



Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 06:19 am GMT

PDB ID : 7NWH
EMDB ID : EMD-12632
Title : Mammalian pre-termination 80S ribosome with eRF1 and eRF3 bound by Blasticidin S.
Authors : Powers, K.T.; Yadav, S.K.N.; Bufton, J.C.; Schaffitzel, C.
Deposited on : 2021-03-16
Resolution : 4.10 Å(reported)
Based on initial model : 5LZT

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

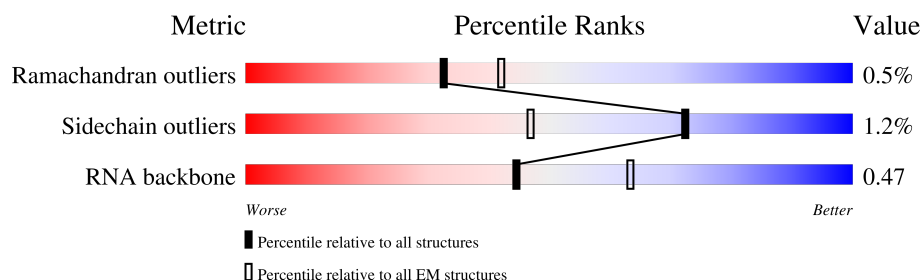
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	249	
2	C	378	
3	d	108	
4	DD	281	
5	dd	56	
6	D	296	
7	e	129	
8	EE	263	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	ee	133	
10	b	226	
11	E	291	
12	f	110	
13	FF	204	
14	ff	68	
15	F	249	
16	g	126	
17	BB	264	
18	GG	263	
19	gg	314	
20	G	242	
21	h	123	
22	HH	191	
23	hh	15	
24	bb	84	
25	H	190	
26	i	107	
27	II	208	
28	ii	437	
29	I	214	
30	j	97	
31	JJ	194	
32	jj	428	
33	J	176	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	k	70	
35	KK	151	
36	L	211	
37	l	51	
38	LL	158	
39	M	218	
40	m	128	
41	MM	123	
42	N	204	
43	n	25	
44	NN	150	
45	O	203	
46	o	142	
47	OO	156	
48	P	199	
49	p	109	
50	PP	145	
51	Q	188	
52	r	137	
53	QQ	158	
54	R	196	
55	s	318	
56	RR	145	
57	S	176	
58	t	196	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	SS	152	
60	T	160	
61	TT	145	
62	U	128	
63	UU	118	
64	V	132	
65	VV	83	
66	W	134	
67	5	3705	
68	WW	139	
69	X	156	
70	7	120	
71	XX	142	
72	Y	134	
73	8	151	
74	YY	146	
75	Z	136	
76	9	1779	
77	ZZ	122	
78	a	147	
79	AA	295	
80	aa	117	
81	B	402	
82	c	115	
83	CC	259	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
84	cc	69	<div><div></div><div>67%</div><div></div><div>84%</div><div></div><div>6%</div><div>10%</div></div>

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 385116 atoms, of which 165738 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	248	Total	C	H	N	O	S	0	0
			3891	1189	1993	389	314	6		

- Molecule 2 is a protein called uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	362	Total	C	H	N	O	S	0	0
			5936	1812	3053	577	480	14		

- Molecule 3 is a protein called eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	107	Total	C	H	N	O	S	0	0
			1818	560	930	171	155	2		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	DD	228	Total	C	H	N	O	S	0	0
			3632	1126	1864	318	316	8		

- Molecule 5 is a protein called S29.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	dd	55	Total	C	H	N	O	S	0	0
			908	286	449	94	74	5		

- Molecule 6 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	D	293	Total	C	H	N	O	S	0	0
			4815	1512	2424	438	427	14		

- Molecule 7 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	e	128	Total	C	H	N	O	S	0	0
			2200	667	1147	216	165	5		

- Molecule 8 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	EE	262	Total	C	H	N	O	S	0	0
			4253	1324	2177	386	358	8		

- Molecule 9 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	ee	55	Total	C	H	N	O	S	0	0
			935	274	492	97	71	1		

- Molecule 10 is a protein called eL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	b	104	Total	C	H	N	O	S	0	0
			1768	527	920	189	129	3		

- Molecule 11 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	216	Total	C	H	N	O	S	0	0
			3617	1115	1888	329	282	3		

- Molecule 12 is a protein called eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	f	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	143	4		

- Molecule 13 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	FF	185	Total	C	H	N	O	S	0	0
			2993	921	1522	277	266	7		

- Molecule 14 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	ff	68	Total	C	H	N	O	S	0	0
			1120	351	565	103	94	7		

- Molecule 15 is a protein called uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	F	225	Total	C	H	N	O	S	0	0
			3870	1205	1995	358	303	9		

- Molecule 16 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	g	114	Total	C	H	N	O	S	0	0
			1905	566	999	187	147	6		

- Molecule 17 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	BB	213	Total	C	H	N	O	S	0	0
			3532	1098	1803	309	308	14		

- Molecule 18 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	GG	237	Total	C	H	N	O	S	0	0
			4005	1200	2082	387	329	7		

- Molecule 19 is a protein called Epididymis tissue sperm binding protein Li 3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	gg	313	Total	C	H	N	O	S	0	0
			4830	1535	2394	424	465	12		

- Molecule 20 is a protein called L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	G	233	Total	C	H	N	O	S	0	0
			3906	1199	2027	361	315	4		

- Molecule 21 is a protein called uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	h	122	Total	C	H	N	O	S	0	0
			2160	640	1147	204	168	1		

- Molecule 22 is a protein called S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	HH	185	Total	C	H	N	O	S	0	0
			3070	952	1582	271	264	1		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	hh	15	Total	C	H	N	O	P	0	0
			478	142	161	54	106	15		

- Molecule 24 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	bb	83	Total	C	H	N	O	S	0	0
			1323	408	672	121	115	7		

- Molecule 25 is a protein called L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	H	190	Total	C	H	N	O	S	0	0
			3113	954	1597	284	272	6		

- Molecule 26 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	i	102	Total	C	H	N	O	S	0	0
			1746	520	916	176	129	5		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	II	206	Total	C	H	N	O	S	0	0
			3459	1058	1773	332	291	5		

- Molecule 28 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	ii	419	Total	C	H	N	O	S	0	0
			6638	2104	3331	562	629	12		

- Molecule 29 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	I	205	Total	C	H	N	O	S	0	0
			3376	1056	1712	321	274	13		

- Molecule 30 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	j	86	Total	C	H	N	O	S	0	0
			1442	434	737	155	111	5		

- Molecule 31 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	JJ	185	Total	C	H	N	O	S	0	0
			3165	969	1640	306	248	2		

- Molecule 32 is a protein called eRF3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	jj	428	Total	C	H	N	O	S	0	0
			6787	2144	3419	580	623	21		

- Molecule 33 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	J	170	Total	C	H	N	O	S	0	0
			2761	861	1399	254	241	6		

- Molecule 34 is a protein called L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	k	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 35 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	KK	96	Total	C	H	N	O	S	0	0
			1646	530	836	143	131	6		

- Molecule 36 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	L	210	Total	C	H	N	O	S	0	0
			3522	1065	1820	354	279	4		

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	1	50	Total	C	H	N	O	S	0	0
			927	286	480	96	64	1		

- Molecule 38 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	LL	143	Total	C	H	N	O	S	0	0
			2425	749	1250	222	198	6		

- Molecule 39 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	M	138	Total	C	H	N	O	S	0	0
			2348	727	1211	221	182	7		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN EL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	m	52	Total	C	H	N	O	S	0	0
			894	266	465	90	67	6		

- Molecule 41 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	MM	117	Total	C	H	N	O	S	0	0
			1847	570	939	161	169	8		

- Molecule 42 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	N	203	Total	C	H	N	O	S	0	0
			3451	1072	1750	359	266	4		

- Molecule 43 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	n	25	Total	C	H	N	O	S	0	0
			525	145	286	64	27	3		

- Molecule 44 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	NN	149	Total	C	H	N	O	S	0	0
			2491	770	1289	228	203	1		

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN UL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	O	199	Total	C	H	N	O	S	0	0
			3408	1051	1778	319	255	5		

- Molecule 46 is a protein called eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	o	104	Total	C	H	N	O	S	0	0
			1771	533	920	174	138	6		

- Molecule 47 is a protein called uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	OO	136	Total	C	H	N	O	S	0	0
			2055	621	1039	199	190	6		

- Molecule 48 is a protein called uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	P	153	Total	C	H	N	O	S	0	0
			2516	777	1274	241	215	9		

- Molecule 49 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	p	91	Total	C	H	N	O	S	0	0
			1466	445	758	136	120	7		

- Molecule 50 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	PP	120	Total	C	H	N	O	S	0	0
			2042	635	1045	187	168	7		

- Molecule 51 is a protein called eL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	Q	187	Total	C	H	N	O	S	0	0
			3149	946	1634	315	250	4		

- Molecule 52 is a protein called eL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	r	124	Total	C	H	N	O	S	0	0
			2045	616	1051	205	167	6		

- Molecule 53 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	QQ	142	Total	C	H	N	O	S	0	0
			2323	717	1195	213	195	3		

- Molecule 54 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	R	180	Total	C	H	N	O	S	0	0
			3172	933	1664	328	238	9		

- Molecule 55 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	s	196	Total	C	H	N	O	S	0	0
			3071	959	1564	263	276	9		

- Molecule 56 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	RR	132	Total	C	H	N	O	S	0	0
			2189	670	1121	199	195	4		

- Molecule 57 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	S	176	Total	C	H	N	O	S	0	0
			2970	930	1508	285	236	11		

- Molecule 58 is a protein called uL12.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	t	153	Total	C	H	N	O	S	0	0
			2375	722	1215	218	217	3		

- Molecule 59 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	SS	144	Total	C	H	N	O	S	0	0
			2437	746	1247	241	202	1		

- Molecule 60 is a protein called eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	T	159	Total	C	H	N	O	S	0	0
			2665	823	1367	252	217	6		

- Molecule 61 is a protein called eS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	TT	141	Total	C	H	N	O	S	0	0
			2229	688	1132	211	195	3		

- Molecule 62 is a protein called L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	U	99	Total	C	H	N	O	S	0	0
			1642	519	833	141	147	2		

- Molecule 63 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	UU	100	Total	C	H	N	O	S	0	0
			1657	498	862	152	141	4		

- Molecule 64 is a protein called eL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	V	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 65 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	VV	83	Total	C	H	N	O	S	0	0
			1273	393	637	117	121	5		

- Molecule 66 is a protein called 60S ribosomal protein L24-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	W	106	Total	C	H	N	O	S	0	0
			1752	538	892	174	144	4		

- Molecule 67 is a RNA chain called 28S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	5	3543	Total	C	H	N	O	P	0	0
			114361	33833	38389	13910	24686	3543		

- Molecule 68 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	WW	129	Total	C	H	N	O	S	0	0
			2114	659	1080	193	176	6		

- Molecule 69 is a protein called uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	X	118	Total	C	H	N	O	S	0	0
			2007	618	1040	181	167	1		

- Molecule 70 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	7	120	Total	C	H	N	O	P	0	0
			3854	1141	1296	456	842	119		

- Molecule 71 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	XX	141	Total	C	H	N	O	S	0	0
			2263	693	1165	219	183	3		

- Molecule 72 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	Y	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 73 is a RNA chain called 5.8S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	8	151	Total	C	H	N	O	P	0	0
			4837	1432	1629	564	1062	150		

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	YY	124	Total	C	H	N	O	S	0	0
			2094	640	1083	198	168	5		

- Molecule 75 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	Z	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 76 is a RNA chain called 18S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	9	1698	Total	C	H	N	O	P	0	0
			54557	16180	18308	6508	11864	1697		

- Molecule 77 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	ZZ	75	Total	C	H	N	O	S	0	0
			1254	382	656	111	104	1		

- Molecule 78 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	a	147	Total	C	H	N	O	S	0	0
			2372	734	1210	239	185	4		

- Molecule 79 is a protein called 40S_SA_C domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	AA	217	Total	C	H	N	O	S	0	0
			3418	1086	1708	300	316	8		

- Molecule 80 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	aa	101	Total	C	H	N	O	S	0	0
			1678	507	864	170	132	5		

- Molecule 81 is a protein called uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	B	394	Total	C	H	N	O	S	0	0
			6482	2020	3310	597	542	13		

- Molecule 82 is a protein called eL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	c	98	Total	C	H	N	O	S	0	0
			1555	481	794	134	140	6		

- Molecule 83 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	CC	221	Total	C	H	N	O	S	0	0
			3522	1111	1806	295	301	9		

- Molecule 84 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	cc	62	Total	C	H	N	O	S	0	0
			1002	297	514	97	92	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
cc	5	HIS	ARG	conflict	UNP G1TIB4

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	dd	1	Total	Zn	0
			1	1	
85	ff	1	Total	Zn	0
			1	1	
85	g	1	Total	Zn	0
			1	1	
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	aa	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

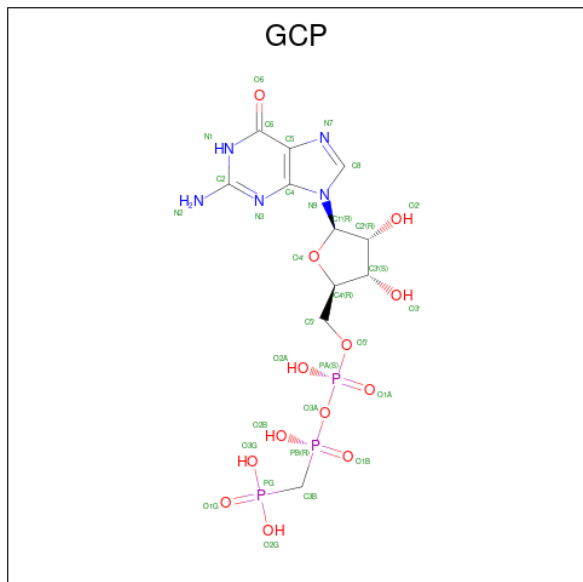
Mol	Chain	Residues	Atoms		AltConf
86	hh	2	Total	Mg	0
			2	2	
86	j	1	Total	Mg	0
			1	1	
86	jj	1	Total	Mg	0
			1	1	
86	o	1	Total	Mg	0
			1	1	
86	P	1	Total	Mg	0
			1	1	
86	V	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	5	189	Total	Mg	0
			189	189	
86	7	4	Total	Mg	0
			4	4	
86	8	10	Total	Mg	0
			10	10	
86	9	70	Total	Mg	0
			70	70	
86	a	1	Total	Mg	0
			1	1	

- Molecule 87 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
87	jj	1	Total	C	H	N	O	P	0
			46	11	14	5	13	3	

- Molecule 88 is BLASTICIDIN S (three-letter code: BLS) (formula: $C_{17}H_{26}N_8O_5$) (labeled as "Ligand of Interest" by depositor).

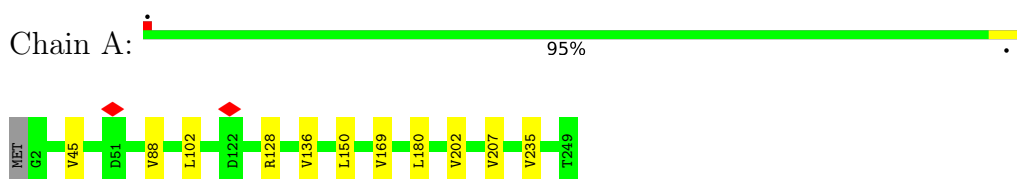


WORLD WIDE
PDB
PROTEIN DATA BANK

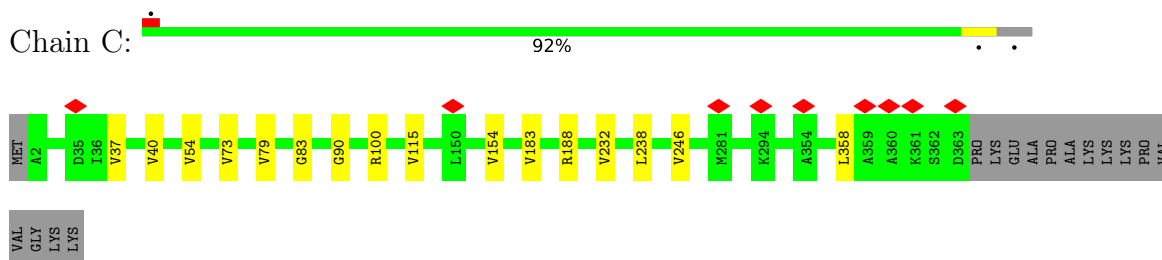
3 Residue-property plots

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

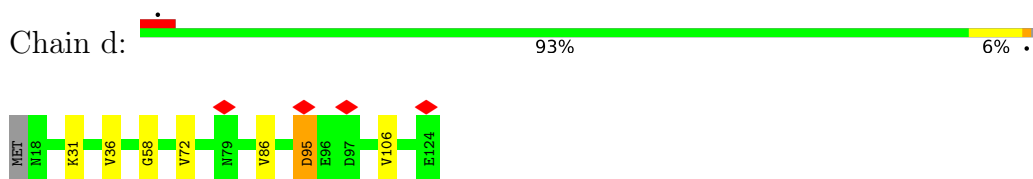
- Molecule 1: 60S ribosomal protein L8



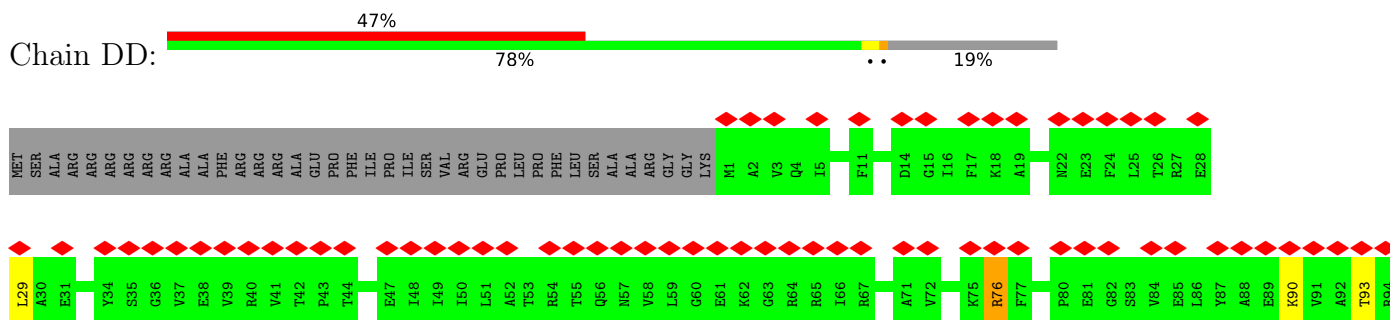
- Molecule 2: uL4



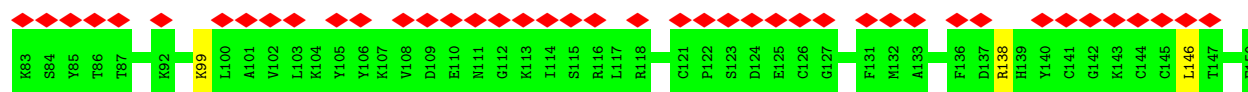
- Molecule 3: eL31



- Molecule 4: 40S ribosomal protein S3

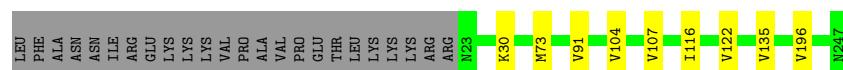


Chain b:  6% 46% 54%



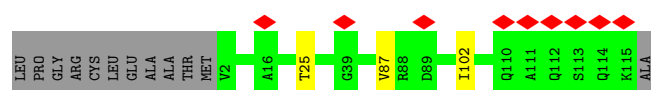
• Molecule 15: uL30

Chain F: 87% 10%



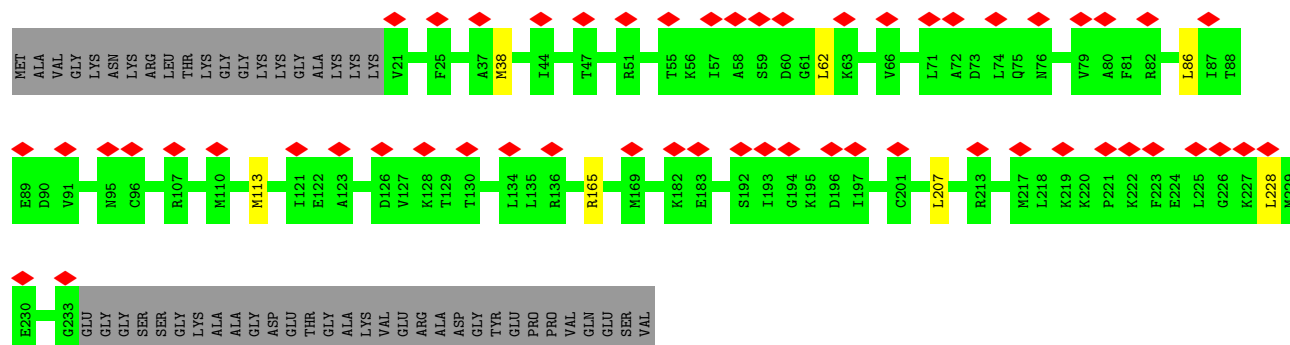
• Molecule 16: 60S ribosomal protein L34

Chain g: 88% 10%



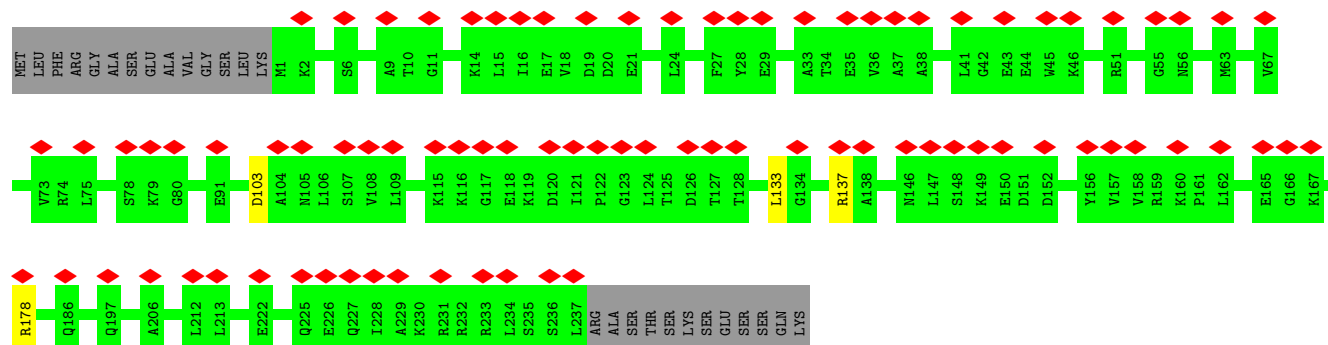
• Molecule 17: 40S ribosomal protein S3a

Chain BB: 78% 19%

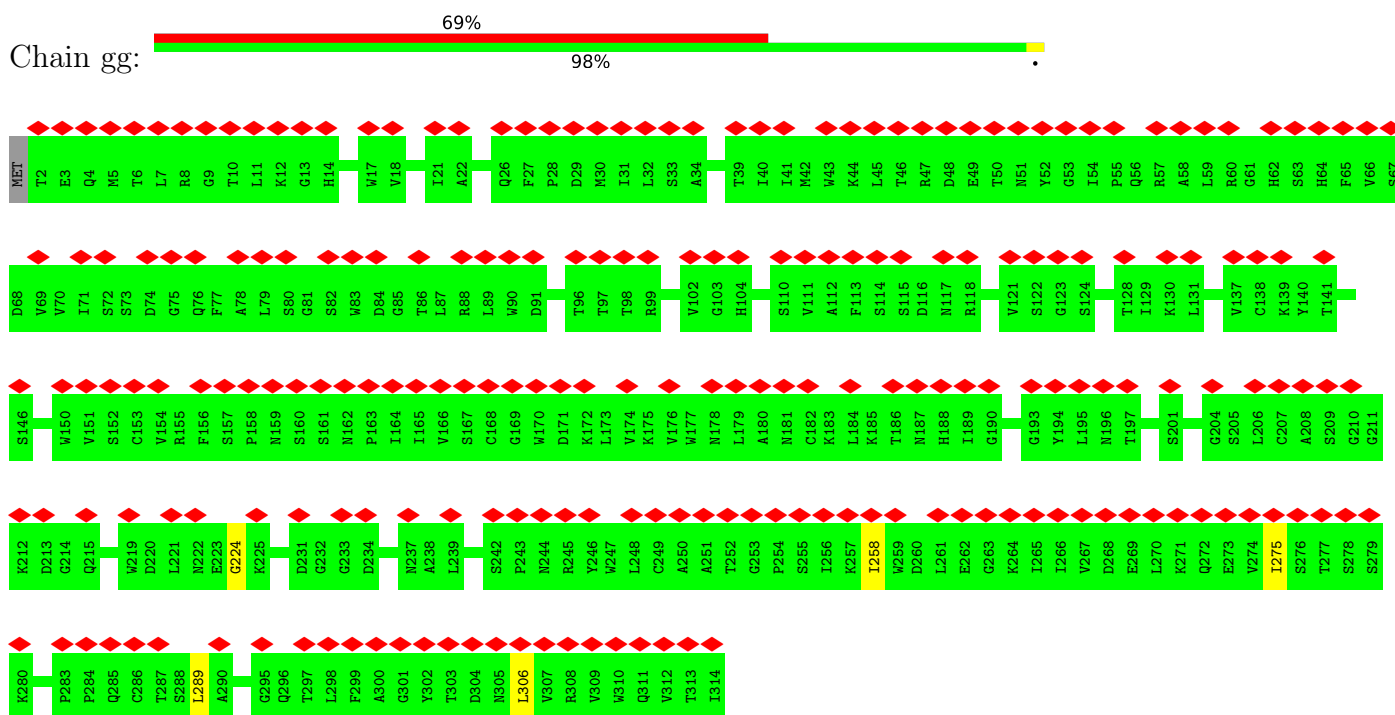


• Molecule 18: 40S ribosomal protein S6

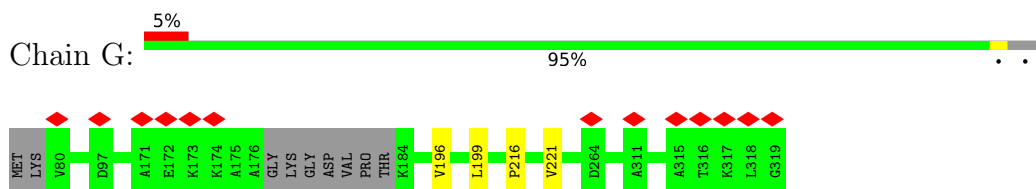
Chain GG: 89% 10%



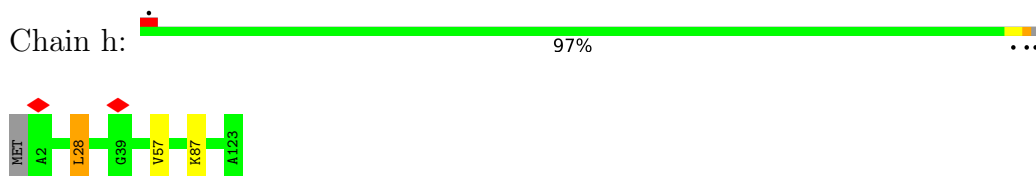
• Molecule 19: Epididymis tissue sperm binding protein Li 3a



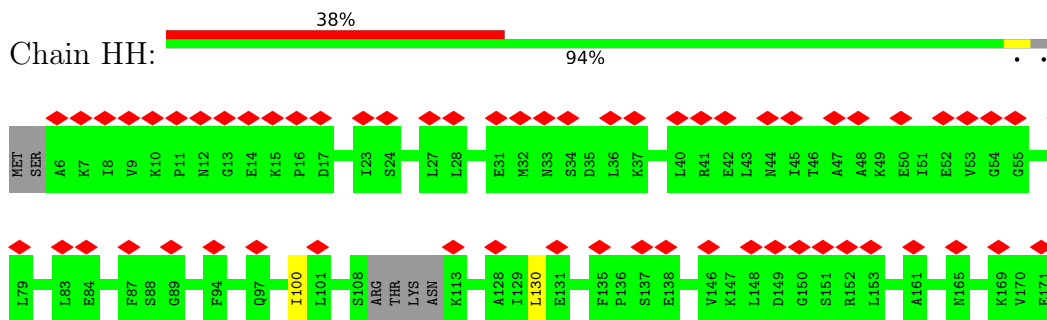
- Molecule 20: L7a



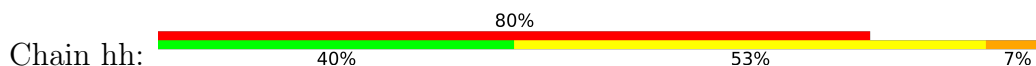
- Molecule 21: uL29

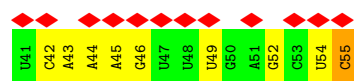


- Molecule 22: S7

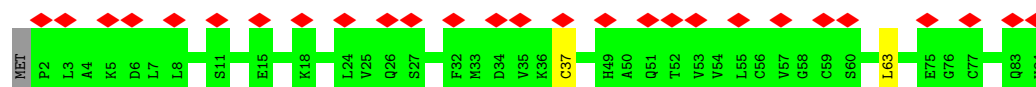


- Molecule 23: mRNA





- Molecule 24: 40S ribosomal protein S27



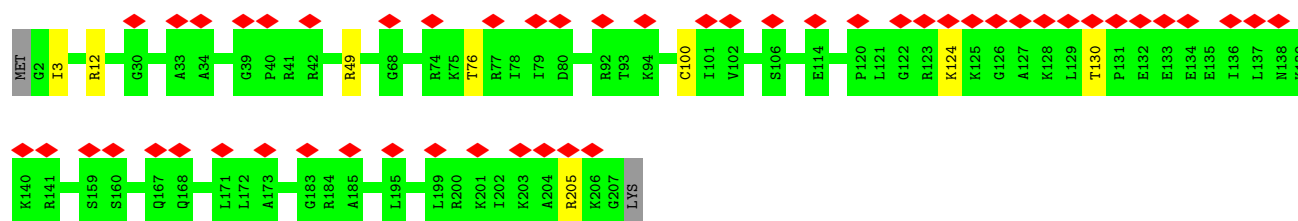
- Molecule 25: L9



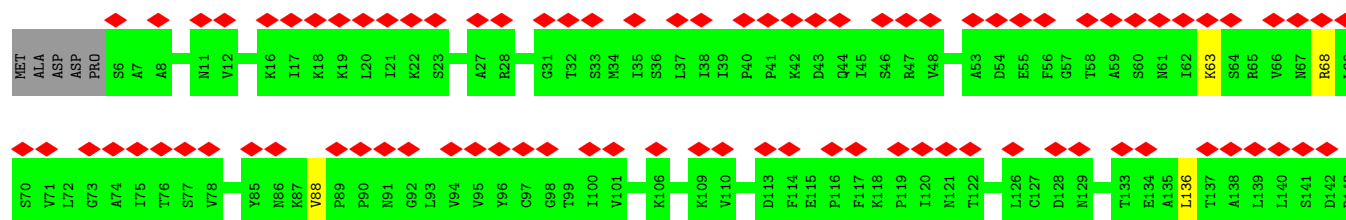
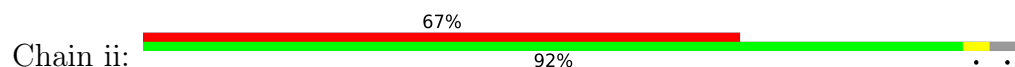
- Molecule 26: 60S ribosomal protein L36

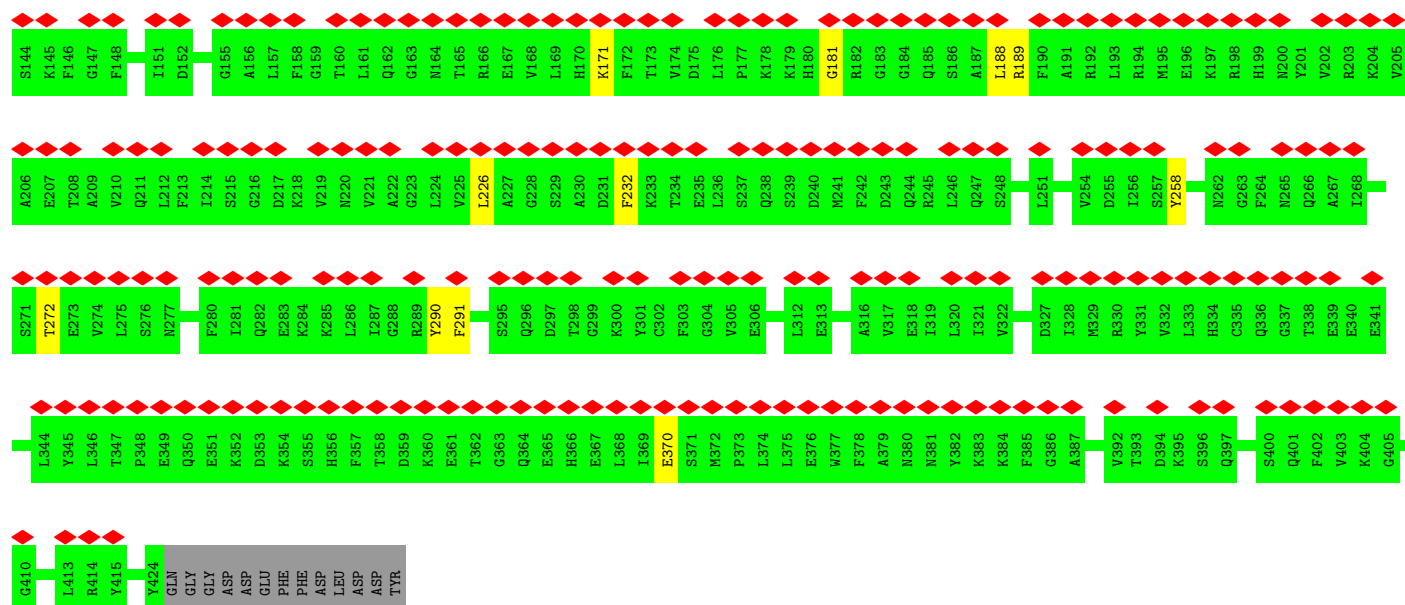


- Molecule 27: 40S ribosomal protein S8



- Molecule 28: Eukaryotic peptide chain release factor subunit 1

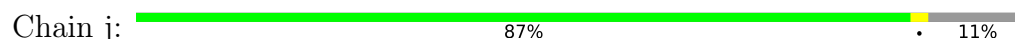




- Molecule 29: 60S ribosomal protein L10



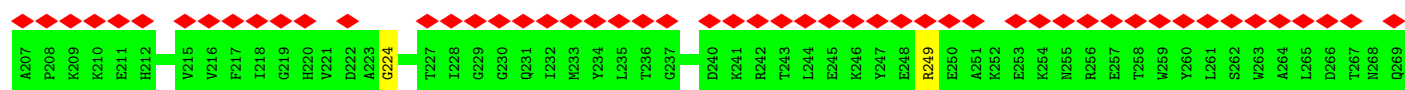
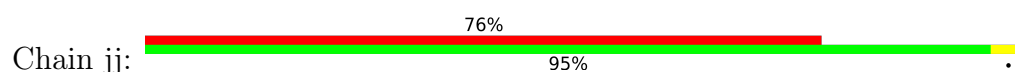
- Molecule 30: Ribosomal protein L37

