	0
86	OHX	5	4059	7/7	0.18	0.98	96,96,96,96	0
85	MG	2	1970	1/1	0.22	0.98	60,60,60,60	0
86	OHX	1	4070	7/7	0.24	0.97	88,88,88,88	0
86	OHX	1	4082	7/7	0.17	0.96	93,93,93,93	0
85	MG	6	1932	1/1	0.18	0.96	37,37,37,37	0
86	OHX	5	4075	7/7	0.25	0.95	91,91,91,91	0
86	OHX	1	4194	7/7	0.20	0.95	114,114,114,114	0
86	OHX	5	4056	7/7	0.20	0.94	87,87,87,87	0
85	MG	1	3563	1/1	0.19	0.94	38,38,38,38	0
85	MG	6	1976	1/1	0.20	0.94	33,33,33,33	0
85	MG	5	3834	1/1	0.18	0.94	31,31,31,31	0
85	MG	1	3448	1/1	0.20	0.93	32,32,32,32	0
86	OHX	5	3939	7/7	0.18	0.92	76,76,76,76	0
85	MG	1	3838	1/1	0.23	0.92	43,43,43,43	0
86	OHX	1	4034	7/7	0.21	0.91	86,86,86,86	0
85	MG	1	3635	1/1	0.28	0.91	55,55,55,55	0
85	MG	2	1976	1/1	0.23	0.91	43,43,43,43	0
86	OHX	2	2122	7/7	0.18	0.90	116,116,116,116	0
86	OHX	2	2169	7/7	0.21	0.90	96,96,96,96	0
85	MG	6	2009	1/1	0.18	0.90	40,40,40,40	0
85	MG	1	3457	1/1	0.20	0.90	21,21,21,21	0
86	OHX	7	226	7/7	0.18	0.89	92,92,92,92	0
86	OHX	5	4223	7/7	0.30	0.88	117,117,117,117	0
86	OHX	6	2050	7/7	0.18	0.87	60,60,60,60	0
85	MG	c8	202	1/1	0.30	0.87	54,54,54,54	0
85	MG	8	205	1/1	0.21	0.86	59,59,59,59	0
85	MG	5	3851	1/1	0.20	0.85	46,46,46,46	0
86	OHX	6	2051	7/7	0.17	0.84	60,60,60,60	0
85	MG	1	3781	1/1	0.18	0.84	39,39,39,39	0
86	OHX	1	4039	7/7	0.19	0.83	98,98,98,98	0
85	MG	5	3614	1/1	0.19	0.83	32,32,32,32	0
86	OHX	5	4107	7/7	0.23	0.83	103,103,103,103	0
85	MG	4	219	1/1	0.18	0.82	45,45,45,45	0
86	OHX	5	4072	7/7	0.16	0.82	96,96,96,96	0
85	MG	5	3420	1/1	0.24	0.82	29,29,29,29	0
86	OHX	5	4106	7/7	0.20	0.82	88,88,88,88	0
86	OHX	5	4187	7/7	0.21	0.81	97,97,97,97	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	6	1941	1/1	0.21	0.81	41,41,41,41	0
85	MG	1	3701	1/1	0.19	0.80	34,34,34,34	0
86	OHX	2	2085	7/7	0.19	0.80	95,95,95,95	0
86	OHX	2	2041	7/7	0.17	0.78	85,85,85,85	0
86	OHX	5	3914	7/7	0.18	0.78	53,53,53,53	0
86	OHX	2	2135	7/7	0.23	0.78	108,108,108,108	0
86	OHX	1	4037	7/7	0.20	0.78	86,86,86,86	0
86	OHX	2	2141	7/7	0.17	0.77	133,133,133,133	0
85	MG	1	3755	1/1	0.18	0.77	18,18,18,18	0
86	OHX	5	3901	7/7	0.18	0.77	37,37,37,37	0
85	MG	5	3889	1/1	0.18	0.77	31,31,31,31	0
86	OHX	1	4084	7/7	0.21	0.76	89,89,89,89	0
86	OHX	5	4076	7/7	0.20	0.76	99,99,99,99	0
85	MG	2	1902	1/1	0.20	0.76	34,34,34,34	0
85	MG	5	3784	1/1	0.20	0.76	22,22,22,22	0
85	MG	4	204	1/1	0.35	0.76	60,60,60,60	0
85	MG	l5	302	1/1	0.29	0.75	54,54,54,54	0
86	OHX	2	2127	7/7	0.17	0.74	115,115,115,115	0
85	MG	2	1920	1/1	0.31	0.74	48,48,48,48	0
86	OHX	4	234	7/7	0.29	0.74	116,116,116,116	0
86	OHX	1	4083	7/7	0.24	0.72	100,100,100,100	0
85	MG	5	3798	1/1	0.18	0.72	62,62,62,62	0
85	MG	1	3557	1/1	0.18	0.72	38,38,38,38	0
85	MG	1	3778	1/1	0.21	0.70	41,41,41,41	0
85	MG	m7	203	1/1	0.24	0.70	26,26,26,26	0
86	OHX	5	3926	7/7	0.19	0.69	59,59,59,59	0
86	OHX	1	4092	7/7	0.39	0.67	88,88,88,88	0
86	OHX	6	2124	7/7	0.17	0.67	87,87,87,87	0
85	MG	m7	202	1/1	0.26	0.66	25,25,25,25	0
85	MG	5	3879	1/1	0.18	0.65	26,26,26,26	0
86	OHX	6	2170	7/7	0.19	0.64	117,117,117,117	0
85	MG	5	3552	1/1	0.26	0.63	23,23,23,23	0
85	MG	1	3800	1/1	0.19	0.63	42,42,42,42	0
85	MG	d2	201	1/1	0.23	0.63	55,55,55,55	0
85	MG	5	3742	1/1	0.35	0.62	32,32,32,32	0
85	MG	5	3768	1/1	0.26	0.62	36,36,36,36	0
85	MG	5	3504	1/1	0.21	0.61	26,26,26,26	0
86	OHX	5	4226	7/7	0.23	0.61	130,130,130,130	0
85	MG	1	3758	1/1	0.23	0.60	23,23,23,23	0
85	MG	5	3487	1/1	0.21	0.59	23,23,23,23	0
86	OHX	5	4162	7/7	0.17	0.59	115,115,115,115	0
86	OHX	2	2105	7/7	0.21	0.59	97,97,97,97	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	5	3775	1/1	0.18	0.59	21,21,21,21	0
86	OHX	1	3870	7/7	0.18	0.59	35,35,35,35	0
85	MG	5	3604	1/1	0.17	0.59	33,33,33,33	0
86	OHX	2	2128	7/7	0.32	0.58	107,107,107,107	0
85	MG	5	3497	1/1	0.20	0.58	21,21,21,21	0
85	MG	5	3658	1/1	0.17	0.58	38,38,38,38	0
85	MG	1	3443	1/1	0.20	0.58	65,65,65,65	0
86	OHX	2	2120	7/7	0.20	0.57	111,111,111,111	0
85	MG	1	3488	1/1	0.23	0.57	42,42,42,42	0
86	OHX	5	4019	7/7	0.18	0.55	84,84,84,84	0
85	MG	1	3651	1/1	0.20	0.53	51,51,51,51	0
86	OHX	5	4113	7/7	0.19	0.51	92,92,92,92	0
85	MG	5	3501	1/1	0.19	0.51	30,30,30,30	0
87	ZN	q0	201	1/1	0.19	0.51	23,23,23,23	0
85	MG	6	2036	1/1	0.30	0.51	62,62,62,62	0
85	MG	2	1916	1/1	0.22	0.50	44,44,44,44	0
85	MG	1	3617	1/1	0.20	0.50	48,48,48,48	0
86	OHX	6	2201	7/7	0.25	0.50	116,116,116,116	0
85	MG	M7	202	1/1	0.26	0.48	26,26,26,26	0
86	OHX	5	4122	7/7	0.17	0.48	114,114,114,114	0
86	OHX	1	3901	7/7	0.17	0.48	65,65,65,65	0
85	MG	1	3668	1/1	0.18	0.48	43,43,43,43	0
85	MG	1	3697	1/1	0.19	0.47	45,45,45,45	0
86	OHX	2	2129	7/7	0.14	0.47	121,121,121,121	0
86	OHX	2	2140	7/7	0.16	0.47	125,125,125,125	0
86	OHX	1	3878	7/7	0.17	0.47	51,51,51,51	0
85	MG	2	2016	1/1	0.31	0.46	59,59,59,59	0
86	OHX	5	4198	7/7	0.20	0.46	98,98,98,98	0
85	MG	6	2205	1/1	0.21	0.46	42,42,42,42	0
86	OHX	5	3931	7/7	0.17	0.45	60,60,60,60	0
85	MG	1	3511	1/1	0.19	0.45	21,21,21,21	0
86	OHX	8	226	7/7	0.14	0.45	115,115,115,115	0
86	OHX	s1	303	7/7	0.25	0.42	128,128,128,128	0
86	OHX	2	2038	7/7	0.15	0.39	97,97,97,97	0
85	MG	5	3550	1/1	0.23	0.39	36,36,36,36	0
85	MG	5	3451	1/1	0.19	0.38	25,25,25,25	0
85	MG	1	3582	1/1	0.28	0.38	30,30,30,30	0
85	MG	5	3556	1/1	0.20	0.36	36,36,36,36	0
86	OHX	2	2181	7/7	0.27	0.36	130,130,130,130	0
85	MG	2	1980	1/1	0.20	0.36	55,55,55,55	0
85	MG	5	3631	1/1	0.22	0.35	33,33,33,33	0
86	OHX	2	2152	7/7	0.14	0.34	145,145,145,145	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	L4	401	1/1	0.17	0.34	32,32,32,32	0
86	OHX	5	4231	7/7	0.17	0.34	137,137,137,137	0
86	OHX	5	4102	7/7	0.17	0.34	82,82,82,82	0
85	MG	1	3693	1/1	0.21	0.34	36,36,36,36	0
85	MG	2	2006	1/1	0.20	0.33	45,45,45,45	0
85	MG	1	3473	1/1	0.21	0.33	18,18,18,18	0
85	MG	5	3722	1/1	0.18	0.33	39,39,39,39	0
86	OHX	2	2148	7/7	0.18	0.33	142,142,142,142	0
85	MG	6	1992	1/1	0.17	0.32	40,40,40,40	0
86	OHX	5	4167	7/7	0.21	0.31	108,108,108,108	0
86	OHX	1	4153	7/7	0.16	0.31	92,92,92,92	0
85	MG	5	3696	1/1	0.18	0.31	36,36,36,36	0
85	MG	6	2003	1/1	0.19	0.31	60,60,60,60	0
85	MG	5	3536	1/1	0.21	0.30	27,27,27,27	0
85	MG	5	3829	1/1	0.21	0.30	59,59,59,59	0
85	MG	5	3745	1/1	0.17	0.30	33,33,33,33	0
85	MG	1	3430	1/1	0.21	0.30	41,41,41,41	0
85	MG	5	3657	1/1	0.21	0.30	30,30,30,30	0
86	OHX	s1	302	7/7	0.18	0.29	67,67,67,67	0
86	OHX	6	2172	7/7	0.23	0.29	114,114,114,114	0
86	OHX	5	4249	7/7	0.17	0.28	109,109,109,109	0
86	OHX	6	2182	7/7	0.30	0.28	109,109,109,109	0
85	MG	5	3789	1/1	0.42	0.28	36,36,36,36	0
86	OHX	5	4143	7/7	0.20	0.27	106,106,106,106	0
85	MG	1	3656	1/1	0.19	0.27	39,39,39,39	0
86	OHX	1	4207	7/7	0.21	0.26	111,111,111,111	0
86	OHX	1	4091	7/7	0.22	0.26	98,98,98,98	0
85	MG	N8	202	1/1	0.23	0.25	37,37,37,37	0
86	OHX	5	4174	7/7	0.21	0.25	109,109,109,109	0
86	OHX	5	4237	7/7	0.14	0.25	116,116,116,116	0
85	MG	1	3501	1/1	0.25	0.24	22,22,22,22	0
85	MG	1	3534	1/1	0.28	0.24	31,31,31,31	0
86	OHX	5	4091	7/7	0.19	0.23	92,92,92,92	0
85	MG	5	3495	1/1	0.19	0.23	26,26,26,26	0
85	MG	1	3696	1/1	0.15	0.23	35,35,35,35	0
85	MG	M3	203	1/1	0.36	0.23	79,79,79,79	0
85	MG	6	1967	1/1	0.19	0.23	59,59,59,59	0
87	ZN	Q0	500	1/1	0.18	0.23	35,35,35,35	0
85	MG	1	3411	1/1	0.21	0.22	33,33,33,33	0
86	OHX	2	2112	7/7	0.16	0.22	130,130,130,130	0
86	OHX	5	4232	7/7	0.18	0.22	82,82,82,82	0
86	OHX	5	4224	7/7	0.22	0.22	113,113,113,113	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	4094	7/7	0.17	0.21	129,129,129,129	0
86	OHX	1	4058	7/7	0.18	0.21	80,80,80,80	0
85	MG	6	1990	1/1	0.21	0.20	58,58,58,58	0
86	OHX	1	4068	7/7	0.23	0.20	78,78,78,78	0
86	OHX	1	4108	7/7	0.18	0.20	97,97,97,97	0
86	OHX	8	221	7/7	0.21	0.20	95,95,95,95	0
85	MG	5	3754	1/1	0.23	0.19	38,38,38,38	0
85	MG	1	3483	1/1	0.23	0.19	39,39,39,39	0
86	OHX	2	2162	7/7	0.21	0.19	126,126,126,126	0
86	OHX	1	3882	7/7	0.16	0.18	53,53,53,53	0
85	MG	1	3567	1/1	0.29	0.18	24,24,24,24	0
85	MG	1	3727	1/1	0.16	0.18	51,51,51,51	0
85	MG	2	1988	1/1	0.23	0.17	62,62,62,62	0
86	OHX	5	4049	7/7	0.20	0.16	83,83,83,83	0
86	OHX	6	2066	7/7	0.16	0.16	94,94,94,94	0