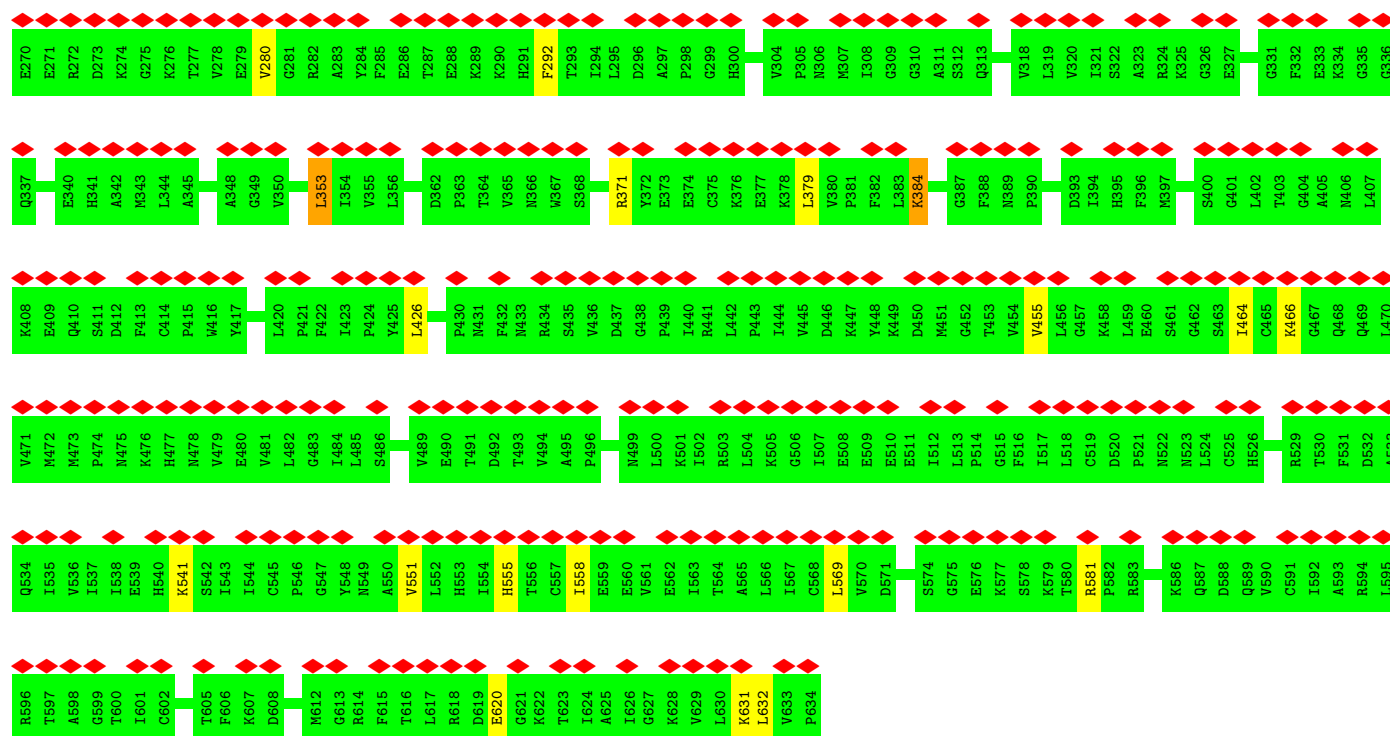


- Molecule 31: 40S ribosomal protein S9

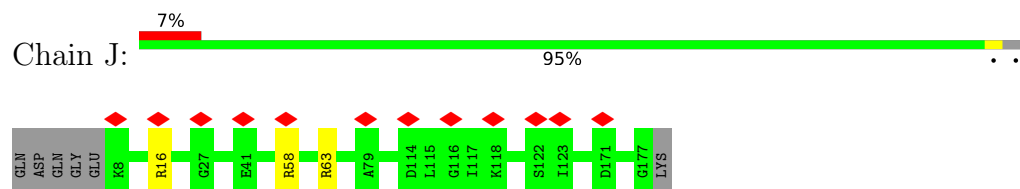


- Molecule 32: eRF3a

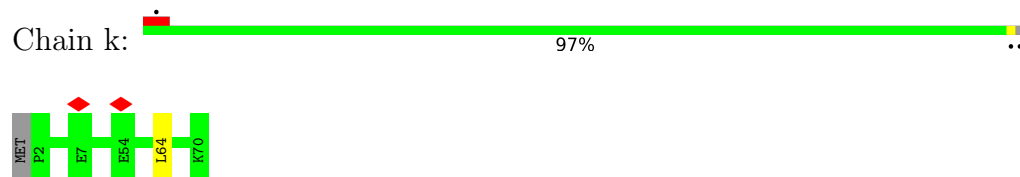




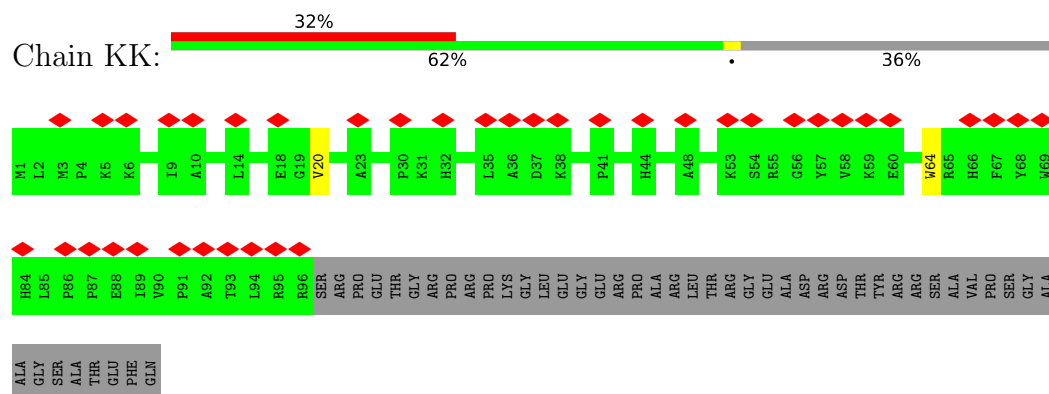
• Molecule 33: 60S ribosomal protein L11



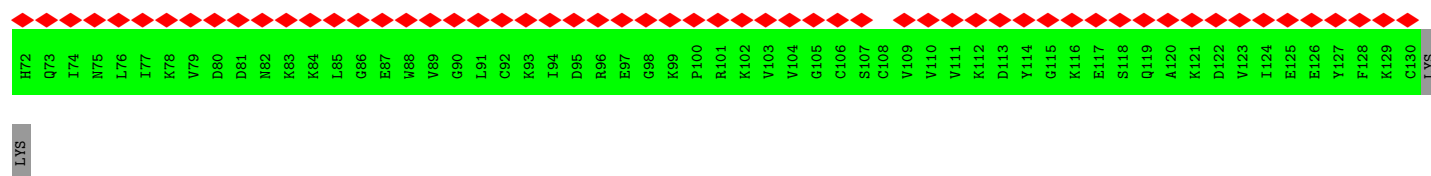
• Molecule 34: L38



• Molecule 35: 40S ribosomal protein S10



- [illegible]



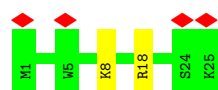
- Molecule 42: Ribosomal protein L15

Chain N: 93% 6%



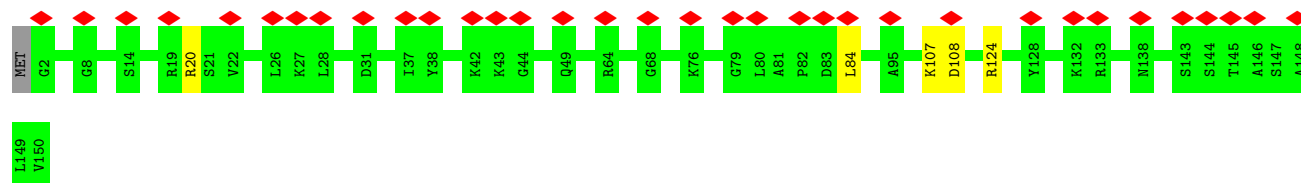
- Molecule 43: 60s ribosomal protein l41

Chain n: 16% 92% 8%



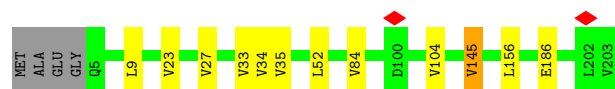
- Molecule 44: ribosomal protein uS15

Chain NN: 23% 96% . .



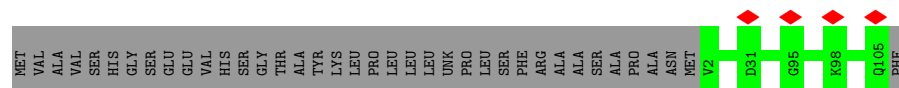
- Molecule 45: 60S RIBOSOMAL PROTEIN UL13

Chain O: 92% 5% .




- Molecule 46: eL42

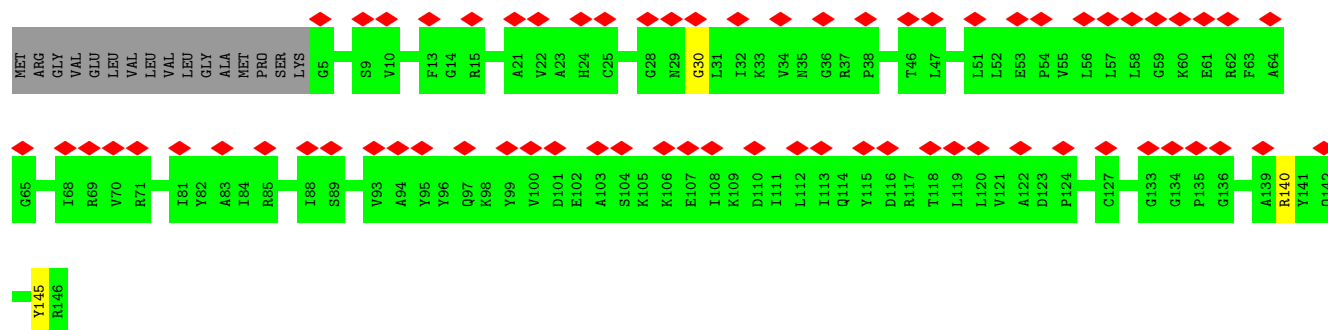
Chain o: 73% 27%




- Molecule 47: uS11

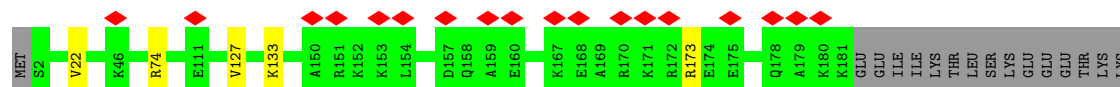
Chain OO: 28% 84% . 13%

Chain QQ: 




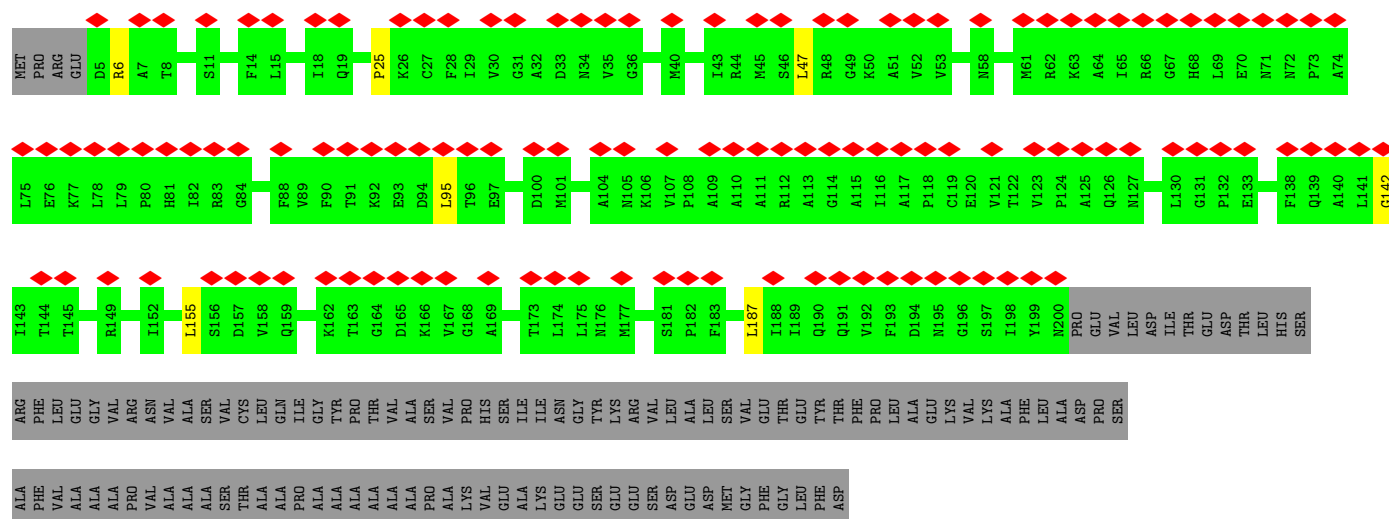
- Molecule 54: 60S ribosomal protein L19

Chain R: 

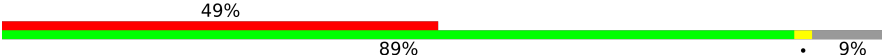


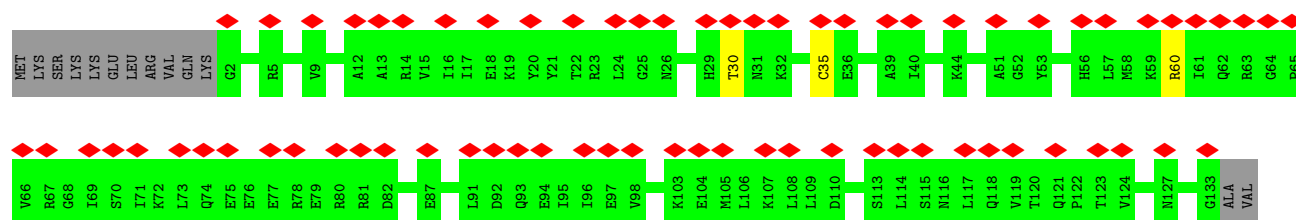
- Molecule 55: 60S acidic ribosomal protein P0

Chain s: 




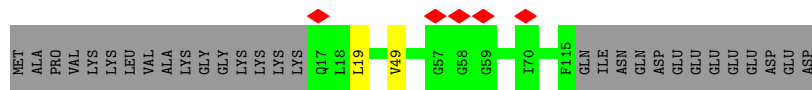
- Molecule 56: 40S ribosomal protein S17

Chain RR: 

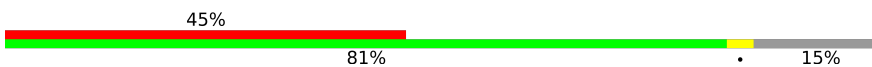


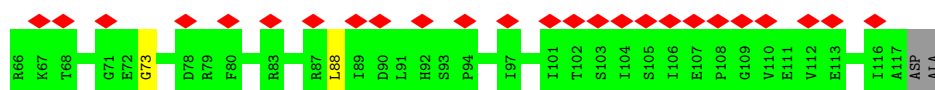
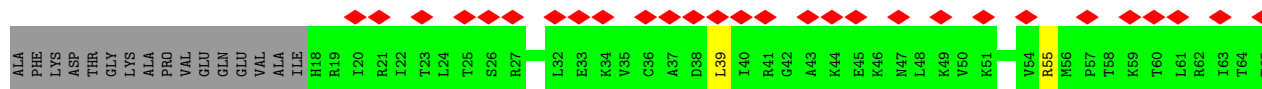
- Molecule 62: L22

Chain U:  76% 23%



- Molecule 63: 40S ribosomal protein S20

Chain UU:  45% 81% 15%



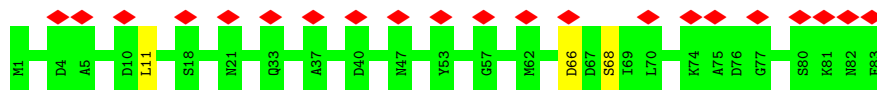
- Molecule 64: eL14

Chain V:  5% 95%




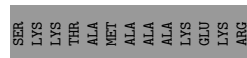
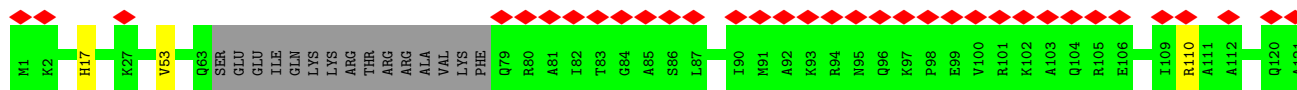
- Molecule 65: 40S ribosomal protein S21

Chain VV:  25% 96%



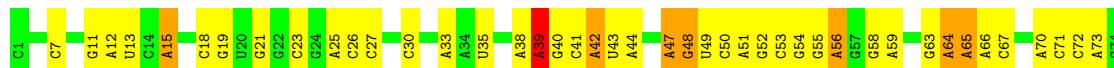
- Molecule 66: 60S ribosomal protein L24-like protein

Chain W:  25% 77% 21%



- Molecule 67: 28S Ribosomal RNA

Chain 5:  50% 39% 7%



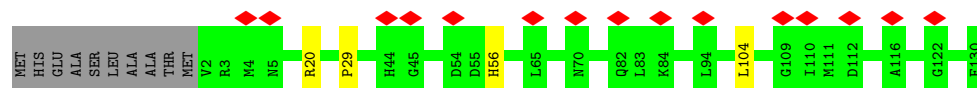


G2897	G2818	A2743	G2855	G2547	C2469	C2393	G2297	A2097	C2019	A1944	U1876	G1797	C
G2901	U2819	A2744	U2856	U2554	C2470	G2394	U2298	G2098	C2022	G1945	G1877	G1798	A
A	C2820	A2745	G2857	G2555	G2471	A2395	A2399	C2299	G2023	G1948	G1879	U1800	
C	C2824	A2746	G2858	G2556	G2472	A2396	A2400	G2100	G2024	A1801	G1880	A1801	
A	A2825	U2747	A2660	A2565	G2473	G2399	A2313	A2103	A2025	G1952	U1882	G1803	
C	U2826	C2748	U2661	G2566	C2474	G2400	G2317	A2104	A2026	U1957	U1883	A1804	
A	G2827	C2749	G2862	G2567	G2475	A2401	G2314	A2105	U1958	U1959	G1884	U1726	
C	G2828	G2750	G2863	C2571	G2476	A2402	G2319	G2106	A1959		U1728	A1805	
A	U2829	G2751	G2864	C2572	G2477	A2403	G2320	A2107	U1960		G1885	U1727	
C		G2752	G2865	U2575	G2478	A2404	G2321	G2108	U1961		U1729	A1811	
A	A2833	G2753	C2670	G2576	U2484	G2405	G2322	A2109	A1962		G1733	G1734	
C	C2834	G2754	C2671	G2577	U2485	G2406	G2323	G2110	A1963		U1735	U1735	
A	A2835		G2866	G2578	U2486		G2324				G1815	G1816	
G3597	U2836	G2758	G2867	G2579	G2487	U2409	G2325	G2113	C1966		G1817	G1817	
C3598	G2837	G2759	G2868	G2580	U2488	C2410	G2326	A	A1967		U1817	G1818	
A3599	U2838	G2760	G2869	G2581	U2489	C2411	G2327	C			G1738	G1819	
	U2839	U2761	G2762	C2582	U2490		G2328	A			G1739	U1820	
A3604	U2840	U2762	G2871	G2583	C2491	G2416	G2329	C			G1740	G1821	
C3605	G2841	U2763	G2881	G2584	C2492	A2417	G2330	A			G1741	U1822	
	G2842	A2764		G2585	G2493	A2418	G2331	C			G1742	G1823	
C3612	U2843	U2769	G2886	G2586	U2494	A2419	G2332	C			G1750	G1824	
U3613	A2844	G2770	G2887	A2587	U2495	C2420	G2333	A			G1753	G1825	
G3614	A2845	G2771	G2888	G2588	U2496	A2421	G2334	C			U1754	G1826	
G3615	G2846	G2772	G2889	G2589		C2422	G2335	A			G1755	G1827	
U3616	G2847		G2890	U2592		A2423	G2336	C			U1756	G1828	
G3617	G2848		U2891	C2593		A2424	G2337	A			U1757	G1829	
C3618	U2849	C2779	U2892	G2601	A2502	G2425	G2338	C			G1758	G1830	
G3619	A2850	G2780	G2893	G2602	G2503	U2426	G2339	C			G1759	G1831	
G3620	G2851	G2781	G2894	C2603	C2504	A2427	G2340	C			G1760	G1832	
A3621	U2852	U2782	A2695	C2604	G2505	A2428	G2341	A			G1761	G1833	
C3622	G2853	A2783	A2696		G2506	A2429	G2342	C			G1762	G1834	
U3623	G2854	G2784	G2897	C2607	C2509	G2430	G2343	A			G1763	G1835	
A3624	G2855	C2785	C2899	G2613	G2510	G2431	G2344	C			G1764	G1836	
G3625	G2856	U2787	U2707	G2614	A2511	G2432	G2345	C			G1765	G1837	
G3626	A2857	G2788	U2708	G2615	A2512	U2433	G2346	C			G1766	G1838	
	U2858	A2789	C2709	G2616	G2513	U2434	G2347	C			A1765	G1839	
A3630	G2859		G2710	G2617	U2514	C2435	G2348	C			A1766	G1840	
U3631	C2860		G2711	G2618	U2515	U2436	G2349	C			A1767	G1841	
C3632			G2712	G2619	C2520	C2437	G2350	C			G1851	G1842	
G3633	G2863		G2713	G2620	G2521	C2438	G2351	C			G1852	G1843	
A3634	A2864		G2714	G2621	G2522	C2439	G2352	C			G1853	G1844	
U3635			G2715	G2622	A2523	U2440	G2353	C			G1854	G1845	
G3636	C2867		G2716		G2524	G2441	G2354	C			G1855	G1846	
	A2871		G2717		G2525	G2442	G2355	C			G1856	G1847	
A3643	G2796		G2718		G2526	G2443	G2356	C			G1857	G1848	
U3644	C2797		G2719		G2527	G2444	U2359	C			G1858	G1849	
U3645	A2798		G2720		G2528	U2445	A2360	C			G1859	G1850	
A3646	G2799		G2721		G2529	G2446	A2361	C			G1860	G1851	
					G2530	G2447	G2362	C			G1861	G1852	
A3649	G2802		G2722		U2630	G2448	G2363	C			G1862	G1853	
C3650	C2803		G2723		U2631	G2449	G2364	C			G1863	G1854	
G3651	G2804		G2724		U2632	G2450	G2365	C			G1864	G1855	
A3652	C2805		A2725		G2633	G2451	A2370	C			G1865	G1856	
U3653	G2806		G2726		G2634	G2452	A2371	C			G1866	G1857	
A3654	A2807		G2727		G2635	G2453	A2372	C			G1867	G1858	
C3655	G2808		G2728		G2636	G2454	A2373	C			G1868	G1859	
	G2809		G2729		G2637	G2455	A2374	C			G1869	G1860	
A2894			G2730		G2638	G2456	A2375	C			G1870	G1861	
A2895	G2814		G2731		G2639	G2457	A2376	C			G1871	G1862	
G3659	A2815		G2732		G2640	G2458	A2377	C			G1872	G1863	
C3660	G2816		G2733		G2641	G2459	A2378	C			G1873	G1864	
			G2734		G2642	G2460	A2379	C			G1874	G1865	
			G2735		G2643	G2461	A2380	C			G1875	G1866	
			G2736		G2644	G2462	A2381	C			G1876	G1867	
			G2737		G2645	G2463	A2382	C			G1877	G1868	
			G2738		G2646	G2464	A2383	C			G1878	G1869	
			G2739		G2647	G2465	A2384	C			G1879	G1870	
			G2740		G2648	G2466	A2385	C			G1880	G1871	
					G2649	G2467	A2386	C			G1881	G1872	
					G2650	G2468	A2387	C			G1882	G1873	
					G2651	G2469	A2388	C			G1883	G1874	
					G2652	G2470	A2389	C			G1884	G1875	
					G2653	G2471	A2390	C			G1885	G1876	
					G2654	G2472	A2391	C			G1886	G1877	
					G2655	G2473	A2392	C			G1887	G1878	
					G2656	G2474	A2393	C			G1888	G1879	
					G2657	G2475	A2394	C			G1889	G1880	
					G2658	G2476	A2395	C			G1890	G1881	
					G2659	G2477	A2396	C			G1891	G1882	
					G2660	G2478	A2397	C			G1892	G1883	
					G2661	G2479	A2398	C			G1893	G1884	
					G2662	G2480	A2399	C			G1894	G1885	
					G2663	G2481	A2400	C			G1895	G1886	
					G2664	G2482	A2401	C			G1896	G1887	
					G2665	G2483	A2402	C			G1897	G1888	
					G2666	G2484	A2403	C			G1898	G1889	
					G2667	G2485	A2404	C			G1899	G1890	
					G2668	G2486	A2405	C			G1900	G1891	
					G2669	G2487	A2406	C			G1901	G1892	
					G2670	G2488	A2407	C			G1902	G1893	
					G2671	G2489	A2408	C			G1903	G1894	
					G2672	G2490	A2409	C			G1904	G1895	
					G2673	G2491	A2410	C			G1905	G1896	
					G2674	G2492	A2411	C			G1906	G1897	
					G2675	G2493	A2412	C			G1907	G1898	
					G2676	G2494	A2413	C			G1908	G1899	
					G2677	G2495	A2414	C			G1909	G1900	
					G2678	G2496	A2415	C			G1910	G1901	
					G2679	G2497	A2416	C			G1911	G1902	
					G2680	G2498	A2417	C			G1912	G1903	
					G2681	G2499	A2418	C			G1913	G1904	
					G2682	G2500	A2419	C			G1914	G1905	
					G2683	G2501	A2420	C			G1915	G1906	
					G2684	G2502	A2421	C			G1916	G1907	
					G2685	G2503	A2422	C			G1917	G1908	
					G2686	G2504	A2423	C			G1918	G1909	
					G2687	G2505	A2424	C			G1919	G1910	
					G2688	G2506	A2425	C			G1920	G1911	
					G2689	G2507	A2426	C			G1921	G1912	
					G2690	G2508	A2427	C			G1922	G1913	
					G2691	G2509	A2428	C			G1923	G1914	
					G2692	G2510	A2429	C			G1924	G1915	
					G2693	G2511	A2430	C			G1925	G1916	
					G2694	G2512	A2431	C			G1926	G1917	
					G2695	G2513	A2432	C			G1927	G1918	
					G2696	G2514	A2433	C			G1928	G1919	
					G2697	G2515	A2434	C			G1929	G1920	
					G2698	G2516	A2435	C			G1930	G1921	
					G2699	G2517	A2436	C			G1931	G1922	
					G2700	G2518	A2437	C			G1932	G1923	
					G2701	G2519	A2438	C			G1933	G1924	
					G2702	G2520	A2439	C			G1934	G1925	
					G2703	G2521	A2440	C			G1935	G1926	
					G2704	G2522	A2441	C			G1936	G1927	
					G2705	G2523	A2442	C			G1937	G1928	
					G2706	G2524	A2443	C			G1938	G19	

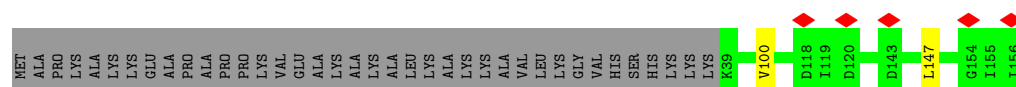
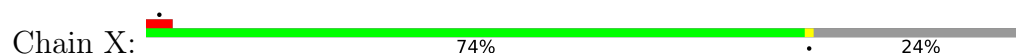




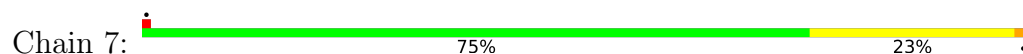
- Molecule 68: Ribosomal protein S15a



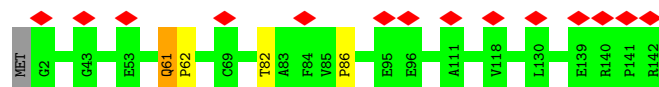
- Molecule 69: uL23



- Molecule 70: 5S Ribosomal RNA



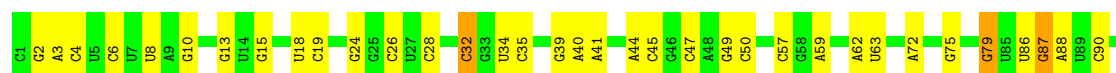
- Molecule 71: 40S ribosomal protein uS12

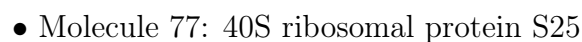


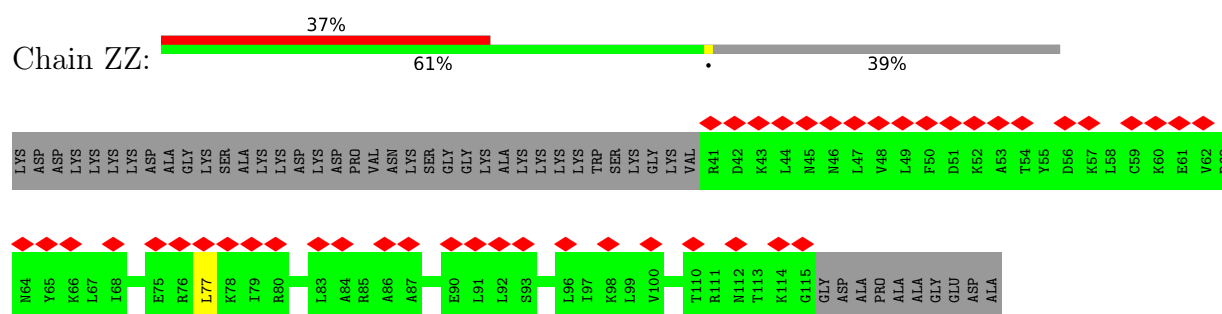
- Molecule 72: Ribosomal protein L26



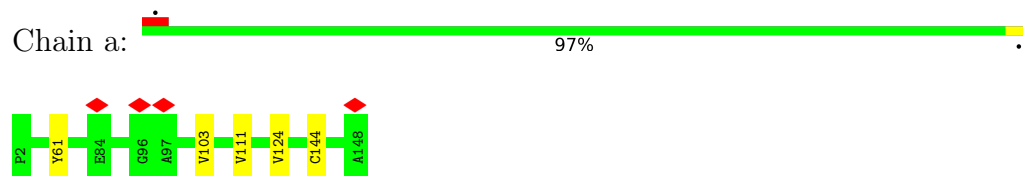
- Molecule 73: 5.8S Ribosomal RNA



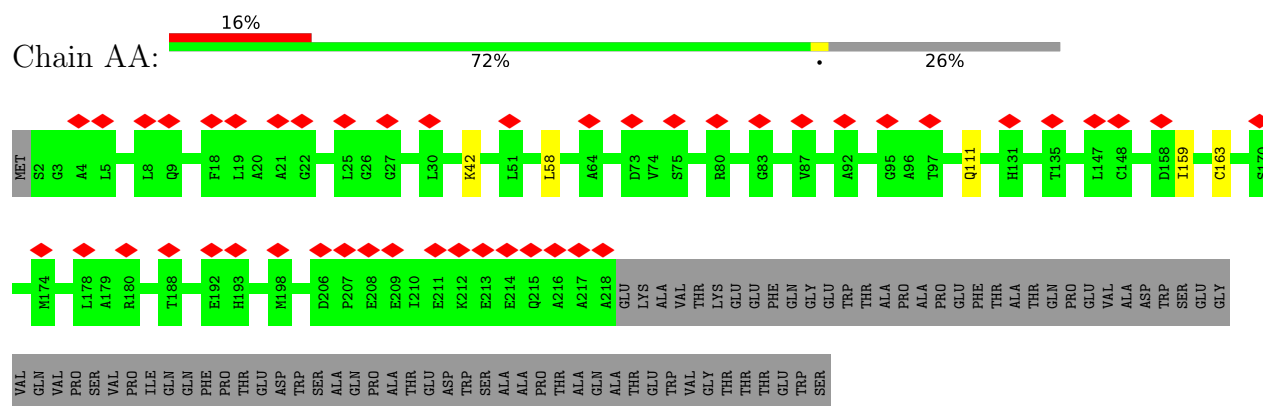




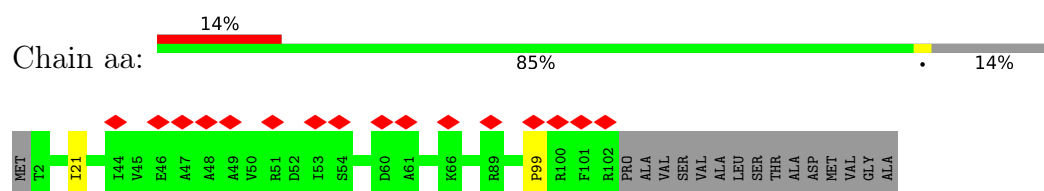
- Molecule 78: 60S ribosomal protein L27a