85	MG	1	3822	1/1	0.15	0.16	48,48,48,48	0
85	MG	1	3675	1/1	0.18	0.16	18,18,18,18	0
86	OHX	6	2145	7/7	0.22	0.14	110,110,110,110	0
85	MG	1	3421	1/1	0.23	0.14	37,37,37,37	0
85	MG	5	3402	1/1	0.18	0.13	16,16,16,16	0
85	MG	4	207	1/1	0.23	0.13	32,32,32,32	0
86	OHX	5	4121	7/7	0.17	0.12	111,111,111,111	0
86	OHX	s4	301	7/7	0.17	0.11	122,122,122,122	0
86	OHX	5	3932	7/7	0.18	0.11	77,77,77,77	0
86	OHX	6	2159	7/7	0.27	0.11	96,96,96,96	0
85	MG	1	3570	1/1	0.19	0.11	13,13,13,13	0
85	MG	1	3467	1/1	0.18	0.10	38,38,38,38	0
86	OHX	1	3871	7/7	0.19	0.10	43,43,43,43	0
85	MG	6	2004	1/1	0.19	0.09	62,62,62,62	0
86	OHX	2	2100	7/7	0.16	0.08	115,115,115,115	0
86	OHX	1	4213	7/7	0.21	0.08	128,128,128,128	0
85	MG	6	1972	1/1	0.17	0.07	46,46,46,46	0
86	OHX	L3	404	7/7	0.28	0.07	128,128,128,128	0
86	OHX	5	3902	7/7	0.20	0.07	43,43,43,43	0
85	MG	5	3645	1/1	0.21	0.07	47,47,47,47	0
86	OHX	5	4242	7/7	0.19	0.07	124,124,124,124	0
86	OHX	O3	202	7/7	0.18	0.07	91,91,91,91	0
85	MG	2	2022	1/1	0.16	0.06	66,66,66,66	0
86	OHX	1	3957	7/7	0.16	0.06	80,80,80,80	0
86	OHX	5	4037	7/7	0.20	0.06	94,94,94,94	0
86	OHX	6	2148	7/7	0.17	0.06	108,108,108,108	0
85	MG	1	3415	1/1	0.24	0.05	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3822	1/1	0.23	0.05	78,78,78,78	0
86	OHX	2	2115	7/7	0.17	0.04	100,100,100,100	0
85	MG	5	3758	1/1	0.19	0.04	46,46,46,46	0
85	MG	5	3635	1/1	0.19	0.04	39,39,39,39	0
85	MG	1	3461	1/1	0.19	0.03	20,20,20,20	0
85	MG	2	1941	1/1	0.17	0.03	50,50,50,50	0
86	OHX	2	2093	7/7	0.21	0.02	94,94,94,94	0
86	OHX	5	3904	7/7	0.18	0.01	47,47,47,47	0
86	OHX	C8	201	7/7	0.16	0.01	91,91,91,91	0
86	OHX	d9	102	7/7	0.20	0.01	117,117,117,117	0
86	OHX	1	4020	7/7	0.14	0.00	127,127,127,127	0
85	MG	5	3728	1/1	0.19	-0.00	20,20,20,20	0
85	MG	1	3819	1/1	0.23	-0.01	42,42,42,42	0
85	MG	5	3885	1/1	0.24	-0.01	59,59,59,59	0
86	OHX	5	4241	7/7	0.34	-0.01	81,81,81,81	0
86	OHX	2	2139	7/7	0.16	-0.01	112,112,112,112	0
85	MG	1	3503	1/1	0.18	-0.02	17,17,17,17	0
85	MG	n0	202	1/1	0.18	-0.02	32,32,32,32	0
86	OHX	1	4186	7/7	0.16	-0.02	120,120,120,120	0
85	MG	Q2	502	1/1	0.17	-0.03	50,50,50,50	0
85	MG	1	3425	1/1	0.22	-0.05	21,21,21,21	0
86	OHX	S8	302	7/7	0.24	-0.05	126,126,126,126	0
86	OHX	5	4052	7/7	0.17	-0.07	83,83,83,83	0
86	OHX	2	2150	7/7	0.18	-0.07	134,134,134,134	0
85	MG	2	1992	1/1	0.35	-0.07	50,50,50,50	0
86	OHX	5	4074	7/7	0.18	-0.08	93,93,93,93	0
86	OHX	5	4042	7/7	0.17	-0.08	100,100,100,100	0
86	OHX	5	4109	7/7	0.30	-0.09	93,93,93,93	0
86	OHX	L4	404	7/7	0.20	-0.11	103,103,103,103	0
85	MG	1	3688	1/1	0.16	-0.11	39,39,39,39	0
86	OHX	1	4105	7/7	0.29	-0.11	101,101,101,101	0
85	MG	5	3486	1/1	0.28	-0.11	28,28,28,28	0
86	OHX	1	4063	7/7	0.18	-0.11	102,102,102,102	0
85	MG	5	3602	1/1	0.19	-0.11	40,40,40,40	0
85	MG	1	3765	1/1	0.18	-0.13	40,40,40,40	0
85	MG	o3	201	1/1	0.19	-0.13	40,40,40,40	0
86	OHX	3	226	7/7	0.15	-0.13	113,113,113,113	0
86	OHX	1	4041	7/7	0.18	-0.14	85,85,85,85	0
85	MG	5	3723	1/1	0.18	-0.16	32,32,32,32	0
86	OHX	2	2171	7/7	0.15	-0.16	110,110,110,110	0
86	OHX	s8	303	7/7	0.28	-0.16	129,129,129,129	0
85	MG	5	3454	1/1	0.15	-0.16	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	2	2178	7/7	0.27	-0.16	141,141,141,141	0
86	OHX	2	2110	7/7	0.14	-0.17	113,113,113,113	0
86	OHX	1	4106	7/7	0.16	-0.17	113,113,113,113	0
85	MG	1	3437	1/1	0.19	-0.18	22,22,22,22	0
86	OHX	6	2117	7/7	0.17	-0.19	108,108,108,108	0
85	MG	5	3404	1/1	0.18	-0.20	32,32,32,32	0
85	MG	2	1966	1/1	0.20	-0.20	49,49,49,49	0
86	OHX	1	3996	7/7	0.22	-0.21	93,93,93,93	0
86	OHX	d4	201	7/7	0.20	-0.21	120,120,120,120	0
86	OHX	2	2168	7/7	0.15	-0.21	135,135,135,135	0
86	OHX	1	3932	7/7	0.16	-0.22	82,82,82,82	0
85	MG	5	3791	1/1	0.19	-0.23	74,74,74,74	0
86	OHX	6	2125	7/7	0.16	-0.23	106,106,106,106	0
85	MG	2	1991	1/1	0.28	-0.23	102,102,102,102	0
85	MG	1	3807	1/1	0.18	-0.23	26,26,26,26	0
86	OHX	6	2137	7/7	0.23	-0.24	101,101,101,101	0
86	OHX	2	2125	7/7	0.20	-0.24	120,120,120,120	0
86	OHX	l3	404	7/7	0.20	-0.24	112,112,112,112	0
86	OHX	1	3888	7/7	0.15	-0.25	56,56,56,56	0
86	OHX	m1	203	7/7	0.31	-0.25	124,124,124,124	0
86	OHX	m0	302	7/7	0.28	-0.26	96,96,96,96	0
85	MG	6	2023	1/1	0.15	-0.26	41,41,41,41	0
86	OHX	1	4143	7/7	0.16	-0.26	107,107,107,107	0
85	MG	2	1948	1/1	0.28	-0.27	57,57,57,57	0
85	MG	n9	3801	1/1	0.18	-0.27	24,24,24,24	0
85	MG	5	3690	1/1	0.16	-0.27	36,36,36,36	0
86	OHX	5	3997	7/7	0.15	-0.28	98,98,98,98	0
85	MG	5	3554	1/1	0.17	-0.28	31,31,31,31	0
86	OHX	5	3949	7/7	0.15	-0.28	84,84,84,84	0
86	OHX	6	2047	7/7	0.18	-0.29	47,47,47,47	0
86	OHX	5	4090	7/7	0.19	-0.31	79,79,79,79	0
86	OHX	1	4093	7/7	0.14	-0.31	109,109,109,109	0
86	OHX	2	2025	7/7	0.16	-0.31	66,66,66,66	0
86	OHX	1	4126	7/7	0.16	-0.31	110,110,110,110	0
85	MG	L8	301	1/1	0.31	-0.32	54,54,54,54	0
86	OHX	5	3988	7/7	0.13	-0.33	97,97,97,97	0
85	MG	4	209	1/1	0.19	-0.33	37,37,37,37	0
86	OHX	5	4081	7/7	0.18	-0.33	87,87,87,87	0
86	OHX	5	4117	7/7	0.17	-0.33	96,96,96,96	0
86	OHX	1	4090	7/7	0.17	-0.33	102,102,102,102	0
86	OHX	n9	3803	7/7	0.17	-0.33	52,52,52,52	0
86	OHX	6	2074	7/7	0.13	-0.34	103,103,103,103	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	5	3460	1/1	0.19	-0.34	24,24,24,24	0
85	MG	6	1905	1/1	0.19	-0.36	49,49,49,49	0
85	MG	O4	201	1/1	0.20	-0.36	45,45,45,45	0
85	MG	1	3621	1/1	0.17	-0.37	32,32,32,32	0
85	MG	6	1988	1/1	0.17	-0.37	36,36,36,36	0
85	MG	1	3754	1/1	0.17	-0.37	29,29,29,29	0
85	MG	5	3609	1/1	0.20	-0.37	24,24,24,24	0
86	OHX	1	3988	7/7	0.17	-0.37	73,73,73,73	0
86	OHX	1	4134	7/7	0.17	-0.37	127,127,127,127	0
85	MG	1	3659	1/1	0.29	-0.38	49,49,49,49	0
85	MG	1	3689	1/1	0.20	-0.39	25,25,25,25	0
86	OHX	6	2192	7/7	0.16	-0.39	130,130,130,130	0
86	OHX	5	4029	7/7	0.18	-0.39	76,76,76,76	0
85	MG	1	3855	1/1	0.16	-0.40	41,41,41,41	0
86	OHX	6	2179	7/7	0.16	-0.40	123,123,123,123	0
86	OHX	6	2158	7/7	0.15	-0.41	112,112,112,112	0
85	MG	d6	102	1/1	0.25	-0.41	47,47,47,47	0
85	MG	q1	101	1/1	0.18	-0.41	39,39,39,39	0
86	OHX	5	3974	7/7	0.17	-0.42	89,89,89,89	0
86	OHX	5	4180	7/7	0.18	-0.42	120,120,120,120	0
86	OHX	5	4120	7/7	0.14	-0.42	118,118,118,118	0
85	MG	1	3867	1/1	0.18	-0.42	21,21,21,21	0
85	MG	5	3494	1/1	0.19	-0.42	23,23,23,23	0
86	OHX	1	4159	7/7	0.15	-0.43	92,92,92,92	0
86	OHX	6	2049	7/7	0.17	-0.43	51,51,51,51	0
86	OHX	5	4041	7/7	0.16	-0.43	126,126,126,126	0
86	OHX	1	3981	7/7	0.18	-0.43	79,79,79,79	0
86	OHX	D9	102	7/7	0.19	-0.43	109,109,109,109	0
85	MG	6	1981	1/1	0.23	-0.44	47,47,47,47	0
86	OHX	1	4005	7/7	0.20	-0.44	79,79,79,79	0
86	OHX	2	2132	7/7	0.15	-0.44	103,103,103,103	0
86	OHX	5	4178	7/7	0.12	-0.44	126,126,126,126	0
85	MG	2	1940	1/1	0.16	-0.45	53,53,53,53	0
85	MG	M1	201	1/1	0.19	-0.45	61,61,61,61	0
85	MG	n6	201	1/1	0.24	-0.45	52,52,52,52	0
85	MG	M7	203	1/1	0.21	-0.46	28,28,28,28	0
85	MG	1	3455	1/1	0.19	-0.46	45,45,45,45	0
85	MG	5	3406	1/1	0.17	-0.46	26,26,26,26	0
86	OHX	2	2070	7/7	0.18	-0.46	89,89,89,89	0
85	MG	8	211	1/1	0.17	-0.46	79,79,79,79	0
85	MG	m6	201	1/1	0.17	-0.46	25,25,25,25	0
86	OHX	1	3869	7/7	0.17	-0.46	38,38,38,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3675	1/1	0.16	-0.46	28,28,28,28	0
86	OHX	6	2146	7/7	0.17	-0.47	109,109,109,109	0
85	MG	s8	301	1/1	0.17	-0.47	45,45,45,45	0
85	MG	5	3810	1/1	0.21	-0.47	32,32,32,32	0
86	OHX	5	4079	7/7	0.19	-0.48	99,99,99,99	0
86	OHX	1	4147	7/7	0.20	-0.48	120,120,120,120	0
85	MG	1	3837	1/1	0.17	-0.49	30,30,30,30	0
86	OHX	1	4137	7/7	0.18	-0.50	89,89,89,89	0
85	MG	1	3641	1/1	0.16	-0.51	32,32,32,32	0
85	MG	2	1973	1/1	0.18	-0.52	57,57,57,57	0
85	MG	2	2000	1/1	0.16	-0.52	53,53,53,53	0
86	OHX	1	3909	7/7	0.15	-0.53	70,70,70,70	0
85	MG	1	3554	1/1	0.20	-0.53	21,21,21,21	0
85	MG	1	3698	1/1	0.17	-0.53	62,62,62,62	0
85	MG	L3	401	1/1	0.16	-0.54	28,28,28,28	0
86	OHX	5	4033	7/7	0.18	-0.54	85,85,85,85	0
85	MG	1	3824	1/1	0.14	-0.54	50,50,50,50	0
86	OHX	5	4078	7/7	0.18	-0.55	78,78,78,78	0
85	MG	5	3744	1/1	0.15	-0.55	25,25,25,25	0
86	OHX	C1	201	7/7	0.17	-0.55	101,101,101,101	0
86	OHX	1	4000	7/7	0.18	-0.56	82,82,82,82	0
85	MG	5	3491	1/1	0.15	-0.56	34,34,34,34	0
85	MG	5	3480	1/1	0.18	-0.56	29,29,29,29	0
86	OHX	5	3905	7/7	0.17	-0.56	45,45,45,45	0
86	OHX	5	4165	7/7	0.16	-0.57	102,102,102,102	0
86	OHX	6	2134	7/7	0.17	-0.57	101,101,101,101	0
85	MG	4	208	1/1	0.16	-0.57	42,42,42,42	0
86	OHX	1	4127	7/7	0.15	-0.57	120,120,120,120	0
85	MG	q3	502	1/1	0.22	-0.57	45,45,45,45	0
86	OHX	2	2033	7/7	0.16	-0.58	75,75,75,75	0
86	OHX	6	2112	7/7	0.17	-0.58	99,99,99,99	0
85	MG	1	3788	1/1	0.17	-0.58	48,48,48,48	0
85	MG	M3	204	1/1	0.23	-0.59	24,24,24,24	0
85	MG	5	3865	1/1	0.17	-0.61	38,38,38,38	0
86	OHX	2	2086	7/7	0.13	-0.61	112,112,112,112	0
86	OHX	5	3973	7/7	0.12	-0.62	62,62,62,62	0
87	ZN	d9	101	1/1	0.13	-0.62	60,60,60,60	0
85	MG	M0	301	1/1	0.16	-0.62	25,25,25,25	0
86	OHX	6	2064	7/7	0.15	-0.63	80,80,80,80	0
85	MG	1	3683	1/1	0.16	-0.63	32,32,32,32	0
86	OHX	1	3922	7/7	0.14	-0.64	77,77,77,77	0
85	MG	5	3621	1/1	0.17	-0.64	46,46,46,46	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	N8	201	1/1	0.16	-0.64	26,26,26,26	0
85	MG	5	3669	1/1	0.15	-0.64	26,26,26,26	0
85	MG	6	1993	1/1	0.16	-0.64	42,42,42,42	0
85	MG	5	3863	1/1	0.16	-0.65	44,44,44,44	0
86	OHX	19	600	7/7	0.15	-0.65	105,105,105,105	0
85	MG	5	3735	1/1	0.16	-0.65	31,31,31,31	0
86	OHX	1	4008	7/7	0.17	-0.65	99,99,99,99	0
86	OHX	15	305	7/7	0.18	-0.65	112,112,112,112	0
86	OHX	1	4120	7/7	0.16	-0.65	105,105,105,105	0
85	MG	5	3752	1/1	0.15	-0.66	36,36,36,36	0
85	MG	6	2006	1/1	0.15	-0.67	46,46,46,46	0
86	OHX	6	2139	7/7	0.14	-0.67	106,106,106,106	0
85	MG	5	3685	1/1	0.14	-0.68	37,37,37,37	0
85	MG	1	4222	1/1	0.14	-0.68	45,45,45,45	0
85	MG	5	4258	1/1	0.18	-0.68	29,29,29,29	0
85	MG	1	3489	1/1	0.17	-0.68	22,22,22,22	0
86	OHX	5	3948	7/7	0.14	-0.69	85,85,85,85	0
85	MG	5	3642	1/1	0.17	-0.70	27,27,27,27	0
86	OHX	6	2143	7/7	0.14	-0.70	117,117,117,117	0
86	OHX	5	4116	7/7	0.18	-0.71	82,82,82,82	0
85	MG	5	3797	1/1	0.18	-0.71	33,33,33,33	0
85	MG	S8	301	1/1	0.16	-0.71	51,51,51,51	0
86	OHX	5	4100	7/7	0.13	-0.71	100,100,100,100	0
86	OHX	2	2107	7/7	0.13	-0.72	96,96,96,96	0
85	MG	5	3866	1/1	0.14	-0.72	31,31,31,31	0
85	MG	L4	403	1/1	0.23	-0.72	25,25,25,25	0
86	OHX	1	3880	7/7	0.16	-0.72	44,44,44,44	0
86	OHX	1	3873	7/7	0.18	-0.73	42,42,42,42	0
86	OHX	2	2101	7/7	0.12	-0.73	116,116,116,116	0
85	MG	1	3620	1/1	0.15	-0.73	55,55,55,55	0
86	OHX	1	4096	7/7	0.14	-0.74	123,123,123,123	0
86	OHX	sR	401	7/7	0.14	-0.74	135,135,135,135	0
86	OHX	1	4107	7/7	0.16	-0.74	98,98,98,98	0
86	OHX	6	2152	7/7	0.16	-0.74	126,126,126,126	0
85	MG	5	3418	1/1	0.17	-0.74	59,59,59,59	0
85	MG	2	1947	1/1	0.18	-0.75	50,50,50,50	0
86	OHX	1	3943	7/7	0.14	-0.75	92,92,92,92	0
86	OHX	2	2058	7/7	0.16	-0.75	103,103,103,103	0
86	OHX	1	4196	7/7	0.14	-0.75	149,149,149,149	0
86	OHX	2	2143	7/7	0.14	-0.75	113,113,113,113	0
85	MG	n0	201	1/1	0.17	-0.76	33,33,33,33	0
85	MG	5	3897	1/1	0.17	-0.78	44,44,44,44	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3403	1/1	0.17	-0.78	27,27,27,27	0
85	MG	1	3633	1/1	0.15	-0.78	35,35,35,35	0
85	MG	5	3691	1/1	0.14	-0.79	38,38,38,38	0
85	MG	L6	201	1/1	0.15	-0.79	35,35,35,35	0
85	MG	M6	201	1/1	0.18	-0.79	39,39,39,39	0
86	OHX	N9	101	7/7	0.17	-0.80	48,48,48,48	0
86	OHX	5	3921	7/7	0.16	-0.80	49,49,49,49	0
86	OHX	8	223	7/7	0.17	-0.81	99,99,99,99	0
85	MG	sM	302	1/1	0.16	-0.81	31,31,31,31	0
86	OHX	1	4072	7/7	0.14	-0.82	103,103,103,103	0
85	MG	5	3816	1/1	0.14	-0.82	37,37,37,37	0
86	OHX	1	3930	7/7	0.14	-0.82	90,90,90,90	0
85	MG	7	210	1/1	0.15	-0.82	28,28,28,28	0
85	MG	5	3753	1/1	0.16	-0.82	42,42,42,42	0
85	MG	5	3893	1/1	0.12	-0.83	95,95,95,95	0
86	OHX	2	2030	7/7	0.15	-0.83	80,80,80,80	0
85	MG	n6	202	1/1	0.17	-0.83	34,34,34,34	0
86	OHX	1	4042	7/7	0.14	-0.83	97,97,97,97	0
86	OHX	1	4047	7/7	0.13	-0.84	85,85,85,85	0
85	MG	l5	303	1/1	0.15	-0.84	51,51,51,51	0
86	OHX	6	2107	7/7	0.17	-0.84	96,96,96,96	0
85	MG	5	3705	1/1	0.16	-0.85	41,41,41,41	0
86	OHX	5	3965	7/7	0.15	-0.85	82,82,82,82	0
86	OHX	2	2145	7/7	0.13	-0.85	133,133,133,133	0
86	OHX	5	3917	7/7	0.16	-0.86	49,49,49,49	0
86	OHX	1	3954	7/7	0.13	-0.86	98,98,98,98	0
85	MG	2	1982	1/1	0.22	-0.87	59,59,59,59	0
86	OHX	1	3921	7/7	0.15	-0.87	79,79,79,79	0
85	MG	1	3407	1/1	0.16	-0.87	34,34,34,34	0
86	OHX	7	216	7/7	0.16	-0.88	73,73,73,73	0
85	MG	1	3486	1/1	0.14	-0.89	39,39,39,39	0
85	MG	5	3716	1/1	0.16	-0.89	44,44,44,44	0
85	MG	1	3608	1/1	0.15	-0.89	50,50,50,50	0
86	OHX	6	2167	7/7	0.12	-0.90	140,140,140,140	0
86	OHX	5	3944	7/7	0.16	-0.90	71,71,71,71	0
85	MG	4	216	1/1	0.11	-0.90	55,55,55,55	0
86	OHX	1	4164	7/7	0.18	-0.91	108,108,108,108	0
86	OHX	1	3939	7/7	0.15	-0.91	84,84,84,84	0
86	OHX	1	3966	7/7	0.13	-0.91	98,98,98,98	0
85	MG	5	3684	1/1	0.14	-0.92	61,61,61,61	0
85	MG	1	3426	1/1	0.16	-0.92	44,44,44,44	0
85	MG	5	3778	1/1	0.16	-0.93	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4033	7/7	0.17	-0.93	103,103,103,103	0
86	OHX	5	4192	7/7	0.13	-0.94	135,135,135,135	0
86	OHX	5	4061	7/7	0.16	-0.94	80,80,80,80	0
85	MG	5	3835	1/1	0.16	-0.94	46,46,46,46	0
85	MG	1	3452	1/1	0.18	-0.95	23,23,23,23	0
86	OHX	5	3906	7/7	0.17	-0.95	49,49,49,49	0
86	OHX	5	3966	7/7	0.14	-0.96	83,83,83,83	0
85	MG	5	3845	1/1	0.15	-0.96	44,44,44,44	0
85	MG	6	2033	1/1	0.19	-0.96	45,45,45,45	0
85	MG	s8	302	1/1	0.16	-0.96	40,40,40,40	0
86	OHX	5	4031	7/7	0.11	-0.96	110,110,110,110	0
86	OHX	6	2155	7/7	0.16	-0.97	93,93,93,93	0
85	MG	5	3714	1/1	0.16	-0.97	42,42,42,42	0
86	OHX	1	3937	7/7	0.12	-0.97	88,88,88,88	0
86	OHX	14	402	7/7	0.20	-0.97	103,103,103,103	0
85	MG	1	3650	1/1	0.16	-0.98	35,35,35,35	0
86	OHX	m0	301	7/7	0.10	-0.98	105,105,105,105	0
86	OHX	8	215	7/7	0.10	-0.98	90,90,90,90	0
85	MG	1	3416	1/1	0.20	-0.99	21,21,21,21	0
86	OHX	6	2154	7/7	0.12	-0.99	117,117,117,117	0
85	MG	5	3859	1/1	0.16	-1.00	44,44,44,44	0
85	MG	1	3719	1/1	0.15	-1.00	30,30,30,30	0
85	MG	1	3547	1/1	0.17	-1.00	32,32,32,32	0
85	MG	5	3617	1/1	0.13	-1.00	32,32,32,32	0
85	MG	1	3777	1/1	0.14	-1.01	55,55,55,55	0
86	OHX	4	222	7/7	0.16	-1.01	46,46,46,46	0
86	OHX	6	2109	7/7	0.14	-1.01	98,98,98,98	0
85	MG	5	3890	1/1	0.10	-1.02	21,21,21,21	0
86	OHX	5	4119	7/7	0.15	-1.02	99,99,99,99	0
85	MG	1	4221	1/1	0.16	-1.02	36,36,36,36	0
86	OHX	5	3919	7/7	0.15	-1.02	53,53,53,53	0
85	MG	1	3714	1/1	0.18	-1.02	25,25,25,25	0
86	OHX	5	3955	7/7	0.13	-1.03	79,79,79,79	0
85	MG	5	3435	1/1	0.16	-1.03	28,28,28,28	0
85	MG	6	1902	1/1	0.16	-1.04	47,47,47,47	0
85	MG	1	3577	1/1	0.18	-1.04	17,17,17,17	0
85	MG	5	3620	1/1	0.16	-1.04	25,25,25,25	0
85	MG	5	3689	1/1	0.15	-1.04	45,45,45,45	0
87	ZN	e1	501	1/1	0.09	-1.05	130,130,130,130	0
86	OHX	2	2090	7/7	0.13	-1.05	89,89,89,89	0
85	MG	1	3445	1/1	0.17	-1.05	39,39,39,39	0
86	OHX	2	2024	7/7	0.16	-1.05	62,62,62,62	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3520	1/1	0.15	-1.06	23,23,23,23	0
86	OHX	2	2048	7/7	0.08	-1.06	104,104,104,104	0
85	MG	5	3801	1/1	0.13	-1.06	50,50,50,50	0
85	MG	1	3759	1/1	0.14	-1.06	35,35,35,35	0
86	OHX	2	2142	7/7	0.10	-1.07	127,127,127,127	0
85	MG	1	3564	1/1	0.17	-1.08	35,35,35,35	0
86	OHX	O7	103	7/7	0.10	-1.08	77,77,77,77	0
86	OHX	8	216	7/7	0.15	-1.10	86,86,86,86	0
86	OHX	1	3919	7/7	0.13	-1.10	79,79,79,79	0
85	MG	1	3782	1/1	0.14	-1.10	46,46,46,46	0
85	MG	1	3717	1/1	0.14	-1.11	56,56,56,56	0
85	MG	5	3809	1/1	0.20	-1.11	62,62,62,62	0
87	ZN	D9	101	1/1	0.10	-1.11	60,60,60,60	0
85	MG	5	4252	1/1	0.15	-1.11	25,25,25,25	0
86	OHX	2	2151	7/7	0.14	-1.11	134,134,134,134	0
86	OHX	4	229	7/7	0.10	-1.13	121,121,121,121	0
86	OHX	4	230	7/7	0.11	-1.13	113,113,113,113	0
86	OHX	1	3944	7/7	0.14	-1.14	87,87,87,87	0
86	OHX	L3	403	7/7	0.16	-1.14	90,90,90,90	0
86	OHX	2	2036	7/7	0.14	-1.15	88,88,88,88	0
86	OHX	1	3931	7/7	0.10	-1.15	68,68,68,68	0
86	OHX	Q2	503	7/7	0.16	-1.17	64,64,64,64	0
86	OHX	5	4013	7/7	0.12	-1.17	129,129,129,129	0
86	OHX	2	2043	7/7	0.10	-1.17	80,80,80,80	0
85	MG	5	3852	1/1	0.18	-1.18	58,58,58,58	0
85	MG	5	3861	1/1	0.15	-1.18	30,30,30,30	0