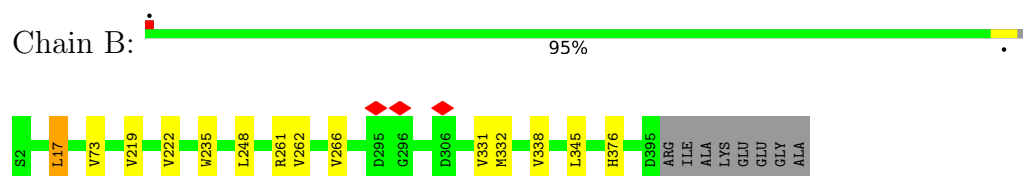
- Molecule 79: 40S_SA_C domain-containing protein



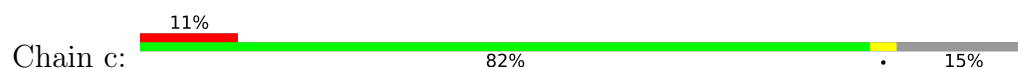
- Molecule 80: 40S ribosomal protein S26

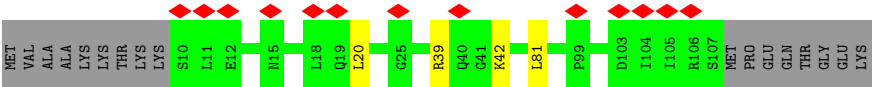


- Molecule 81: uL3

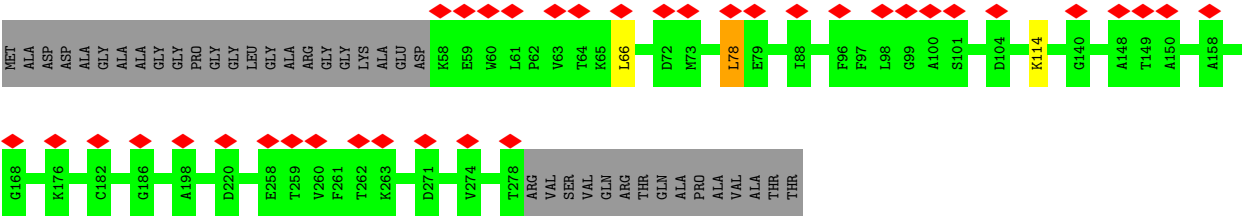
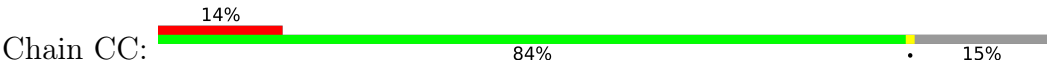


- Molecule 82: eL30

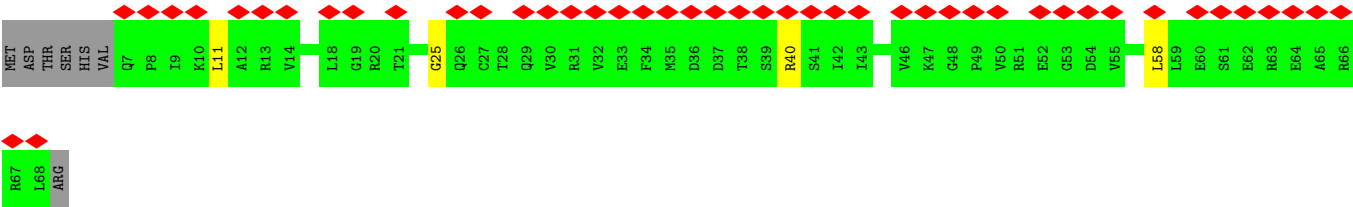
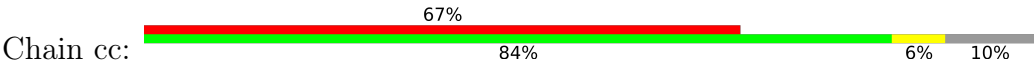




• Molecule 83: 40S ribosomal protein S2



• Molecule 84: 40S ribosomal protein S28



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.92	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	79000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	1.11	10/1936 (0.5%)	0.97	2/2596 (0.1%)
2	C	1.10	13/2937 (0.4%)	0.98	4/3946 (0.1%)
3	d	1.02	4/903 (0.4%)	0.95	0/1216
4	DD	0.59	0/1796	1.01	5/2417 (0.2%)
5	dd	0.64	0/470	0.96	0/623
6	D	0.83	0/2437	0.87	2/3264 (0.1%)
7	e	1.18	5/1071 (0.5%)	0.97	0/1429
8	EE	0.59	0/2118	0.90	3/2849 (0.1%)
9	ee	0.67	0/447	0.91	0/587
10	b	0.82	0/861	0.91	0/1138
11	E	0.88	3/1762 (0.2%)	0.93	2/2362 (0.1%)
12	f	1.14	3/895 (0.3%)	0.96	1/1198 (0.1%)
13	FF	0.55	0/1492	0.92	1/2005 (0.0%)
14	ff	0.57	0/567	1.04	1/753 (0.1%)
15	F	1.17	7/1911 (0.4%)	0.96	1/2549 (0.0%)
16	g	0.93	1/916 (0.1%)	0.96	1/1220 (0.1%)
17	BB	0.58	0/1756	0.90	5/2350 (0.2%)
18	GG	0.54	0/1946	0.89	1/2590 (0.0%)
19	gg	0.46	0/2493	0.83	1/3394 (0.0%)
20	G	0.88	1/1910 (0.1%)	0.92	1/2569 (0.0%)
21	h	0.91	1/1021 (0.1%)	0.97	2/1348 (0.1%)
22	HH	0.61	1/1510 (0.1%)	0.88	4/2022 (0.2%)
23	hh	0.67	0/353	1.37	3/547 (0.5%)
24	bb	0.56	0/665	0.84	2/891 (0.2%)
25	H	0.94	1/1535 (0.1%)	0.88	1/2063 (0.0%)
26	i	0.90	2/841 (0.2%)	0.94	0/1112
27	II	0.62	0/1715	0.88	1/2287 (0.0%)
28	ii	0.56	0/3361	0.98	10/4519 (0.2%)
29	I	1.01	3/1702 (0.2%)	0.89	0/2272
30	j	1.05	1/720 (0.1%)	1.00	0/952
31	JJ	0.68	0/1550	0.86	0/2069
32	jj	0.57	0/3435	0.95	8/4633 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	J	0.77	0/1385	0.92	1/1852 (0.1%)
34	k	0.85	0/575	0.88	1/761 (0.1%)
35	KK	0.55	0/834	0.90	1/1125 (0.1%)
36	L	0.91	3/1733 (0.2%)	0.96	0/2316
37	l	0.93	0/459	0.92	1/608 (0.2%)
38	LL	0.68	0/1195	0.85	0/1597
39	M	0.94	0/1158	0.92	0/1547
40	m	0.85	0/435	0.85	0/575
41	MM	0.43	0/918	0.75	1/1233 (0.1%)
42	N	1.14	6/1746 (0.3%)	0.97	2/2338 (0.1%)
43	n	0.71	0/240	1.29	2/305 (0.7%)
44	NN	0.63	0/1226	0.88	1/1649 (0.1%)
45	O	1.16	12/1662 (0.7%)	1.01	1/2222 (0.0%)
46	o	0.85	0/864	0.93	0/1140
47	OO	0.61	0/1029	0.94	1/1380 (0.1%)
48	P	1.07	3/1268 (0.2%)	0.91	0/1700
49	p	1.03	2/718 (0.3%)	0.89	0/953
50	PP	0.62	0/1017	1.03	2/1358 (0.1%)
51	Q	1.13	5/1539 (0.3%)	1.00	0/2054
52	r	0.99	0/1010	0.94	1/1354 (0.1%)
53	QQ	0.56	0/1146	0.92	1/1534 (0.1%)
54	R	0.87	3/1524 (0.2%)	1.01	1/2013 (0.0%)
55	s	0.55	0/1530	0.92	3/2064 (0.1%)
56	RR	0.58	0/1082	0.87	1/1452 (0.1%)
57	S	1.08	7/1501 (0.5%)	0.93	2/2012 (0.1%)
58	t	0.52	1/1174 (0.1%)	0.90	2/1582 (0.1%)
59	SS	0.56	0/1208	1.03	2/1618 (0.1%)
60	T	1.03	3/1326 (0.2%)	0.97	1/1770 (0.1%)
61	TT	0.55	0/1115	0.87	1/1493 (0.1%)
62	U	0.80	1/823 (0.1%)	0.91	1/1104 (0.1%)
63	UU	0.62	0/805	0.98	2/1081 (0.2%)
64	V	1.12	1/993 (0.1%)	0.96	0/1332
65	VV	0.60	0/643	0.81	0/860
66	W	0.87	1/873 (0.1%)	0.89	0/1158
67	5	1.40	348/84975 (0.4%)	1.67	1993/132516 (1.5%)
68	WW	0.73	0/1051	0.87	0/1406
69	X	0.95	1/984 (0.1%)	0.95	1/1323 (0.1%)
70	7	1.29	6/2858 (0.2%)	1.49	26/4455 (0.6%)
71	XX	0.73	0/1116	0.88	0/1490
72	Y	1.01	1/1132 (0.1%)	0.98	3/1504 (0.2%)
73	8	1.37	9/3581 (0.3%)	1.65	76/5577 (1.4%)
74	YY	0.53	0/1028	0.82	0/1366
75	Z	0.92	1/1130 (0.1%)	0.93	1/1507 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	9	0.91	11/40524 (0.0%)	1.44	428/63134 (0.7%)
77	ZZ	0.50	0/604	0.93	0/810
78	a	1.18	6/1191 (0.5%)	0.94	0/1590
79	AA	0.61	0/1747	0.80	0/2374
80	aa	0.69	0/828	0.86	0/1109
81	B	1.05	11/3240 (0.3%)	0.95	2/4339 (0.0%)
82	c	0.85	0/771	1.09	4/1034 (0.4%)
83	CC	0.73	0/1753	0.92	2/2369 (0.1%)
84	cc	0.61	0/490	1.07	3/656 (0.5%)
All	All	1.10	498/234789 (0.2%)	1.37	2633/343469 (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
3	d	0	1
53	QQ	0	1
67	5	0	7
71	XX	0	1
76	9	0	1
79	AA	0	1
All	All	0	12

All (498) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	2836	A	N9-C4	-8.41	1.32	1.37
67	5	1637	A	N9-C4	-8.35	1.32	1.37
67	5	1907	A	N9-C4	-8.30	1.32	1.37
48	P	119	VAL	CB-CG1	-7.97	1.36	1.52
67	5	2849	A	N9-C4	-7.93	1.33	1.37
67	5	1518	A	N9-C4	-7.76	1.33	1.37
67	5	39	A	N7-C5	-7.61	1.34	1.39
81	B	262	VAL	CB-CG2	-7.56	1.36	1.52
67	5	1352	C	N1-C6	-7.55	1.32	1.37
67	5	42	A	N9-C4	-7.33	1.33	1.37
67	5	1917	A	N9-C4	-7.30	1.33	1.37
2	C	37	VAL	CB-CG2	-7.27	1.37	1.52
11	E	165	VAL	CB-CG1	-7.25	1.37	1.52
67	5	2818	C	N1-C6	-7.23	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	2844	A	N9-C4	-7.21	1.33	1.37
67	5	1655	C	N1-C6	-7.14	1.32	1.37
12	f	29	LYS	CA-CB	-7.12	1.38	1.53
67	5	4380	A	C6-N6	-7.12	1.28	1.33
67	5	3842	C	N1-C6	-7.12	1.32	1.37
45	O	84	VAL	CB-CG1	-7.11	1.38	1.52
67	5	1888	A	N9-C4	-7.06	1.33	1.37
67	5	3621	A	N9-C4	-7.05	1.33	1.37
67	5	2786	C	N1-C6	-7.04	1.32	1.37
67	5	1928	C	N1-C6	-7.00	1.32	1.37
67	5	65	A	N9-C4	-6.97	1.33	1.37
81	B	332	MET	CA-CB	-6.95	1.38	1.53
67	5	2072	C	N1-C6	-6.94	1.32	1.37
67	5	2785	C	N1-C6	-6.92	1.32	1.37
67	5	1505	C	N1-C6	-6.89	1.33	1.37
67	5	4214	A	C6-N6	-6.81	1.28	1.33
67	5	1661	C	N1-C6	-6.81	1.33	1.37
67	5	2579	G	N9-C4	-6.80	1.32	1.38
67	5	1331	C	N1-C6	-6.75	1.33	1.37
67	5	2317	C	N1-C6	-6.73	1.33	1.37
15	F	107	VAL	CB-CG2	-6.72	1.38	1.52
67	5	4206	C	N1-C6	-6.72	1.33	1.37
67	5	2423	A	N9-C4	-6.71	1.33	1.37
67	5	1503	A	N9-C4	-6.70	1.33	1.37
67	5	2335	C	N1-C6	-6.70	1.33	1.37
67	5	1520	C	N1-C6	-6.69	1.33	1.37
11	E	178	VAL	CB-CG2	-6.69	1.38	1.52
67	5	2410	C	N1-C6	-6.66	1.33	1.37
67	5	2334	C	N1-C6	-6.66	1.33	1.37
67	5	2025	A	C6-N6	-6.65	1.28	1.33
67	5	2446	C	N1-C6	-6.65	1.33	1.37
67	5	1633	G	N9-C8	-6.60	1.33	1.37
73	8	103	A	N7-C5	-6.60	1.35	1.39
67	5	1332	C	N1-C6	-6.58	1.33	1.37
67	5	3928	A	N9-C4	-6.57	1.33	1.37
67	5	1535	C	C4-C5	-6.57	1.37	1.43
67	5	1662	C	N1-C6	-6.57	1.33	1.37
67	5	1885	G	N9-C8	-6.55	1.33	1.37
54	R	127	VAL	CB-CG1	-6.53	1.39	1.52
2	C	232	VAL	CB-CG2	-6.52	1.39	1.52
12	f	84	VAL	CB-CG1	-6.51	1.39	1.52
67	5	63	G	N9-C8	-6.51	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	54	VAL	CB-CG1	-6.51	1.39	1.52
67	5	355	A	C5-C6	-6.49	1.35	1.41
67	5	1323	A	N9-C4	-6.49	1.33	1.37
45	O	27	VAL	CB-CG2	-6.47	1.39	1.52
67	5	1357	C	N1-C6	-6.46	1.33	1.37
67	5	1892	A	C6-N6	-6.46	1.28	1.33
67	5	1670	G	N9-C8	-6.45	1.33	1.37
67	5	4424	A	N9-C4	-6.44	1.33	1.37
67	5	338	A	N9-C4	-6.44	1.33	1.37
2	C	246	VAL	CB-CG1	-6.41	1.39	1.52
70	7	97	G	N9-C4	-6.40	1.32	1.38
67	5	418	A	C6-N6	-6.39	1.28	1.33
67	5	1686	C	N1-C6	-6.38	1.33	1.37
67	5	4219	A	N9-C4	-6.37	1.34	1.37
7	e	98	GLU	CB-CG	-6.36	1.40	1.52
67	5	1458	C	N1-C6	-6.34	1.33	1.37
67	5	2346	C	N1-C6	-6.34	1.33	1.37
15	F	135	VAL	CB-CG1	-6.34	1.39	1.52
67	5	3782	C	N1-C6	-6.32	1.33	1.37
1	A	136	VAL	CB-CG2	-6.32	1.39	1.52
67	5	1610	C	N1-C6	-6.30	1.33	1.37
67	5	2360	A	N9-C4	-6.30	1.34	1.37
67	5	1867	A	N9-C4	-6.26	1.34	1.37
67	5	2053	C	N1-C6	-6.26	1.33	1.37
67	5	4536	C	N3-C4	-6.25	1.29	1.33
67	5	3635	A	N9-C4	-6.25	1.34	1.37
67	5	3855	C	N1-C6	-6.25	1.33	1.37
67	5	1323	A	C5-C6	-6.23	1.35	1.41
67	5	2323	C	N1-C6	-6.23	1.33	1.37
67	5	1917	A	C6-N6	-6.22	1.28	1.33
81	B	266	VAL	CB-CG1	-6.22	1.39	1.52
67	5	4547	C	N1-C6	-6.22	1.33	1.37
67	5	2441	C	N1-C6	-6.21	1.33	1.37
42	N	121	VAL	CB-CG1	-6.20	1.39	1.52
67	5	100	C	N1-C6	-6.20	1.33	1.37
67	5	350	C	N1-C6	-6.20	1.33	1.37
67	5	83	C	N1-C6	-6.18	1.33	1.37
67	5	3820	G	N9-C8	-6.18	1.33	1.37
2	C	115	VAL	CB-CG1	-6.18	1.39	1.52
67	5	2460	A	N9-C4	-6.17	1.34	1.37
67	5	2349	A	C6-N6	-6.17	1.29	1.33
73	8	57	C	N1-C6	-6.16	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	4707	A	N9-C4	-6.15	1.34	1.37
67	5	941	C	N1-C6	-6.14	1.33	1.37
67	5	1913	C	N1-C6	-6.14	1.33	1.37
67	5	5043	A	N9-C4	-6.14	1.34	1.37
51	Q	81	VAL	CB-CG2	-6.13	1.40	1.52
73	8	40	A	N3-C4	-6.13	1.31	1.34
1	A	45	VAL	CB-CG1	-6.12	1.40	1.52
2	C	115	VAL	CB-CG2	-6.12	1.40	1.52
67	5	1857	C	N1-C6	-6.11	1.33	1.37
67	5	4507	A	N9-C4	-6.11	1.34	1.37
67	5	1535	C	N1-C6	-6.10	1.33	1.37
67	5	4766	C	N1-C6	-6.09	1.33	1.37
78	a	144	CYS	CA-CB	-6.09	1.40	1.53
45	O	84	VAL	CB-CG2	-6.09	1.40	1.52
76	9	1245	G	N9-C4	6.07	1.42	1.38
67	5	1898	C	N1-C6	-6.06	1.33	1.37
76	9	52	G	N9-C4	-6.05	1.33	1.38
81	B	222	VAL	CB-CG2	-6.05	1.40	1.52
67	5	4525	C	N1-C6	-6.04	1.33	1.37
45	O	145	VAL	CB-CG1	-6.03	1.40	1.52
67	5	1628	C	C4-C5	-6.03	1.38	1.43
81	B	219	VAL	CB-CG1	-6.03	1.40	1.52
67	5	67	C	N1-C6	-6.02	1.33	1.37
67	5	71	C	N1-C6	-6.01	1.33	1.37
67	5	4592	C	N1-C6	-6.00	1.33	1.37
25	H	57	VAL	CB-CG2	-5.98	1.40	1.52
67	5	3691	G	N9-C8	-5.98	1.33	1.37
67	5	2437	C	N1-C6	-5.97	1.33	1.37
48	P	119	VAL	CB-CG2	-5.97	1.40	1.52
67	5	1322	A	N9-C4	-5.95	1.34	1.37
57	S	38	VAL	CB-CG2	-5.94	1.40	1.52
67	5	4373	G	N9-C8	-5.94	1.33	1.37
21	h	57	VAL	CB-CG1	-5.93	1.40	1.52
42	N	89	VAL	CB-CG1	-5.93	1.40	1.52
67	5	3854	C	N1-C6	-5.93	1.33	1.37
67	5	4559	A	N9-C4	-5.93	1.34	1.37
49	p	11	VAL	CB-CG1	-5.93	1.40	1.52
67	5	1641	G	N9-C4	-5.92	1.33	1.38
11	E	178	VAL	CB-CG1	-5.92	1.40	1.52
1	A	88	VAL	CB-CG2	-5.91	1.40	1.52
67	5	4536	C	N1-C6	-5.91	1.33	1.37
64	V	57	VAL	CB-CG2	-5.91	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	8	40	A	N9-C4	-5.90	1.34	1.37
15	F	91	VAL	CB-CG2	-5.89	1.40	1.52
67	5	1525	A	N9-C4	-5.89	1.34	1.37
67	5	2340	C	N1-C6	-5.89	1.33	1.37
45	O	23	VAL	CB-CG1	-5.88	1.40	1.52
67	5	2068	C	N1-C6	-5.88	1.33	1.37
67	5	2779	C	N1-C6	-5.88	1.33	1.37
2	C	154	VAL	CB-CG1	-5.86	1.40	1.52
67	5	2078	C	C4-C5	-5.86	1.38	1.43
67	5	1340	C	N1-C6	-5.85	1.33	1.37
67	5	1065	G	N9-C4	-5.85	1.33	1.38
67	5	51	A	C5-C6	-5.85	1.35	1.41
67	5	299	C	N1-C6	-5.84	1.33	1.37
70	7	95	C	N1-C6	-5.84	1.33	1.37
67	5	4984	C	N1-C6	-5.83	1.33	1.37
67	5	64	A	C5-C6	-5.82	1.35	1.41
67	5	2397	G	N1-C2	-5.82	1.33	1.37
67	5	2780	C	N1-C6	-5.82	1.33	1.37
67	5	1590	C	N1-C6	-5.81	1.33	1.37
67	5	41	C	N1-C6	-5.81	1.33	1.37
67	5	2068	C	C4-C5	-5.80	1.38	1.43
67	5	4688	C	C4-C5	-5.79	1.38	1.43
73	8	41	A	N9-C4	-5.79	1.34	1.37
67	5	4444	C	N1-C6	-5.78	1.33	1.37
1	A	202	VAL	CB-CG2	-5.78	1.40	1.52
67	5	1665	C	N1-C6	-5.77	1.33	1.37
45	O	35	VAL	CB-CG2	-5.77	1.40	1.52
57	S	31	ARG	CA-CB	-5.76	1.41	1.53
67	5	3858	C	N1-C6	-5.75	1.33	1.37
67	5	3882	C	N1-C6	-5.75	1.33	1.37
67	5	5004	C	C4-C5	-5.75	1.38	1.43
67	5	2815	A	C5-C6	-5.74	1.35	1.41
67	5	2604	C	N1-C6	-5.74	1.33	1.37
51	Q	86	VAL	CB-CG1	-5.74	1.40	1.52
57	S	12	VAL	CB-CG2	-5.74	1.40	1.52
67	5	4938	A	N9-C4	-5.74	1.34	1.37
67	5	2785	C	N3-C4	-5.73	1.29	1.33
58	t	19	GLY	C-O	-5.72	1.14	1.23
67	5	1653	A	C5-C6	-5.72	1.35	1.41
67	5	4170	A	C6-N1	-5.71	1.31	1.35
67	5	4380	A	C5-C6	-5.71	1.35	1.41
67	5	3650	C	C4-C5	-5.71	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	1679	A	N3-C4	-5.70	1.31	1.34
67	5	4767	C	N1-C6	-5.70	1.33	1.37
67	5	2532	C	N1-C6	-5.70	1.33	1.37
67	5	3727	A	N9-C4	-5.70	1.34	1.37
67	5	2464	C	N1-C6	-5.70	1.33	1.37
76	9	1853	C	N1-C6	-5.70	1.33	1.37
29	I	38	ARG	CA-CB	-5.70	1.41	1.53
78	a	124	VAL	CB-CG1	-5.68	1.41	1.52
67	5	293	G	N9-C8	-5.68	1.33	1.37
67	5	3852	A	N9-C4	-5.68	1.34	1.37
67	5	4662	C	N1-C6	-5.67	1.33	1.37
2	C	40	VAL	CB-CG1	-5.66	1.41	1.52
67	5	1350	C	N1-C6	-5.66	1.33	1.37
67	5	1938	C	N1-C6	-5.66	1.33	1.37
67	5	2739	C	N1-C6	-5.66	1.33	1.37
67	5	4305	G	N7-C5	-5.66	1.35	1.39
81	B	266	VAL	CB-CG2	-5.65	1.41	1.52
67	5	4487	A	N9-C4	-5.65	1.34	1.37
51	Q	47	VAL	CB-CG2	-5.64	1.41	1.52
67	5	4223	C	N1-C6	-5.64	1.33	1.37
67	5	418	A	C6-N1	-5.63	1.31	1.35
76	9	813	A	N9-C4	-5.63	1.34	1.37
67	5	410	A	N9-C4	-5.63	1.34	1.37
1	A	88	VAL	CB-CG1	-5.62	1.41	1.52
67	5	4716	C	N1-C6	-5.62	1.33	1.37
73	8	26	C	C4-C5	-5.62	1.38	1.43
67	5	3864	C	N1-C6	-5.62	1.33	1.37
67	5	94	A	N9-C4	-5.61	1.34	1.37
67	5	1900	C	N1-C6	-5.61	1.33	1.37
75	Z	74	VAL	CB-CG1	-5.61	1.41	1.52
67	5	3643	A	N9-C4	-5.60	1.34	1.37
67	5	1499	C	N1-C6	-5.60	1.33	1.37
67	5	2858	A	N9-C4	-5.60	1.34	1.37
67	5	1515	A	C6-N6	-5.60	1.29	1.33
42	N	192	TRP	CB-CG	-5.59	1.40	1.50
36	L	70	VAL	CB-CG1	-5.58	1.41	1.52
67	5	2351	C	N1-C6	-5.58	1.33	1.37
7	e	45	VAL	CB-CG2	-5.58	1.41	1.52
15	F	122	VAL	CB-CG2	-5.57	1.41	1.52
67	5	4393	G	N9-C8	-5.57	1.33	1.37
45	O	104	VAL	CB-CG2	-5.57	1.41	1.52
76	9	1383	A	N9-C4	-5.57	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	4319	C	N1-C6	-5.57	1.33	1.37
48	P	24	VAL	CB-CG2	-5.56	1.41	1.52
67	5	4519	C	N1-C6	-5.56	1.33	1.37
67	5	27	C	N1-C6	-5.55	1.33	1.37
67	5	2392	C	C4-C5	-5.55	1.38	1.43
67	5	3896	C	N1-C6	-5.55	1.33	1.37
67	5	4562	C	N1-C6	-5.54	1.33	1.37
67	5	2783	A	N9-C4	-5.54	1.34	1.37
67	5	3911	C	C4-C5	-5.54	1.38	1.43
67	5	4710	C	N1-C6	-5.52	1.33	1.37
2	C	183	VAL	CB-CG1	-5.52	1.41	1.52
67	5	2836	A	C5-C6	-5.51	1.36	1.41
67	5	1626	G	N9-C4	-5.51	1.33	1.38
67	5	3633	C	N1-C6	-5.51	1.33	1.37
67	5	3893	C	N1-C6	-5.51	1.33	1.37
2	C	79	VAL	CB-CG1	-5.50	1.41	1.52
67	5	1666	C	N1-C6	-5.50	1.33	1.37
67	5	4428	A	N9-C4	-5.50	1.34	1.37
3	d	72	VAL	CB-CG1	-5.50	1.41	1.52
67	5	53	C	N1-C6	-5.49	1.33	1.37
72	Y	58	VAL	CB-CG1	-5.49	1.41	1.52
67	5	41	C	C4-C5	-5.49	1.38	1.43
67	5	2783	A	C6-N6	-5.49	1.29	1.33
67	5	38	A	C5-C6	-5.48	1.36	1.41
67	5	2051	C	C4-C5	-5.48	1.38	1.43
67	5	5016	A	C5-C6	-5.48	1.36	1.41
67	5	1898	C	C4-C5	-5.48	1.38	1.43
81	B	262	VAL	CB-CG1	-5.47	1.41	1.52
67	5	56	A	N9-C4	-5.47	1.34	1.37
67	5	3910	C	C4-C5	-5.47	1.38	1.43
67	5	4561	C	N1-C6	-5.47	1.33	1.37
81	B	73	VAL	CB-CG2	-5.47	1.41	1.52
81	B	331	VAL	CB-CG2	-5.46	1.41	1.52
67	5	1662	C	C4-C5	-5.46	1.38	1.43
67	5	1327	C	C4-C5	-5.46	1.38	1.43
67	5	3702	A	N9-C4	-5.46	1.34	1.37
67	5	2772	C	N1-C6	-5.45	1.33	1.37
67	5	1580	C	C4-C5	-5.45	1.38	1.43
67	5	1893	C	N1-C6	-5.45	1.33	1.37
67	5	1872	G	N9-C4	-5.44	1.33	1.38
67	5	3687	A	N9-C4	-5.44	1.34	1.37
3	d	106	VAL	CB-CG1	-5.44	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	1847	C	N1-C6	-5.44	1.33	1.37
67	5	1306	C	C4-C5	-5.43	1.38	1.43
1	A	202	VAL	CB-CG1	-5.43	1.41	1.52
67	5	4502	C	N1-C6	-5.43	1.33	1.37
29	I	96	VAL	CB-CG2	-5.42	1.41	1.52
67	5	2745	A	N9-C4	-5.42	1.34	1.37
67	5	3909	C	C4-N4	-5.42	1.29	1.33
67	5	1427	A	N9-C4	-5.42	1.34	1.37
7	e	79	VAL	CB-CG1	-5.42	1.41	1.52
67	5	2641	A	N9-C4	-5.42	1.34	1.37
73	8	18	U	N1-C2	-5.42	1.33	1.38
76	9	1563	G	N9-C4	-5.42	1.33	1.38
78	a	124	VAL	CB-CG2	-5.42	1.41	1.52
67	5	1397	A	C6-N6	-5.41	1.29	1.33
67	5	1888	A	N3-C4	-5.41	1.31	1.34
67	5	2290	C	N1-C6	-5.41	1.33	1.37
67	5	4724	A	C6-N6	-5.41	1.29	1.33
67	5	1648	C	N1-C6	-5.41	1.33	1.37
67	5	1654	G	N9-C8	-5.41	1.34	1.37
67	5	1631	A	N9-C8	-5.41	1.33	1.37
57	S	67	VAL	CB-CG1	-5.40	1.41	1.52
67	5	2849	A	C5-C4	-5.40	1.34	1.38
67	5	3879	G	N9-C4	-5.39	1.33	1.38
7	e	45	VAL	CB-CG1	-5.39	1.41	1.52
81	B	235	TRP	CB-CG	-5.39	1.40	1.50
67	5	1469	C	N1-C6	-5.39	1.33	1.37
67	5	1535	C	C4-N4	-5.39	1.29	1.33
67	5	2743	A	C6-N6	-5.38	1.29	1.33
2	C	183	VAL	CB-CG2	-5.38	1.41	1.52
67	5	1628	C	N1-C6	-5.38	1.33	1.37
45	O	23	VAL	CB-CG2	-5.38	1.41	1.52
57	S	39	VAL	CB-CG2	-5.38	1.41	1.52
67	5	2791	C	N1-C6	-5.38	1.33	1.37
67	5	4590	A	N9-C4	-5.37	1.34	1.37
67	5	360	A	C6-N6	-5.36	1.29	1.33
67	5	1577	G	N9-C8	-5.36	1.34	1.37
67	5	4170	A	C6-N6	-5.36	1.29	1.33
67	5	210	C	N1-C6	-5.35	1.33	1.37
67	5	289	C	N1-C6	-5.35	1.33	1.37
67	5	1879	C	C4-C5	-5.35	1.38	1.43
1	A	235	VAL	CB-CG2	-5.35	1.41	1.52
67	5	33	A	N9-C4	-5.35	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	410	A	C6-N6	-5.34	1.29	1.33
67	5	4564	A	N9-C4	-5.34	1.34	1.37
67	5	2071	A	N9-C8	-5.33	1.33	1.37
67	5	1632	A	N7-C5	-5.33	1.36	1.39
67	5	238	C	N1-C6	-5.33	1.33	1.37
73	8	105	C	N1-C6	-5.32	1.33	1.37
51	Q	148	VAL	CB-CG2	-5.32	1.41	1.52
57	S	62	VAL	CB-CG2	-5.32	1.41	1.52
67	5	355	A	N9-C4	-5.32	1.34	1.37
67	5	4565	C	C4-C5	-5.32	1.38	1.43
78	a	111	VAL	CB-CG1	-5.32	1.41	1.52
67	5	2509	C	C4-C5	-5.32	1.38	1.43
67	5	4087	G	N9-C4	-5.31	1.33	1.38
67	5	2797	C	N1-C6	-5.30	1.33	1.37
76	9	1469	A	N9-C4	5.30	1.41	1.37
67	5	1541	C	N1-C6	-5.30	1.33	1.37
16	g	87	VAL	CB-CG2	-5.30	1.41	1.52
30	j	70	VAL	CB-CG2	-5.30	1.41	1.52
67	5	3876	A	C6-N1	-5.29	1.31	1.35
45	O	34	VAL	CB-CG1	-5.29	1.41	1.52
67	5	1346	C	N1-C6	-5.29	1.33	1.37
67	5	3774	A	C5-C6	-5.29	1.36	1.41
70	7	10	C	N1-C6	-5.29	1.33	1.37
15	F	116	ILE	CB-CG2	-5.28	1.36	1.52
67	5	4184	G	N9-C4	-5.28	1.33	1.38
49	p	64	VAL	CB-CG2	-5.28	1.41	1.52
54	R	22	VAL	CB-CG1	-5.28	1.41	1.52
67	5	1920	C	N1-C6	-5.28	1.33	1.37
67	5	2392	C	N1-C6	-5.28	1.33	1.37
67	5	1908	A	C5-C6	-5.27	1.36	1.41
67	5	2770	C	N1-C6	-5.27	1.33	1.37
29	I	126	VAL	CB-CG1	-5.27	1.41	1.52
26	i	76	ARG	CB-CG	-5.27	1.38	1.52
67	5	3672	G	N9-C4	-5.27	1.33	1.38
67	5	1599	G	N1-C2	-5.27	1.33	1.37
67	5	2422	C	N1-C6	-5.27	1.33	1.37
15	F	104	VAL	CB-CG1	-5.26	1.41	1.52
70	7	97	G	C2-N3	-5.26	1.28	1.32
60	T	76	VAL	CB-CG2	-5.26	1.41	1.52
67	5	92	C	N1-C6	-5.26	1.33	1.37
67	5	2268	A	N9-C4	-5.26	1.34	1.37
67	5	2851	G	N9-C8	-5.26	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	4186	A	N3-C4	-5.26	1.31	1.34
67	5	3655	C	N1-C6	-5.25	1.33	1.37
45	O	35	VAL	CB-CG1	-5.25	1.41	1.52
81	B	338	VAL	CB-CG1	-5.25	1.41	1.52
67	5	2075	G	N9-C8	-5.25	1.34	1.37
66	W	53	VAL	CB-CG2	-5.24	1.41	1.52
67	5	4533	A	C5-C6	-5.24	1.36	1.41
67	5	1387	A	C5-C6	-5.24	1.36	1.41
67	5	1521	C	C4-C5	-5.24	1.38	1.43
67	5	1879	C	N1-C6	-5.24	1.34	1.37
60	T	76	VAL	CB-CG1	-5.23	1.41	1.52
67	5	422	C	C4-C5	-5.23	1.38	1.43
67	5	2529	A	N9-C4	-5.23	1.34	1.37
67	5	4080	C	N1-C6	-5.23	1.34	1.37
15	F	135	VAL	CB-CG2	-5.23	1.41	1.52
67	5	222	C	N1-C6	-5.23	1.34	1.37
42	N	25	VAL	CB-CG2	-5.23	1.41	1.52
67	5	1795	A	C6-N6	-5.23	1.29	1.33
67	5	1339	U	C2-N3	-5.22	1.34	1.37
67	5	1668	A	C6-N1	-5.22	1.31	1.35
45	O	33	VAL	CB-CG2	-5.22	1.41	1.52
78	a	103	VAL	CB-CG2	-5.21	1.42	1.52
67	5	1942	A	N9-C4	-5.21	1.34	1.37
67	5	1884	C	N1-C6	-5.21	1.34	1.37
67	5	3859	G	N9-C8	-5.21	1.34	1.37
67	5	2881	A	N9-C4	-5.20	1.34	1.37
67	5	2069	A	N9-C4	-5.20	1.34	1.37
1	A	207	VAL	CB-CG2	-5.20	1.42	1.52
36	L	25	TRP	CB-CG	-5.20	1.40	1.50
22	HH	100	ILE	C-N	5.20	1.46	1.34
67	5	4653	C	N1-C6	-5.19	1.34	1.37
67	5	4671	C	N1-C6	-5.19	1.34	1.37
67	5	4883	C	N1-C6	-5.19	1.34	1.37
67	5	362	A	N9-C4	-5.18	1.34	1.37
67	5	1313	C	N1-C6	-5.18	1.34	1.37
67	5	4485	C	N1-C6	-5.18	1.34	1.37
67	5	1524	A	N9-C4	-5.18	1.34	1.37
67	5	3869	C	N1-C6	-5.18	1.34	1.37
67	5	3700	C	N1-C6	-5.17	1.34	1.37
3	d	86	VAL	CB-CG1	-5.17	1.42	1.52
67	5	26	C	N1-C6	-5.17	1.34	1.37
67	5	414	C	N1-C6	-5.17	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	2393	C	N1-C6	-5.17	1.34	1.37
67	5	4982	A	N9-C4	-5.17	1.34	1.37
67	5	4715	C	C4-C5	-5.17	1.38	1.43
67	5	81	C	C4-C5	-5.16	1.38	1.43
67	5	1331	C	C4-C5	-5.16	1.38	1.43
67	5	87	A	N9-C8	-5.15	1.33	1.37
76	9	628	A	N9-C4	-5.15	1.34	1.37
67	5	323	C	N1-C6	-5.14	1.34	1.37
67	5	33	A	C6-N6	-5.14	1.29	1.33
67	5	357	U	N1-C6	-5.14	1.33	1.38
7	e	79	VAL	CB-CG2	-5.14	1.42	1.52
67	5	1895	G	N9-C8	-5.14	1.34	1.37
67	5	2338	C	N1-C6	-5.14	1.34	1.37
42	N	59	TYR	CD1-CE1	-5.14	1.31	1.39
67	5	4325	A	C6-N6	-5.14	1.29	1.33
54	R	22	VAL	CB-CG2	-5.13	1.42	1.52
67	5	1631	A	N9-C4	-5.13	1.34	1.37
67	5	4979	A	C5-C6	-5.13	1.36	1.41
70	7	111	C	N1-C6	-5.13	1.34	1.37
67	5	1659	U	N1-C2	-5.13	1.33	1.38
67	5	1785	C	N1-C6	-5.13	1.34	1.37
67	5	2397	G	C6-N1	-5.13	1.35	1.39
67	5	4318	C	N1-C6	-5.13	1.34	1.37
12	f	84	VAL	CB-CG2	-5.12	1.42	1.52
67	5	4720	C	N1-C6	-5.12	1.34	1.37
67	5	332	C	C4-C5	-5.12	1.38	1.43
67	5	4313	A	N9-C4	-5.12	1.34	1.37
67	5	4533	A	N7-C5	-5.12	1.36	1.39
67	5	21	G	N9-C8	-5.11	1.34	1.37
67	5	1674	C	C4-C5	-5.11	1.38	1.43
67	5	1669	A	C6-N6	-5.11	1.29	1.33
67	5	2039	G	N1-C2	-5.11	1.33	1.37
67	5	2853	C	N1-C6	-5.11	1.34	1.37
67	5	2279	A	N9-C4	-5.11	1.34	1.37
67	5	1857	C	C4-C5	-5.10	1.38	1.43
67	5	4761	G	N9-C4	-5.10	1.33	1.38
67	5	4466	C	N1-C6	-5.10	1.34	1.37
69	X	100	VAL	CB-CG1	-5.10	1.42	1.52
2	C	73	VAL	CB-CG2	-5.10	1.42	1.52
36	L	79	GLU	CB-CG	-5.10	1.42	1.52
67	5	2438	A	C5-C6	-5.10	1.36	1.41
67	5	39	A	C8-N7	-5.10	1.27	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	422	C	N1-C6	-5.10	1.34	1.37
67	5	3654	G	N3-C4	-5.10	1.31	1.35
1	A	235	VAL	CB-CG1	-5.09	1.42	1.52
20	G	196	VAL	CB-CG2	-5.09	1.42	1.52
51	Q	82	VAL	CB-CG2	-5.09	1.42	1.52
67	5	2458	C	N1-C6	-5.08	1.34	1.37
67	5	47	A	N9-C4	-5.08	1.34	1.37
67	5	1681	G	N9-C8	-5.08	1.34	1.37
67	5	4561	C	N3-C4	-5.08	1.30	1.33
67	5	4195	G	C6-N1	-5.08	1.35	1.39
57	S	38	VAL	CB-CG1	-5.08	1.42	1.52
45	O	33	VAL	CB-CG1	-5.07	1.42	1.52
67	5	4386	C	N1-C6	-5.07	1.34	1.37
73	8	140	C	N1-C6	-5.07	1.34	1.37
2	C	37	VAL	CB-CG1	-5.07	1.42	1.52
67	5	1354	A	C6-N6	-5.07	1.29	1.33
67	5	4862	G	N9-C4	-5.07	1.33	1.38
67	5	941	C	C4-C5	-5.07	1.38	1.43
67	5	2078	C	N1-C6	-5.07	1.34	1.37
67	5	5050	C	N1-C6	-5.07	1.34	1.37
62	U	49	VAL	CB-CG2	-5.06	1.42	1.52
67	5	2802	C	N1-C6	-5.06	1.34	1.37
67	5	1279	A	N9-C4	-5.06	1.34	1.37
67	5	1788	A	N9-C4	-5.05	1.34	1.37
67	5	4456	C	N1-C6	-5.05	1.34	1.37
67	5	39	A	C5-C6	-5.05	1.36	1.41
67	5	4507	A	N3-C4	-5.05	1.31	1.34
67	5	4488	A	N9-C4	-5.05	1.34	1.37
70	7	14	C	N1-C6	-5.05	1.34	1.37
67	5	358	C	N1-C6	-5.04	1.34	1.37
76	9	1200	A	N9-C4	-5.04	1.34	1.37
67	5	1276	C	N1-C6	-5.04	1.34	1.37
67	5	4582	C	N1-C6	-5.04	1.34	1.37
60	T	75	VAL	CB-CG1	-5.04	1.42	1.52
67	5	1521	C	N1-C6	-5.04	1.34	1.37
67	5	2321	G	N9-C4	-5.03	1.33	1.38
67	5	2409	U	N1-C6	-5.03	1.33	1.38
67	5	3846	C	N1-C6	-5.03	1.34	1.37
1	A	169	VAL	CB-CG1	-5.03	1.42	1.52
67	5	2295	C	N1-C6	-5.03	1.34	1.37
67	5	4535	A	N3-C4	-5.03	1.31	1.34
67	5	4508	C	C4-C5	-5.03	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	N	155	VAL	CB-CG2	-5.03	1.42	1.52
67	5	101	A	C5-C6	-5.03	1.36	1.41
67	5	1507	C	C4-C5	-5.03	1.39	1.43
67	5	1855	G	N9-C8	-5.03	1.34	1.37
67	5	2381	A	N9-C4	-5.02	1.34	1.37
67	5	2461	G	N9-C8	-5.02	1.34	1.37
3	d	36	VAL	CB-CG2	-5.02	1.42	1.52
67	5	1518	A	C6-N6	-5.02	1.29	1.33
67	5	3653	A	N7-C5	-5.02	1.36	1.39
67	5	1460	C	C4-C5	-5.02	1.39	1.43
67	5	2449	A	C6-N6	-5.02	1.29	1.33
67	5	2583	C	N1-C6	-5.02	1.34	1.37
67	5	4313	A	N3-C4	-5.02	1.31	1.34
76	9	330	G	N9-C4	-5.02	1.33	1.38
67	5	1396	G	N9-C8	-5.01	1.34	1.37
76	9	1719	A	N9-C4	-5.01	1.34	1.37
67	5	3903	A	C5-C6	-5.01	1.36	1.41
26	i	77	VAL	CB-CG2	-5.01	1.42	1.52
67	5	3747	A	N9-C4	-5.00	1.34	1.37
67	5	79	C	N1-C6	-5.00	1.34	1.37
67	5	1908	A	C6-N6	-5.00	1.29	1.33
78	a	61	TYR	CE1-CZ	-5.00	1.32	1.38