86	OHX	6	2132	7/7	0.15	-1.18	100,100,100,100	0
85	MG	5	3771	1/1	0.19	-1.19	55,55,55,55	0
85	MG	L3	402	1/1	0.15	-1.20	43,43,43,43	0
86	OHX	1	4075	7/7	0.15	-1.20	113,113,113,113	0
85	MG	M7	204	1/1	0.17	-1.21	27,27,27,27	0
86	OHX	5	3956	7/7	0.15	-1.21	76,76,76,76	0
86	OHX	2	2049	7/7	0.10	-1.21	94,94,94,94	0
85	MG	1	3816	1/1	0.15	-1.21	38,38,38,38	0
86	OHX	5	4026	7/7	0.16	-1.21	83,83,83,83	0
86	OHX	6	2142	7/7	0.15	-1.21	108,108,108,108	0
85	MG	6	2026	1/1	0.10	-1.22	69,69,69,69	0
86	OHX	1	3893	7/7	0.15	-1.23	52,52,52,52	0
86	OHX	6	2057	7/7	0.14	-1.23	63,63,63,63	0
85	MG	M5	302	1/1	0.13	-1.23	46,46,46,46	0
86	OHX	1	4168	7/7	0.12	-1.23	161,161,161,161	0
85	MG	n8	201	1/1	0.14	-1.23	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3492	1/1	0.17	-1.24	42,42,42,42	0
86	OHX	1	3970	7/7	0.12	-1.24	94,94,94,94	0
87	ZN	q3	501	1/1	0.11	-1.25	50,50,50,50	0
85	MG	6	2002	1/1	0.15	-1.25	43,43,43,43	0
85	MG	1	3491	1/1	0.16	-1.25	23,23,23,23	0
85	MG	n3	202	1/1	0.14	-1.25	35,35,35,35	0
86	OHX	5	4118	7/7	0.15	-1.26	94,94,94,94	0
86	OHX	6	2120	7/7	0.12	-1.26	93,93,93,93	0
85	MG	5	3641	1/1	0.17	-1.26	47,47,47,47	0
86	OHX	6	2118	7/7	0.10	-1.26	89,89,89,89	0
85	MG	2	2005	1/1	0.10	-1.27	59,59,59,59	0
86	OHX	1	4117	7/7	0.12	-1.27	136,136,136,136	0
86	OHX	5	4094	7/7	0.15	-1.28	101,101,101,101	0
85	MG	6	1982	1/1	0.12	-1.29	31,31,31,31	0
85	MG	6	1969	1/1	0.13	-1.30	49,49,49,49	0
86	OHX	5	3947	7/7	0.14	-1.30	72,72,72,72	0
86	OHX	6	2073	7/7	0.13	-1.30	99,99,99,99	0
85	MG	5	3428	1/1	0.17	-1.30	21,21,21,21	0
85	MG	4	202	1/1	0.18	-1.31	48,48,48,48	0
85	MG	L4	402	1/1	0.18	-1.32	51,51,51,51	0
85	MG	M3	201	1/1	0.12	-1.33	37,37,37,37	0
86	OHX	3	219	7/7	0.07	-1.34	96,96,96,96	0
86	OHX	2	2118	7/7	0.16	-1.35	129,129,129,129	0
85	MG	2	1994	1/1	0.15	-1.35	60,60,60,60	0
85	MG	1	3682	1/1	0.16	-1.35	50,50,50,50	0
86	OHX	5	4009	7/7	0.16	-1.35	74,74,74,74	0
85	MG	o4	201	1/1	0.16	-1.36	41,41,41,41	0
86	OHX	5	4166	7/7	0.12	-1.36	120,120,120,120	0
86	OHX	5	4001	7/7	0.15	-1.36	79,79,79,79	0
85	MG	1	3498	1/1	0.16	-1.36	20,20,20,20	0
86	OHX	C5	201	7/7	0.13	-1.37	136,136,136,136	0
86	OHX	2	2124	7/7	0.10	-1.37	116,116,116,116	0
86	OHX	1	4074	7/7	0.12	-1.37	105,105,105,105	0
86	OHX	5	3983	7/7	0.16	-1.37	77,77,77,77	0
86	OHX	5	3910	7/7	0.17	-1.37	48,48,48,48	0
86	OHX	5	3915	7/7	0.15	-1.37	53,53,53,53	0
85	MG	5	3663	1/1	0.14	-1.38	35,35,35,35	0
86	OHX	1	4027	7/7	0.09	-1.38	112,112,112,112	0
86	OHX	1	3889	7/7	0.14	-1.38	56,56,56,56	0
85	MG	1	4218	1/1	0.17	-1.38	17,17,17,17	0
85	MG	2	1908	1/1	0.17	-1.39	60,60,60,60	0
86	OHX	5	3987	7/7	0.10	-1.39	80,80,80,80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3624	1/1	0.17	-1.39	18,18,18,18	0
85	MG	4	218	1/1	0.14	-1.40	34,34,34,34	0
85	MG	8	204	1/1	0.15	-1.40	42,42,42,42	0
86	OHX	5	3975	7/7	0.14	-1.40	75,75,75,75	0
85	MG	1	3626	1/1	0.16	-1.41	39,39,39,39	0
85	MG	1	3666	1/1	0.12	-1.41	30,30,30,30	0
86	OHX	2	2079	7/7	0.13	-1.41	107,107,107,107	0
86	OHX	l3	403	7/7	0.14	-1.42	87,87,87,87	0
85	MG	5	3543	1/1	0.16	-1.42	23,23,23,23	0
86	OHX	o2	201	7/7	0.11	-1.42	78,78,78,78	0
86	OHX	5	4005	7/7	0.12	-1.42	80,80,80,80	0
85	MG	1	3428	1/1	0.12	-1.43	41,41,41,41	0
86	OHX	2	2089	7/7	0.16	-1.43	100,100,100,100	0
86	OHX	5	4054	7/7	0.15	-1.43	86,86,86,86	0
85	MG	5	3782	1/1	0.11	-1.44	64,64,64,64	0
85	MG	5	3436	1/1	0.14	-1.44	36,36,36,36	0
85	MG	M9	201	1/1	0.14	-1.44	52,52,52,52	0
85	MG	5	3701	1/1	0.14	-1.44	56,56,56,56	0
86	OHX	1	4001	7/7	0.13	-1.44	133,133,133,133	0
85	MG	6	1995	1/1	0.15	-1.44	32,32,32,32	0
85	MG	1	3802	1/1	0.14	-1.44	74,74,74,74	0
85	MG	5	3777	1/1	0.11	-1.45	45,45,45,45	0
86	OHX	2	2068	7/7	0.07	-1.45	113,113,113,113	0
86	OHX	3	215	7/7	0.12	-1.46	79,79,79,79	0
85	MG	5	3819	1/1	0.17	-1.48	47,47,47,47	0
86	OHX	5	3929	7/7	0.14	-1.48	50,50,50,50	0
86	OHX	1	3875	7/7	0.15	-1.49	41,41,41,41	0
86	OHX	5	4124	7/7	0.12	-1.49	119,119,119,119	0
86	OHX	1	4054	7/7	0.14	-1.49	94,94,94,94	0
85	MG	6	1962	1/1	0.14	-1.50	37,37,37,37	0
86	OHX	5	4024	7/7	0.12	-1.50	95,95,95,95	0
85	MG	1	3581	1/1	0.16	-1.50	29,29,29,29	0
86	OHX	l5	304	7/7	0.11	-1.51	116,116,116,116	0
86	OHX	6	2105	7/7	0.14	-1.51	97,97,97,97	0
85	MG	5	3489	1/1	0.16	-1.52	42,42,42,42	0
86	OHX	5	4018	7/7	0.10	-1.53	101,101,101,101	0
85	MG	5	3425	1/1	0.16	-1.53	30,30,30,30	0
86	OHX	1	4044	7/7	0.08	-1.53	109,109,109,109	0
86	OHX	5	3979	7/7	0.10	-1.54	76,76,76,76	0
86	OHX	1	4087	7/7	0.13	-1.54	120,120,120,120	0
85	MG	5	3870	1/1	0.12	-1.54	39,39,39,39	0
85	MG	M7	206	1/1	0.15	-1.54	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	6	2024	1/1	0.15	-1.54	40,40,40,40	0
87	ZN	Q3	501	1/1	0.11	-1.54	47,47,47,47	0
86	OHX	5	4135	7/7	0.15	-1.55	109,109,109,109	0
86	OHX	2	2106	7/7	0.14	-1.55	111,111,111,111	0
86	OHX	c3	201	7/7	0.24	-1.55	122,122,122,122	0
85	MG	2	2184	1/1	0.11	-1.55	78,78,78,78	0
87	ZN	q2	501	1/1	0.06	-1.55	59,59,59,59	0
86	OHX	c5	201	7/7	0.17	-1.55	127,127,127,127	0
86	OHX	1	4097	7/7	0.12	-1.55	115,115,115,115	0
86	OHX	1	3995	7/7	0.14	-1.55	81,81,81,81	0
85	MG	5	3849	1/1	0.15	-1.56	40,40,40,40	0
85	MG	5	3660	1/1	0.12	-1.56	39,39,39,39	0
86	OHX	1	4004	7/7	0.17	-1.56	72,72,72,72	0
86	OHX	c1	202	7/7	0.15	-1.56	108,108,108,108	0
86	OHX	2	2037	7/7	0.09	-1.56	71,71,71,71	0
86	OHX	5	4240	7/7	0.16	-1.57	192,192,192,192	0
85	MG	sM	301	1/1	0.12	-1.57	33,33,33,33	0
86	OHX	1	3904	7/7	0.14	-1.57	70,70,70,70	0
87	ZN	O7	101	1/1	0.13	-1.57	25,25,25,25	0
86	OHX	2	2078	7/7	0.10	-1.57	100,100,100,100	0
86	OHX	1	3971	7/7	0.12	-1.58	75,75,75,75	0
86	OHX	1	4029	7/7	0.11	-1.58	102,102,102,102	0
85	MG	5	3455	1/1	0.16	-1.59	82,82,82,82	0
86	OHX	1	3986	7/7	0.05	-1.59	93,93,93,93	0
86	OHX	5	3918	7/7	0.14	-1.59	56,56,56,56	0
86	OHX	1	3928	7/7	0.12	-1.59	72,72,72,72	0
86	OHX	5	4077	7/7	0.09	-1.60	136,136,136,136	0
86	OHX	1	3978	7/7	0.09	-1.60	101,101,101,101	0
86	OHX	6	2202	7/7	0.06	-1.60	159,159,159,159	0
86	OHX	5	4104	7/7	0.12	-1.60	107,107,107,107	0
85	MG	5	3718	1/1	0.15	-1.61	49,49,49,49	0
87	ZN	E1	501	1/1	0.10	-1.61	100,100,100,100	0
85	MG	5	3818	1/1	0.07	-1.61	51,51,51,51	0
86	OHX	6	2054	7/7	0.15	-1.61	69,69,69,69	0
86	OHX	5	4046	7/7	0.17	-1.62	78,78,78,78	0
85	MG	5	3712	1/1	0.14	-1.62	38,38,38,38	0
86	OHX	5	4206	7/7	0.13	-1.62	121,121,121,121	0
86	OHX	1	3905	7/7	0.14	-1.63	52,52,52,52	0
86	OHX	6	2067	7/7	0.11	-1.64	70,70,70,70	0
86	OHX	5	4017	7/7	0.13	-1.64	128,128,128,128	0
86	OHX	O2	201	7/7	0.12	-1.65	74,74,74,74	0
85	MG	1	3449	1/1	0.13	-1.65	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4138	7/7	0.13	-1.65	111,111,111,111	0
86	OHX	5	4040	7/7	0.13	-1.65	103,103,103,103	0
86	OHX	6	2141	7/7	0.09	-1.65	127,127,127,127	0
86	OHX	1	4121	7/7	0.16	-1.65	102,102,102,102	0
85	MG	5	3720	1/1	0.15	-1.65	31,31,31,31	0
86	OHX	6	2065	7/7	0.12	-1.66	78,78,78,78	0
86	OHX	2	2069	7/7	0.10	-1.67	125,125,125,125	0
86	OHX	2	2121	7/7	0.10	-1.67	116,116,116,116	0
85	MG	1	3499	1/1	0.17	-1.67	52,52,52,52	0
85	MG	5	3611	1/1	0.13	-1.68	22,22,22,22	0
86	OHX	1	3948	7/7	0.14	-1.69	90,90,90,90	0
86	OHX	5	3958	7/7	0.14	-1.69	71,71,71,71	0
85	MG	14	401	1/1	0.16	-1.69	28,28,28,28	0
86	OHX	1	4038	7/7	0.05	-1.70	119,119,119,119	0
85	MG	1	3686	1/1	0.11	-1.71	44,44,44,44	0
86	OHX	1	4110	7/7	0.14	-1.71	92,92,92,92	0
86	OHX	6	2101	7/7	0.10	-1.72	134,134,134,134	0
86	OHX	5	3933	7/7	0.13	-1.72	60,60,60,60	0
86	OHX	1	3885	7/7	0.15	-1.73	55,55,55,55	0
86	OHX	1	4045	7/7	0.12	-1.73	94,94,94,94	0
85	MG	1	3731	1/1	0.13	-1.73	40,40,40,40	0
86	OHX	1	3886	7/7	0.15	-1.74	53,53,53,53	0
85	MG	1	3771	1/1	0.07	-1.74	36,36,36,36	0
86	OHX	1	4016	7/7	0.08	-1.74	105,105,105,105	0
86	OHX	5	3908	7/7	0.15	-1.74	39,39,39,39	0
85	MG	1	3763	1/1	0.14	-1.74	38,38,38,38	0
87	ZN	o7	501	1/1	0.11	-1.74	29,29,29,29	0
86	OHX	1	4100	7/7	0.11	-1.74	116,116,116,116	0
86	OHX	6	2100	7/7	0.12	-1.75	127,127,127,127	0
85	MG	1	3649	1/1	0.13	-1.76	19,19,19,19	0
86	OHX	2	2044	7/7	0.12	-1.76	96,96,96,96	0
86	OHX	1	4088	7/7	0.14	-1.77	104,104,104,104	0
85	MG	5	3628	1/1	0.16	-1.78	32,32,32,32	0
86	OHX	6	2115	7/7	0.18	-1.78	95,95,95,95	0
85	MG	4	212	1/1	0.15	-1.78	29,29,29,29	0
85	MG	6	1915	1/1	0.13	-1.78	57,57,57,57	0
85	MG	5	3447	1/1	0.14	-1.79	29,29,29,29	0
85	MG	1	3833	1/1	0.09	-1.80	40,40,40,40	0
85	MG	5	3888	1/1	0.14	-1.80	32,32,32,32	0
85	MG	5	3878	1/1	0.18	-1.80	27,27,27,27	0
86	OHX	1	3952	7/7	0.10	-1.81	90,90,90,90	0
86	OHX	1	3927	7/7	0.13	-1.81	56,56,56,56	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4030	7/7	0.14	-1.81	94,94,94,94	0
86	OHX	M5	304	7/7	0.13	-1.82	91,91,91,91	0
85	MG	1	3422	1/1	0.15	-1.82	23,23,23,23	0
86	OHX	5	3923	7/7	0.15	-1.83	57,57,57,57	0
86	OHX	4	223	7/7	0.12	-1.83	77,77,77,77	0
85	MG	4	213	1/1	0.18	-1.83	50,50,50,50	0
85	MG	5	3513	1/1	0.16	-1.84	27,27,27,27	0
85	MG	N3	203	1/1	0.10	-1.84	40,40,40,40	0
85	MG	1	3750	1/1	0.10	-1.85	38,38,38,38	0
86	OHX	1	4012	7/7	0.15	-1.85	101,101,101,101	0
86	OHX	2	2040	7/7	0.10	-1.85	79,79,79,79	0
86	OHX	1	4024	7/7	0.16	-1.85	94,94,94,94	0
86	OHX	6	2056	7/7	0.14	-1.86	57,57,57,57	0
85	MG	5	3699	1/1	0.15	-1.86	30,30,30,30	0
86	OHX	M0	303	7/7	0.13	-1.86	86,86,86,86	0
85	MG	1	3753	1/1	0.12	-1.87	44,44,44,44	0
86	OHX	1	3997	7/7	0.12	-1.87	111,111,111,111	0
85	MG	5	3417	1/1	0.14	-1.87	21,21,21,21	0
86	OHX	5	4101	7/7	0.12	-1.87	121,121,121,121	0
85	MG	1	3664	1/1	0.14	-1.88	39,39,39,39	0
87	ZN	d6	101	1/1	0.12	-1.90	48,48,48,48	0
86	OHX	1	3994	7/7	0.16	-1.90	92,92,92,92	0
86	OHX	6	2096	7/7	0.11	-1.91	105,105,105,105	0
86	OHX	1	3907	7/7	0.14	-1.91	61,61,61,61	0
86	OHX	5	4133	7/7	0.15	-1.91	102,102,102,102	0
86	OHX	2	2104	7/7	0.11	-1.92	169,169,169,169	0
85	MG	1	3712	1/1	0.12	-1.93	41,41,41,41	0
85	MG	5	3651	1/1	0.14	-1.93	31,31,31,31	0
86	OHX	1	3968	7/7	0.16	-1.93	65,65,65,65	0
85	MG	5	3694	1/1	0.13	-1.93	35,35,35,35	0
85	MG	8	208	1/1	0.15	-1.93	34,34,34,34	0
85	MG	5	3632	1/1	0.14	-1.94	30,30,30,30	0
86	OHX	2	2027	7/7	0.13	-1.94	69,69,69,69	0
86	OHX	5	4036	7/7	0.10	-1.94	105,105,105,105	0
86	OHX	2	2050	7/7	0.11	-1.95	95,95,95,95	0
85	MG	1	3602	1/1	0.15	-1.95	21,21,21,21	0
86	OHX	5	4131	7/7	0.13	-1.96	147,147,147,147	0
86	OHX	2	2054	7/7	0.12	-1.96	107,107,107,107	0
86	OHX	5	3962	7/7	0.10	-1.96	73,73,73,73	0
86	OHX	m5	302	7/7	0.11	-1.97	98,98,98,98	0
85	MG	1	3636	1/1	0.14	-1.97	43,43,43,43	0
85	MG	1	3690	1/1	0.16	-1.97	49,49,49,49	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	2	2182	1/1	0.14	-1.98	54,54,54,54	0
86	OHX	n3	203	7/7	0.10	-1.98	69,69,69,69	0
86	OHX	6	2150	7/7	0.15	-1.98	115,115,115,115	0
85	MG	5	3761	1/1	0.16	-1.99	64,64,64,64	0
85	MG	c1	201	1/1	0.14	-1.99	41,41,41,41	0
86	OHX	5	4098	7/7	0.13	-1.99	114,114,114,114	0
85	MG	5	3692	1/1	0.14	-2.00	39,39,39,39	0
86	OHX	6	2077	7/7	0.14	-2.01	92,92,92,92	0
86	OHX	5	4088	7/7	0.15	-2.01	91,91,91,91	0
85	MG	5	3800	1/1	0.13	-2.01	35,35,35,35	0
86	OHX	6	2110	7/7	0.15	-2.01	93,93,93,93	0
85	MG	1	3424	1/1	0.12	-2.02	37,37,37,37	0
85	MG	1	3723	1/1	0.12	-2.03	43,43,43,43	0
86	OHX	1	4057	7/7	0.15	-2.03	114,114,114,114	0
86	OHX	SR	401	7/7	0.07	-2.03	136,136,136,136	0
85	MG	L2	301	1/1	0.11	-2.03	26,26,26,26	0
86	OHX	1	3902	7/7	0.14	-2.03	59,59,59,59	0
85	MG	5	3767	1/1	0.14	-2.04	29,29,29,29	0
85	MG	2	1985	1/1	0.15	-2.04	45,45,45,45	0
85	MG	5	3708	1/1	0.16	-2.04	36,36,36,36	0
86	OHX	7	222	7/7	0.06	-2.05	89,89,89,89	0
86	OHX	1	3879	7/7	0.17	-2.05	50,50,50,50	0
85	MG	8	202	1/1	0.14	-2.05	47,47,47,47	0
86	OHX	1	3949	7/7	0.09	-2.06	78,78,78,78	0
85	MG	M0	302	1/1	0.10	-2.06	37,37,37,37	0
86	OHX	2	2130	7/7	0.13	-2.06	150,150,150,150	0
86	OHX	1	3940	7/7	0.10	-2.07	80,80,80,80	0
86	OHX	1	4002	7/7	0.08	-2.07	115,115,115,115	0
85	MG	5	3603	1/1	0.16	-2.08	19,19,19,19	0
86	OHX	6	2128	7/7	0.12	-2.09	109,109,109,109	0
85	MG	1	3601	1/1	0.16	-2.09	18,18,18,18	0
86	OHX	1	3913	7/7	0.14	-2.09	72,72,72,72	0
86	OHX	5	3943	7/7	0.16	-2.09	64,64,64,64	0
86	OHX	3	221	7/7	0.08	-2.10	102,102,102,102	0
86	OHX	5	3954	7/7	0.13	-2.10	74,74,74,74	0
85	MG	2	1964	1/1	0.12	-2.11	117,117,117,117	0
86	OHX	5	4011	7/7	0.12	-2.11	82,82,82,82	0
86	OHX	1	4089	7/7	0.09	-2.11	159,159,159,159	0
85	MG	5	3740	1/1	0.14	-2.11	34,34,34,34	0
85	MG	6	2034	1/1	0.13	-2.11	50,50,50,50	0
86	OHX	2	2039	7/7	0.12	-2.12	83,83,83,83	0
86	OHX	1	4101	7/7	0.12	-2.12	122,122,122,122	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	3936	7/7	0.13	-2.13	76,76,76,76	0
85	MG	5	3459	1/1	0.14	-2.13	23,23,23,23	0
86	OHX	5	3996	7/7	0.14	-2.13	78,78,78,78	0
86	OHX	2	2028	7/7	0.13	-2.13	62,62,62,62	0
85	MG	5	3484	1/1	0.15	-2.14	42,42,42,42	0
86	OHX	C3	202	7/7	0.12	-2.16	131,131,131,131	0
85	MG	5	3839	1/1	0.15	-2.16	30,30,30,30	0
85	MG	1	3828	1/1	0.12	-2.17	35,35,35,35	0
85	MG	5	3599	1/1	0.14	-2.17	31,31,31,31	0
85	MG	7	211	1/1	0.14	-2.17	46,46,46,46	0
86	OHX	5	4073	7/7	0.14	-2.18	93,93,93,93	0
86	OHX	6	2089	7/7	0.10	-2.19	108,108,108,108	0
86	OHX	2	2056	7/7	0.11	-2.19	93,93,93,93	0
86	OHX	1	4015	7/7	0.12	-2.20	98,98,98,98	0
86	OHX	5	4083	7/7	0.16	-2.20	94,94,94,94	0
86	OHX	6	2129	7/7	0.10	-2.22	113,113,113,113	0
86	OHX	5	3961	7/7	0.07	-2.22	72,72,72,72	0
85	MG	1	3406	1/1	0.14	-2.22	26,26,26,26	0
86	OHX	1	4095	7/7	0.15	-2.22	95,95,95,95	0
86	OHX	1	4078	7/7	0.12	-2.22	101,101,101,101	0
85	MG	6	2025	1/1	0.12	-2.23	52,52,52,52	0
86	OHX	2	2047	7/7	0.07	-2.23	94,94,94,94	0
86	OHX	6	2122	7/7	0.08	-2.23	115,115,115,115	0
87	ZN	D6	500	1/1	0.08	-2.24	67,67,67,67	0
85	MG	5	4256	1/1	0.15	-2.25	23,23,23,23	0
85	MG	M5	301	1/1	0.13	-2.25	43,43,43,43	0
85	MG	1	3478	1/1	0.14	-2.25	36,36,36,36	0
86	OHX	6	2052	7/7	0.15	-2.26	56,56,56,56	0
86	OHX	1	3912	7/7	0.15	-2.27	66,66,66,66	0
86	OHX	2	2114	7/7	0.15	-2.27	124,124,124,124	0
86	OHX	6	2071	7/7	0.10	-2.27	96,96,96,96	0
85	MG	1	3584	1/1	0.14	-2.27	31,31,31,31	0
85	MG	5	3759	1/1	0.14	-2.28	32,32,32,32	0
86	OHX	1	3989	7/7	0.14	-2.29	72,72,72,72	0
86	OHX	5	3970	7/7	0.11	-2.29	77,77,77,77	0
85	MG	n8	202	1/1	0.15	-2.29	19,19,19,19	0
85	MG	6	1974	1/1	0.15	-2.29	45,45,45,45	0
86	OHX	2	2157	7/7	0.13	-2.30	195,195,195,195	0
85	MG	1	3645	1/1	0.07	-2.30	54,54,54,54	0
86	OHX	O7	104	7/7	0.12	-2.30	75,75,75,75	0
86	OHX	c8	203	7/7	0.07	-2.31	113,113,113,113	0
85	MG	1	3866	1/1	0.15	-2.31	49,49,49,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3794	1/1	0.09	-2.32	45,45,45,45	0
86	OHX	6	2116	7/7	0.12	-2.33	100,100,100,100	0
85	MG	1	3846	1/1	0.16	-2.33	24,24,24,24	0
86	OHX	5	4008	7/7	0.09	-2.34	64,64,64,64	0
86	OHX	3	222	7/7	0.10	-2.35	119,119,119,119	0
86	OHX	5	3968	7/7	0.14	-2.36	74,74,74,74	0
85	MG	5	3407	1/1	0.12	-2.36	32,32,32,32	0
85	MG	5	3715	1/1	0.13	-2.39	58,58,58,58	0
85	MG	5	3527	1/1	0.16	-2.39	26,26,26,26	0
85	MG	O7	102	1/1	0.15	-2.40	32,32,32,32	0
85	MG	1	3611	1/1	0.11	-2.41	36,36,36,36	0
86	OHX	1	4018	7/7	0.14	-2.41	93,93,93,93	0
86	OHX	2	2095	7/7	0.06	-2.41	132,132,132,132	0
85	MG	1	3783	1/1	0.13	-2.42	36,36,36,36	0
86	OHX	6	2070	7/7	0.11	-2.44	67,67,67,67	0
86	OHX	6	2097	7/7	0.08	-2.44	119,119,119,119	0
86	OHX	1	4139	7/7	0.14	-2.45	87,87,87,87	0
86	OHX	6	2123	7/7	0.11	-2.45	114,114,114,114	0
86	OHX	7	221	7/7	0.11	-2.45	82,82,82,82	0
86	OHX	1	3918	7/7	0.14	-2.46	72,72,72,72	0
85	MG	6	1994	1/1	0.05	-2.47	51,51,51,51	0
86	OHX	5	3995	7/7	0.12	-2.47	86,86,86,86	0
86	OHX	2	2057	7/7	0.10	-2.47	105,105,105,105	0
86	OHX	6	2164	7/7	0.09	-2.48	153,153,153,153	0
85	MG	1	4220	1/1	0.10	-2.48	23,23,23,23	0
85	MG	1	3662	1/1	0.10	-2.49	22,22,22,22	0
85	MG	5	3840	1/1	0.06	-2.51	43,43,43,43	0
85	MG	5	3703	1/1	0.09	-2.51	32,32,32,32	0
86	OHX	1	3963	7/7	0.08	-2.51	88,88,88,88	0
86	OHX	5	4045	7/7	0.14	-2.51	95,95,95,95	0
86	OHX	4	225	7/7	0.10	-2.52	97,97,97,97	0
85	MG	5	3854	1/1	0.13	-2.52	54,54,54,54	0
85	MG	m7	205	1/1	0.13	-2.53	26,26,26,26	0
87	ZN	Q2	501	1/1	0.05	-2.54	63,63,63,63	0
85	MG	5	3461	1/1	0.17	-2.54	29,29,29,29	0
86	OHX	6	2062	7/7	0.12	-2.55	71,71,71,71	0
85	MG	m7	201	1/1	0.14	-2.55	24,24,24,24	0