All (2633) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	3911	C	C6-N1-C2	-12.96	115.12	120.30
67	5	1535	C	C5-C4-N4	-12.52	111.44	120.20
67	5	1081	C	C6-N1-C2	-12.39	115.34	120.30
67	5	4723	A	C6-N1-C2	-12.38	111.17	118.60
67	5	143	C	O4'-C1'-N1	12.29	118.03	108.20
73	8	103	A	N1-C6-N6	12.25	125.95	118.60
67	5	38	A	N1-C6-N6	11.79	125.67	118.60
76	9	1215	C	C6-N1-C2	-11.57	115.67	120.30
67	5	3653	A	C8-N9-C4	-11.47	101.21	105.80
67	5	3910	C	C6-N1-C2	-11.29	115.78	120.30
67	5	41	C	N1-C2-O2	11.10	125.56	118.90
67	5	3653	A	C8-N9-C1'	-11.09	107.75	127.70
67	5	1308	C	C6-N1-C2	-11.07	115.87	120.30
67	5	2579	G	N3-C4-N9	-11.02	119.39	126.00
67	5	5004	C	C5-C4-N4	-10.98	112.52	120.20
70	7	97	G	N3-C4-N9	-10.67	119.60	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	3909	C	N3-C4-C5	10.65	126.16	121.90
67	5	2465	C	N1-C2-O2	10.52	125.21	118.90
67	5	1628	C	C5-C4-N4	-10.34	112.96	120.20
67	5	1081	C	C2-N1-C1'	10.32	130.15	118.80
67	5	30	C	N1-C2-O2	10.31	125.09	118.90
67	5	1653	A	N1-C6-N6	10.18	124.71	118.60
67	5	4536	C	N3-C2-O2	-10.12	114.82	121.90
67	5	2799	G	C4-N9-C1'	10.11	139.64	126.50
67	5	1812	C	C2-N1-C1'	10.07	129.88	118.80
67	5	2785	C	N1-C2-O2	10.00	124.90	118.90
67	5	355	A	N1-C6-N6	10.00	124.60	118.60
67	5	5004	C	N3-C4-N4	9.95	124.97	118.00
67	5	51	A	N1-C6-N6	9.92	124.55	118.60
67	5	1191	C	C6-N1-C2	-9.92	116.33	120.30
67	5	4980	C	C5-C4-N4	-9.89	113.27	120.20
76	9	876	C	N1-C2-O2	9.87	124.82	118.90
67	5	4378	A	O4'-C1'-N9	9.80	116.04	108.20
67	5	64	A	N1-C6-N6	9.78	124.47	118.60
67	5	4533	A	N1-C6-N6	9.77	124.46	118.60
67	5	4723	A	C5-C6-N1	9.72	122.56	117.70
67	5	1580	C	C2-N1-C1'	9.72	129.49	118.80
67	5	106	A	N1-C6-N6	9.70	124.42	118.60
67	5	3911	C	C2-N1-C1'	9.69	129.45	118.80
67	5	294	G	C8-N9-C1'	-9.67	114.43	127.00
67	5	39	A	C8-N9-C4	-9.67	101.93	105.80
67	5	64	A	C5-C6-N6	-9.65	115.98	123.70
67	5	1587	G	C8-N9-C4	-9.64	102.54	106.40
67	5	2068	C	C5-C4-N4	-9.59	113.49	120.20
67	5	38	A	C6-C5-N7	-9.58	125.60	132.30
67	5	1680	G	N1-C2-N2	-9.58	107.58	116.20
67	5	3860	A	N1-C6-N6	-9.52	112.89	118.60
76	9	1513	C	N3-C2-O2	-9.51	115.25	121.90
76	9	1458	G	O5'-P-OP1	-9.50	97.15	105.70
76	9	52	G	N3-C4-C5	9.47	133.33	128.60
67	5	1898	C	C5-C4-N4	-9.45	113.59	120.20
67	5	50	C	C5-C4-N4	-9.44	113.59	120.20
67	5	1065	G	N3-C4-N9	-9.42	120.35	126.00
67	5	3653	A	C4-N9-C1'	9.36	143.14	126.30
67	5	2025	A	C5-C6-N1	9.35	122.37	117.70
67	5	1541	C	C2-N1-C1'	9.35	129.08	118.80
67	5	39	A	C8-N9-C1'	-9.34	110.90	127.70
67	5	4279	A	N1-C6-N6	9.30	124.18	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4528	G	C8-N9-C4	-9.29	102.68	106.40
67	5	5016	A	N1-C6-N6	9.24	124.14	118.60
67	5	4536	C	N1-C2-O2	9.20	124.42	118.90
76	9	672	A	O4'-C1'-N9	9.16	115.53	108.20
67	5	1521	C	C5-C4-N4	-9.15	113.79	120.20
67	5	2815	A	C5-C6-N6	-9.15	116.38	123.70
67	5	1507	C	C6-N1-C2	-9.13	116.65	120.30
67	5	299	C	N1-C2-O2	9.09	124.35	118.90
67	5	1535	C	N3-C4-C5	9.08	125.53	121.90
67	5	1674	C	N1-C2-O2	9.08	124.35	118.90
67	5	1076	C	N3-C2-O2	-9.08	115.54	121.90
67	5	90	G	C8-N9-C4	-9.06	102.78	106.40
67	5	2799	G	C8-N9-C1'	-9.06	115.23	127.00
67	5	2540	C	C6-N1-C2	-9.04	116.68	120.30
76	9	140	U	C6-N1-C2	-9.04	115.58	121.00
67	5	1675	C	N3-C2-O2	-9.00	115.60	121.90
76	9	524	U	C5-C4-O4	-8.98	120.51	125.90
76	9	1245	G	N3-C4-C5	-8.96	124.12	128.60
8	EE	48	LEU	CB-CG-CD1	8.95	126.22	111.00
67	5	2078	C	C2-N1-C1'	8.95	128.65	118.80
76	9	1096	G	N3-C2-N2	8.90	126.13	119.90
67	5	1928	C	C6-N1-C2	8.89	123.86	120.30
67	5	1651	G	N1-C2-N2	-8.86	108.23	116.20
67	5	3650	C	C2-N1-C1'	8.86	128.55	118.80
76	9	1563	G	N3-C4-C5	8.85	133.02	128.60
67	5	3749	C	C2-N1-C1'	8.83	128.52	118.80
67	5	1623	A	N1-C6-N6	8.82	123.89	118.60
67	5	2410	C	C2-N1-C1'	8.79	128.47	118.80
67	5	2833	A	O4'-C1'-N9	8.79	115.23	108.20
67	5	1081	C	C6-N1-C1'	-8.79	110.26	120.80
67	5	1580	C	C6-N1-C2	-8.78	116.79	120.30
67	5	1632	A	C8-N9-C4	-8.75	102.30	105.80
67	5	1938	C	C6-N1-C2	8.73	123.79	120.30
67	5	2465	C	C2-N1-C1'	8.69	128.35	118.80
67	5	1648	C	N1-C2-O2	8.68	124.11	118.90
67	5	2815	A	C4-C5-N7	8.68	115.04	110.70
67	5	2346	C	O4'-C1'-N1	8.65	115.12	108.20
67	5	4971	A	N1-C6-N6	-8.65	113.41	118.60
67	5	3882	C	C6-N1-C2	-8.64	116.84	120.30
76	9	1490	G	N3-C4-C5	-8.63	124.28	128.60
67	5	3774	A	N1-C6-N6	8.63	123.78	118.60
67	5	356	G	C2-N3-C4	-8.63	107.59	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1851	G	C4-N9-C1'	8.62	137.71	126.50
67	5	3876	A	N1-C6-N6	-8.62	113.43	118.60
76	9	1513	C	N1-C2-O2	8.60	124.06	118.90
67	5	1648	C	N3-C2-O2	-8.59	115.88	121.90
67	5	355	A	C5-C6-N6	-8.58	116.83	123.70
67	5	2393	C	C5-C4-N4	-8.57	114.20	120.20
76	9	1254	C	O4'-C1'-N1	8.57	115.05	108.20
67	5	1465	G	C4-N9-C1'	8.56	137.63	126.50
67	5	1928	C	N3-C4-C5	8.55	125.32	121.90
67	5	3917	A	C5-C6-N6	-8.53	116.88	123.70
73	8	103	A	C6-C5-N7	-8.52	126.33	132.30
67	5	1318	C	C5-C4-N4	-8.50	114.25	120.20
76	9	1096	G	N1-C2-N2	-8.50	108.55	116.20
67	5	3945	A	P-O3'-C3'	8.50	129.90	119.70
82	c	20	LEU	CA-CB-CG	8.49	134.82	115.30
67	5	1941	A	N1-C6-N6	-8.49	113.51	118.60
67	5	2410	C	C6-N1-C1'	-8.48	110.63	120.80
76	9	1532	C	C2-N1-C1'	8.46	128.11	118.80
67	5	3909	C	C6-N1-C2	8.45	123.68	120.30
67	5	1872	G	C2-N3-C4	-8.45	107.68	111.90
76	9	1658	G	C4-C5-N7	8.45	114.18	110.80
76	9	524	U	N3-C4-O4	8.43	125.30	119.40
76	9	1416	C	C2-N1-C1'	8.43	128.07	118.80
76	9	1562	C	C6-N1-C2	8.41	123.66	120.30
67	5	4533	A	C5-C6-N6	-8.41	116.97	123.70
67	5	5016	A	C5-C6-N6	-8.40	116.98	123.70
67	5	1680	G	N3-C2-N2	8.39	125.78	119.90
67	5	1065	G	N3-C4-C5	8.39	132.79	128.60
67	5	4618	G	C8-N9-C4	-8.35	103.06	106.40
67	5	4463	U	O4'-C1'-N1	8.35	114.88	108.20
67	5	4193	C	C2-N1-C1'	8.34	127.97	118.80
76	9	1495	G	O4'-C1'-N9	-8.34	101.53	108.20
67	5	1675	C	C6-N1-C2	-8.33	116.97	120.30
76	9	1603	G	C8-N9-C1'	-8.32	116.19	127.00
67	5	968	C	N1-C2-O2	8.31	123.89	118.90
76	9	1219	C	C2-N1-C1'	8.31	127.94	118.80
67	5	3910	C	C2-N1-C1'	8.30	127.93	118.80
67	5	1515	A	C5-C6-N1	8.28	121.84	117.70
76	9	1218	C	C6-N1-C2	-8.26	116.99	120.30
76	9	1638	G	P-O3'-C3'	8.25	129.60	119.70
67	5	1675	C	N1-C2-O2	8.25	123.85	118.90
76	9	1490	G	N3-C4-N9	8.24	130.95	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4448	G	C2-N3-C4	-8.24	107.78	111.90
76	9	909	G	N3-C4-N9	8.23	130.94	126.00
67	5	3774	A	C5-C6-N6	-8.22	117.12	123.70
67	5	3737	A	N1-C6-N6	8.20	123.52	118.60
67	5	2527	A	N1-C6-N6	-8.19	113.68	118.60
67	5	143	C	C6-N1-C2	-8.15	117.04	120.30
76	9	1019	C	C6-N1-C2	-8.15	117.04	120.30
67	5	38	A	N9-C4-C5	-8.14	102.54	105.80
67	5	2815	A	N1-C6-N6	8.14	123.48	118.60
67	5	159	C	C2-N1-C1'	8.13	127.75	118.80
67	5	4626	A	N1-C6-N6	-8.13	113.72	118.60
67	5	3749	C	C6-N1-C2	-8.11	117.06	120.30
76	9	1658	G	C6-C5-N7	-8.11	125.53	130.40
67	5	978	G	O4'-C1'-N9	8.10	114.68	108.20
67	5	384	A	N1-C6-N6	-8.09	113.75	118.60
76	9	1563	G	C8-N9-C4	8.08	109.63	106.40
67	5	294	G	C4-N9-C1'	8.07	137.00	126.50
76	9	1603	G	C4-N9-C1'	8.07	136.99	126.50
67	5	1812	C	C6-N1-C1'	-8.07	111.12	120.80
67	5	159	C	N3-C4-N4	8.06	123.64	118.00
67	5	1924	C	N1-C2-O2	8.06	123.73	118.90
67	5	2499	C	N3-C2-O2	-8.05	116.27	121.90
67	5	1675	C	C2-N1-C1'	8.05	127.65	118.80
67	5	1191	C	N3-C2-O2	-8.03	116.28	121.90
76	9	347	G	N3-C2-N2	-8.02	114.28	119.90
67	5	1515	A	C6-N1-C2	-8.01	113.79	118.60
67	5	1851	G	C8-N9-C1'	-8.01	116.58	127.00
76	9	1305	C	N3-C2-O2	-8.01	116.29	121.90
67	5	4723	A	N1-C2-N3	8.00	133.30	129.30
67	5	30	C	N3-C2-O2	-7.99	116.31	121.90
67	5	1662	C	C2-N1-C1'	7.99	127.58	118.80
67	5	1674	C	N3-C2-O2	-7.99	116.31	121.90
67	5	1986	U	P-O3'-C3'	7.97	129.27	119.70
67	5	3749	C	N3-C2-O2	-7.97	116.32	121.90
67	5	1662	C	N1-C2-O2	7.97	123.68	118.90
67	5	1653	A	N9-C4-C5	-7.97	102.61	105.80
67	5	352	G	O4'-C1'-N9	-7.96	101.83	108.20
67	5	2411	C	C2-N1-C1'	7.95	127.54	118.80
67	5	2509	C	C2-N1-C1'	7.94	127.53	118.80
67	5	3917	A	C6-N1-C2	-7.93	113.84	118.60
67	5	1577	G	O4'-C1'-N9	7.91	114.53	108.20
67	5	1651	G	C4-N9-C1'	7.90	136.78	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	3910	C	N3-C2-O2	-7.89	116.37	121.90
67	5	2671	C	N3-C2-O2	-7.89	116.38	121.90
67	5	956	A	N1-C6-N6	-7.88	113.87	118.60
67	5	1501	C	O4'-C1'-N1	7.88	114.50	108.20
67	5	4338	G	C2-N3-C4	-7.87	107.97	111.90
67	5	2274	C	C6-N1-C2	-7.85	117.16	120.30
67	5	2670	C	N1-C2-O2	7.84	123.61	118.90
67	5	1847	C	C2-N1-C1'	7.82	127.41	118.80
67	5	1651	G	C6-C5-N7	-7.81	125.71	130.40
76	9	909	G	N3-C4-C5	-7.81	124.70	128.60
67	5	2860	C	N3-C4-N4	7.80	123.46	118.00
67	5	1465	G	C8-N9-C1'	-7.78	116.89	127.00
67	5	3774	A	N9-C4-C5	-7.78	102.69	105.80
67	5	302	C	N1-C2-O2	7.77	123.56	118.90
67	5	4555	U	O4'-C1'-N1	7.77	114.42	108.20
67	5	1327	C	N1-C2-O2	7.76	123.56	118.90
67	5	38	A	C5-C6-N6	-7.75	117.50	123.70
67	5	1794	A	C8-N9-C4	-7.75	102.70	105.80
67	5	2299	G	C8-N9-C4	-7.75	103.30	106.40
67	5	3650	C	C5-C4-N4	-7.74	114.78	120.20
67	5	106	A	C8-N9-C1'	-7.74	113.77	127.70
4	DD	29	LEU	CB-CG-CD2	-7.73	97.86	111.00
67	5	4279	A	C5-C6-N6	-7.73	117.52	123.70
67	5	4214	A	C5-C6-N1	7.73	121.56	117.70
67	5	1323	A	C5-C6-N6	-7.71	117.53	123.70
67	5	2802	C	N3-C2-O2	-7.71	116.50	121.90
67	5	159	C	C6-N1-C1'	-7.71	111.55	120.80
67	5	2337	C	C6-N1-C2	-7.71	117.22	120.30
67	5	4362	A	C8-N9-C4	-7.71	102.72	105.80
76	9	1019	C	C2-N1-C1'	7.70	127.27	118.80
67	5	4654	C	N1-C2-O2	7.69	123.52	118.90
67	5	955	G	N1-C2-N2	-7.68	109.29	116.20
67	5	2068	C	N3-C4-N4	7.67	123.37	118.00
67	5	2781	G	C8-N9-C1'	-7.67	117.02	127.00
67	5	1868	A	N1-C6-N6	7.67	123.20	118.60
67	5	2579	G	N3-C4-C5	7.67	132.44	128.60
76	9	350	C	C5-C4-N4	-7.66	114.84	120.20
67	5	2853	C	C6-N1-C2	7.66	123.36	120.30
67	5	1646	A	C6-N1-C2	-7.65	114.01	118.60
67	5	727	C	C6-N1-C2	-7.64	117.24	120.30
67	5	1651	G	C8-N9-C1'	-7.64	117.06	127.00
67	5	1682	A	C6-N1-C2	-7.64	114.02	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	50	C	N3-C4-C5	7.64	124.95	121.90
67	5	1327	C	C2-N1-C1'	7.62	127.19	118.80
67	5	2465	C	C6-N1-C1'	-7.62	111.65	120.80
67	5	2291	G	C2-N3-C4	-7.62	108.09	111.90
67	5	4654	C	C2-N1-C1'	7.61	127.17	118.80
76	9	1055	A	N1-C6-N6	7.61	123.16	118.60
67	5	2025	A	C5-C6-N6	-7.60	117.62	123.70
67	5	3866	C	C2-N1-C1'	7.60	127.16	118.80
67	5	1870	C	N3-C4-C5	7.58	124.93	121.90
67	5	106	A	C4-N9-C1'	7.58	139.95	126.30
76	9	1219	C	C5-C6-N1	7.58	124.79	121.00
67	5	1191	C	O4'-C1'-N1	7.57	114.26	108.20
67	5	1576	G	C8-N9-C1'	-7.57	117.16	127.00
67	5	2093	G	O4'-C1'-N9	7.57	114.25	108.20
67	5	3871	A	C6-N1-C2	-7.57	114.06	118.60
67	5	2785	C	N3-C2-O2	-7.56	116.61	121.90
67	5	299	C	N3-C2-O2	-7.56	116.61	121.90
67	5	2815	A	N9-C4-C5	-7.56	102.78	105.80
76	9	319	C	C2-N1-C1'	-7.55	110.49	118.80
67	5	3911	C	N3-C2-O2	-7.55	116.61	121.90
67	5	1357	C	N1-C2-O2	7.55	123.43	118.90
73	8	15	G	C2-N3-C4	-7.55	108.12	111.90
67	5	83	C	N3-C4-C5	7.55	124.92	121.90
67	5	292	G	C8-N9-C1'	-7.55	117.19	127.00
67	5	38	A	C4-C5-N7	7.54	114.47	110.70
67	5	38	A	C8-N9-C1'	-7.54	114.13	127.70
67	5	2277	C	N1-C2-O2	7.53	123.42	118.90
67	5	3749	C	N1-C2-O2	7.53	123.42	118.90
70	7	11	A	C8-N9-C4	7.53	108.81	105.80
67	5	1323	A	N1-C6-N6	7.52	123.11	118.60
67	5	4583	C	O4'-C1'-N1	7.52	114.21	108.20
67	5	1931	C	C2-N1-C1'	7.51	127.07	118.80
67	5	106	A	C6-C5-N7	-7.51	127.04	132.30
67	5	39	A	C4-N9-C1'	7.51	139.81	126.30
67	5	51	A	C6-C5-N7	-7.51	127.05	132.30
76	9	1825	A	O4'-C1'-N9	7.50	114.20	108.20
67	5	64	A	N9-C4-C5	-7.50	102.80	105.80
67	5	2781	G	C4-N9-C1'	7.50	136.24	126.50
67	5	106	A	O4'-C1'-N9	-7.49	102.21	108.20
67	5	332	C	N3-C4-C5	7.49	124.89	121.90
73	8	44	A	C5-C6-N6	-7.49	117.71	123.70
67	5	292	G	C4-N9-C1'	7.48	136.22	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1357	C	C2-N1-C1'	7.48	127.02	118.80
67	5	2335	C	N1-C2-O2	7.47	123.38	118.90
67	5	4688	C	C5-C4-N4	-7.47	114.97	120.20
67	5	1674	C	C5-C4-N4	-7.47	114.97	120.20
76	9	1250	A	O4'-C1'-N9	-7.46	102.23	108.20
76	9	1715	A	N1-C6-N6	7.46	123.08	118.60
67	5	293	G	C8-N9-C1'	-7.46	117.31	127.00
67	5	1599	G	N1-C2-N2	-7.46	109.49	116.20
67	5	1589	C	N1-C2-O2	7.45	123.37	118.90
67	5	2078	C	C6-N1-C1'	-7.45	111.87	120.80
67	5	2319	C	C5-C4-N4	-7.43	115.00	120.20
67	5	1235	G	N3-C4-N9	-7.43	121.54	126.00
67	5	1879	C	C5-C4-N4	-7.43	115.00	120.20
67	5	384	A	O4'-C1'-N9	7.41	114.13	108.20
67	5	1327	C	C5-C4-N4	-7.41	115.02	120.20
67	5	39	A	N1-C6-N6	7.40	123.04	118.60
67	5	408	A	C8-N9-C4	-7.40	102.84	105.80
67	5	2815	A	C6-C5-N7	-7.39	127.13	132.30
67	5	1670	G	N3-C2-N2	7.39	125.07	119.90
76	9	998	A	O4'-C1'-N9	7.38	114.11	108.20
67	5	264	C	C5-C4-N4	-7.38	115.03	120.20
67	5	38	A	C4-N9-C1'	7.36	139.55	126.30
73	8	15	G	C8-N9-C1'	-7.36	117.43	127.00
67	5	3774	A	C8-N9-C1'	-7.36	114.46	127.70
67	5	3887	C	C6-N1-C2	7.36	123.24	120.30
67	5	2039	G	C8-N9-C1'	-7.35	117.44	127.00
73	8	44	A	N1-C6-N6	7.35	123.01	118.60
76	9	1849	G	C4-N9-C1'	7.35	136.06	126.50
67	5	112	C	C2-N1-C1'	7.34	126.88	118.80
67	5	3771	C	C2-N1-C1'	7.34	126.88	118.80
70	7	36	C	N1-C2-O2	7.34	123.30	118.90
76	9	1245	G	N3-C4-N9	7.33	130.40	126.00
67	5	38	A	O4'-C1'-N9	-7.33	102.34	108.20
67	5	2025	A	C8-N9-C4	7.33	108.73	105.80
67	5	4603	C	C2-N1-C1'	7.32	126.85	118.80
67	5	332	C	C5-C4-N4	-7.32	115.08	120.20
76	9	350	C	N3-C4-C5	7.31	124.83	121.90
22	HH	72	PHE	CB-CG-CD2	-7.31	115.68	120.80
67	5	671	G	N3-C4-N9	-7.30	121.62	126.00
76	9	1216	C	N3-C4-N4	-7.29	112.89	118.00
67	5	303	C	N3-C2-O2	-7.29	116.80	121.90
67	5	3916	G	N3-C4-C5	-7.29	124.96	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	386	A	N1-C6-N6	7.29	122.97	118.60
76	9	603	C	N3-C4-C5	7.29	124.81	121.90
67	5	1456	C	N3-C4-C5	7.27	124.81	121.90
67	5	4215	C	N3-C4-C5	7.27	124.81	121.90
33	J	63	ARG	NE-CZ-NH2	-7.27	116.66	120.30
67	5	2003	G	O5'-P-OP2	-7.27	99.16	105.70
67	5	4717	A	C5-C6-N6	-7.27	117.88	123.70
76	9	876	C	N3-C2-O2	-7.27	116.81	121.90
67	5	1864	G	N3-C4-C5	-7.27	124.97	128.60
67	5	1665	C	N1-C2-O2	7.26	123.26	118.90
67	5	4331	G	N1-C2-N2	-7.26	109.66	116.20
67	5	1580	C	N3-C2-O2	-7.26	116.82	121.90
67	5	356	G	N1-C2-N2	-7.26	109.67	116.20
67	5	1580	C	C6-N1-C1'	-7.26	112.09	120.80
67	5	2785	C	C6-N1-C1'	-7.26	112.09	120.80
67	5	81	C	N1-C2-O2	7.26	123.25	118.90
32	jj	353	LEU	CB-CG-CD2	7.26	123.34	111.00
67	5	2024	G	N3-C4-N9	-7.26	121.65	126.00
67	5	386	A	C6-C5-N7	-7.25	127.22	132.30
67	5	4525	C	N1-C2-O2	7.25	123.25	118.90
76	9	363	A	O4'-C1'-N9	7.25	114.00	108.20
67	5	1235	G	C2-N3-C4	-7.25	108.28	111.90
67	5	1081	C	C5-C6-N1	7.25	124.62	121.00
67	5	4868	G	N3-C4-C5	-7.25	124.98	128.60
67	5	3748	A	C6-N1-C2	-7.24	114.25	118.60
67	5	747	A	N1-C6-N6	7.24	122.94	118.60
67	5	2411	C	C6-N1-C1'	-7.24	112.11	120.80
73	8	26	C	C5-C4-N4	-7.24	115.13	120.20
67	5	1868	A	C8-N9-C4	-7.24	102.90	105.80
67	5	2731	C	N1-C2-O2	7.24	123.24	118.90
76	9	1811	C	N1-C2-O2	7.23	123.24	118.90
67	5	1327	C	C6-N1-C1'	-7.22	112.14	120.80
67	5	1646	A	N1-C2-N3	7.21	132.91	129.30
67	5	80	C	N1-C2-O2	7.21	123.22	118.90
67	5	1892	A	C5-C6-N1	7.20	121.30	117.70
28	ii	189	ARG	CG-CD-NE	7.20	126.92	111.80
67	5	1534	A	O4'-C1'-N9	7.20	113.96	108.20
67	5	3919	C	C6-N1-C2	-7.20	117.42	120.30
67	5	2499	C	N1-C2-O2	7.20	123.22	118.90
76	9	1216	C	O4'-C1'-N1	7.19	113.95	108.20
67	5	218	A	O4'-C1'-N9	-7.19	102.45	108.20
67	5	1427	A	N1-C6-N6	7.19	122.91	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1535	C	N3-C4-N4	7.18	123.03	118.00
67	5	1653	A	C6-C5-N7	-7.18	127.27	132.30
67	5	4179	G	C4-N9-C1'	7.18	135.83	126.50
76	9	813	A	O5'-P-OP1	-7.18	99.24	105.70
76	9	347	G	N3-C4-N9	-7.17	121.69	126.00
67	5	4911	A	O4'-C1'-N9	-7.17	102.47	108.20
76	9	1438	A	C5-C6-N6	-7.17	117.97	123.70
73	8	79	G	C4-N9-C1'	7.16	135.81	126.50
67	5	2458	C	N1-C2-O2	7.16	123.19	118.90
67	5	4971	A	O4'-C1'-N9	7.16	113.93	108.20
73	8	103	A	C5-C6-N6	-7.16	117.97	123.70
67	5	351	C	C2-N1-C1'	7.15	126.67	118.80
67	5	1343	A	C6-N1-C2	-7.15	114.31	118.60
67	5	5004	C	C2-N1-C1'	7.14	126.66	118.80
67	5	2815	A	C5-N7-C8	-7.14	100.33	103.90
67	5	1191	C	C6-N1-C1'	7.13	129.36	120.80
67	5	4513	A	C5-C6-N6	-7.13	118.00	123.70
67	5	2397	G	N1-C2-N2	-7.12	109.79	116.20
67	5	3845	A	C6-N1-C2	-7.12	114.33	118.60
67	5	2078	C	C6-N1-C2	-7.12	117.45	120.30
76	9	826	A	N1-C6-N6	-7.11	114.33	118.60
67	5	159	C	C5-C4-N4	-7.11	115.22	120.20
67	5	2850	A	C6-N1-C2	-7.11	114.34	118.60
67	5	4166	G	N3-C2-N2	7.11	124.87	119.90
67	5	1306	C	C2-N1-C1'	7.10	126.61	118.80
67	5	4456	C	N3-C2-O2	-7.10	116.93	121.90
67	5	2802	C	N1-C2-O2	7.09	123.16	118.90
67	5	4087	G	N3-C4-N9	-7.09	121.74	126.00
76	9	4	C	N3-C4-C5	7.09	124.74	121.90
17	BB	113	MET	CG-SD-CE	-7.09	88.86	100.20
67	5	4645	C	N1-C2-O2	7.08	123.15	118.90
76	9	329	G	C4-N9-C1'	7.08	135.70	126.50
32	jj	384	LYS	CB-CG-CD	7.07	129.99	111.60
67	5	1938	C	N3-C4-C5	7.07	124.73	121.90
67	5	11	G	C4-N9-C1'	7.06	135.68	126.50
67	5	2381	A	N1-C6-N6	-7.06	114.36	118.60
22	HH	72	PHE	CB-CG-CD1	7.06	125.74	120.80
67	5	351	C	C6-N1-C2	-7.05	117.48	120.30
67	5	356	G	N1-C2-N3	7.05	128.13	123.90
67	5	1859	C	C5-C4-N4	-7.05	115.26	120.20
73	8	19	C	N1-C2-O2	7.05	123.13	118.90
67	5	1357	C	C6-N1-C1'	-7.05	112.34	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1674	C	C2-N1-C1'	7.04	126.55	118.80
67	5	4945	G	C8-N9-C1'	-7.04	117.84	127.00
67	5	1794	A	N7-C8-N9	7.04	117.32	113.80
67	5	4345	C	N3-C2-O2	-7.04	116.97	121.90
67	5	301	G	C2-N3-C4	-7.04	108.38	111.90
67	5	2320	G	C2-N3-C4	-7.04	108.38	111.90
73	8	96	C	C5-C4-N4	-7.04	115.27	120.20
67	5	1594	C	C5-C4-N4	-7.03	115.28	120.20
67	5	4435	U	O5'-P-OP1	-7.03	99.38	105.70
67	5	1456	C	C5-C4-N4	-7.02	115.28	120.20
13	FF	19	LEU	N-CA-C	-7.02	92.04	111.00
67	5	2302	C	N1-C2-O2	7.02	123.11	118.90
67	5	4394	A	N1-C6-N6	7.02	122.81	118.60
67	5	81	C	C2-N1-C1'	7.02	126.52	118.80
28	ii	232	PHE	CB-CG-CD1	7.02	125.71	120.80
67	5	4981	G	C8-N9-C1'	-7.01	117.89	127.00
67	5	2659	A	N1-C6-N6	7.01	122.81	118.60
67	5	1662	C	C6-N1-C1'	-7.01	112.39	120.80
67	5	1847	C	C6-N1-C2	-7.00	117.50	120.30
70	7	95	C	C2-N1-C1'	7.00	126.50	118.80
67	5	55	G	C4-N9-C1'	7.00	135.60	126.50
67	5	3911	C	N3-C4-N4	7.00	122.90	118.00
76	9	1219	C	C6-N1-C1'	-7.00	112.40	120.80
67	5	4193	C	C6-N1-C1'	-6.99	112.42	120.80
67	5	1238	A	N1-C6-N6	-6.99	114.41	118.60
67	5	1879	C	N1-C2-O2	6.99	123.09	118.90
67	5	1981	G	N3-C4-N9	-6.98	121.81	126.00
67	5	4485	C	C2-N1-C1'	6.98	126.48	118.80
67	5	1626	G	C2-N3-C4	-6.98	108.41	111.90
67	5	1237	C	C5-C4-N4	-6.97	115.32	120.20
67	5	2393	C	C6-N1-C1'	-6.97	112.43	120.80
67	5	4669	A	C6-N1-C2	-6.97	114.42	118.60
67	5	2509	C	C5-C4-N4	-6.97	115.32	120.20
67	5	1271	G	C8-N9-C4	-6.96	103.61	106.40
67	5	4180	G	C4-N9-C1'	6.96	135.55	126.50
76	9	1648	G	O4'-C1'-N9	6.96	113.77	108.20
67	5	238	C	C6-N1-C2	-6.96	117.52	120.30
67	5	2393	C	N1-C2-O2	6.96	123.07	118.90
67	5	51	A	C5-C6-N6	-6.95	118.14	123.70
76	9	319	C	O4'-C1'-N1	6.95	113.76	108.20
76	9	1191	C	N3-C4-C5	6.95	124.68	121.90
67	5	1064	G	C4-N9-C1'	6.95	135.53	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	66	A	O4'-C1'-N9	6.95	113.76	108.20
67	5	2836	A	C2-N3-C4	-6.95	107.13	110.60
76	9	689	U	O4'-C1'-N1	-6.95	102.64	108.20
67	5	1985	G	C4-N9-C1'	6.94	135.53	126.50
76	9	876	C	C2-N1-C1'	6.94	126.43	118.80
67	5	363	A	N1-C6-N6	-6.94	114.44	118.60
67	5	1529	G	C4-N9-C1'	6.93	135.51	126.50
67	5	2860	C	C5-C4-N4	-6.93	115.34	120.20
67	5	1931	C	C6-N1-C1'	-6.93	112.49	120.80
67	5	5069	U	O4'-C1'-N1	6.93	113.74	108.20
67	5	1077	C	N3-C2-O2	-6.92	117.05	121.90
67	5	1890	G	C4-C5-N7	6.92	113.57	110.80
67	5	2847	G	O4'-C1'-N9	6.92	113.74	108.20
73	8	41	A	O4'-C1'-N9	6.92	113.74	108.20
67	5	302	C	N3-C2-O2	-6.92	117.05	121.90
67	5	4215	C	C6-N1-C2	6.92	123.07	120.30
73	8	103	A	C4-C5-C6	6.92	120.46	117.00
67	5	2693	G	C8-N9-C1'	-6.92	118.01	127.00
67	5	4179	G	C8-N9-C1'	-6.92	118.01	127.00
67	5	3650	C	C6-N1-C1'	-6.91	112.50	120.80
67	5	3774	A	O4'-C1'-N9	-6.91	102.67	108.20
67	5	4868	G	C4-N9-C1'	6.91	135.49	126.50
67	5	2367	A	N1-C6-N6	-6.91	114.45	118.60
67	5	2621	A	C5-C6-N1	6.90	121.15	117.70
67	5	3633	C	C2-N1-C1'	6.90	126.39	118.80
67	5	3909	C	C2-N3-C4	-6.90	116.45	119.90
76	9	1450	G	N3-C4-C5	6.90	132.05	128.60
67	5	4382	G	C8-N9-C4	-6.90	103.64	106.40
67	5	41	C	N3-C2-O2	-6.89	117.08	121.90
73	8	26	C	C2-N1-C1'	6.89	126.38	118.80
76	9	1460	C	C6-N1-C2	-6.89	117.55	120.30
70	7	97	G	N3-C4-C5	6.89	132.04	128.60
67	5	1327	C	N3-C2-O2	-6.88	117.08	121.90
67	5	1847	C	C6-N1-C1'	-6.88	112.55	120.80
67	5	4705	A	C5-C6-N1	6.87	121.14	117.70
67	5	2878	G	C6-C5-N7	-6.87	126.28	130.40
67	5	4375	C	N3-C2-O2	-6.87	117.09	121.90
73	8	26	C	N1-C2-O2	6.87	123.02	118.90
67	5	163	A	C5-C6-N6	-6.86	118.21	123.70
67	5	1191	C	N1-C2-N3	6.86	124.00	119.20
67	5	1237	C	O4'-C1'-N1	6.86	113.69	108.20
67	5	70	A	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(°)
67	5	4919	G	N9-C4-C5	-6.85	102.66	105.40
67	5	1329	G	C4-N9-C1'	6.85	135.41	126.50
67	5	173	C	O4'-C1'-N1	6.85	113.68	108.20
67	5	2799	G	N3-C4-C5	-6.84	125.18	128.60
67	5	2750	G	N1-C2-N2	-6.84	110.05	116.20
67	5	84	A	N1-C6-N6	6.84	122.70	118.60
67	5	4179	G	C8-N9-C4	-6.84	103.67	106.40
67	5	4985	U	C6-N1-C2	-6.84	116.90	121.00
67	5	2393	C	C2-N1-C1'	6.83	126.31	118.80
67	5	4528	G	N7-C8-N9	6.82	116.51	113.10
67	5	4696	C	C5-C4-N4	-6.82	115.42	120.20
67	5	2784	C	C5-C4-N4	-6.82	115.42	120.20
67	5	2836	A	N1-C6-N6	6.82	122.69	118.60
67	5	3737	A	C5-C6-N6	-6.82	118.25	123.70
76	9	1513	C	C6-N1-C2	-6.82	117.57	120.30
67	5	2603	C	C5-C4-N4	-6.82	115.43	120.20
67	5	1665	C	N3-C2-O2	-6.82	117.13	121.90
73	8	79	G	C8-N9-C1'	-6.82	118.14	127.00
76	9	1055	A	C5-C6-N6	-6.82	118.25	123.70
67	5	2856	C	N3-C4-C5	6.81	124.62	121.90
67	5	1541	C	C6-N1-C1'	-6.81	112.63	120.80
76	9	501	C	N3-C2-O2	-6.81	117.14	121.90
67	5	3685	C	C2-N1-C1'	6.80	126.28	118.80
67	5	2603	C	C2-N1-C1'	6.80	126.28	118.80
67	5	4862	G	N3-C4-C5	6.80	132.00	128.60
76	9	1715	A	C5-C6-N6	-6.80	118.26	123.70
67	5	3866	C	N1-C2-O2	6.79	122.98	118.90
67	5	4902	C	N1-C2-O2	6.79	122.97	118.90
76	9	1416	C	C6-N1-C1'	-6.79	112.66	120.80
76	9	1532	C	N1-C2-O2	6.78	122.97	118.90
67	5	1308	C	C2-N1-C1'	6.78	126.26	118.80
67	5	1985	G	P-O3'-C3'	6.78	127.84	119.70
76	9	475	C	C6-N1-C2	6.78	123.01	120.30
67	5	2848	G	C2-N3-C4	-6.78	108.51	111.90
67	5	4738	C	C5-C4-N4	-6.78	115.45	120.20
76	9	1216	C	C5-C4-N4	6.78	124.94	120.20
67	5	1623	A	C5-C6-N6	-6.78	118.28	123.70
67	5	1641	G	N3-C4-C5	6.78	131.99	128.60
73	8	103	A	C8-N9-C4	-6.77	103.09	105.80
67	5	4671	C	C6-N1-C1'	-6.77	112.67	120.80
67	5	1580	C	N3-C4-N4	6.77	122.74	118.00
76	9	1318	G	C8-N9-C1'	-6.77	118.20	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	2785	C	C2-N1-C1'	6.77	126.24	118.80
76	9	480	G	C4-N9-C1'	6.76	135.29	126.50
67	5	4945	G	C4-N9-C1'	6.76	135.28	126.50
67	5	2039	G	C4-N9-C1'	6.75	135.28	126.50
67	5	1237	C	C6-N1-C1'	-6.75	112.70	120.80
76	9	1219	C	C6-N1-C2	-6.75	117.60	120.30
67	5	1624	G	O4'-C1'-N9	6.75	113.60	108.20
67	5	3911	C	C6-N1-C1'	-6.75	112.70	120.80
67	5	355	A	C6-C5-N7	-6.74	127.58	132.30
67	5	1599	G	N3-C2-N2	6.74	124.62	119.90
67	5	351	C	N3-C2-O2	-6.74	117.19	121.90
67	5	1926	C	C2-N1-C1'	6.74	126.21	118.80
67	5	4392	G	N1-C6-O6	-6.74	115.86	119.90
76	9	1318	G	C4-N9-C1'	6.73	135.25	126.50
67	5	5004	C	C6-N1-C1'	-6.73	112.73	120.80
67	5	1529	G	C8-N9-C1'	-6.72	118.26	127.00
67	5	3879	G	N3-C4-C5	6.71	131.96	128.60
73	8	105	C	C5-C4-N4	-6.71	115.50	120.20
67	5	1653	A	C8-N9-C1'	-6.71	115.62	127.70
67	5	3653	A	C4-C5-C6	6.71	120.36	117.00
67	5	4579	U	C5-C4-O4	-6.71	121.87	125.90
76	9	1490	G	C2-N3-C4	6.71	115.25	111.90
67	5	2851	G	C8-N9-C1'	-6.71	118.28	127.00
76	9	1219	C	C5-C4-N4	-6.71	115.51	120.20
67	5	1628	C	N3-C4-N4	6.70	122.69	118.00
67	5	4458	C	C5-C4-N4	-6.70	115.51	120.20
67	5	336	A	C5-C6-N1	6.70	121.05	117.70
67	5	355	A	C4-C5-N7	6.70	114.05	110.70
67	5	2789	A	N1-C6-N6	6.70	122.62	118.60
76	9	1663	A	P-O3'-C3'	6.69	127.73	119.70
67	5	1674	C	N3-C4-C5	6.69	124.58	121.90
67	5	302	C	C2-N1-C1'	6.69	126.16	118.80
67	5	1641	G	C2-N3-C4	-6.69	108.55	111.90
67	5	4773	C	O4'-C1'-N1	-6.69	102.85	108.20
67	5	1076	C	C6-N1-C2	-6.68	117.63	120.30
67	5	3623	C	C6-N1-C1'	-6.68	112.78	120.80
76	9	1603	G	N3-C4-N9	6.68	130.01	126.00
67	5	1315	C	N3-C4-C5	6.68	124.57	121.90
67	5	2057	A	N1-C6-N6	-6.68	114.59	118.60
67	5	4886	C	C6-N1-C2	-6.67	117.63	120.30
67	5	3646	A	C5-C6-N6	-6.67	118.37	123.70
67	5	1898	C	N3-C4-C5	6.67	124.57	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	3760	A	N1-C6-N6	-6.66	114.60	118.60
76	9	1824	A	C5'-C4'-O4'	6.66	117.09	109.10
67	5	1794	A	C5-N7-C8	-6.66	100.57	103.90
67	5	1733	G	N1-C2-N2	-6.66	110.21	116.20
67	5	741	C	C6-N1-C2	-6.65	117.64	120.30
67	5	4278	C	C5-C4-N4	-6.65	115.54	120.20
17	BB	86	LEU	CA-CB-CG	6.65	130.59	115.30
76	9	465	A	N1-C6-N6	6.65	122.59	118.60
76	9	1760	G	N3-C4-N9	-6.65	122.01	126.00
67	5	323	C	N1-C2-O2	6.64	122.88	118.90
67	5	2846	G	N3-C4-C5	-6.64	125.28	128.60
67	5	352	G	C8-N9-C1'	-6.64	118.37	127.00
67	5	2465	C	N3-C2-O2	-6.64	117.25	121.90
67	5	4701	A	O4'-C1'-N9	6.64	113.51	108.20
76	9	810	A	N9-C1'-C2'	-6.64	104.70	112.00
76	9	1389	C	C6-N1-C2	-6.63	117.65	120.30
67	5	1885	G	C8-N9-C1'	-6.63	118.38	127.00
67	5	2758	G	C8-N9-C1'	-6.63	118.38	127.00
67	5	4705	A	C6-N1-C2	-6.63	114.62	118.60
2	C	238	LEU	CA-CB-CG	6.62	130.54	115.30
67	5	2261	G	N3-C4-C5	6.62	131.91	128.60
67	5	4516	G	N3-C4-N9	-6.62	122.03	126.00
67	5	2458	C	C2-N1-C1'	6.62	126.08	118.80
67	5	72	C	N3-C4-C5	6.62	124.55	121.90
67	5	1883	G	C2-N3-C4	-6.62	108.59	111.90
67	5	4434	C	C2-N1-C1'	6.62	126.08	118.80
76	9	1539	U	O4'-C1'-N1	6.62	113.49	108.20
67	5	2299	G	N3-C4-C5	-6.62	125.29	128.60
67	5	3867	A	N1-C6-N6	6.61	122.57	118.60
76	9	123	G	C4-N9-C1'	6.61	135.10	126.50
67	5	361	C	O4'-C1'-N1	6.61	113.49	108.20
67	5	3749	C	C6-N1-C1'	-6.61	112.87	120.80
67	5	2838	G	C8-N9-C4	-6.61	103.76	106.40
84	cc	58	LEU	CA-CB-CG	6.60	130.48	115.30
67	5	2851	G	C4-N9-C1'	6.60	135.08	126.50
76	9	1501	C	N1-C2-O2	6.60	122.86	118.90
67	5	1584	G	C2-N3-C4	-6.60	108.60	111.90
67	5	2277	C	C2-N1-C1'	6.59	126.05	118.80
67	5	2078	C	C5-C4-N4	-6.59	115.59	120.20
67	5	2850	A	C5-C6-N1	6.59	120.99	117.70
67	5	2694	G	O4'-C1'-N9	-6.59	102.93	108.20
67	5	84	A	C5-C6-N6	-6.58	118.43	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1610	C	C5-C4-N4	-6.58	115.59	120.20
73	8	26	C	N3-C4-C5	6.58	124.53	121.90
67	5	1331	C	C5-C4-N4	-6.58	115.60	120.20
67	5	1864	G	N3-C4-N9	6.57	129.94	126.00
76	9	501	C	N1-C2-O2	6.57	122.84	118.90
67	5	4392	G	C8-N9-C4	-6.57	103.77	106.40
67	5	1543	G	N1-C2-N2	-6.57	110.29	116.20
67	5	4189	U	C5-C4-O4	-6.57	121.96	125.90
67	5	4529	G	C4-N9-C1'	6.57	135.04	126.50
67	5	3910	C	C6-N1-C1'	-6.57	112.92	120.80
67	5	4667	C	N3-C2-O2	-6.57	117.31	121.90
67	5	81	C	C5-C4-N4	-6.56	115.61	120.20
67	5	1682	A	N1-C2-N3	6.56	132.58	129.30
67	5	3633	C	N1-C2-O2	6.56	122.83	118.90
67	5	54	G	C8-N9-C1'	-6.55	118.48	127.00
67	5	4180	G	C8-N9-C1'	-6.55	118.48	127.00
67	5	4256	A	N1-C6-N6	6.55	122.53	118.60
67	5	4510	A	N1-C6-N6	6.55	122.53	118.60
67	5	2075	G	C8-N9-C1'	-6.55	118.48	127.00
67	5	2629	C	N1-C2-O2	6.54	122.83	118.90
76	9	1637	A	O4'-C1'-N9	-6.54	102.97	108.20
67	5	1520	C	C2-N1-C1'	6.54	125.99	118.80
67	5	1573	G	O4'-C1'-N9	6.54	113.43	108.20
67	5	2834	C	O4'-C1'-N1	-6.54	102.97	108.20
67	5	2671	C	C6-N1-C2	-6.53	117.69	120.30
67	5	418	A	C6-N1-C2	-6.53	114.68	118.60
67	5	352	G	C4-N9-C1'	6.53	134.99	126.50
67	5	1237	C	C2-N1-C1'	6.53	125.98	118.80
67	5	89	C	C6-N1-C2	-6.53	117.69	120.30
67	5	2290	C	O4'-C1'-N1	6.53	113.42	108.20
67	5	4715	C	N1-C2-O2	6.53	122.82	118.90
76	9	1191	C	C5-C4-N4	-6.53	115.63	120.20
67	5	1926	C	N1-C2-O2	6.53	122.81	118.90
67	5	2074	C	C5-C4-N4	-6.53	115.63	120.20
67	5	2802	C	C6-N1-C2	-6.53	117.69	120.30
76	9	1526	G	N3-C2-N2	-6.52	115.34	119.90
67	5	2835	A	C8-N9-C4	-6.52	103.19	105.80
76	9	1181	A	N1-C6-N6	6.52	122.51	118.60
67	5	1670	G	N1-C2-N2	-6.51	110.34	116.20
76	9	168	C	C2-N1-C1'	6.51	125.97	118.80
35	KK	70	TYR	CA-CB-CG	6.51	125.77	113.40
67	5	2834	C	C6-N1-C1'	-6.51	112.99	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1465	G	C6-C5-N7	-6.51	126.50	130.40
67	5	1306	C	C5-C4-N4	-6.51	115.64	120.20
67	5	3882	C	O4'-C1'-N1	6.50	113.40	108.20
67	5	3872	A	C6-N1-C2	-6.50	114.70	118.60
67	5	4654	C	C6-N1-C1'	-6.50	113.00	120.80
67	5	4981	G	N3-C2-N2	6.50	124.45	119.90
67	5	958	G	C2-N3-C4	-6.50	108.65	111.90
67	5	2320	G	N1-C2-N2	-6.50	110.35	116.20
67	5	4345	C	N1-C2-O2	6.50	122.80	118.90
67	5	1623	A	C6-C5-N7	-6.50	127.75	132.30
67	5	4533	A	C6-C5-N7	-6.50	127.75	132.30
67	5	66	A	N1-C6-N6	-6.50	114.70	118.60
67	5	1305	C	C2-N1-C1'	6.49	125.94	118.80
67	5	2012	A	O4'-C1'-N9	6.49	113.39	108.20
76	9	974	C	C6-N1-C2	-6.49	117.70	120.30
67	5	3782	C	C5-C4-N4	-6.49	115.66	120.20
67	5	4981	G	C4-N9-C1'	6.49	134.94	126.50
67	5	1655	C	C2-N1-C1'	6.48	125.93	118.80
76	9	1532	C	C6-N1-C1'	-6.48	113.02	120.80
67	5	360	A	C5-N7-C8	-6.48	100.66	103.90
76	9	1834	A	N1-C6-N6	6.48	122.49	118.60
67	5	98	A	N1-C6-N6	-6.48	114.71	118.60
67	5	1373	A	N1-C6-N6	6.47	122.48	118.60
67	5	1623	A	C5-N7-C8	-6.47	100.66	103.90
67	5	11	G	C8-N9-C1'	-6.47	118.59	127.00
67	5	1306	C	N1-C2-O2	6.47	122.78	118.90
67	5	1643	A	C6-N1-C2	-6.47	114.72	118.60
67	5	314	G	C8-N9-C4	-6.47	103.81	106.40
67	5	1853	G	C2-N3-C4	-6.46	108.67	111.90
67	5	4680	G	N1-C2-N2	-6.46	110.38	116.20
67	5	2850	A	C8-N9-C4	-6.46	103.22	105.80
67	5	2743	A	C5-C6-N1	6.46	120.93	117.70
61	TT	66	LEU	CA-CB-CG	6.46	130.15	115.30
67	5	4717	A	C5-C6-N1	6.46	120.93	117.70
67	5	2335	C	C2-N1-C1'	6.45	125.90	118.80
76	9	1230	C	C6-N1-C2	-6.45	117.72	120.30
76	9	1452	A	O5'-P-OP1	-6.45	99.89	105.70
67	5	30	C	C2-N1-C1'	6.45	125.89	118.80
67	5	2533	C	C2-N1-C1'	6.45	125.89	118.80
63	UU	73	GLY	N-CA-C	-6.45	96.99	113.10
67	5	1342	A	C8-N9-C4	-6.44	103.22	105.80
67	5	1427	A	N9-C4-C5	-6.44	103.22	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	3903	A	C5-C6-N6	-6.44	118.55	123.70
67	5	4746	C	N3-C4-N4	6.44	122.51	118.00
67	5	3898	G	C2-N3-C4	-6.44	108.68	111.90
70	7	57	C	C2-N1-C1'	6.44	125.88	118.80
67	5	1836	G	N1-C2-N2	-6.43	110.41	116.20
57	S	84	TYR	CB-CG-CD2	6.43	124.86	121.00
67	5	3923	A	C6-N1-C2	-6.43	114.74	118.60
67	5	4529	G	C8-N9-C1'	-6.43	118.64	127.00
67	5	4980	C	N3-C4-N4	6.43	122.50	118.00
76	9	563	G	C4-N9-C1'	6.43	134.86	126.50
76	9	1658	G	N9-C4-C5	-6.43	102.83	105.40
67	5	2320	G	C8-N9-C1'	-6.42	118.65	127.00
84	cc	11	LEU	CB-CG-CD2	-6.42	100.08	111.00
76	9	84	A	C4-N9-C1'	6.42	137.86	126.30
67	5	2577	C	N1-C2-O2	6.42	122.75	118.90
67	5	4924	C	N1-C2-O2	6.42	122.75	118.90
73	8	72	A	N1-C6-N6	6.42	122.45	118.60
73	8	79	G	O4'-C1'-N9	-6.42	103.06	108.20
67	5	360	A	C5-C6-N1	6.42	120.91	117.70
67	5	2856	C	C5-C4-N4	-6.42	115.71	120.20
76	9	1226	G	C8-N9-C4	-6.42	103.83	106.40
67	5	40	G	N3-C4-C5	6.41	131.81	128.60
67	5	4169	G	C2-N3-C4	-6.41	108.69	111.90
84	cc	25	GLY	N-CA-C	-6.41	97.08	113.10
67	5	387	G	N3-C4-N9	6.41	129.84	126.00
67	5	1298	C	N1-C2-O2	6.41	122.74	118.90
67	5	1682	A	C5-C6-N6	-6.40	118.58	123.70
67	5	2540	C	C2-N1-C1'	6.40	125.84	118.80
67	5	3771	C	C6-N1-C2	-6.40	117.74	120.30
67	5	2841	G	C8-N9-C4	-6.40	103.84	106.40
67	5	3683	C	N3-C4-C5	6.40	124.46	121.90
67	5	4456	C	N1-C2-O2	6.40	122.74	118.90
67	5	666	G	N3-C2-N2	-6.40	115.42	119.90
67	5	2785	C	N3-C4-C5	6.40	124.46	121.90
76	9	1849	G	C8-N9-C1'	-6.40	118.68	127.00
67	5	39	A	C5-C6-N6	-6.39	118.58	123.70
67	5	112	C	C6-N1-C1'	-6.39	113.13	120.80
67	5	63	G	C8-N9-C1'	-6.39	118.69	127.00
67	5	1924	C	C2-N1-C1'	6.39	125.83	118.80
76	9	1219	C	N3-C4-N4	6.39	122.47	118.00
67	5	2057	A	C5-C6-N1	6.39	120.89	117.70
67	5	4305	G	C6-C5-N7	-6.38	126.57	130.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4667	C	N1-C2-O2	6.38	122.73	118.90
76	9	995	G	N3-C2-N2	6.38	124.36	119.90
67	5	1662	C	N3-C2-O2	-6.38	117.44	121.90
67	5	2349	A	C5-C6-N1	6.38	120.89	117.70
67	5	4533	A	C4-C5-N7	6.38	113.89	110.70
67	5	3911	C	C5-C6-N1	6.38	124.19	121.00
67	5	1739	G	C4-N9-C1'	6.37	134.78	126.50
67	5	4389	C	C2-N1-C1'	6.37	125.81	118.80
67	5	65	A	O4'-C1'-N9	6.37	113.30	108.20
67	5	1520	C	C6-N1-C1'	-6.37	113.16	120.80
67	5	4688	C	C2-N1-C1'	6.37	125.80	118.80
67	5	3917	A	C5-C6-N1	6.36	120.88	117.70
67	5	4195	G	N1-C2-N2	-6.36	110.47	116.20
67	5	4527	G	C8-N9-C1'	-6.36	118.73	127.00
67	5	1733	G	N3-C2-N2	6.36	124.35	119.90
67	5	1864	G	C4-N9-C1'	6.36	134.76	126.50
67	5	2863	G	C2-N3-C4	-6.36	108.72	111.90
67	5	4549	G	N1-C2-N2	-6.35	110.48	116.20
73	8	41	A	N9-C4-C5	6.35	108.34	105.80
76	9	1638	G	C4-N9-C1'	-6.35	118.24	126.50
67	5	2638	G	N3-C4-C5	6.34	131.77	128.60
67	5	4726	G	N3-C4-N9	-6.34	122.19	126.00
76	9	1305	C	N1-C2-O2	6.34	122.71	118.90
57	S	84	TYR	CB-CG-CD1	-6.34	117.19	121.00
67	5	1944	A	C5-C6-N6	-6.34	118.63	123.70
67	5	4088	C	N1-C2-O2	6.34	122.70	118.90
76	9	987	A	O4'-C1'-N9	-6.34	103.13	108.20
67	5	108	A	N1-C6-N6	6.34	122.40	118.60
76	9	1294	G	N3-C4-N9	6.34	129.80	126.00
67	5	3622	C	C5-C4-N4	-6.33	115.77	120.20
76	9	1490	G	C4-N9-C1'	6.33	134.73	126.50
67	5	4165	C	C6-N1-C2	-6.33	117.77	120.30
67	5	4862	G	N3-C4-N9	-6.33	122.20	126.00
67	5	666	G	N3-C4-N9	-6.33	122.20	126.00
76	9	1095	U	C5-C6-N1	6.33	125.86	122.70
67	5	4278	C	C2-N1-C1'	6.33	125.76	118.80
76	9	42	A	O4'-C1'-N9	6.33	113.26	108.20
67	5	386	A	C5-C6-N6	-6.32	118.64	123.70
67	5	1331	C	C2-N1-C1'	6.32	125.76	118.80
67	5	2834	C	C2-N1-C1'	6.32	125.75	118.80
76	9	52	G	C2-N3-C4	-6.32	108.74	111.90
67	5	2519	U	O4'-C1'-N1	6.32	113.26	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	2354	G	N1-C2-N2	-6.32	110.51	116.20
67	5	3903	A	C4-C5-N7	6.32	113.86	110.70
76	9	1717	C	N1-C2-O2	6.32	122.69	118.90
67	5	1535	C	C6-N1-C2	6.32	122.83	120.30
67	5	1887	G	C8-N9-C1'	-6.32	118.79	127.00
67	5	4680	G	C4-N9-C1'	6.32	134.71	126.50
67	5	4881	U	N1-C1'-C2'	-6.32	105.05	112.00
67	5	5016	A	C4-C5-N7	6.31	113.86	110.70
67	5	4124	G	C8-N9-C1'	-6.31	118.79	127.00
67	5	1629	G	C8-N9-C1'	-6.31	118.80	127.00
73	8	141	C	N3-C2-O2	-6.31	117.48	121.90
67	5	2784	C	N3-C4-C5	6.31	124.42	121.90
67	5	1589	C	C2-N1-C1'	6.31	125.74	118.80
73	8	6	C	N3-C2-O2	-6.30	117.49	121.90
67	5	3882	C	C2-N1-C1'	6.30	125.73	118.80
67	5	23	C	N1-C1'-C2'	-6.30	105.07	112.00
28	ii	226	LEU	CB-CG-CD1	6.30	121.71	111.00
67	5	353	A	C8-N9-C1'	-6.30	116.36	127.70
67	5	2659	A	C5-C6-N6	-6.30	118.66	123.70
67	5	1580	C	N1-C2-O2	6.30	122.68	118.90
67	5	2406	G	C8-N9-C1'	-6.30	118.81	127.00
67	5	163	A	C5-C6-N1	6.29	120.85	117.70
67	5	1924	C	N3-C2-O2	-6.29	117.50	121.90
67	5	1574	G	N1-C2-N2	-6.29	110.54	116.20
67	5	1640	C	N3-C4-C5	6.29	124.42	121.90
67	5	1235	G	C5-C6-O6	6.29	132.37	128.60
67	5	1529	G	C8-N9-C4	-6.28	103.89	106.40
76	9	1526	G	N1-C2-N2	6.28	121.85	116.20
67	5	4166	G	N1-C2-N2	-6.28	110.55	116.20
67	5	1967	A	C5-C6-N6	-6.28	118.68	123.70
67	5	3893	C	N1-C2-O2	6.27	122.66	118.90
67	5	1373	A	C6-C5-N7	-6.27	127.91	132.30
67	5	1373	A	N9-C4-C5	-6.27	103.29	105.80
67	5	1651	G	N3-C2-N2	6.27	124.29	119.90
67	5	2638	G	N3-C4-N9	-6.27	122.24	126.00
67	5	3598	C	O4'-C1'-N1	6.27	113.21	108.20
67	5	2025	A	N9-C4-C5	-6.27	103.29	105.80
67	5	4375	C	C6-N1-C2	-6.26	117.80	120.30
41	MM	33	ARG	C-N-CA	6.26	135.44	122.30
67	5	324	A	C5-C6-N1	6.26	120.83	117.70
67	5	4447	C	C5-C4-N4	-6.26	115.82	120.20
67	5	494	C	N3-C4-N4	-6.25	113.62	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	55	G	C8-N9-C1'	-6.25	118.87	127.00
67	5	4561	C	C6-N1-C1'	-6.25	113.30	120.80
67	5	2838	G	C6-C5-N7	-6.25	126.65	130.40
67	5	4444	C	N1-C2-O2	6.25	122.65	118.90
67	5	1944	A	C5-C6-N1	6.25	120.82	117.70
67	5	2533	C	C6-N1-C1'	-6.25	113.30	120.80
67	5	4948	C	C5-C4-N4	-6.25	115.83	120.20
76	9	1498	A	O4'-C1'-N9	6.25	113.20	108.20
67	5	1739	G	N3-C4-C5	-6.24	125.48	128.60
76	9	1148	A	N1-C6-N6	6.24	122.34	118.60
67	5	1812	C	C6-N1-C2	-6.24	117.81	120.30
67	5	4451	G	N1-C2-N2	-6.24	110.59	116.20
67	5	4561	C	C2-N1-C1'	6.24	125.66	118.80
67	5	2041	A	N1-C6-N6	-6.23	114.86	118.60
67	5	1623	A	C4-C5-N7	6.23	113.81	110.70
67	5	3897	G	C2-N3-C4	-6.23	108.78	111.90
83	CC	66	LEU	CA-CB-CG	6.23	129.63	115.30
67	5	719	C	N1-C2-O2	6.23	122.64	118.90
67	5	1535	C	C2-N3-C4	-6.23	116.79	119.90
67	5	1674	C	C6-N1-C1'	-6.23	113.33	120.80
67	5	4434	C	C6-N1-C1'	-6.23	113.33	120.80
67	5	1387	A	C5-C6-N6	-6.23	118.72	123.70
67	5	4761	G	N3-C4-C5	6.23	131.71	128.60
67	5	4624	A	C6-N1-C2	-6.22	114.87	118.60
76	9	1603	G	O4'-C1'-N9	6.22	113.17	108.20
28	ii	68	ARG	NE-CZ-NH2	6.22	123.41	120.30
67	5	4579	U	C2-N1-C1'	6.22	125.16	117.70
76	9	140	U	C2-N1-C1'	6.22	125.16	117.70
67	5	2406	G	C4-N9-C1'	6.21	134.58	126.50
76	9	1389	C	C2-N1-C1'	6.21	125.63	118.80
67	5	83	C	C6-N1-C2	6.21	122.78	120.30
76	9	171	A	C5-C6-N6	-6.21	118.73	123.70