85	MG	5	3787	1/1	0.13	-2.55	33,33,33,33	0
85	MG	5	3444	1/1	0.14	-2.55	21,21,21,21	0
85	MG	5	3600	1/1	0.11	-2.55	50,50,50,50	0
86	OHX	6	2058	7/7	0.13	-2.56	61,61,61,61	0
86	OHX	5	4063	7/7	0.14	-2.57	106,106,106,106	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3950	7/7	0.10	-2.57	89,89,89,89	0
86	OHX	1	3975	7/7	0.10	-2.57	88,88,88,88	0
86	OHX	1	4112	7/7	0.12	-2.57	102,102,102,102	0
86	OHX	6	2106	7/7	0.10	-2.57	92,92,92,92	0
86	OHX	5	3911	7/7	0.16	-2.57	44,44,44,44	0
86	OHX	5	4028	7/7	0.15	-2.58	73,73,73,73	0
86	OHX	1	4003	7/7	0.14	-2.58	90,90,90,90	0
86	OHX	1	3911	7/7	0.14	-2.58	70,70,70,70	0
86	OHX	2	2091	7/7	0.12	-2.60	100,100,100,100	0
86	OHX	6	2099	7/7	0.10	-2.60	124,124,124,124	0
85	MG	1	4223	1/1	0.15	-2.60	20,20,20,20	0
85	MG	5	3795	1/1	0.11	-2.61	42,42,42,42	0
86	OHX	5	4064	7/7	0.08	-2.61	125,125,125,125	0
85	MG	6	2016	1/1	0.12	-2.62	38,38,38,38	0
86	OHX	2	2055	7/7	0.10	-2.62	100,100,100,100	0
86	OHX	1	4154	7/7	0.15	-2.62	109,109,109,109	0
85	MG	1	3793	1/1	0.11	-2.63	73,73,73,73	0
85	MG	5	3674	1/1	0.13	-2.63	33,33,33,33	0
85	MG	5	3510	1/1	0.11	-2.64	20,20,20,20	0
86	OHX	2	2065	7/7	0.13	-2.65	87,87,87,87	0
86	OHX	5	3969	7/7	0.10	-2.66	76,76,76,76	0
85	MG	5	3831	1/1	0.07	-2.66	59,59,59,59	0
86	OHX	5	4071	7/7	0.17	-2.66	106,106,106,106	0
86	OHX	2	2074	7/7	0.06	-2.66	111,111,111,111	0
85	MG	12	302	1/1	0.11	-2.66	28,28,28,28	0
86	OHX	5	3991	7/7	0.10	-2.68	69,69,69,69	0
86	OHX	1	3906	7/7	0.12	-2.68	57,57,57,57	0
86	OHX	2	2082	7/7	0.12	-2.69	110,110,110,110	0
86	OHX	5	4007	7/7	0.11	-2.69	101,101,101,101	0
86	OHX	5	4002	7/7	0.13	-2.70	58,58,58,58	0
86	OHX	5	3980	7/7	0.10	-2.70	81,81,81,81	0
86	OHX	q2	502	7/7	0.12	-2.71	67,67,67,67	0
85	MG	1	3724	1/1	0.11	-2.71	43,43,43,43	0
85	MG	1	3642	1/1	0.12	-2.72	36,36,36,36	0
85	MG	1	3640	1/1	0.14	-2.72	28,28,28,28	0
85	MG	5	3654	1/1	0.10	-2.73	35,35,35,35	0
85	MG	1	3779	1/1	0.16	-2.73	24,24,24,24	0
86	OHX	1	3920	7/7	0.11	-2.74	70,70,70,70	0
85	MG	5	3843	1/1	0.16	-2.75	25,25,25,25	0
86	OHX	3	224	7/7	0.14	-2.75	132,132,132,132	0
85	MG	5	3437	1/1	0.11	-2.76	45,45,45,45	0
86	OHX	o7	502	7/7	0.12	-2.77	80,80,80,80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	M5	303	7/7	0.11	-2.77	68,68,68,68	0
86	OHX	5	3936	7/7	0.12	-2.77	54,54,54,54	0
86	OHX	5	4025	7/7	0.09	-2.78	88,88,88,88	0
86	OHX	1	4036	7/7	0.11	-2.78	87,87,87,87	0
86	OHX	5	3957	7/7	0.09	-2.78	65,65,65,65	0
86	OHX	2	2133	7/7	0.11	-2.79	119,119,119,119	0
85	MG	5	3440	1/1	0.10	-2.79	31,31,31,31	0
85	MG	N3	202	1/1	0.08	-2.79	51,51,51,51	0
86	OHX	1	3947	7/7	0.14	-2.79	70,70,70,70	0
85	MG	5	3750	1/1	0.14	-2.80	34,34,34,34	0
86	OHX	2	2094	7/7	0.11	-2.80	119,119,119,119	0
86	OHX	5	4032	7/7	0.14	-2.80	88,88,88,88	0
86	OHX	1	3956	7/7	0.13	-2.82	86,86,86,86	0
86	OHX	1	4059	7/7	0.10	-2.82	117,117,117,117	0
85	MG	1	3477	1/1	0.10	-2.83	30,30,30,30	0
86	OHX	6	2086	7/7	0.12	-2.83	88,88,88,88	0
86	OHX	5	3930	7/7	0.12	-2.84	48,48,48,48	0
86	OHX	1	3899	7/7	0.13	-2.84	48,48,48,48	0
86	OHX	5	4022	7/7	0.09	-2.86	87,87,87,87	0
86	OHX	6	2153	7/7	0.14	-2.86	118,118,118,118	0
85	MG	5	3830	1/1	0.09	-2.87	46,46,46,46	0
85	MG	6	1984	1/1	0.14	-2.87	70,70,70,70	0
85	MG	1	3823	1/1	0.11	-2.87	30,30,30,30	0
86	OHX	1	4010	7/7	0.13	-2.87	82,82,82,82	0
85	MG	1	3681	1/1	0.09	-2.88	56,56,56,56	0
86	OHX	5	3986	7/7	0.11	-2.88	72,72,72,72	0
85	MG	1	3692	1/1	0.13	-2.89	25,25,25,25	0
86	OHX	1	4077	7/7	0.10	-2.89	97,97,97,97	0
86	OHX	2	2098	7/7	0.07	-2.90	126,126,126,126	0
86	OHX	5	3934	7/7	0.13	-2.91	62,62,62,62	0
86	OHX	1	4014	7/7	0.13	-2.92	104,104,104,104	0
85	MG	12	301	1/1	0.18	-2.92	43,43,43,43	0
86	OHX	5	3953	7/7	0.10	-2.93	55,55,55,55	0
86	OHX	5	3981	7/7	0.11	-2.93	71,71,71,71	0
85	MG	M7	205	1/1	0.14	-2.96	34,34,34,34	0
85	MG	5	3733	1/1	0.13	-2.97	32,32,32,32	0
86	OHX	5	3941	7/7	0.10	-2.97	67,67,67,67	0
86	OHX	5	3963	7/7	0.14	-2.98	77,77,77,77	0
86	OHX	4	228	7/7	0.13	-2.98	96,96,96,96	0
86	OHX	1	3898	7/7	0.11	-3.00	55,55,55,55	0
85	MG	5	3769	1/1	0.21	-3.00	86,86,86,86	0
85	MG	1	3780	1/1	0.15	-3.00	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4175	7/7	0.13	-3.01	86,86,86,86	0
86	OHX	1	4062	7/7	0.06	-3.01	133,133,133,133	0
86	OHX	1	3964	7/7	0.09	-3.02	90,90,90,90	0
86	OHX	2	2032	7/7	0.12	-3.02	89,89,89,89	0
85	MG	5	3666	1/1	0.13	-3.03	21,21,21,21	0
86	OHX	5	4043	7/7	0.15	-3.05	96,96,96,96	0
86	OHX	5	4111	7/7	0.14	-3.06	104,104,104,104	0
86	OHX	1	3923	7/7	0.10	-3.06	69,69,69,69	0
86	OHX	5	4003	7/7	0.13	-3.07	95,95,95,95	0
85	MG	5	3719	1/1	0.16	-3.08	31,31,31,31	0
86	OHX	2	2061	7/7	0.12	-3.10	84,84,84,84	0
85	MG	5	3860	1/1	0.13	-3.10	51,51,51,51	0
86	OHX	5	4197	7/7	0.14	-3.10	92,92,92,92	0
86	OHX	2	2088	7/7	0.09	-3.10	101,101,101,101	0
85	MG	1	3857	1/1	0.13	-3.11	59,59,59,59	0
86	OHX	2	2081	7/7	0.09	-3.11	127,127,127,127	0
86	OHX	6	2135	7/7	0.09	-3.12	116,116,116,116	0
85	MG	5	3711	1/1	0.10	-3.12	51,51,51,51	0
86	OHX	2	2096	7/7	0.11	-3.12	121,121,121,121	0
86	OHX	1	4119	7/7	0.15	-3.12	103,103,103,103	0
86	OHX	1	4051	7/7	0.10	-3.14	99,99,99,99	0
86	OHX	5	4096	7/7	0.13	-3.15	115,115,115,115	0
86	OHX	6	2078	7/7	0.11	-3.15	76,76,76,76	0
86	OHX	1	4109	7/7	0.09	-3.16	120,120,120,120	0
86	OHX	5	3920	7/7	0.14	-3.17	51,51,51,51	0
85	MG	1	3772	1/1	0.14	-3.18	47,47,47,47	0
86	OHX	1	4022	7/7	0.14	-3.18	105,105,105,105	0
85	MG	1	3603	1/1	0.14	-3.21	24,24,24,24	0
85	MG	5	3408	1/1	0.11	-3.21	17,17,17,17	0
85	MG	1	3830	1/1	0.14	-3.21	16,16,16,16	0
86	OHX	1	3938	7/7	0.13	-3.23	58,58,58,58	0
85	MG	1	3605	1/1	0.14	-3.23	29,29,29,29	0
86	OHX	5	4038	7/7	0.08	-3.23	105,105,105,105	0
86	OHX	o3	203	7/7	0.08	-3.24	88,88,88,88	0
85	MG	5	3820	1/1	0.11	-3.25	52,52,52,52	0
86	OHX	5	3922	7/7	0.15	-3.26	53,53,53,53	0
86	OHX	6	2082	7/7	0.06	-3.27	83,83,83,83	0
85	MG	1	3446	1/1	0.08	-3.27	31,31,31,31	0
85	MG	6	1978	1/1	0.13	-3.27	67,67,67,67	0
85	MG	1	3427	1/1	0.13	-3.28	27,27,27,27	0
86	OHX	2	2052	7/7	0.14	-3.29	83,83,83,83	0
86	OHX	6	2063	7/7	0.11	-3.30	71,71,71,71	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2083	7/7	0.08	-3.31	114,114,114,114	0
85	MG	6	2017	1/1	0.11	-3.32	58,58,58,58	0
86	OHX	6	2085	7/7	0.10	-3.32	109,109,109,109	0
86	OHX	1	4056	7/7	0.09	-3.34	112,112,112,112	0
86	OHX	1	3998	7/7	0.09	-3.35	96,96,96,96	0
86	OHX	6	2069	7/7	0.10	-3.36	79,79,79,79	0
86	OHX	5	3977	7/7	0.11	-3.36	81,81,81,81	0
86	OHX	8	222	7/7	0.07	-3.37	114,114,114,114	0
86	OHX	2	2076	7/7	0.13	-3.37	115,115,115,115	0
86	OHX	6	2083	7/7	0.11	-3.37	98,98,98,98	0
86	OHX	2	2059	7/7	0.08	-3.38	91,91,91,91	0
85	MG	1	3831	1/1	0.11	-3.38	39,39,39,39	0
85	MG	5	3682	1/1	0.16	-3.39	22,22,22,22	0
85	MG	1	3812	1/1	0.14	-3.39	27,27,27,27	0
86	OHX	5	3989	7/7	0.14	-3.40	62,62,62,62	0
86	OHX	1	4080	7/7	0.10	-3.41	106,106,106,106	0
86	OHX	7	223	7/7	0.08	-3.42	106,106,106,106	0
85	MG	5	3837	1/1	0.14	-3.43	40,40,40,40	0
86	OHX	5	4006	7/7	0.11	-3.46	87,87,87,87	0
85	MG	1	3476	1/1	0.15	-3.46	21,21,21,21	0
86	OHX	1	3884	7/7	0.12	-3.46	50,50,50,50	0
86	OHX	5	4085	7/7	0.10	-3.47	95,95,95,95	0
85	MG	5	3664	1/1	0.12	-3.47	37,37,37,37	0
86	OHX	5	4068	7/7	0.13	-3.48	81,81,81,81	0
86	OHX	1	3974	7/7	0.10	-3.48	86,86,86,86	0
86	OHX	2	2131	7/7	0.12	-3.49	93,93,93,93	0
86	OHX	1	3916	7/7	0.13	-3.50	71,71,71,71	0
85	MG	1	3744	1/1	0.12	-3.50	29,29,29,29	0
85	MG	1	3497	1/1	0.11	-3.51	33,33,33,33	0
86	OHX	5	4084	7/7	0.10	-3.52	112,112,112,112	0
86	OHX	1	4181	7/7	0.09	-3.53	192,192,192,192	0
85	MG	2	2002	1/1	0.10	-3.54	87,87,87,87	0
86	OHX	2	2097	7/7	0.08	-3.55	131,131,131,131	0
86	OHX	1	4006	7/7	0.10	-3.55	102,102,102,102	0
86	OHX	5	3916	7/7	0.13	-3.56	51,51,51,51	0
85	MG	2	1942	1/1	0.10	-3.57	63,63,63,63	0
86	OHX	6	2068	7/7	0.09	-3.57	71,71,71,71	0
85	MG	5	3857	1/1	0.12	-3.58	37,37,37,37	0
86	OHX	2	2067	7/7	0.10	-3.58	114,114,114,114	0
85	MG	O3	201	1/1	0.10	-3.60	28,28,28,28	0
86	OHX	1	3976	7/7	0.10	-3.61	80,80,80,80	0