76	9	662	G	O4'-C1'-N9	-6.21	103.23	108.20
76	9	106	C	N1-C2-O2	6.21	122.62	118.90
67	5	4305	G	C4-C5-N7	6.20	113.28	110.80
67	5	4305	G	C8-N9-C4	-6.19	103.92	106.40
76	9	1566	G	C4-N9-C1'	-6.19	118.45	126.50
67	5	364	G	C4-C5-N7	6.19	113.28	110.80
76	9	1781	A	N1-C6-N6	6.19	122.32	118.60
67	5	1868	A	N7-C8-N9	6.19	116.89	113.80
67	5	2838	G	N7-C8-N9	6.19	116.20	113.10
76	9	1666	C	C6-N1-C2	6.19	122.78	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	64	A	C4-C5-N7	6.19	113.79	110.70
32	jj	426	LEU	CA-CB-CG	6.19	129.53	115.30
67	5	2399	G	N3-C4-C5	-6.19	125.51	128.60
76	9	621	C	N1-C2-O2	6.19	122.61	118.90
67	5	3869	C	C5-C4-N4	-6.19	115.87	120.20
67	5	1803	G	C8-N9-C1'	-6.18	118.96	127.00
67	5	4528	G	C4-N9-C1'	6.18	134.54	126.50
67	5	4696	C	N3-C4-N4	6.18	122.33	118.00
76	9	1438	A	N1-C6-N6	6.18	122.31	118.60
67	5	924	C	O4'-C1'-N1	6.18	113.14	108.20
67	5	2335	C	C6-N1-C1'	-6.18	113.38	120.80
67	5	3820	G	C8-N9-C1'	-6.18	118.97	127.00
67	5	4454	G	N1-C2-N2	-6.18	110.64	116.20
67	5	1629	G	C6-C5-N7	-6.17	126.69	130.40
67	5	2894	A	C5-C6-N1	6.17	120.79	117.70
67	5	4363	A	C5-C6-N1	6.17	120.79	117.70
76	9	621	C	N3-C2-O2	-6.17	117.58	121.90
76	9	1267	C	O4'-C1'-N1	6.17	113.14	108.20
67	5	101	A	C5-C6-N6	-6.17	118.77	123.70
67	5	1880	G	C6-C5-N7	-6.17	126.70	130.40
67	5	1985	G	C8-N9-C1'	-6.17	118.98	127.00
67	5	2657	G	O4'-C1'-N9	-6.17	103.27	108.20
67	5	299	C	C2-N1-C1'	6.16	125.58	118.80
67	5	40	G	C2-N3-C4	-6.16	108.82	111.90
67	5	2670	C	C2-N1-C1'	6.16	125.58	118.80
76	9	1474	A	C4-C5-N7	-6.16	107.62	110.70
32	jj	292	PHE	CB-CG-CD2	-6.16	116.49	120.80
67	5	2639	U	O4'-C1'-N1	6.16	113.13	108.20
76	9	102	A	O4'-C1'-N9	6.16	113.13	108.20
76	9	1860	A	C5-C6-N1	6.16	120.78	117.70
76	9	480	G	C8-N9-C1'	-6.16	119.00	127.00
67	5	3653	A	N7-C8-N9	6.16	116.88	113.80
67	5	4337	C	C5-C4-N4	-6.16	115.89	120.20
76	9	1842	C	C6-N1-C2	-6.16	117.84	120.30
67	5	1653	A	C5-C6-N6	-6.15	118.78	123.70
67	5	4375	C	N1-C2-O2	6.15	122.59	118.90
67	5	263	G	C8-N9-C1'	-6.15	119.00	127.00
67	5	4380	A	C5-C6-N1	6.15	120.77	117.70
67	5	4561	C	N1-C2-O2	6.15	122.59	118.90
76	9	1806	A	N1-C6-N6	6.15	122.29	118.60
67	5	1759	G	C8-N9-C4	-6.15	103.94	106.40
67	5	1342	A	N7-C8-N9	6.14	116.87	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	2694	G	C8-N9-C1'	-6.14	119.01	127.00
67	5	3860	A	C5-C6-N6	6.14	128.62	123.70
67	5	3816	A	O4'-C1'-N9	6.14	113.11	108.20
67	5	2878	G	C8-N9-C1'	-6.14	119.02	127.00
67	5	1854	G	N1-C2-N2	-6.14	110.68	116.20
67	5	4331	G	N3-C2-N2	6.14	124.20	119.90
67	5	2443	G	C4-N9-C1'	6.13	134.47	126.50
67	5	1690	C	C2-N1-C1'	6.13	125.54	118.80
67	5	11	G	N3-C4-C5	-6.13	125.54	128.60
67	5	4443	C	C5-C4-N4	-6.13	115.91	120.20
67	5	1484	G	N3-C2-N2	6.12	124.19	119.90
76	9	1793	A	C5-C6-N6	-6.12	118.80	123.70
67	5	1910	G	C4-N9-C1'	6.12	134.46	126.50
67	5	289	C	C2-N1-C1'	6.12	125.53	118.80
67	5	4717	A	C6-N1-C2	-6.12	114.93	118.60
76	9	123	G	N3-C4-N9	6.12	129.67	126.00
67	5	38	A	C5-N7-C8	-6.12	100.84	103.90
67	5	2096	G	N1-C6-O6	-6.12	116.23	119.90
76	9	1065	G	N3-C2-N2	6.12	124.18	119.90
76	9	1534	C	C6-N1-C2	-6.12	117.85	120.30
67	5	3771	C	C5-C6-N1	6.11	124.06	121.00
76	9	84	A	N1-C6-N6	6.11	122.27	118.60
76	9	1294	G	C4-N9-C1'	6.11	134.45	126.50
70	7	101	A	C8-N9-C4	-6.11	103.36	105.80
67	5	3904	G	O4'-C1'-N9	6.11	113.09	108.20
67	5	4279	A	N9-C4-C5	-6.11	103.36	105.80
76	9	1216	C	C2-N1-C1'	-6.11	112.08	118.80
76	9	674	C	N3-C4-C5	6.11	124.34	121.90
67	5	3687	A	C5-C6-N6	-6.11	118.82	123.70
67	5	4661	G	N1-C2-N3	6.11	127.56	123.90
67	5	353	A	N1-C6-N6	6.10	122.26	118.60
67	5	2046	G	C4-N9-C1'	6.10	134.43	126.50
67	5	1458	C	C5-C4-N4	-6.10	115.93	120.20
67	5	1870	C	C2-N3-C4	-6.10	116.85	119.90
67	5	1670	G	N3-C4-N9	6.10	129.66	126.00
67	5	3893	C	N3-C2-O2	-6.10	117.63	121.90
76	9	670	A	C8-N9-C4	-6.10	103.36	105.80
76	9	995	G	N1-C2-N2	-6.10	110.71	116.20
67	5	355	A	N9-C4-C5	-6.10	103.36	105.80
67	5	1929	A	C8-N9-C1'	-6.10	116.73	127.70
67	5	2024	G	N3-C4-C5	6.10	131.65	128.60
76	9	1658	G	N3-C4-N9	6.10	129.66	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	3771	C	C6-N1-C1'	-6.09	113.49	120.80
67	5	4550	G	N1-C2-N2	-6.09	110.72	116.20
76	9	1414	A	N1-C6-N6	6.09	122.26	118.60
67	5	1331	C	C6-N1-C1'	-6.09	113.49	120.80
6	D	109	LEU	CB-CG-CD1	-6.09	100.64	111.00
67	5	356	G	C8-N9-C1'	-6.09	119.08	127.00
67	5	1734	G	C2-N3-C4	-6.09	108.85	111.90
72	Y	27	ARG	NE-CZ-NH1	-6.09	117.25	120.30
70	7	29	C	N1-C2-O2	6.09	122.55	118.90
67	5	1880	G	N3-C2-N2	6.09	124.16	119.90
76	9	1245	G	O4'-C1'-N9	6.09	113.07	108.20
67	5	2290	C	N3-C2-O2	-6.09	117.64	121.90
67	5	2867	C	C6-N1-C2	-6.09	117.86	120.30
67	5	2802	C	C2-N1-C1'	6.08	125.49	118.80
67	5	4651	A	C6-N1-C2	-6.08	114.95	118.60
67	5	4710	C	C6-N1-C2	-6.08	117.87	120.30
67	5	2746	A	N1-C6-N6	6.08	122.25	118.60
67	5	3719	A	N1-C6-N6	6.08	122.25	118.60
67	5	415	G	C8-N9-C1'	-6.08	119.10	127.00
67	5	3633	C	C6-N1-C1'	-6.08	113.51	120.80
67	5	4942	C	P-O3'-C3'	6.08	126.99	119.70
59	SS	137	LYS	CA-CB-CG	6.08	126.77	113.40
67	5	355	A	C5-N7-C8	-6.08	100.86	103.90
67	5	1836	G	O4'-C1'-N9	6.08	113.06	108.20
67	5	1916	G	C4-N9-C1'	6.08	134.40	126.50
67	5	2379	A	C8-N9-C1'	-6.08	116.77	127.70
67	5	2878	G	N1-C2-N2	-6.08	110.73	116.20
67	5	3687	A	N1-C6-N6	6.08	122.25	118.60
67	5	3924	C	C2-N1-C1'	6.08	125.48	118.80
67	5	2014	C	O4'-C1'-N1	6.07	113.06	108.20
67	5	4284	C	C6-N1-C2	-6.07	117.87	120.30
76	9	915	G	C8-N9-C1'	-6.07	119.11	127.00
67	5	1521	C	N3-C4-N4	6.07	122.25	118.00
67	5	2277	C	C6-N1-C1'	-6.07	113.52	120.80
67	5	1890	G	C5-N7-C8	-6.07	101.27	104.30
67	5	4388	A	N1-C6-N6	-6.06	114.96	118.60
67	5	2324	C	C2-N1-C1'	6.06	125.47	118.80
67	5	3636	C	N1-C2-O2	6.06	122.53	118.90
67	5	1576	G	C4-N9-C1'	6.06	134.37	126.50
67	5	4087	G	N3-C4-C5	6.06	131.63	128.60
76	9	1014	G	C8-N9-C1'	-6.06	119.12	127.00
67	5	105	A	C4-C5-N7	6.06	113.73	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	2619	G	N1-C2-N2	-6.05	110.75	116.20
67	5	1065	G	C6-C5-N7	6.05	134.03	130.40
67	5	1957	U	C2-N1-C1'	-6.05	110.44	117.70
67	5	2860	C	C6-N1-C1'	-6.05	113.54	120.80
76	9	1466	G	N3-C4-N9	-6.05	122.37	126.00
76	9	1584	G	C4-N9-C1'	6.05	134.37	126.50
67	5	3929	G	C4-N9-C1'	6.05	134.36	126.50
67	5	1206	C	N1-C2-O2	6.05	122.53	118.90
67	5	5016	A	C6-C5-N7	-6.05	128.07	132.30
76	9	84	A	C4-C5-C6	6.05	120.02	117.00
67	5	1318	C	N3-C4-N4	6.04	122.23	118.00
67	5	2319	C	N3-C4-C5	6.04	124.32	121.90
73	8	103	A	N7-C8-N9	6.04	116.82	113.80
76	9	909	G	C5-C6-O6	-6.04	124.97	128.60
67	5	1869	G	C8-N9-C1'	-6.04	119.15	127.00
67	5	3845	A	C5-C6-N1	6.04	120.72	117.70
67	5	3866	C	N3-C2-O2	-6.04	117.67	121.90
76	9	84	A	C8-N9-C1'	-6.04	116.83	127.70
76	9	1055	A	C6-C5-N7	-6.04	128.07	132.30
76	9	1265	A	O4'-C1'-N9	6.04	113.03	108.20
67	5	2406	G	C8-N9-C4	-6.04	103.98	106.40
67	5	2511	A	O4'-C1'-N9	6.04	113.03	108.20
67	5	1629	G	C2-N3-C4	-6.04	108.88	111.90
67	5	4472	G	C4-N9-C1'	6.04	134.35	126.50
67	5	4513	A	C5-C6-N1	6.04	120.72	117.70
67	5	1859	C	N3-C4-N4	6.04	122.23	118.00
76	9	1717	C	C2-N1-C1'	6.04	125.44	118.80
67	5	3635	A	C8-N9-C4	6.04	108.21	105.80
67	5	3901	A	C8-N9-C1'	-6.04	116.84	127.70
67	5	4097	G	C2-N3-C4	-6.03	108.88	111.90
67	5	968	C	N3-C2-O2	-6.03	117.68	121.90
67	5	2345	G	N1-C2-N2	-6.03	110.77	116.20
67	5	294	G	N1-C2-N2	-6.03	110.77	116.20
67	5	4681	A	C8-N9-C4	6.03	108.21	105.80
67	5	41	C	C6-N1-C1'	-6.03	113.57	120.80
67	5	1926	C	N3-C2-O2	-6.03	117.68	121.90
67	5	351	C	N1-C2-O2	6.03	122.52	118.90
67	5	1989	G	N1-C2-N2	-6.03	110.78	116.20
67	5	2393	C	N3-C4-C5	6.02	124.31	121.90
67	5	2799	G	N1-C2-N3	6.02	127.51	123.90
67	5	4661	G	C2-N3-C4	-6.02	108.89	111.90
67	5	4945	G	C6-C5-N7	-6.02	126.79	130.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	293	G	C4-N9-C1'	6.02	134.32	126.50
67	5	1333	A	C6-N1-C2	-6.02	114.99	118.60
67	5	4427	G	C8-N9-C1'	-6.02	119.17	127.00
67	5	1801	A	C5-C6-N6	-6.02	118.89	123.70
67	5	48	G	N1-C2-N2	-6.01	110.79	116.20
67	5	2448	G	N1-C2-N2	-6.01	110.79	116.20
67	5	1663	C	C2-N1-C1'	6.01	125.41	118.80
67	5	1729	A	C5-C6-N1	6.01	120.70	117.70
67	5	1794	A	C8-N9-C1'	-6.01	116.88	127.70
67	5	1916	G	C8-N9-C1'	-6.01	119.19	127.00
67	5	2613	C	N3-C4-C5	6.01	124.30	121.90
76	9	1257	G	C8-N9-C1'	6.01	134.81	127.00
4	DD	218	LEU	CA-CB-CG	6.01	129.12	115.30
67	5	1065	G	C4-N9-C1'	-6.01	118.69	126.50
67	5	2622	G	C4-N9-C1'	6.00	134.31	126.50
67	5	3650	C	N1-C2-O2	6.00	122.50	118.90
76	9	1584	G	C8-N9-C1'	-6.00	119.19	127.00
32	jj	632	LEU	CB-CG-CD1	-6.00	100.80	111.00
67	5	1458	C	C6-N1-C2	6.00	122.70	120.30
67	5	2659	A	N9-C4-C5	-6.00	103.40	105.80
67	5	2860	C	C6-N1-C2	-6.00	117.90	120.30
67	5	418	A	C8-N9-C1'	-6.00	116.90	127.70
67	5	3774	A	C4-N9-C1'	6.00	137.10	126.30
67	5	3774	A	C4-C5-N7	6.00	113.70	110.70
76	9	501	C	C6-N1-C2	-6.00	117.90	120.30
67	5	1329	G	N3-C4-C5	-6.00	125.60	128.60
76	9	1566	G	C8-N9-C1'	5.99	134.79	127.00
67	5	1371	A	N1-C6-N6	5.99	122.19	118.60
67	5	2321	G	C2-N3-C4	-5.99	108.91	111.90
67	5	2379	A	O4'-C1'-N9	-5.99	103.41	108.20
67	5	3887	C	N3-C4-C5	5.99	124.30	121.90
67	5	2613	C	C5-C4-N4	-5.99	116.01	120.20
67	5	3650	C	N3-C2-O2	-5.99	117.71	121.90
18	GG	133	LEU	CA-CB-CG	5.99	129.06	115.30
67	5	1653	A	C4-C5-N7	5.98	113.69	110.70
67	5	2640	G	C8-N9-C1'	-5.98	119.22	127.00
67	5	2848	G	N1-C6-O6	5.98	123.49	119.90
67	5	2040	A	N1-C6-N6	5.98	122.19	118.60
67	5	1655	C	C6-N1-C1'	-5.98	113.62	120.80
76	9	1798	C	N1-C2-O2	5.98	122.49	118.90
67	5	323	C	N3-C2-O2	-5.98	117.71	121.90
67	5	1323	A	C4-C5-N7	5.98	113.69	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4936	G	N3-C4-C5	5.98	131.59	128.60
67	5	1681	G	N1-C2-N2	-5.98	110.82	116.20
76	9	171	A	N1-C6-N6	5.98	122.19	118.60
67	5	1091	C	N1-C2-O2	5.97	122.48	118.90
67	5	2050	G	C4-N9-C1'	5.97	134.27	126.50
73	8	72	A	N9-C4-C5	-5.97	103.41	105.80
76	9	330	G	N3-C4-C5	5.97	131.59	128.60
67	5	2458	C	N3-C2-O2	-5.97	117.72	121.90
67	5	2804	C	C2-N1-C1'	5.97	125.37	118.80
67	5	4193	C	N1-C2-O2	5.97	122.48	118.90
67	5	418	A	C5-C6-N1	5.97	120.68	117.70
67	5	1651	G	N1-C2-N3	5.97	127.48	123.90
67	5	1580	C	C5-C4-N4	-5.96	116.03	120.20
67	5	1608	G	C4-N9-C1'	5.96	134.25	126.50
67	5	2419	C	N1-C2-O2	5.96	122.48	118.90
67	5	4984	C	N3-C4-C5	5.96	124.29	121.90
67	5	1663	C	C5-C4-N4	-5.96	116.03	120.20
67	5	1938	C	C5-C4-N4	-5.96	116.03	120.20
67	5	2419	C	N3-C2-O2	-5.96	117.73	121.90
67	5	4654	C	N3-C2-O2	-5.96	117.73	121.90
67	5	41	C	C2-N1-C1'	5.96	125.36	118.80
67	5	3917	A	N1-C6-N6	5.96	122.17	118.60
67	5	4560	C	C6-N1-C2	5.96	122.68	120.30
67	5	4716	C	N3-C4-C5	5.96	124.28	121.90
76	9	1488	C	C2-N1-C1'	5.96	125.36	118.80
67	5	1681	G	N3-C2-N2	5.96	124.07	119.90
67	5	2878	G	C4-N9-C1'	5.96	134.24	126.50
67	5	1931	C	N3-C4-N4	5.95	122.17	118.00
67	5	2392	C	C2-N1-C1'	5.95	125.35	118.80
76	9	168	C	C6-N1-C2	-5.95	117.92	120.30
67	5	2758	G	C4-N9-C1'	5.95	134.24	126.50
67	5	3835	C	C6-N1-C2	-5.95	117.92	120.30
67	5	4510	A	C8-N9-C1'	-5.95	116.99	127.70
76	9	1416	C	C5-C6-N1	5.95	123.98	121.00
67	5	54	G	C4-N9-C1'	5.95	134.23	126.50
76	9	1760	G	C5-C6-O6	5.95	132.17	128.60
76	9	1834	A	C6-C5-N7	-5.95	128.14	132.30
67	5	1879	C	C2-N1-C1'	5.95	125.34	118.80
76	9	480	G	O5'-P-OP2	-5.95	100.35	105.70
67	5	4746	C	C2-N1-C1'	5.94	125.34	118.80
67	5	2355	G	N1-C2-N2	-5.94	110.85	116.20
76	9	1566	G	O4'-C1'-N9	5.94	112.95	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1628	C	N3-C4-C5	5.94	124.28	121.90
76	9	1603	G	N1-C2-N2	-5.94	110.86	116.20
67	5	284	G	N3-C4-C5	-5.94	125.63	128.60
67	5	4511	A	O4'-C1'-N9	5.94	112.95	108.20
67	5	1868	A	C5-C6-N6	-5.93	118.95	123.70
67	5	1958	A	N1-C6-N6	-5.93	115.04	118.60
67	5	4291	G	C4-N9-C1'	5.93	134.21	126.50
67	5	4533	A	C5-N7-C8	-5.93	100.93	103.90
67	5	4902	C	C2-N1-C1'	5.93	125.32	118.80
67	5	285	G	C2-N3-C4	-5.93	108.94	111.90
67	5	1300	G	N3-C4-N9	-5.93	122.44	126.00
67	5	51	A	C4-C5-N7	5.93	113.66	110.70
67	5	2435	G	N3-C4-C5	5.93	131.56	128.60
67	5	3727	A	C8-N9-C4	5.93	108.17	105.80
55	s	47	LEU	CA-CB-CG	5.92	128.92	115.30
67	5	1888	A	N1-C6-N6	-5.92	115.05	118.60
67	5	2579	G	C5-C6-O6	5.92	132.15	128.60
76	9	1735	A	N1-C6-N6	5.92	122.15	118.60
67	5	11	G	N3-C4-N9	5.92	129.55	126.00
73	8	15	G	C4-N9-C1'	5.92	134.20	126.50
55	s	155	LEU	CA-CB-CG	5.92	128.91	115.30
67	5	2784	C	C6-N1-C1'	-5.92	113.70	120.80
67	5	3685	C	C6-N1-C1'	-5.91	113.70	120.80
76	9	29	G	C8-N9-C4	-5.91	104.03	106.40
67	5	421	C	N3-C4-C5	5.91	124.27	121.90
67	5	342	G	N3-C4-C5	-5.91	125.64	128.60
76	9	159	A	N1-C6-N6	-5.91	115.05	118.60
67	5	360	A	C5-C6-N6	-5.91	118.97	123.70
67	5	1283	G	C2-N3-C4	-5.91	108.95	111.90
73	8	39	G	C2-N3-C4	-5.91	108.95	111.90
67	5	1635	C	N3-C4-C5	5.91	124.26	121.90
67	5	1880	G	N1-C2-N2	-5.91	110.89	116.20
73	8	6	C	N1-C2-O2	5.91	122.44	118.90
76	9	563	G	C8-N9-C1'	-5.91	119.32	127.00
67	5	4667	C	C2-N1-C1'	5.90	125.29	118.80
67	5	3867	A	C5-C6-N6	-5.90	118.98	123.70
76	9	1083	A	O4'-C1'-N9	5.90	112.92	108.20
76	9	1180	C	C6-N1-C2	5.90	122.66	120.30
67	5	3612	C	N3-C2-O2	-5.90	117.77	121.90
67	5	3691	G	C2-N3-C4	-5.90	108.95	111.90
67	5	4671	C	C2-N1-C1'	5.90	125.29	118.80
76	9	604	A	O4'-C1'-N9	-5.90	103.48	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	9	1181	A	C5-C6-N6	-5.90	118.98	123.70
67	5	4298	A	C6-N1-C2	-5.89	115.06	118.60
67	5	1390	G	N1-C2-N2	-5.89	110.90	116.20
67	5	1988	G	C2-N3-C4	-5.89	108.95	111.90
76	9	390	C	C2-N1-C1'	5.89	125.28	118.80
76	9	480	G	N3-C4-N9	5.89	129.54	126.00
67	5	489	C	N3-C4-C5	5.89	124.26	121.90
67	5	2392	C	N1-C2-O2	5.89	122.43	118.90
67	5	2724	G	N3-C4-C5	5.89	131.54	128.60
67	5	4179	G	N7-C8-N9	5.89	116.05	113.10
67	5	4427	G	N1-C2-N2	-5.89	110.90	116.20
76	9	123	G	C8-N9-C1'	-5.89	119.34	127.00
67	5	429	A	C5-C6-N6	-5.89	118.99	123.70
67	5	1546	C	N3-C4-C5	5.89	124.25	121.90
67	5	4582	C	N3-C2-O2	-5.89	117.78	121.90
76	9	1223	A	C8-N9-C4	5.89	108.16	105.80
67	5	1896	A	C8-N9-C1'	-5.88	117.11	127.70
76	9	1603	G	C6-C5-N7	-5.88	126.87	130.40
16	g	25	THR	CA-CB-CG2	-5.88	104.17	112.40
67	5	422	C	C5-C4-N4	-5.88	116.08	120.20
67	5	1576	G	C8-N9-C4	-5.88	104.05	106.40
67	5	1895	G	C8-N9-C1'	-5.88	119.36	127.00
67	5	1296	G	O4'-C1'-N9	5.88	112.90	108.20
67	5	422	C	N1-C2-O2	5.88	122.42	118.90
67	5	98	A	C5-C6-N1	5.87	120.64	117.70
67	5	2693	G	C4-N9-C1'	5.87	134.13	126.50
67	5	2335	C	N3-C2-O2	-5.87	117.79	121.90
67	5	1654	G	N3-C2-N2	5.87	124.01	119.90
67	5	2670	C	N3-C2-O2	-5.87	117.79	121.90
67	5	4738	C	N3-C4-N4	5.87	122.11	118.00
76	9	1498	A	C5-C6-N1	5.87	120.63	117.70
67	5	4510	A	C4-N9-C1'	5.87	136.86	126.30
67	5	1589	C	C5-C4-N4	-5.87	116.09	120.20
67	5	3826	C	C6-N1-C2	-5.87	117.95	120.30
67	5	4978	G	N3-C2-N2	5.87	124.01	119.90
67	5	499	G	N3-C2-N2	5.86	124.00	119.90
76	9	1294	G	N3-C2-N2	5.86	124.00	119.90
67	5	1589	C	N3-C4-C5	5.86	124.25	121.90
76	9	594	A	O4'-C1'-N9	5.86	112.89	108.20
8	EE	48	LEU	CB-CG-CD2	-5.86	101.04	111.00
67	5	38	A	C4-C5-C6	5.86	119.93	117.00
67	5	298	G	C8-N9-C1'	-5.86	119.38	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	339	C	C2-N1-C1'	5.85	125.24	118.80
67	5	2748	C	C6-N1-C2	5.85	122.64	120.30
67	5	4407	G	C8-N9-C1'	-5.85	119.39	127.00
67	5	4528	G	N3-C4-C5	-5.85	125.67	128.60
76	9	909	G	C2-N3-C4	5.85	114.83	111.90
73	8	45	C	N3-C2-O2	-5.85	117.81	121.90
76	9	1658	G	N1-C6-O6	5.85	123.41	119.90
67	5	283	G	C4-N9-C1'	5.85	134.10	126.50
76	9	1335	G	C4-C5-N7	5.85	113.14	110.80
76	9	52	G	N3-C4-N9	-5.84	122.49	126.00
67	5	294	G	N9-C4-C5	-5.84	103.06	105.40
67	5	2277	C	C5-C4-N4	-5.84	116.11	120.20
67	5	2627	C	C2-N1-C1'	5.84	125.22	118.80
67	5	4645	C	C2-N1-C1'	5.84	125.22	118.80
73	8	45	C	N1-C2-O2	5.84	122.40	118.90
67	5	1460	C	C5-C4-N4	-5.84	116.11	120.20
67	5	2397	G	C2-N3-C4	-5.84	108.98	111.90
67	5	3901	A	C4-N9-C1'	5.84	136.81	126.30
67	5	4917	C	N1-C2-O2	5.84	122.40	118.90
76	9	140	U	C6-N1-C1'	-5.84	113.03	121.20
67	5	90	G	N7-C8-N9	5.84	116.02	113.10
67	5	1931	C	C5-C4-N4	-5.84	116.11	120.20
67	5	295	A	O4'-C1'-N9	5.83	112.87	108.20
67	5	1976	G	N3-C4-C5	5.83	131.52	128.60
67	5	2724	G	C2-N3-C4	-5.83	108.98	111.90
82	c	39	ARG	CG-CD-NE	5.83	124.05	111.80
67	5	1667	A	C5-C6-N1	5.83	120.61	117.70
67	5	3899	G	C8-N9-C4	-5.83	104.07	106.40
67	5	4278	C	C6-N1-C1'	-5.83	113.81	120.80
67	5	4324	A	C5-C6-N1	5.83	120.61	117.70
67	5	3866	C	C6-N1-C1'	-5.83	113.81	120.80
67	5	3619	G	N3-C4-C5	5.83	131.51	128.60
67	5	1064	G	C8-N9-C1'	-5.82	119.43	127.00
67	5	1506	G	N1-C2-N2	-5.82	110.96	116.20
67	5	2443	G	C6-C5-N7	-5.82	126.91	130.40
67	5	1854	G	C2-N3-C4	-5.82	108.99	111.90
67	5	437	G	C4-N9-C1'	5.82	134.07	126.50
67	5	1553	A	C5-C6-N6	-5.82	119.04	123.70
76	9	1501	C	C2-N1-C1'	5.82	125.20	118.80
67	5	4537	C	O4'-C1'-N1	5.82	112.86	108.20
76	9	674	C	C6-N1-C2	5.82	122.63	120.30
4	DD	138	VAL	CG1-CB-CG2	5.82	120.21	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	hh	44	A	O5'-P-OP1	-5.82	100.46	105.70
67	5	55	G	C8-N9-C4	-5.82	104.07	106.40
67	5	2282	A	N1-C6-N6	-5.82	115.11	118.60
67	5	3873	G	C4-N9-C1'	5.82	134.06	126.50
76	9	1529	C	O4'-C1'-N1	5.82	112.85	108.20
67	5	1541	C	N1-C2-O2	5.82	122.39	118.90
76	9	639	C	C2-N1-C1'	5.82	125.20	118.80
67	5	4204	C	C6-N1-C2	-5.81	117.97	120.30
76	9	82	G	C4-N9-C1'	5.81	134.06	126.50
54	R	173	ARG	CA-CB-CG	5.81	126.19	113.40
67	5	2539	C	C6-N1-C1'	-5.81	113.83	120.80
76	9	1438	A	N9-C4-C5	-5.81	103.47	105.80
70	7	82	G	C8-N9-C4	-5.81	104.08	106.40
76	9	1294	G	C8-N9-C1'	-5.81	119.45	127.00
67	5	3850	C	N1-C2-O2	5.81	122.38	118.90
67	5	4472	G	C8-N9-C1'	-5.81	119.45	127.00
67	5	83	C	C5-C4-N4	-5.80	116.14	120.20
67	5	1529	G	N1-C2-N2	-5.80	110.98	116.20
67	5	1541	C	N3-C2-O2	-5.80	117.84	121.90
67	5	4293	U	O4'-C1'-N1	5.80	112.84	108.20
67	5	1608	G	C8-N9-C1'	-5.80	119.46	127.00
67	5	4510	A	C6-C5-N7	-5.80	128.24	132.30
67	5	1353	G	C8-N9-C1'	-5.80	119.46	127.00
67	5	4694	G	C4-N9-C1'	5.80	134.04	126.50
67	5	4979	A	C5-C6-N6	-5.80	119.06	123.70
67	5	1520	C	N1-C2-O2	5.80	122.38	118.90
67	5	1780	A	C5-C6-N1	5.80	120.60	117.70
67	5	1202	C	N1-C1'-C2'	-5.80	105.62	112.00
67	5	4486	C	N3-C4-N4	5.80	122.06	118.00
76	9	84	A	C6-C5-N7	-5.79	128.24	132.30
76	9	1661	A	P-O3'-C3'	5.79	126.65	119.70
67	5	335	A	C5-C6-N1	5.79	120.60	117.70
67	5	1218	G	C8-N9-C4	5.79	108.72	106.40
67	5	1895	G	N3-C2-N2	5.79	123.95	119.90
67	5	2731	C	N3-C2-O2	-5.79	117.85	121.90
67	5	4710	C	C2-N1-C1'	5.79	125.17	118.80