85	MG	1	3565	1/1	0.15	-3.61	27,27,27,27	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3738	1/1	0.13	-3.61	24,24,24,24	0
85	MG	m5	301	1/1	0.10	-3.63	45,45,45,45	0
86	OHX	6	2095	7/7	0.11	-3.64	100,100,100,100	0
86	OHX	5	4000	7/7	0.10	-3.64	94,94,94,94	0
86	OHX	1	3890	7/7	0.14	-3.65	53,53,53,53	0
86	OHX	1	4028	7/7	0.12	-3.65	92,92,92,92	0
86	OHX	1	3910	7/7	0.09	-3.65	66,66,66,66	0
85	MG	1	3433	1/1	0.11	-3.65	29,29,29,29	0
86	OHX	1	4069	7/7	0.07	-3.65	119,119,119,119	0
85	MG	5	3450	1/1	0.14	-3.66	20,20,20,20	0
86	OHX	1	3962	7/7	0.09	-3.66	59,59,59,59	0
86	OHX	6	2079	7/7	0.08	-3.68	88,88,88,88	0
86	OHX	6	2061	7/7	0.12	-3.70	65,65,65,65	0
86	OHX	1	3958	7/7	0.11	-3.71	75,75,75,75	0
85	MG	5	3806	1/1	0.11	-3.71	30,30,30,30	0
85	MG	1	3558	1/1	0.16	-3.73	40,40,40,40	0
85	MG	5	3724	1/1	0.16	-3.74	28,28,28,28	0
85	MG	1	3729	1/1	0.14	-3.74	61,61,61,61	0
86	OHX	5	3952	7/7	0.11	-3.75	83,83,83,83	0
85	MG	1	3764	1/1	0.11	-3.76	42,42,42,42	0
85	MG	5	3774	1/1	0.13	-3.77	27,27,27,27	0
86	OHX	5	4014	7/7	0.09	-3.82	77,77,77,77	0
86	OHX	1	4021	7/7	0.13	-3.83	99,99,99,99	0
86	OHX	1	3896	7/7	0.11	-3.84	52,52,52,52	0
85	MG	1	3710	1/1	0.13	-3.85	25,25,25,25	0
85	MG	5	3678	1/1	0.13	-3.85	37,37,37,37	0
85	MG	1	3672	1/1	0.13	-3.85	36,36,36,36	0
85	MG	2	1999	1/1	0.12	-3.86	83,83,83,83	0
86	OHX	2	2029	7/7	0.13	-3.86	75,75,75,75	0
86	OHX	1	3895	7/7	0.14	-3.86	54,54,54,54	0
86	OHX	6	2166	7/7	0.11	-3.87	115,115,115,115	0
86	OHX	1	3993	7/7	0.11	-3.89	84,84,84,84	0
86	OHX	1	3908	7/7	0.11	-3.90	54,54,54,54	0
86	OHX	1	3987	7/7	0.10	-3.93	80,80,80,80	0
86	OHX	l3	402	7/7	0.07	-3.93	79,79,79,79	0
86	OHX	7	220	7/7	0.13	-3.93	76,76,76,76	0
86	OHX	1	4011	7/7	0.10	-3.97	89,89,89,89	0
86	OHX	5	4128	7/7	0.12	-3.98	112,112,112,112	0
85	MG	6	2008	1/1	0.13	-3.99	41,41,41,41	0
86	OHX	1	3946	7/7	0.12	-4.03	71,71,71,71	0
85	MG	1	3438	1/1	0.14	-4.03	36,36,36,36	0
85	MG	5	3704	1/1	0.14	-4.03	41,41,41,41	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4026	7/7	0.07	-4.03	116,116,116,116	0
86	OHX	1	4032	7/7	0.12	-4.06	108,108,108,108	0
85	MG	6	1970	1/1	0.13	-4.06	49,49,49,49	0
86	OHX	5	4103	7/7	0.10	-4.08	123,123,123,123	0
86	OHX	1	4052	7/7	0.07	-4.10	108,108,108,108	0
86	OHX	5	4060	7/7	0.09	-4.10	113,113,113,113	0
86	OHX	5	4065	7/7	0.12	-4.12	91,91,91,91	0
85	MG	1	3775	1/1	0.14	-4.14	29,29,29,29	0
85	MG	5	3597	1/1	0.12	-4.14	28,28,28,28	0
85	MG	1	3760	1/1	0.14	-4.14	30,30,30,30	0
86	OHX	1	3881	7/7	0.13	-4.15	46,46,46,46	0
85	MG	5	3430	1/1	0.13	-4.15	27,27,27,27	0
86	OHX	2	2072	7/7	0.06	-4.15	100,100,100,100	0
85	MG	5	3485	1/1	0.11	-4.16	41,41,41,41	0
86	OHX	1	3933	7/7	0.12	-4.18	86,86,86,86	0
85	MG	1	3468	1/1	0.10	-4.18	37,37,37,37	0
86	OHX	5	4016	7/7	0.14	-4.19	87,87,87,87	0
86	OHX	2	2060	7/7	0.08	-4.19	99,99,99,99	0
86	OHX	6	2108	7/7	0.12	-4.19	88,88,88,88	0
85	MG	5	3779	1/1	0.15	-4.19	38,38,38,38	0
86	OHX	1	3985	7/7	0.11	-4.20	69,69,69,69	0
86	OHX	1	3961	7/7	0.11	-4.22	72,72,72,72	0
85	MG	1	3745	1/1	0.12	-4.23	39,39,39,39	0
85	MG	6	1930	1/1	0.14	-4.25	46,46,46,46	0
85	MG	1	3695	1/1	0.10	-4.26	36,36,36,36	0
86	OHX	1	3965	7/7	0.12	-4.27	85,85,85,85	0
86	OHX	7	217	7/7	0.12	-4.29	68,68,68,68	0
86	OHX	5	4048	7/7	0.10	-4.30	94,94,94,94	0
86	OHX	2	2045	7/7	0.09	-4.30	82,82,82,82	0
86	OHX	2	2073	7/7	0.07	-4.32	95,95,95,95	0
86	OHX	8	220	7/7	0.07	-4.33	101,101,101,101	0
85	MG	5	3817	1/1	0.12	-4.33	33,33,33,33	0
86	OHX	1	3984	7/7	0.11	-4.33	94,94,94,94	0
86	OHX	1	3925	7/7	0.11	-4.34	66,66,66,66	0
86	OHX	5	4055	7/7	0.11	-4.37	86,86,86,86	0
86	OHX	2	2063	7/7	0.10	-4.38	95,95,95,95	0
86	OHX	5	3925	7/7	0.12	-4.39	46,46,46,46	0
86	OHX	1	3960	7/7	0.10	-4.40	78,78,78,78	0
86	OHX	4	224	7/7	0.09	-4.40	93,93,93,93	0
86	OHX	1	3892	7/7	0.11	-4.41	56,56,56,56	0
85	MG	5	3698	1/1	0.10	-4.41	44,44,44,44	0
85	MG	1	3732	1/1	0.09	-4.42	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3705	1/1	0.12	-4.42	47,47,47,47	0
85	MG	1	3480	1/1	0.15	-4.43	57,57,57,57	0
86	OHX	5	4168	7/7	0.07	-4.44	154,154,154,154	0
86	OHX	1	4040	7/7	0.10	-4.45	114,114,114,114	0
85	MG	5	3749	1/1	0.09	-4.46	38,38,38,38	0
86	OHX	2	2077	7/7	0.11	-4.46	98,98,98,98	0
85	MG	1	3811	1/1	0.12	-4.46	40,40,40,40	0
85	MG	1	3665	1/1	0.10	-4.47	37,37,37,37	0
86	OHX	1	3980	7/7	0.14	-4.50	87,87,87,87	0
85	MG	5	3492	1/1	0.12	-4.50	22,22,22,22	0
86	OHX	1	3967	7/7	0.15	-4.53	82,82,82,82	0
86	OHX	1	3999	7/7	0.07	-4.53	105,105,105,105	0
86	OHX	5	4196	7/7	0.12	-4.54	65,65,65,65	0
86	OHX	5	3924	7/7	0.12	-4.55	52,52,52,52	0
86	OHX	5	3946	7/7	0.12	-4.59	62,62,62,62	0
86	OHX	5	4051	7/7	0.15	-4.61	88,88,88,88	0
86	OHX	1	3887	7/7	0.13	-4.63	49,49,49,49	0
86	OHX	5	4097	7/7	0.13	-4.63	93,93,93,93	0
85	MG	1	3606	1/1	0.11	-4.63	42,42,42,42	0
86	OHX	2	2066	7/7	0.12	-4.65	89,89,89,89	0
85	MG	1	3746	1/1	0.14	-4.65	50,50,50,50	0
85	MG	1	3706	1/1	0.07	-4.65	30,30,30,30	0
86	OHX	5	4080	7/7	0.09	-4.68	95,95,95,95	0
86	OHX	5	4050	7/7	0.07	-4.68	111,111,111,111	0
85	MG	6	1973	1/1	0.14	-4.70	43,43,43,43	0
86	OHX	2	2051	7/7	0.09	-4.71	91,91,91,91	0
85	MG	1	3434	1/1	0.13	-4.72	34,34,34,34	0
86	OHX	1	4009	7/7	0.10	-4.72	93,93,93,93	0
86	OHX	2	2042	7/7	0.11	-4.72	79,79,79,79	0
86	OHX	5	3982	7/7	0.08	-4.74	63,63,63,63	0
86	OHX	6	2138	7/7	0.11	-4.78	100,100,100,100	0
85	MG	1	3442	1/1	0.15	-4.79	19,19,19,19	0
86	OHX	2	2111	7/7	0.09	-4.80	93,93,93,93	0
86	OHX	1	3929	7/7	0.10	-4.83	63,63,63,63	0
86	OHX	6	2102	7/7	0.07	-4.84	96,96,96,96	0
86	OHX	1	4064	7/7	0.07	-4.87	123,123,123,123	0
86	OHX	1	3990	7/7	0.11	-4.89	97,97,97,97	0
86	OHX	1	4019	7/7	0.12	-4.90	89,89,89,89	0
85	MG	1	3715	1/1	0.12	-4.91	31,31,31,31	0
86	OHX	8	218	7/7	0.12	-4.94	97,97,97,97	0
86	OHX	3	218	7/7	0.11	-4.95	81,81,81,81	0
86	OHX	5	4023	7/7	0.08	-4.97	89,89,89,89	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	4013	7/7	0.08	-4.97	105,105,105,105	0
85	MG	1	3453	1/1	0.17	-5.00	37,37,37,37	0
85	MG	7	214	1/1	0.15	-5.00	54,54,54,54	0
86	OHX	6	2149	7/7	0.14	-5.00	87,87,87,87	0
86	OHX	1	3969	7/7	0.10	-5.02	80,80,80,80	0
86	OHX	5	3998	7/7	0.08	-5.04	91,91,91,91	0
85	MG	1	3628	1/1	0.11	-5.07	52,52,52,52	0
85	MG	5	3637	1/1	0.11	-5.08	35,35,35,35	0
86	OHX	5	4086	7/7	0.14	-5.11	98,98,98,98	0
85	MG	1	3864	1/1	0.16	-5.13	33,33,33,33	0
86	OHX	5	4035	7/7	0.14	-5.14	102,102,102,102	0
86	OHX	5	3972	7/7	0.10	-5.17	66,66,66,66	0
86	OHX	5	4123	7/7	0.16	-5.17	116,116,116,116	0
85	MG	5	3739	1/1	0.10	-5.18	31,31,31,31	0
86	OHX	5	3960	7/7	0.12	-5.21	61,61,61,61	0
86	OHX	5	3993	7/7	0.13	-5.22	66,66,66,66	0
86	OHX	1	3991	7/7	0.12	-5.28	92,92,92,92	0
86	OHX	1	4030	7/7	0.08	-5.28	103,103,103,103	0
86	OHX	6	2092	7/7	0.09	-5.32	94,94,94,94	0
85	MG	5	3616	1/1	0.14	-5.33	36,36,36,36	0
86	OHX	5	4129	7/7	0.07	-5.33	114,114,114,114	0
85	MG	1	3691	1/1	0.14	-5.33	28,28,28,28	0
86	OHX	5	3950	7/7	0.13	-5.33	67,67,67,67	0
86	OHX	3	216	7/7	0.14	-5.36	87,87,87,87	0
86	OHX	5	3937	7/7	0.12	-5.36	62,62,62,62	0
85	MG	6	1989	1/1	0.13	-5.37	60,60,60,60	0
86	OHX	5	3992	7/7	0.10	-5.37	81,81,81,81	0
86	OHX	6	2131	7/7	0.09	-5.38	119,119,119,119	0
86	OHX	5	4215	7/7	0.11	-5.38	85,85,85,85	0
86	OHX	5	3984	7/7	0.12	-5.38	71,71,71,71	0
86	OHX	1	3934	7/7	0.10	-5.40	68,68,68,68	0
86	OHX	6	2119	7/7	0.07	-5.40	107,107,107,107	0
85	MG	5	3725	1/1	0.07	-5.41	41,41,41,41	0
86	OHX	M6	202	7/7	0.09	-5.42	80,80,80,80	0
85	MG	1	3852	1/1	0.16	-5.47	43,43,43,43	0
86	OHX	5	4057	7/7	0.07	-5.48	105,105,105,105	0
86	OHX	5	4153	7/7	0.10	-5.51	95,95,95,95	0
86	OHX	6	2060	7/7	0.11	-5.52	69,69,69,69	0
86	OHX	5	4015	7/7	0.10	-5.55	83,83,83,83	0
86	OHX	1	3983	7/7	0.08	-5.59	89,89,89,89	0
85	MG	5	3804	1/1	0.08	-5.61	27,27,27,27	0
85	MG	5	3688	1/1	0.13	-5.62	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	2	2071	7/7	0.08	-5.66	108,108,108,108	0
85	MG	5	3747	1/1	0.11	-5.75	47,47,47,47	0
86	OHX	5	3967	7/7	0.10	-5.79	70,70,70,70	0
86	OHX	5	4021	7/7	0.09	-5.79	90,90,90,90	0
86	OHX	1	3951	7/7	0.11	-5.79	72,72,72,72	0