76	9	1373	C	C6-N1-C2	5.79	122.62	120.30
67	5	1271	G	N3-C4-C5	-5.79	125.70	128.60
67	5	2088	A	N1-C6-N6	5.79	122.07	118.60
67	5	3636	C	N3-C2-O2	-5.79	117.85	121.90
76	9	1250	A	N1-C6-N6	5.79	122.07	118.60
67	5	2746	A	C5-C6-N6	-5.79	119.07	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4550	G	C8-N9-C4	-5.79	104.08	106.40
67	5	1427	A	C8-N9-C4	5.79	108.11	105.80
67	5	1589	C	C6-N1-C1'	-5.79	113.86	120.80
67	5	4506	C	C2-N1-C1'	5.79	125.16	118.80
67	5	4176	C	N3-C4-C5	5.78	124.21	121.90
76	9	1337	C	O4'-C1'-N1	5.78	112.83	108.20
67	5	2438	A	C4-C5-N7	5.78	113.59	110.70
67	5	2836	A	N3-C4-C5	5.78	130.84	126.80
73	8	6	C	C2-N1-C1'	5.78	125.15	118.80
76	9	1603	G	N9-C4-C5	-5.78	103.09	105.40
67	5	409	G	C6-C5-N7	-5.77	126.94	130.40
67	5	955	G	N3-C2-N2	5.77	123.94	119.90
67	5	81	C	N3-C4-N4	5.77	122.04	118.00
67	5	4525	C	C2-N1-C1'	5.77	125.15	118.80
76	9	351	G	N3-C4-N9	-5.77	122.54	126.00
67	5	1371	A	C5-C6-N6	-5.77	119.08	123.70
67	5	4324	A	C5-C6-N6	-5.77	119.08	123.70
67	5	4603	C	N1-C2-O2	5.77	122.36	118.90
17	BB	165	ARG	CG-CD-NE	5.77	123.91	111.80
67	5	353	A	C4-N9-C1'	5.77	136.68	126.30
67	5	2586	G	O4'-C1'-N9	-5.77	103.59	108.20
70	7	95	C	C6-N1-C1'	-5.77	113.88	120.80
67	5	2325	C	C2-N1-C1'	5.76	125.14	118.80
83	CC	78	LEU	CB-CG-CD2	5.76	120.80	111.00
67	5	1585	C	N3-C2-O2	-5.76	117.87	121.90
67	5	1893	C	N1-C2-O2	5.76	122.36	118.90
67	5	2630	U	P-O3'-C3'	5.76	126.62	119.70
76	9	998	A	N1-C6-N6	-5.76	115.14	118.60
1	A	150	LEU	CA-CB-CG	5.76	128.55	115.30
28	ii	290	TYR	CB-CG-CD2	5.76	124.46	121.00
67	5	1640	C	N1-C2-O2	5.76	122.36	118.90
67	5	4567	G	C8-N9-C4	-5.76	104.09	106.40
67	5	962	C	C6-N1-C1'	-5.76	113.89	120.80
67	5	3916	G	N3-C4-N9	5.76	129.46	126.00
67	5	4701	A	C4-N9-C1'	-5.76	115.93	126.30
76	9	1394	G	C8-N9-C1'	-5.76	119.51	127.00
76	9	1470	C	O4'-C1'-N1	5.76	112.81	108.20
67	5	301	G	N1-C2-N2	-5.76	111.02	116.20
67	5	3864	C	C2-N3-C4	-5.76	117.02	119.90
67	5	4980	C	N3-C4-C5	5.76	124.20	121.90
67	5	2750	G	N3-C2-N2	5.75	123.93	119.90
67	5	1183	C	N3-C2-O2	-5.75	117.87	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1308	C	C5-C6-N1	5.75	123.88	121.00
67	5	4362	A	N1-C6-N6	-5.75	115.15	118.60
67	5	4680	G	C8-N9-C1'	-5.75	119.52	127.00
67	5	4407	G	C4-N9-C1'	5.75	133.97	126.50
67	5	4583	C	C6-N1-C2	-5.75	118.00	120.30
67	5	3704	U	C6-N1-C2	-5.75	117.55	121.00
76	9	501	C	C2-N1-C1'	5.75	125.12	118.80
67	5	4367	G	N1-C2-N2	-5.75	111.03	116.20
67	5	163	A	C4-C5-N7	5.74	113.57	110.70
67	5	3879	G	C2-N3-C4	-5.74	109.03	111.90
59	SS	45	LEU	CA-CB-CG	5.74	128.51	115.30
67	5	671	G	N3-C4-C5	5.74	131.47	128.60
67	5	222	C	C5-C4-N4	-5.74	116.18	120.20
67	5	1896	A	C4-N9-C1'	5.74	136.63	126.30
67	5	4386	C	N3-C4-N4	-5.74	113.98	118.00
67	5	1178	G	O4'-C1'-N9	5.73	112.79	108.20
67	5	1587	G	N7-C8-N9	5.73	115.97	113.10
67	5	4910	A	O4'-C1'-N9	-5.73	103.61	108.20
76	9	989	C	C5-C4-N4	-5.73	116.19	120.20
21	h	28	LEU	CB-CG-CD2	-5.73	101.26	111.00
67	5	4485	C	N3-C2-O2	-5.73	117.89	121.90
67	5	4622	A	C6-N1-C2	-5.73	115.16	118.60
70	7	97	G	C2-N3-C4	-5.72	109.04	111.90
76	9	915	G	C4-N9-C1'	5.72	133.94	126.50
67	5	2429	A	C5-C6-N1	5.72	120.56	117.70
67	5	4486	C	C5-C4-N4	-5.72	116.19	120.20
67	5	1657	G	C8-N9-C4	-5.72	104.11	106.40
67	5	168	C	N1-C2-O2	5.72	122.33	118.90
67	5	1575	A	C8-N9-C1'	-5.72	117.41	127.70
70	7	48	G	C4-C5-N7	5.72	113.09	110.80
67	5	3691	G	N1-C2-N2	-5.72	111.05	116.20
67	5	23	C	N3-C4-C5	5.72	124.19	121.90
67	5	968	C	C2-N1-C1'	5.72	125.09	118.80
76	9	82	G	C8-N9-C1'	-5.72	119.57	127.00
67	5	56	A	N3-C4-N9	-5.71	122.83	127.40
67	5	221	C	C2-N1-C1'	5.71	125.09	118.80
67	5	2805	C	C2-N1-C1'	5.71	125.09	118.80
67	5	3866	C	C6-N1-C2	-5.71	118.01	120.30
67	5	4669	A	C5-C6-N1	5.71	120.56	117.70
76	9	1250	A	C8-N9-C1'	-5.71	117.41	127.70
67	5	2579	G	C2-N3-C4	-5.71	109.04	111.90
76	9	948	C	C6-N1-C2	-5.71	118.02	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4434	C	N1-C2-O2	5.71	122.33	118.90
67	5	977	C	O4'-C1'-N1	5.71	112.77	108.20
67	5	3859	G	C8-N9-C1'	-5.71	119.58	127.00
67	5	3871	A	C8-N9-C1'	-5.71	117.42	127.70
67	5	4305	G	N7-C8-N9	5.71	115.95	113.10
73	8	125	C	O4'-C1'-N1	5.71	112.77	108.20
67	5	4291	G	C8-N9-C1'	-5.71	119.58	127.00
67	5	2467	U	O4'-C1'-N1	5.70	112.76	108.20
67	5	105	A	N9-C4-C5	-5.70	103.52	105.80
67	5	1929	A	C4-N9-C1'	5.70	136.56	126.30
76	9	1658	G	C5-C6-O6	-5.70	125.18	128.60
67	5	4878	C	N1-C2-O2	5.70	122.32	118.90
67	5	41	C	N3-C4-C5	5.70	124.18	121.90
67	5	3685	C	N1-C2-O2	5.70	122.32	118.90
67	5	3746	A	C5-C6-N6	-5.70	119.14	123.70
67	5	4448	G	N3-C4-C5	5.70	131.45	128.60
67	5	23	C	C5-C4-N4	-5.70	116.21	120.20
67	5	106	A	C4-C5-C6	5.70	119.85	117.00
67	5	4915	G	N3-C4-C5	5.69	131.45	128.60
67	5	969	C	C6-N1-C2	-5.69	118.02	120.30
67	5	3748	A	N1-C2-N3	5.69	132.15	129.30
67	5	4171	C	C6-N1-C2	5.69	122.58	120.30
28	ii	232	PHE	CB-CG-CD2	-5.69	116.82	120.80
67	5	105	A	C5-N7-C8	-5.69	101.06	103.90
67	5	2074	C	N3-C4-C5	5.69	124.17	121.90
76	9	47	G	C2-N3-C4	-5.69	109.06	111.90
67	5	101	A	N9-C4-C5	-5.69	103.53	105.80
67	5	1920	C	C6-N1-C1'	-5.68	113.98	120.80
67	5	1983	A	O4'-C1'-N9	5.68	112.75	108.20
76	9	1055	A	C4-C5-N7	5.68	113.54	110.70
67	5	4193	C	C5-C4-N4	-5.68	116.22	120.20
67	5	4710	C	N3-C2-O2	-5.68	117.92	121.90
67	5	1880	G	C4-N9-C1'	5.68	133.88	126.50
73	8	125	C	N1-C1'-C2'	5.68	121.38	114.00
73	8	135	C	C6-N1-C2	-5.68	118.03	120.30
76	9	639	C	C6-N1-C2	-5.68	118.03	120.30
67	5	18	C	C2-N1-C1'	5.68	125.05	118.80
67	5	2815	A	C8-N9-C1'	-5.68	117.48	127.70
67	5	148	A	N1-C6-N6	5.68	122.00	118.60
67	5	2051	C	C5-C4-N4	-5.68	116.23	120.20
67	5	3929	G	C8-N9-C1'	-5.68	119.62	127.00
76	9	11	A	C8-N9-C4	5.68	108.07	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	9	1695	A	N1-C6-N6	5.68	122.01	118.60
67	5	945	U	O4'-C1'-N1	5.67	112.74	108.20
67	5	4230	C	N3-C2-O2	-5.67	117.93	121.90
67	5	4631	G	N3-C4-N9	5.67	129.41	126.00
76	9	1060	A	O4'-C1'-N9	5.67	112.74	108.20
67	5	1830	G	C4-N9-C1'	5.67	133.88	126.50
67	5	3857	G	N3-C2-N2	5.67	123.87	119.90
67	5	651	C	C2-N1-C1'	5.67	125.04	118.80
67	5	713	C	N3-C2-O2	-5.67	117.93	121.90
67	5	4549	G	N3-C2-N2	5.67	123.87	119.90
76	9	1257	G	C4-N9-C1'	-5.67	119.13	126.50
67	5	1585	C	O4'-C1'-N1	5.67	112.73	108.20
67	5	1627	G	C6-C5-N7	-5.67	127.00	130.40
76	9	504	G	N3-C2-N2	5.67	123.87	119.90
67	5	4415	A	N9-C1'-C2'	-5.67	105.77	112.00
67	5	90	G	C4-N9-C1'	5.66	133.86	126.50
76	9	1247	C	O4'-C1'-N1	-5.66	103.67	108.20
67	5	2509	C	C6-N1-C1'	-5.66	114.01	120.80
67	5	1633	G	P-O3'-C3'	5.66	126.49	119.70
67	5	1660	U	O4'-C1'-N1	5.66	112.73	108.20
67	5	21	G	N3-C2-N2	5.66	123.86	119.90
67	5	1506	G	N3-C2-N2	5.66	123.86	119.90
67	5	3891	A	C5-C6-N1	5.66	120.53	117.70
76	9	1425	G	C4-N9-C1'	5.66	133.85	126.50
67	5	1843	A	C5-C6-N1	5.66	120.53	117.70
76	9	1327	G	O5'-P-OP2	-5.66	100.61	105.70
67	5	336	A	C6-N1-C2	-5.65	115.21	118.60
67	5	1899	G	C6-C5-N7	-5.65	127.01	130.40
73	8	41	A	N3-C4-N9	-5.65	122.88	127.40
67	5	294	G	N3-C2-N2	5.65	123.86	119.90
67	5	3632	C	C2-N1-C1'	5.65	125.02	118.80
67	5	4211	C	P-O3'-C3'	5.65	126.48	119.70
72	Y	94	THR	CA-CB-CG2	-5.65	104.49	112.40
67	5	2789	A	N9-C4-C5	-5.65	103.54	105.80
67	5	4363	A	C5-C6-N6	-5.65	119.18	123.70
67	5	4286	C	C2-N1-C1'	5.65	125.01	118.80
67	5	54	G	N1-C2-N2	-5.65	111.12	116.20
67	5	3834	C	C2-N1-C1'	5.65	125.01	118.80
67	5	263	G	C4-N9-C1'	5.64	133.84	126.50
76	9	613	G	C8-N9-C4	-5.64	104.14	106.40
76	9	1610	G	C4-N9-C1'	5.64	133.84	126.50
67	5	4525	C	N3-C2-O2	-5.64	117.95	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	8	32	C	N1-C2-O2	5.64	122.29	118.90
60	T	145	GLY	N-CA-C	5.64	127.20	113.10
76	9	603	C	C6-N1-C2	5.64	122.56	120.30
67	5	2068	C	C5-C6-N1	5.64	123.82	121.00
11	E	128	LEU	CB-CG-CD2	-5.64	101.42	111.00
67	5	41	C	C5-C4-N4	-5.64	116.25	120.20
67	5	1234	G	C2-N3-C4	-5.64	109.08	111.90
67	5	1541	C	C5-C4-N4	-5.64	116.25	120.20
67	5	1510	G	C8-N9-C1'	-5.64	119.67	127.00
67	5	1738	A	C5-C6-N6	-5.64	119.19	123.70
67	5	3901	A	C6-C5-N7	-5.64	128.35	132.30
76	9	624	C	C6-N1-C2	-5.64	118.05	120.30
67	5	1314	C	O4'-C1'-N1	5.63	112.71	108.20
67	5	1321	G	N1-C2-N2	-5.63	111.13	116.20
67	5	2896	G	C8-N9-C4	-5.63	104.15	106.40
67	5	4091	G	N3-C4-C5	-5.63	125.78	128.60
67	5	4502	C	O4'-C1'-N1	5.63	112.71	108.20
67	5	4681	A	N9-C4-C5	-5.63	103.55	105.80
67	5	352	G	C6-C5-N7	-5.63	127.02	130.40
67	5	364	G	C6-C5-N7	-5.63	127.02	130.40
67	5	4517	A	C8-N9-C4	-5.63	103.55	105.80
67	5	166	C	N3-C4-C5	5.63	124.15	121.90
67	5	1373	A	C5-C6-N6	-5.63	119.20	123.70
67	5	4189	U	N3-C4-O4	5.63	123.34	119.40
76	9	547	G	C8-N9-C1'	-5.63	119.68	127.00
67	5	1607	C	C2-N1-C1'	5.63	124.99	118.80
67	5	1654	G	N9-C4-C5	-5.63	103.15	105.40
67	5	3858	C	C2-N1-C1'	5.63	124.99	118.80
76	9	35	C	N3-C4-C5	5.63	124.15	121.90
67	5	1191	C	C5-C4-N4	5.63	124.14	120.20
67	5	2543	A	N1-C6-N6	5.63	121.97	118.60
67	5	3617	G	N3-C4-C5	5.63	131.41	128.60
67	5	1358	G	O4'-C1'-N9	-5.62	103.70	108.20
67	5	1998	A	O4'-C1'-N9	-5.62	103.70	108.20
67	5	4945	G	N1-C2-N2	-5.62	111.14	116.20
73	8	47	C	C2-N1-C1'	5.62	124.99	118.80
67	5	942	G	N1-C2-N2	-5.62	111.14	116.20
67	5	1515	A	C5-C6-N6	-5.62	119.20	123.70
67	5	2022	C	N3-C4-C5	5.62	124.15	121.90
67	5	2672	C	C2-N1-C1'	5.62	124.98	118.80
67	5	3911	C	C5-C4-N4	-5.62	116.26	120.20
67	5	719	C	C2-N1-C1'	5.62	124.98	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1812	C	N1-C2-O2	5.62	122.27	118.90
67	5	2754	G	C2-N3-C4	-5.62	109.09	111.90
67	5	3871	A	C5-C6-N1	5.62	120.51	117.70
76	9	347	G	N1-C2-N2	5.62	121.26	116.20
67	5	4516	G	C8-N9-C4	-5.62	104.15	106.40
67	5	4917	C	C6-N1-C1'	-5.61	114.06	120.80
67	5	1306	C	C6-N1-C1'	-5.61	114.07	120.80
67	5	1764	G	C4-N9-C1'	5.61	133.79	126.50
67	5	1895	G	C4-N9-C1'	5.61	133.79	126.50
67	5	2337	C	N3-C2-O2	-5.61	117.97	121.90
73	8	28	C	C2-N1-C1'	5.61	124.97	118.80
67	5	1323	A	C5-N7-C8	-5.61	101.10	103.90
67	5	1812	C	C5-C4-N4	-5.61	116.27	120.20
73	8	44	A	C6-C5-N7	-5.61	128.38	132.30
34	k	64	LEU	CA-CB-CG	5.61	128.19	115.30
76	9	1740	C	C5-C4-N4	-5.61	116.28	120.20
76	9	1019	C	C6-N1-C1'	-5.60	114.08	120.80
67	5	298	G	C4-N9-C1'	5.60	133.78	126.50
67	5	955	G	C4-N9-C1'	5.60	133.78	126.50
67	5	1586	G	C8-N9-C4	-5.60	104.16	106.40
67	5	1739	G	C8-N9-C1'	-5.60	119.72	127.00
67	5	2071	A	C5-C6-N1	5.60	120.50	117.70
67	5	2889	G	C4-N9-C1'	5.60	133.78	126.50
67	5	4479	A	O4'-C1'-N9	5.60	112.68	108.20
67	5	4291	G	O4'-C1'-N9	5.60	112.68	108.20
67	5	4533	A	N9-C4-C5	-5.60	103.56	105.80
67	5	4640	C	C5-C4-N4	-5.60	116.28	120.20
76	9	329	G	C8-N9-C1'	-5.60	119.72	127.00
67	5	1924	C	C6-N1-C1'	-5.60	114.08	120.80
67	5	38	A	N3-C4-N9	5.59	131.88	127.40
67	5	386	A	C4-C5-N7	5.59	113.50	110.70
67	5	418	A	N1-C2-N3	5.59	132.10	129.30
67	5	4671	C	C5-C4-N4	-5.59	116.28	120.20
67	5	1484	G	N3-C4-N9	5.59	129.36	126.00
67	5	1537	A	C5-C6-N1	5.59	120.50	117.70
67	5	1675	C	C6-N1-C1'	-5.59	114.09	120.80
67	5	2081	C	C2-N1-C1'	5.59	124.95	118.80
67	5	2282	A	C8-N9-C4	-5.59	103.56	105.80
67	5	3820	G	C4-N9-C1'	5.59	133.77	126.50
76	9	1414	A	O4'-C1'-N9	-5.59	103.73	108.20
67	5	364	G	N9-C4-C5	-5.59	103.16	105.40
67	5	3871	A	N1-C2-N3	5.59	132.09	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4949	G	N3-C2-N2	-5.59	115.99	119.90
67	5	364	G	O4'-C1'-N9	5.59	112.67	108.20
67	5	100	C	N3-C4-C5	5.59	124.14	121.90
67	5	2443	G	N3-C4-C5	-5.59	125.81	128.60
73	8	26	C	N3-C2-O2	-5.59	117.99	121.90
76	9	1014	G	N9-C4-C5	-5.59	103.17	105.40
67	5	656	C	C6-N1-C2	5.58	122.53	120.30
67	5	4213	A	C4-N9-C1'	5.58	136.35	126.30
67	5	4503	A	C5-C6-N1	5.58	120.49	117.70
67	5	1321	G	C4-N9-C1'	5.58	133.76	126.50
67	5	1872	G	N1-C2-N2	-5.58	111.18	116.20
67	5	1890	G	C6-C5-N7	-5.58	127.05	130.40
76	9	1262	C	O4'-C1'-N1	5.58	112.67	108.20
67	5	1458	C	N3-C4-C5	5.58	124.13	121.90
67	5	2355	G	N3-C2-N2	5.58	123.81	119.90
67	5	352	G	C4-C5-N7	5.58	113.03	110.80
67	5	2853	C	N3-C4-C5	5.58	124.13	121.90
67	5	3924	C	C5-C4-N4	-5.58	116.30	120.20
67	5	3924	C	N1-C2-O2	5.58	122.25	118.90
76	9	1250	A	C4-N9-C1'	5.58	136.34	126.30
67	5	1218	G	C4-N9-C1'	-5.58	119.25	126.50
67	5	1329	G	C8-N9-C1'	-5.58	119.75	127.00
67	5	4631	G	C4-N9-C1'	5.58	133.75	126.50
76	9	1205	C	N3-C2-O2	-5.58	118.00	121.90
76	9	1223	A	N9-C4-C5	-5.58	103.57	105.80
76	9	1275	G	O4'-C1'-N9	5.58	112.66	108.20
67	5	1816	C	C6-N1-C2	-5.57	118.07	120.30
67	5	3816	A	C8-N9-C4	-5.57	103.57	105.80
67	5	5050	C	N3-C2-O2	-5.57	118.00	121.90
67	5	923	C	N3-C4-C5	5.57	124.13	121.90
67	5	1451	G	C8-N9-C4	-5.57	104.17	106.40
67	5	4380	A	C5-C6-N6	-5.57	119.24	123.70
76	9	1501	C	N3-C2-O2	-5.57	118.00	121.90
67	5	1920	C	C2-N1-C1'	5.57	124.93	118.80
67	5	81	C	N3-C2-O2	-5.57	118.00	121.90
67	5	1507	C	C5-C6-N1	5.57	123.78	121.00
67	5	1632	A	O4'-C1'-N9	5.57	112.66	108.20
67	5	4682	U	O4'-C1'-N1	5.57	112.65	108.20
67	5	4969	C	C6-N1-C2	-5.57	118.07	120.30
73	8	148	A	C6-N1-C2	-5.57	115.26	118.60
76	9	1389	C	N3-C2-O2	-5.57	118.00	121.90
67	5	4681	A	N1-C6-N6	5.56	121.94	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	9	1856	C	C5-C4-N4	-5.56	116.31	120.20
67	5	2577	C	N3-C4-C5	5.56	124.12	121.90
67	5	4186	A	N1-C2-N3	5.56	132.08	129.30
67	5	4279	A	C4-C5-N7	5.56	113.48	110.70
73	8	47	C	N3-C4-N4	5.56	121.89	118.00
67	5	1065	G	C5-C6-O6	5.56	131.94	128.60
67	5	1794	A	C4-N9-C1'	5.56	136.30	126.30
67	5	2379	A	N9-C4-C5	-5.56	103.58	105.80
73	8	28	C	C6-N1-C2	-5.56	118.08	120.30
73	8	44	A	C4-C5-N7	5.56	113.48	110.70
76	9	140	U	C5-C6-N1	5.56	125.48	122.70
56	RR	60	ARG	CA-CB-CG	5.55	125.62	113.40
67	5	1575	A	C4-N9-C1'	5.55	136.30	126.30
67	5	1663	C	N3-C4-N4	5.55	121.89	118.00
67	5	2591	A	C5-C6-N6	-5.55	119.26	123.70
67	5	3774	A	C6-C5-N7	-5.55	128.41	132.30
67	5	4523	A	N1-C6-N6	-5.55	115.27	118.60
76	9	473	A	C5-C6-N1	5.55	120.48	117.70
76	9	1216	C	C6-N1-C1'	5.55	127.47	120.80
67	5	1502	G	N3-C4-C5	5.55	131.38	128.60
17	BB	62	LEU	CB-CG-CD2	-5.55	101.56	111.00
42	N	14	LYS	CD-CE-NZ	5.55	124.47	111.70
67	5	1739	G	N3-C4-N9	5.55	129.33	126.00
67	5	4310	A	C5-C6-N1	5.55	120.48	117.70
76	9	1610	G	N3-C4-N9	5.55	129.33	126.00
67	5	284	G	N3-C4-N9	5.55	129.33	126.00
67	5	2050	G	C8-N9-C1'	-5.55	119.79	127.00
67	5	4868	G	C8-N9-C4	-5.55	104.18	106.40
67	5	1967	A	N1-C6-N6	5.55	121.93	118.60
76	9	1354	G	N3-C2-N2	5.55	123.78	119.90
67	5	234	G	N3-C4-C5	5.55	131.37	128.60
67	5	1316	G	N1-C2-N2	-5.55	111.21	116.20
67	5	1890	G	N1-C6-O6	5.55	123.23	119.90
67	5	3704	U	N1-C2-O2	-5.55	118.92	122.80
67	5	4091	G	N3-C4-N9	5.55	129.33	126.00
67	5	4444	C	C2-N1-C1'	5.55	124.90	118.80
76	9	659	G	C4-N9-C1'	5.55	133.71	126.50
76	9	1618	C	O5'-P-OP1	-5.55	100.71	105.70
67	5	1455	G	C4-N9-C1'	5.54	133.71	126.50
67	5	409	G	C8-N9-C4	-5.54	104.18	106.40
67	5	1670	G	C8-N9-C1'	-5.54	119.79	127.00
67	5	4618	G	N7-C8-N9	5.54	115.87	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1350	C	C6-N1-C2	-5.54	118.08	120.30
73	8	103	A	C5-N7-C8	-5.54	101.13	103.90
76	9	391	C	C6-N1-C1'	-5.54	114.15	120.80
67	5	382	G	C8-N9-C1'	-5.54	119.80	127.00
67	5	1910	G	C8-N9-C1'	-5.54	119.80	127.00
67	5	4384	U	C5-C4-O4	-5.54	122.58	125.90
67	5	4487	A	C5-C6-N6	-5.54	119.27	123.70
67	5	1404	G	N3-C4-N9	-5.54	122.68	126.00
67	5	3612	C	C2-N1-C1'	5.54	124.89	118.80
67	5	4124	G	C4-N9-C1'	5.54	133.70	126.50
76	9	1464	C	C2-N1-C1'	-5.54	112.71	118.80
67	5	2410	C	N1-C2-O2	5.54	122.22	118.90
76	9	1798	C	C2-N1-C1'	5.54	124.89	118.80
24	bb	63	LEU	CB-CG-CD2	-5.53	101.59	111.00
67	5	1397	A	C5-C6-N1	5.53	120.47	117.70
67	5	4155	C	N1-C2-O2	5.53	122.22	118.90
21	h	87	LYS	CD-CE-NZ	-5.53	98.98	111.70
67	5	1274	A	N1-C6-N6	5.53	121.92	118.60
67	5	4427	G	C4-N9-C1'	5.53	133.69	126.50
67	5	2302	C	C2-N1-C1'	5.53	124.88	118.80
67	5	1795	A	C5-C6-N1	5.53	120.46	117.70
76	9	1755	C	N1-C2-O2	5.53	122.22	118.90
67	5	1373	A	C8-N9-C1'	-5.53	117.75	127.70
67	5	1520	C	C5-C4-N4	-5.53	116.33	120.20
67	5	1878	G	C8-N9-C4	-5.53	104.19	106.40
67	5	4749	C	N3-C4-C5	5.52	124.11	121.90
67	5	707	C	N1-C2-O2	5.52	122.21	118.90
67	5	4631	G	C6-C5-N7	-5.52	127.09	130.40
70	7	57	C	C6-N1-C1'	-5.52	114.17	120.80
67	5	2423	A	N1-C6-N6	5.52	121.91	118.60
67	5	4560	C	N3-C4-C5	5.52	124.11	121.90
70	7	36	C	C2-N1-C1'	5.52	124.87	118.80
67	5	285	G	N1-C2-N2	-5.52	111.23	116.20
67	5	1503	A	O4'-C1'-N9	5.52	112.61	108.20
67	5	2025	A	C4-C5-C6	-5.52	114.24	117.00
67	5	323	C	C2-N1-C1'	5.52	124.87	118.80
67	5	3646	A	N1-C6-N6	5.51	121.91	118.60
67	5	1322	A	O4'-C1'-N9	-5.51	103.79	108.20
76	9	293	C	O4'-C1'-N1	5.51	112.61	108.20
67	5	1887	G	C4-N9-C1'	5.51	133.66	126.50
67	5	5008	C	C5-C4-N4	-5.51	116.34	120.20
76	9	911	C	N3-C4-C5	5.51	124.11	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	240	G	C4-N9-C1'	5.51	133.66	126.50
76	9	223	C	C2-N1-C1'	5.51	124.86	118.80
76	9	1793	A	C5-C6-N1	5.51	120.45	117.70
67	5	2318	G	N1-C2-N2	-5.51	111.24	116.20
67	5	3864	C	N3-C4-C5	5.51	124.10	121.90
73	8	13	G	N1-C2-N3	5.51	127.20	123.90
67	5	4316	G	C8-N9-C4	-5.51	104.20	106.40
76	9	41	G	O4'-C1'-N9	5.51	112.61	108.20
67	5	1982	G	C8-N9-C4	-5.50	104.20	106.40
67	5	2051	C	C2-N1-C1'	5.50	124.86	118.80
67	5	2420	A	N1-C6-N6	5.50	121.90	118.60
67	5	4097	G	N3-C4-C5	5.50	131.35	128.60
67	5	385	A	O4'-C1'-N9	5.50	112.60	108.20
67	5	2332	A	C5-N7-C8	-5.50	101.15	103.90
67	5	2511	A	C8-N9-C4	-5.50	103.60	105.80
76	9	1860	A	C6-N1-C2	-5.50	115.30	118.60
67	5	303	C	C6-N1-C2	-5.50	118.10	120.30
67	5	408	A	N7-C8-N9	5.50	116.55	113.80
67	5	1404	G	N3-C4-C5	5.50	131.35	128.60
67	5	2878	G	N3-C2-N2	5.50	123.75	119.90
67	5	3871	A	C4-N9-C1'	5.50	136.20	126.30
67	5	4195	G	C4-N9-C1'	5.50	133.65	126.50
73	8	135	C	C2-N1-C1'	5.50	124.85	118.80
76	9	429	C	N1-C2-O2	5.50	122.20	118.90
67	5	1384	C	C6-N1-C2	-5.50	118.10	120.30
17	BB	228	LEU	CA-CB-CG	5.50	127.94	115.30
67	5	1887	G	N1-C2-N2	-5.50	111.25	116.20
67	5	2036	C	C2-N1-C1'	5.50	124.84	118.80
67	5	2715	G	C2-N3-C4	-5.50	109.15	111.90
67	5	4497	U	O4'-C1'-N1	5.50	112.60	108.20
67	5	4764	A	C8-N9-C4	5.50	108.00	105.80
67	5	4942	C	N3-C2-O2	-5.50	118.05	121.90
76	9	319	C	C6-N1-C1'	5.50	127.39	120.80
67	5	2793	G	C2-N3-C4	-5.50	109.15	111.90
67	5	3719	A	C5-C6-N6	-5.50	119.30	123.70
76	9	347	G	N3-C4-C5	5.50	131.35	128.60
67	5	452	A	N1-C6-N6	5.49	121.90	118.60
67	5	2435	G	N3-C4-N9	-5.49	122.70	126.00
67	5	2438	A	C5-N7-C8	-5.49	101.15	103.90
67	5	3923	A	C5-C6-N1	5.49	120.45	117.70