86	OHX	6	2084	7/7	0.10	-5.80	96,96,96,96	0
86	OHX	2	2053	7/7	0.07	-5.81	94,94,94,94	0
85	MG	5	3668	1/1	0.12	-5.83	29,29,29,29	0
85	MG	7	212	1/1	0.15	-5.93	64,64,64,64	0
86	OHX	6	2075	7/7	0.09	-5.94	69,69,69,69	0
86	OHX	5	4095	7/7	0.11	-5.96	104,104,104,104	0
85	MG	5	3452	1/1	0.14	-6.00	35,35,35,35	0
86	OHX	1	4158	7/7	0.15	-6.04	84,84,84,84	0
85	MG	5	3496	1/1	0.12	-6.08	39,39,39,39	0
85	MG	1	3441	1/1	0.09	-6.09	30,30,30,30	0
86	OHX	5	3994	7/7	0.07	-6.11	102,102,102,102	0
86	OHX	5	4047	7/7	0.09	-6.16	97,97,97,97	0
86	OHX	2	2084	7/7	0.07	-6.23	111,111,111,111	0
86	OHX	1	3959	7/7	0.09	-6.25	71,71,71,71	0
86	OHX	5	4130	7/7	0.09	-6.26	95,95,95,95	0
86	OHX	6	2111	7/7	0.10	-6.27	104,104,104,104	0
85	MG	5	3650	1/1	0.11	-6.29	22,22,22,22	0
86	OHX	1	3941	7/7	0.11	-6.33	76,76,76,76	0
85	MG	5	3838	1/1	0.13	-6.33	53,53,53,53	0
85	MG	1	3740	1/1	0.07	-6.34	49,49,49,49	0
86	OHX	5	3935	7/7	0.10	-6.35	56,56,56,56	0
85	MG	1	3678	1/1	0.16	-6.35	36,36,36,36	0
86	OHX	5	3959	7/7	0.12	-6.38	58,58,58,58	0
86	OHX	6	2091	7/7	0.12	-6.43	94,94,94,94	0
86	OHX	6	2098	7/7	0.09	-6.49	103,103,103,103	0
85	MG	1	3787	1/1	0.15	-6.50	46,46,46,46	0
85	MG	1	3632	1/1	0.12	-6.52	50,50,50,50	0
86	OHX	5	4058	7/7	0.08	-6.55	109,109,109,109	0
86	OHX	3	220	7/7	0.05	-6.57	101,101,101,101	0
86	OHX	1	3942	7/7	0.12	-6.58	78,78,78,78	0
85	MG	1	3616	1/1	0.14	-6.58	32,32,32,32	0
86	OHX	6	2103	7/7	0.10	-6.59	88,88,88,88	0
86	OHX	7	219	7/7	0.08	-6.63	76,76,76,76	0
86	OHX	2	2064	7/7	0.09	-6.65	104,104,104,104	0
85	MG	5	3483	1/1	0.11	-6.66	34,34,34,34	0
86	OHX	1	3979	7/7	0.07	-6.67	87,87,87,87	0
85	MG	5	3736	1/1	0.10	-6.69	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3914	7/7	0.11	-6.71	58,58,58,58	0
86	OHX	m6	202	7/7	0.09	-6.75	73,73,73,73	0
85	MG	1	3464	1/1	0.14	-6.75	31,31,31,31	0
85	MG	1	3676	1/1	0.12	-6.76	59,59,59,59	0
86	OHX	1	3917	7/7	0.10	-6.79	70,70,70,70	0
85	MG	5	3636	1/1	0.10	-6.80	40,40,40,40	0
86	OHX	5	3942	7/7	0.08	-6.85	75,75,75,75	0
86	OHX	1	4035	7/7	0.10	-6.86	99,99,99,99	0
86	OHX	3	217	7/7	0.08	-6.90	86,86,86,86	0
85	MG	1	3524	1/1	0.14	-6.92	20,20,20,20	0
85	MG	1	3829	1/1	0.14	-6.95	47,47,47,47	0
86	OHX	5	4067	7/7	0.08	-6.97	105,105,105,105	0
86	OHX	5	3927	7/7	0.12	-6.98	59,59,59,59	0
85	MG	5	3891	1/1	0.15	-7.00	64,64,64,64	0
86	OHX	1	4099	7/7	0.13	-7.02	115,115,115,115	0
86	OHX	2	2102	7/7	0.07	-7.03	110,110,110,110	0
86	OHX	6	2087	7/7	0.07	-7.05	91,91,91,91	0
86	OHX	6	2072	7/7	0.10	-7.08	67,67,67,67	0
85	MG	1	3803	1/1	0.10	-7.09	41,41,41,41	0
86	OHX	1	3977	7/7	0.09	-7.09	85,85,85,85	0
86	OHX	5	3971	7/7	0.08	-7.09	65,65,65,65	0
86	OHX	6	2094	7/7	0.08	-7.09	105,105,105,105	0
86	OHX	2	2046	7/7	0.08	-7.13	86,86,86,86	0
86	OHX	5	3990	7/7	0.07	-7.17	84,84,84,84	0
86	OHX	1	4043	7/7	0.11	-7.18	88,88,88,88	0
86	OHX	1	3955	7/7	0.09	-7.29	80,80,80,80	0
85	MG	1	3741	1/1	0.13	-7.32	43,43,43,43	0
86	OHX	6	2090	7/7	0.06	-7.41	90,90,90,90	0
85	MG	6	2032	1/1	0.10	-7.43	56,56,56,56	0
86	OHX	5	3945	7/7	0.10	-7.56	61,61,61,61	0
86	OHX	6	2076	7/7	0.08	-7.63	86,86,86,86	0
85	MG	5	3836	1/1	0.12	-7.64	22,22,22,22	0
85	MG	1	3657	1/1	0.11	-7.66	23,23,23,23	0
86	OHX	6	2080	7/7	0.08	-7.68	79,79,79,79	0
86	OHX	5	3964	7/7	0.12	-7.69	66,66,66,66	0
85	MG	6	2007	1/1	0.12	-7.75	50,50,50,50	0
86	OHX	6	2093	7/7	0.06	-7.84	87,87,87,87	0
85	MG	6	2010	1/1	0.10	-7.85	36,36,36,36	0
85	MG	1	3435	1/1	0.10	-7.86	32,32,32,32	0
86	OHX	5	4087	7/7	0.09	-7.95	105,105,105,105	0
86	OHX	6	2104	7/7	0.08	-7.99	100,100,100,100	0
85	MG	5	3765	1/1	0.07	-8.00	46,46,46,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	5	4012	7/7	0.09	-8.02	82,82,82,82	0
86	OHX	1	3926	7/7	0.11	-8.12	72,72,72,72	0
86	OHX	8	217	7/7	0.08	-8.37	102,102,102,102	0
86	OHX	5	4069	7/7	0.11	-8.46	108,108,108,108	0
86	OHX	1	3972	7/7	0.12	-8.47	107,107,107,107	0
86	OHX	5	4010	7/7	0.05	-8.51	88,88,88,88	0
86	OHX	7	218	7/7	0.10	-8.57	84,84,84,84	0
86	OHX	5	4213	7/7	0.09	-8.60	166,166,166,166	0
86	OHX	5	4034	7/7	0.10	-8.63	86,86,86,86	0
85	MG	5	3826	1/1	0.09	-8.69	29,29,29,29	0
86	OHX	1	3945	7/7	0.10	-8.82	82,82,82,82	0
86	OHX	5	4070	7/7	0.10	-8.85	98,98,98,98	0
85	MG	5	3792	1/1	0.07	-8.97	32,32,32,32	0
86	OHX	6	2088	7/7	0.08	-9.25	95,95,95,95	0
86	OHX	5	3928	7/7	0.11	-9.26	55,55,55,55	0
85	MG	1	3725	1/1	0.10	-9.28	35,35,35,35	0
85	MG	1	3845	1/1	0.13	-9.29	43,43,43,43	0
86	OHX	1	3973	7/7	0.10	-9.49	82,82,82,82	0
85	MG	5	3702	1/1	0.12	-9.67	44,44,44,44	0
86	OHX	1	4048	7/7	0.13	-9.75	86,86,86,86	0
86	OHX	6	2081	7/7	0.09	-9.81	78,78,78,78	0
86	OHX	5	4020	7/7	0.10	-9.84	85,85,85,85	0
85	MG	5	3488	1/1	0.11	-10.00	41,41,41,41	0
86	OHX	1	4007	7/7	0.11	-10.02	90,90,90,90	0
85	MG	6	1986	1/1	0.10	-10.04	39,39,39,39	0
86	OHX	5	4066	7/7	0.07	-10.26	97,97,97,97	0
85	MG	5	3653	1/1	0.10	-10.51	46,46,46,46	0
85	MG	4	210	1/1	0.09	-10.62	43,43,43,43	0
85	MG	1	3638	1/1	0.08	-10.66	49,49,49,49	0
85	MG	1	3770	1/1	0.14	-10.71	75,75,75,75	0
86	OHX	5	3978	7/7	0.10	-10.83	65,65,65,65	0
85	MG	5	3760	1/1	0.10	-10.87	35,35,35,35	0
86	OHX	5	3976	7/7	0.09	-10.95	85,85,85,85	0
85	MG	5	3788	1/1	0.09	-10.97	39,39,39,39	0
85	MG	5	3824	1/1	0.10	-11.57	37,37,37,37	0
86	OHX	5	3985	7/7	0.08	-12.02	71,71,71,71	0
85	MG	1	3440	1/1	0.14	-12.07	31,31,31,31	0
85	MG	5	3741	1/1	0.08	-12.09	46,46,46,46	0
86	OHX	1	3935	7/7	0.09	-12.12	68,68,68,68	0
86	OHX	6	2130	7/7	0.07	-12.94	96,96,96,96	0
85	MG	5	3794	1/1	0.14	-13.00	64,64,64,64	0
85	MG	5	3895	1/1	0.13	-13.00	51,51,51,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3687	1/1	0.07	-13.71	45,45,45,45	0
85	MG	8	210	1/1	0.05	-13.89	50,50,50,50	0
85	MG	5	3601	1/1	0.09	-13.98	35,35,35,35	0
85	MG	5	3862	1/1	0.10	-14.30	33,33,33,33	0
86	OHX	1	4055	7/7	0.08	-14.54	104,104,104,104	0
85	MG	1	3671	1/1	0.09	-14.77	40,40,40,40	0
85	MG	1	3639	1/1	0.09	-15.33	56,56,56,56	0
85	MG	5	3812	1/1	0.07	-15.39	74,74,74,74	0
86	OHX	5	4004	7/7	0.09	-15.45	69,69,69,69	0
85	MG	5	3686	1/1	0.10	-17.14	32,32,32,32	0
86	OHX	6	2114	7/7	0.11	-17.19	102,102,102,102	0
86	OHX	1	3992	7/7	0.08	-17.20	94,94,94,94	0
85	MG	5	3808	1/1	0.11	-17.86	59,59,59,59	0
85	MG	6	2001	1/1	0.10	-18.71	80,80,80,80	0
85	MG	5	3781	1/1	0.17	-19.00	64,64,64,64	0
85	MG	5	3471	1/1	0.14	-19.67	40,40,40,40	0
85	MG	4	215	1/1	0.12	-23.73	60,60,60,60	0
85	MG	5	3679	1/1	0.12	-29.03	28,28,28,28	0
86	OHX	2	2062	7/7	0.07	-36.09	105,105,105,105	0
85	MG	5	3464	1/1	0.13	-59.00	30,30,30,30	0
85	MG	5	3850	1/1	0.10	-161.00	56,56,56,56	0
85	MG	6	1979	1/1	0.25	-	51,51,51,51	0
85	MG	6	1999	1/1	0.32	-	87,87,87,87	0
85	MG	6	2045	1/1	0.36	-	63,63,63,63	0
85	MG	5	3773	1/1	0.28	-	83,83,83,83	0
85	MG	3	208	1/1	0.11	-	66,66,66,66	0
85	MG	1	3841	1/1	0.25	-	37,37,37,37	0
85	MG	5	3876	1/1	0.27	-	39,39,39,39	0
85	MG	1	3737	1/1	0.17	-	54,54,54,54	0
85	MG	1	3840	1/1	0.24	-	39,39,39,39	0
85	MG	1	3465	1/1	0.26	-	41,41,41,41	0
85	MG	1	3490	1/1	0.25	-	51,51,51,51	0
85	MG	5	3799	1/1	0.10	-	39,39,39,39	0
85	MG	1	3851	1/1	0.15	-	50,50,50,50	0
85	MG	2	2021	1/1	0.45	-	61,61,61,61	0
85	MG	6	2041	1/1	0.52	-	65,65,65,65	0
85	MG	5	3615	1/1	0.29	-	30,30,30,30	0
85	MG	1	3703	1/1	0.09	-	49,49,49,49	0
85	MG	6	2044	1/1	0.38	-	44,44,44,44	0
85	MG	1	3613	1/1	0.28	-	36,36,36,36	0
85	MG	2	1996	1/1	0.42	-	48,48,48,48	0
86	OHX	2	2159	7/7	0.11	-	260,260,260,260	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	1924	1/1	0.61	-	87,87,87,87	0
85	MG	1	3500	1/1	0.26	-	51,51,51,51	0
85	MG	5	3883	1/1	0.13	-	48,48,48,48	0
85	MG	4	201	1/1	0.34	-	50,50,50,50	0
85	MG	1	3756	1/1	0.22	-	91,91,91,91	0
85	MG	1	3627	1/1	0.33	-	58,58,58,58	0
85	MG	5	3886	1/1	0.50	-	80,80,80,80	0
85	MG	5	3500	1/1	0.16	-	45,45,45,45	0
85	MG	8	212	1/1	0.22	-	47,47,47,47	0
85	MG	2	1954	1/1	0.57	-	87,87,87,87	0
85	MG	1	3792	1/1	0.18	-	58,58,58,58	0
85	MG	5	3873	1/1	0.39	-	47,47,47,47	0
85	MG	4	217	1/1	0.14	-	48,48,48,48	0
85	MG	1	3795	1/1	0.20	-	51,51,51,51	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.