67	5	4485	C	N1-C2-O2	5.49	122.20	118.90
67	5	707	C	N3-C2-O2	-5.49	118.06	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	928	C	C5-C4-N4	-5.49	116.36	120.20
76	9	1828	C	N3-C4-C5	5.49	124.10	121.90
67	5	1342	A	C5-N7-C8	-5.49	101.16	103.90
67	5	1898	C	N3-C4-N4	5.49	121.84	118.00
67	5	4527	G	C4-N9-C1'	5.49	133.64	126.50
73	8	10	G	C6-C5-N7	-5.49	127.11	130.40
76	9	1215	C	N3-C4-C5	-5.49	119.70	121.90
67	5	437	G	C8-N9-C1'	-5.49	119.87	127.00
67	5	2001	G	C4-N9-C1'	-5.49	119.37	126.50
76	9	1806	A	C5-C6-N6	-5.49	119.31	123.70
76	9	11	A	N1-C6-N6	5.48	121.89	118.60
76	9	853	C	C6-N1-C2	-5.48	118.11	120.30
67	5	1064	G	N3-C4-C5	-5.48	125.86	128.60
67	5	1629	G	C4-N9-C1'	5.48	133.63	126.50
67	5	4183	G	C8-N9-C1'	5.48	134.13	127.00
70	7	34	C	C5-C4-N4	-5.48	116.36	120.20
76	9	1580	A	C8-N9-C4	-5.48	103.61	105.80
76	9	1715	A	C4-C5-N7	5.48	113.44	110.70
50	PP	40	ARG	NE-CZ-NH2	-5.48	117.56	120.30
67	5	1352	C	N3-C4-C5	5.48	124.09	121.90
67	5	2878	G	C4-C5-N7	5.48	112.99	110.80
67	5	1283	G	N3-C4-N9	-5.48	122.71	126.00
67	5	2351	C	O4'-C1'-N1	5.48	112.58	108.20
67	5	3934	G	C8-N9-C4	-5.48	104.21	106.40
76	9	1852	C	C6-N1-C2	-5.48	118.11	120.30
42	N	22	LEU	CB-CG-CD2	-5.48	101.69	111.00
67	5	285	G	C5-C6-O6	5.47	131.88	128.60
72	Y	113	LYS	CA-CB-CG	5.47	125.44	113.40
12	f	46	ARG	NE-CZ-NH2	-5.47	117.56	120.30
67	5	1357	C	N3-C2-O2	-5.47	118.07	121.90
67	5	2603	C	N3-C4-N4	5.47	121.83	118.00
28	ii	290	TYR	CB-CG-CD1	-5.47	117.72	121.00
67	5	1626	G	N3-C4-N9	-5.47	122.72	126.00
67	5	1857	C	C5-C4-N4	-5.47	116.37	120.20
67	5	1938	C	C6-N1-C1'	-5.47	114.24	120.80
67	5	2871	A	N1-C6-N6	5.47	121.88	118.60
67	5	3612	C	N1-C2-O2	5.47	122.18	118.90
67	5	339	C	C6-N1-C1'	-5.47	114.24	120.80
67	5	5004	C	C6-N1-C2	-5.47	118.11	120.30
67	5	3909	C	C5-C4-N4	-5.47	116.37	120.20
67	5	4333	C	C5-C4-N4	-5.47	116.37	120.20
67	5	4868	G	C8-N9-C1'	-5.47	119.89	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	418	A	C4-N9-C1'	5.46	136.13	126.30
67	5	1803	G	C8-N9-C4	5.46	108.58	106.40
67	5	2739	C	N3-C4-C5	5.46	124.08	121.90
67	5	4213	A	C8-N9-C4	-5.46	103.61	105.80
67	5	3857	G	N3-C4-C5	-5.46	125.87	128.60
67	5	4598	C	C5-C4-N4	-5.46	116.38	120.20
76	9	672	A	N1-C6-N6	5.46	121.88	118.60
67	5	651	C	C6-N1-C1'	-5.46	114.25	120.80
67	5	4335	C	N3-C4-C5	5.46	124.08	121.90
76	9	1490	G	C8-N9-C1'	-5.46	119.90	127.00
67	5	1777	C	C2-N1-C1'	5.46	124.80	118.80
67	5	1945	G	C8-N9-C4	-5.46	104.22	106.40
67	5	4513	A	C6-N1-C2	-5.46	115.33	118.60
70	7	97	G	N3-C2-N2	-5.46	116.08	119.90
67	5	229	G	C4-C5-N7	5.46	112.98	110.80
67	5	2001	G	C8-N9-C1'	5.46	134.09	127.00
67	5	80	C	N3-C2-O2	-5.45	118.08	121.90
73	8	150	C	N3-C4-N4	-5.45	114.18	118.00
76	9	215	G	N3-C4-C5	5.45	131.33	128.60
76	9	1760	G	N1-C6-O6	-5.45	116.63	119.90
76	9	1245	G	C2-N3-C4	5.45	114.63	111.90
32	jj	569	LEU	CA-CB-CG	5.45	127.84	115.30
76	9	1226	G	N7-C8-N9	5.45	115.83	113.10
76	9	1230	C	O4'-C1'-N1	5.45	112.56	108.20
67	5	39	A	C4-C5-C6	5.45	119.72	117.00
67	5	2622	G	C8-N9-C1'	-5.45	119.92	127.00
67	5	3760	A	C5-C6-N6	5.45	128.06	123.70
67	5	3840	U	O4'-C1'-N1	5.45	112.56	108.20
67	5	1941	A	C5-C6-N6	5.45	128.06	123.70
67	5	2381	A	C5-C6-N6	5.45	128.06	123.70
67	5	3696	C	C2-N1-C1'	5.45	124.79	118.80
76	9	545	A	N1-C6-N6	5.45	121.87	118.60
82	c	42	LYS	CD-CE-NZ	5.44	124.22	111.70
4	DD	76	ARG	NE-CZ-NH1	5.44	123.02	120.30
32	jj	379	LEU	CB-CG-CD2	-5.44	101.75	111.00
67	5	39	A	N7-C8-N9	5.44	116.52	113.80
67	5	199	G	O4'-C1'-N9	5.44	112.55	108.20
67	5	2435	G	C2-N3-C4	-5.44	109.18	111.90
67	5	4277	G	N3-C4-N9	5.44	129.27	126.00
67	5	4668	U	O5'-P-OP1	-5.44	100.80	105.70
67	5	4701	A	C8-N9-C1'	5.44	137.50	127.70
73	8	8	U	C2-N1-C1'	5.44	124.23	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	9	1294	G	N3-C4-C5	-5.44	125.88	128.60
67	5	39	A	C6-C5-N7	-5.44	128.49	132.30
67	5	1884	C	N1-C2-O2	5.44	122.16	118.90
70	7	36	C	C6-N1-C1'	-5.44	114.27	120.80
67	5	4204	C	C2-N1-C1'	5.44	124.78	118.80
67	5	111	C	C6-N1-C2	-5.44	118.12	120.30
67	5	283	G	C8-N9-C1'	-5.44	119.93	127.00
67	5	749	G	C2-N3-C4	-5.44	109.18	111.90
67	5	2006	U	O4'-C1'-N1	5.44	112.55	108.20
67	5	2815	A	C4-N9-C1'	5.44	136.09	126.30
76	9	123	G	N3-C4-C5	-5.44	125.88	128.60
76	9	1849	G	C6-C5-N7	-5.44	127.14	130.40
67	5	1811	G	N3-C4-N9	-5.43	122.74	126.00
67	5	4088	C	N3-C2-O2	-5.43	118.10	121.90
67	5	4579	U	N3-C4-O4	5.43	123.20	119.40
76	9	1638	G	C8-N9-C1'	5.43	134.06	127.00
67	5	3835	C	C2-N1-C1'	5.43	124.78	118.80
67	5	4604	G	C8-N9-C1'	-5.43	119.94	127.00
67	5	1629	G	N1-C6-O6	5.43	123.16	119.90
67	5	1573	G	C8-N9-C4	-5.43	104.23	106.40
67	5	2276	A	C5-C6-N6	-5.43	119.36	123.70
67	5	3630	A	N1-C6-N6	-5.43	115.34	118.60
67	5	4412	C	C2-N1-C1'	5.43	124.77	118.80
70	7	15	C	C2-N1-C1'	5.43	124.77	118.80
76	9	1527	C	C6-N1-C2	5.43	122.47	120.30
76	9	1860	A	C5-C6-N6	-5.43	119.36	123.70
67	5	962	C	C6-N1-C2	-5.43	118.13	120.30
67	5	3617	G	N3-C4-N9	-5.43	122.74	126.00
67	5	4374	U	O4'-C1'-N1	-5.43	103.86	108.20
67	5	1216	C	C6-N1-C2	5.42	122.47	120.30
67	5	4511	A	N1-C6-N6	-5.42	115.35	118.60
8	EE	162	ILE	CG1-CB-CG2	-5.42	99.47	111.40
67	5	2895	A	C5-C6-N6	-5.42	119.36	123.70
67	5	3692	A	C5-C6-N6	-5.42	119.36	123.70
73	8	96	C	N3-C4-N4	5.42	121.80	118.00
73	8	121	G	C2-N3-C4	-5.42	109.19	111.90
67	5	1553	A	N1-C6-N6	5.42	121.85	118.60
67	5	1883	G	O4'-C1'-N9	-5.42	103.86	108.20
67	5	2429	A	C6-N1-C2	-5.42	115.35	118.60
67	5	4179	G	N3-C2-N2	5.42	123.69	119.90
76	9	1274	G	N3-C2-N2	5.42	123.69	119.90
67	5	4726	G	C2-N3-C4	-5.42	109.19	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4169	G	N1-C2-N2	-5.42	111.32	116.20
67	5	4517	A	C6-N1-C2	-5.42	115.35	118.60
67	5	4945	G	N9-C4-C5	-5.42	103.23	105.40
76	9	587	A	O4'-C1'-N9	-5.42	103.86	108.20
67	5	315	G	O4'-C1'-N9	5.42	112.53	108.20
67	5	713	C	N1-C2-O2	5.42	122.15	118.90
67	5	2860	C	C2-N1-C1'	5.42	124.76	118.80
76	9	1327	G	C4-N9-C1'	5.42	133.54	126.50
67	5	89	C	N3-C2-O2	-5.42	118.11	121.90
67	5	4744	A	O4'-C1'-N9	-5.42	103.87	108.20
67	5	210	C	N3-C4-C5	5.41	124.07	121.90
67	5	2379	A	C4-N9-C1'	5.41	136.04	126.30
67	5	4239	A	C5-C6-N6	-5.41	119.37	123.70
73	8	41	A	N1-C6-N6	-5.41	115.35	118.60
73	8	148	A	C5-C6-N1	5.41	120.41	117.70
67	5	1803	G	N9-C4-C5	-5.41	103.23	105.40
67	5	1549	G	C8-N9-C4	-5.41	104.24	106.40
67	5	1584	G	N1-C6-O6	5.41	123.15	119.90
67	5	4087	G	C4-N9-C1'	-5.41	119.47	126.50
67	5	4330	G	N3-C4-C5	-5.41	125.89	128.60
67	5	352	G	C2-N3-C4	-5.41	109.19	111.90
67	5	1788	A	O4'-C1'-N9	5.41	112.53	108.20
67	5	1842	G	N3-C2-N2	5.41	123.69	119.90
67	5	4550	G	N1-C2-N3	5.41	127.14	123.90
67	5	55	G	N3-C4-C5	-5.41	125.90	128.60
76	9	669	A	C8-N9-C1'	-5.41	117.97	127.70
67	5	1310	C	N1-C2-O2	5.41	122.14	118.90
67	5	2871	A	C5-C6-N6	-5.41	119.38	123.70
70	7	109	U	C2-N1-C1'	5.41	124.19	117.70
73	8	26	C	C6-N1-C1'	-5.41	114.31	120.80
67	5	4394	A	C5-C6-N6	-5.40	119.38	123.70
67	5	1651	G	N3-C4-N9	5.40	129.24	126.00
67	5	1626	G	N3-C4-C5	5.40	131.30	128.60
76	9	1394	G	O4'-C1'-N9	-5.40	103.88	108.20
67	5	2478	C	C6-N1-C2	-5.40	118.14	120.30
67	5	2691	U	C6-N1-C2	-5.40	117.76	121.00
67	5	4092	G	C4-N9-C1'	5.40	133.52	126.50
67	5	4978	G	N1-C2-N2	-5.40	111.34	116.20
67	5	1589	C	N3-C2-O2	-5.40	118.12	121.90
67	5	2591	A	N1-C6-N6	5.40	121.84	118.60
76	9	1280	G	N3-C4-N9	5.40	129.24	126.00
76	9	1413	G	C8-N9-C1'	-5.40	119.98	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1577	G	C4-N9-C1'	5.39	133.51	126.50
67	5	4522	G	C4-C5-N7	5.39	112.96	110.80
76	9	1666	C	C6-N1-C1'	-5.39	114.33	120.80
76	9	1588	A	C5-C6-N6	5.39	128.01	123.70
67	5	1510	G	C4-N9-C1'	5.39	133.51	126.50
67	5	1893	C	O4'-C1'-N1	5.39	112.51	108.20
67	5	3783	A	O4'-C1'-N9	5.39	112.51	108.20
76	9	391	C	C2-N1-C1'	5.39	124.73	118.80
67	5	401	G	N3-C4-C5	-5.39	125.91	128.60
67	5	1346	C	N3-C4-C5	5.39	124.06	121.90
67	5	3903	A	C5-N7-C8	-5.39	101.21	103.90
67	5	4623	G	N7-C8-N9	5.39	115.79	113.10
67	5	2615	C	C6-N1-C2	-5.39	118.14	120.30
67	5	75	G	N1-C2-N2	-5.38	111.35	116.20
67	5	3857	G	N3-C4-N9	5.38	129.23	126.00
67	5	2321	G	N3-C4-C5	5.38	131.29	128.60
67	5	2509	C	N1-C2-O2	5.38	122.13	118.90
67	5	3705	G	C4-N9-C1'	5.38	133.50	126.50
76	9	435	A	N1-C6-N6	-5.38	115.37	118.60
76	9	886	A	N1-C6-N6	-5.38	115.37	118.60
67	5	1594	C	N3-C4-C5	5.38	124.05	121.90
67	5	1668	A	N1-C6-N6	-5.38	115.37	118.60
67	5	1552	G	C2-N3-C4	-5.38	109.21	111.90
67	5	1573	G	N9-C1'-C2'	5.38	120.99	114.00
67	5	643	C	C6-N1-C2	5.38	122.45	120.30
67	5	2033	A	C5-C6-N6	-5.38	119.40	123.70
67	5	4978	G	C8-N9-C1'	-5.38	120.01	127.00
67	5	4688	C	C6-N1-C1'	-5.38	114.35	120.80
73	8	150	C	C6-N1-C2	5.38	122.45	120.30
76	9	1798	C	N3-C2-O2	-5.38	118.14	121.90
67	5	3752	C	N1-C2-O2	5.37	122.12	118.90
67	5	1308	C	C6-N1-C1'	-5.37	114.35	120.80
67	5	1310	C	C2-N1-C1'	5.37	124.71	118.80
67	5	4701	A	N1-C6-N6	-5.37	115.38	118.60
67	5	2539	C	C2-N1-C1'	5.37	124.71	118.80
67	5	2640	G	C4-N9-C1'	5.37	133.48	126.50
67	5	2847	G	C8-N9-C4	-5.37	104.25	106.40
67	5	732	A	C5-C6-N6	-5.37	119.41	123.70
69	X	147	LEU	CB-CG-CD2	-5.37	101.87	111.00
76	9	1425	G	C8-N9-C1'	-5.37	120.02	127.00
67	5	2544	G	C8-N9-C1'	-5.37	120.02	127.00
67	5	2654	C	C2-N1-C1'	5.37	124.70	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	7	29	C	N3-C4-C5	5.37	124.05	121.90
67	5	1411(C)	C	C6-N1-C2	-5.37	118.15	120.30
67	5	4317	A	C6-N1-C2	-5.37	115.38	118.60
76	9	52	G	C8-N9-C4	5.37	108.55	106.40
76	9	1335	G	N3-C2-N2	5.37	123.66	119.90
76	9	1664	A	N1-C6-N6	-5.37	115.38	118.60
67	5	917	A	N1-C6-N6	5.36	121.82	118.60
67	5	1529	G	N7-C8-N9	5.36	115.78	113.10
67	5	3882	C	N3-C2-O2	-5.36	118.15	121.90
67	5	2670	C	C5-C4-N4	-5.36	116.45	120.20
76	9	1563	G	N9-C4-C5	-5.36	103.26	105.40
67	5	221	C	C6-N1-C1'	-5.36	114.37	120.80
76	9	390	C	C6-N1-C1'	-5.36	114.37	120.80
32	jj	292	PHE	CB-CG-CD1	5.36	124.55	120.80
67	5	1619	G	C4-N9-C1'	5.36	133.47	126.50
67	5	1803	G	C2-N3-C4	-5.36	109.22	111.90
67	5	2438	A	C5-C6-N6	-5.36	119.42	123.70
67	5	2621	A	C5-C6-N6	-5.36	119.41	123.70
67	5	3654	G	C2-N3-C4	-5.36	109.22	111.90
67	5	666	G	C4-N9-C1'	-5.36	119.54	126.50
67	5	1577	G	C8-N9-C1'	-5.36	120.04	127.00
67	5	52	G	C8-N9-C1'	-5.35	120.04	127.00
67	5	343	C	C2-N1-C1'	5.35	124.69	118.80
67	5	1282	G	C6-C5-N7	-5.35	127.19	130.40
67	5	3665	G	C8-N9-C1'	-5.35	120.04	127.00
67	5	33	A	C5-N7-C8	-5.35	101.22	103.90
67	5	51	A	N9-C4-C5	-5.35	103.66	105.80
67	5	66	A	C8-N9-C4	-5.35	103.66	105.80
67	5	135	G	N3-C2-N2	5.35	123.64	119.90
67	5	3813	A	C8-N9-C1'	-5.35	118.07	127.70
67	5	4603	C	C6-N1-C1'	-5.35	114.38	120.80
76	9	1014	G	C6-C5-N7	-5.35	127.19	130.40
67	5	320	C	O4'-C1'-N1	5.35	112.48	108.20
73	8	47	C	C6-N1-C2	-5.35	118.16	120.30
76	9	1019	C	C5-C6-N1	5.35	123.67	121.00
67	5	1655	C	N1-C2-O2	5.34	122.11	118.90
67	5	1794	A	N1-C6-N6	5.34	121.81	118.60
67	5	2603	C	N1-C2-O2	5.34	122.11	118.90
67	5	4522	G	N3-C2-N2	5.34	123.64	119.90
67	5	1690	C	N1-C2-O2	5.34	122.11	118.90
67	5	3857	G	C8-N9-C4	-5.34	104.26	106.40
67	5	707	C	C2-N1-C1'	5.34	124.68	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	2824	C	N1-C2-O2	5.34	122.11	118.90
67	5	3894	A	C8-N9-C1'	-5.34	118.09	127.70
67	5	4485	C	C6-N1-C2	-5.34	118.16	120.30
76	9	1474	A	N1-C6-N6	-5.34	115.40	118.60
76	9	1702	G	N1-C6-O6	-5.34	116.69	119.90
43	n	18	ARG	CG-CD-NE	5.34	123.01	111.80
67	5	356	G	C4-N9-C1'	5.34	133.44	126.50
67	5	414	C	O4'-C1'-N1	5.34	112.47	108.20
67	5	1541	C	N3-C4-N4	5.34	121.74	118.00
67	5	2737	C	C5-C4-N4	-5.34	116.46	120.20
63	UU	39	LEU	CA-CB-CG	-5.34	103.03	115.30
67	5	90	G	C8-N9-C1'	-5.34	120.06	127.00
67	5	4565	C	C6-N1-C2	-5.34	118.17	120.30
67	5	1875	C	C5-C4-N4	-5.33	116.47	120.20
67	5	2863	G	N1-C2-N3	5.33	127.10	123.90
67	5	686	A	C5-C6-N6	-5.33	119.43	123.70
67	5	2318	G	N3-C2-N2	5.33	123.63	119.90
67	5	2468	U	P-O3'-C3'	5.33	126.10	119.70
67	5	2518	G	C2-N3-C4	-5.33	109.23	111.90
73	8	19	C	N3-C2-O2	-5.33	118.17	121.90
67	5	1842	G	N1-C2-N2	-5.33	111.40	116.20
67	5	1729	A	C6-N1-C2	-5.33	115.40	118.60
76	9	1079	C	C5-C4-N4	-5.33	116.47	120.20
67	5	4194	U	C5-C4-O4	5.33	129.10	125.90
73	8	141	C	C6-N1-C2	-5.33	118.17	120.30
67	5	1081	C	C2-N3-C4	5.33	122.56	119.90
67	5	3850	C	N3-C2-O2	-5.33	118.17	121.90
67	5	4388	A	C6-N1-C2	-5.33	115.40	118.60
50	PP	60	LEU	CB-CG-CD2	5.32	120.05	111.00
67	5	228	C	N3-C2-O2	-5.32	118.17	121.90
67	5	4541	G	C2-N3-C4	-5.32	109.24	111.90
67	5	4645	C	C6-N1-C1'	-5.32	114.41	120.80
67	5	2359	U	P-O3'-C3'	5.32	126.08	119.70
67	5	4305	G	C5-N7-C8	-5.32	101.64	104.30
76	9	884	C	C6-N1-C2	5.32	122.43	120.30
45	O	52	LEU	CA-CB-CG	5.32	127.53	115.30
67	5	2748	C	C2-N3-C4	-5.32	117.24	119.90
67	5	3867	A	N9-C4-C5	-5.32	103.67	105.80
67	5	221	C	N1-C2-O2	5.32	122.09	118.90
67	5	285	G	N1-C2-N3	5.32	127.09	123.90
67	5	1561	G	C8-N9-C1'	-5.32	120.09	127.00
67	5	2748	C	N3-C4-C5	5.32	124.03	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4087	G	C2-N3-C4	-5.32	109.24	111.90
67	5	1641	G	N3-C4-N9	-5.32	122.81	126.00
67	5	2493	G	C4-N9-C1'	5.32	133.41	126.50
67	5	4256	A	C5-C6-N6	-5.32	119.45	123.70
2	C	100	ARG	CG-CD-NE	5.31	122.96	111.80
67	5	1836	G	C8-N9-C1'	-5.31	120.09	127.00
67	5	4553	A	C8-N9-C1'	-5.31	118.14	127.70
76	9	1659	U	C6-N1-C2	-5.31	117.81	121.00
67	5	106	A	N9-C4-C5	-5.31	103.68	105.80
67	5	1830	G	C8-N9-C1'	-5.31	120.10	127.00
67	5	1846	G	N3-C4-C5	-5.31	125.94	128.60
67	5	1998	A	N1-C6-N6	5.31	121.79	118.60
67	5	2792	C	N3-C2-O2	-5.31	118.18	121.90
67	5	4298	A	C5-C6-N1	5.31	120.36	117.70
67	5	2276	A	C6-N1-C2	-5.31	115.42	118.60
76	9	1327	G	C8-N9-C1'	-5.31	120.10	127.00
76	9	925	G	N3-C4-N9	-5.31	122.82	126.00
76	9	1294	G	N1-C2-N2	-5.31	111.42	116.20
67	5	131	C	C2-N1-C1'	5.30	124.64	118.80
67	5	1610	C	N3-C4-C5	5.30	124.02	121.90
67	5	2693	G	N1-C2-N2	-5.30	111.43	116.20
67	5	2607	C	C2-N1-C1'	5.30	124.63	118.80
55	s	6	ARG	NE-CZ-NH1	5.30	122.95	120.30
67	5	1279	A	N1-C6-N6	5.30	121.78	118.60
73	8	148	A	C5-C6-N6	-5.30	119.46	123.70
58	t	15	LEU	CA-CB-CG	5.30	127.49	115.30
67	5	1789	C	N3-C4-C5	5.30	124.02	121.90
76	9	897	U	O4'-C1'-N1	5.30	112.44	108.20
76	9	1395	C	C5'-C4'-O4'	5.30	115.46	109.10
67	5	1546	C	C5-C4-N4	-5.30	116.49	120.20
67	5	3665	G	C2-N3-C4	-5.30	109.25	111.90
67	5	4214	A	C6-N1-C2	-5.30	115.42	118.60
67	5	241	G	C4-N9-C1'	5.30	133.38	126.50
67	5	2379	A	N1-C6-N6	5.30	121.78	118.60
67	5	4581	G	C2-N3-C4	-5.30	109.25	111.90
67	5	2050	G	C6-C5-N7	-5.29	127.22	130.40
67	5	2093	G	P-O3'-C3'	5.29	126.05	119.70
67	5	2404	A	C5-C6-N1	5.29	120.35	117.70
76	9	1314	U	C2-N1-C1'	5.29	124.05	117.70
67	5	240	G	C8-N9-C1'	-5.29	120.12	127.00
67	5	3649	A	C5-C6-N6	-5.29	119.47	123.70
76	9	1515	G	C8-N9-C4	-5.29	104.28	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	148	A	N9-C4-C5	-5.29	103.68	105.80
76	9	677	G	C4-N9-C1'	5.29	133.38	126.50
76	9	1394	G	C4-N9-C1'	5.29	133.38	126.50
67	5	1869	G	C4-N9-C1'	5.29	133.38	126.50
67	5	4622	A	C5-C6-N1	5.29	120.34	117.70
76	9	480	G	C6-C5-N7	-5.29	127.23	130.40
67	5	2664	G	N3-C4-N9	-5.29	122.83	126.00
67	5	53	C	N1-C2-O2	5.29	122.07	118.90
67	5	3649	A	C5-C6-N1	5.29	120.34	117.70
67	5	3916	G	C4-N9-C1'	5.29	133.37	126.50
67	5	3841	C	N3-C4-C5	5.28	124.01	121.90
67	5	4723	A	N3-C4-C5	-5.28	123.10	126.80
70	7	115	A	C5-C6-N1	5.28	120.34	117.70
67	5	409	G	N7-C8-N9	5.28	115.74	113.10
67	5	969	C	N3-C2-O2	-5.28	118.20	121.90
67	5	2603	C	C6-N1-C1'	-5.28	114.47	120.80
67	5	2772	C	N1-C2-O2	5.28	122.07	118.90
20	G	199	LEU	CB-CG-CD2	-5.28	102.03	111.00
67	5	4902	C	C6-N1-C1'	-5.28	114.47	120.80
67	5	4487	A	N1-C6-N6	5.28	121.77	118.60
67	5	4604	G	C4-N9-C1'	5.28	133.36	126.50
67	5	4920	C	N1-C1'-C2'	-5.28	106.20	112.00
76	9	1389	C	N1-C2-O2	5.28	122.06	118.90
76	9	1715	A	N9-C4-C5	-5.28	103.69	105.80
76	9	656	G	C4-N9-C1'	5.27	133.36	126.50
67	5	1065	G	N1-C6-O6	-5.27	116.74	119.90
67	5	1316	G	C8-N9-C1'	-5.27	120.14	127.00
67	5	2010	A	O4'-C1'-N9	5.27	112.42	108.20
67	5	2848	G	C5-C6-N1	-5.27	108.86	111.50
76	9	11	A	N9-C4-C5	-5.27	103.69	105.80
76	9	1603	G	N3-C2-N2	5.27	123.59	119.90
67	5	2807	A	C5-C6-N1	5.27	120.34	117.70
76	9	611	G	N3-C4-N9	5.27	129.16	126.00
11	E	208	GLY	N-CA-C	5.27	126.28	113.10
67	5	1277	G	C2-N3-C4	-5.27	109.27	111.90
67	5	3807	A	C5-C6-N1	5.27	120.33	117.70
67	5	4183	G	N3-C4-N9	-5.27	122.84	126.00
73	8	87	G	C2-N3-C4	-5.27	109.27	111.90
76	9	1740	C	N3-C4-N4	5.27	121.69	118.00
67	5	344	A	C6-N1-C2	-5.27	115.44	118.60
67	5	1651	G	C2-N3-C4	-5.27	109.27	111.90
67	5	1929	A	C6-N1-C2	-5.27	115.44	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4370	G	C8-N9-C1'	-5.27	120.15	127.00
67	5	4506	C	C6-N1-C2	-5.27	118.19	120.30
76	9	1757	G	C4-N9-C1'	5.27	133.35	126.50
67	5	301	G	N1-C2-N3	5.27	127.06	123.90
67	5	1561	G	N3-C4-N9	5.27	129.16	126.00
76	9	1454	A	C5-C6-N6	5.27	127.91	123.70
76	9	1619	A	C5-C6-N6	-5.27	119.49	123.70
67	5	434	A	C5-C6-N6	-5.26	119.49	123.70
67	5	1300	G	N3-C4-C5	5.26	131.23	128.60
67	5	2726	G	C4-C5-N7	5.26	112.91	110.80
67	5	3945	A	O3'-P-O5'	5.26	114.00	104.00
76	9	1699	A	N9-C4-C5	-5.26	103.69	105.80
73	8	50	C	N3-C2-O2	-5.26	118.22	121.90
76	9	1147	C	C5-C4-N4	-5.26	116.52	120.20
76	9	1330	G	N3-C4-N9	-5.26	122.84	126.00
73	8	141	C	C2-N1-C1'	5.26	124.59	118.80
76	9	853	C	N3-C2-O2	-5.26	118.22	121.90
67	5	2259	G	C8-N9-C1'	-5.26	120.16	127.00
67	5	2850	A	N7-C8-N9	5.26	116.43	113.80
67	5	4578	G	C4-N9-C1'	5.26	133.34	126.50
67	5	4695	C	C6-N1-C2	5.26	122.40	120.30
76	9	18	C	N3-C4-N4	5.26	121.68	118.00
67	5	2403	A	C8-N9-C4	-5.26	103.70	105.80
67	5	3691	G	N1-C2-N3	5.26	127.06	123.90
76	9	1513	C	C5-C4-N4	5.26	123.88	120.20
81	B	17	LEU	CB-CG-CD2	-5.26	102.06	111.00
62	U	19	LEU	CB-CG-CD2	5.26	119.94	111.00
67	5	344	A	C5-C6-N1	5.26	120.33	117.70
67	5	353	A	N9-C4-C5	-5.26	103.70	105.80
67	5	4179	G	C6-C5-N7	-5.26	127.25	130.40
67	5	106	A	C5-N7-C8	-5.25	101.27	103.90
67	5	2840	A	C6-N1-C2	-5.25	115.45	118.60
67	5	1329	G	N7-C8-N9	5.25	115.73	113.10
67	5	1383	G	C8-N9-C4	-5.25	104.30	106.40
67	5	1857	C	N3-C4-C5	5.25	124.00	121.90
67	5	1916	G	N1-C2-N2	-5.25	111.47	116.20
67	5	2289	C	C5-C4-N4	-5.25	116.52	120.20
76	9	291	G	C4-N9-C1'	5.25	133.33	126.50
67	5	2737	C	C2-N1-C1'	5.25	124.58	118.80
76	9	1858	G	C6-C5-N7	-5.25	127.25	130.40
67	5	384	A	C5-C6-N6	5.25	127.90	123.70
67	5	1910	G	C8-N9-C4	-5.25	104.30	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4462	C	N1-C2-O2	5.25	122.05	118.90
76	9	1055	A	C8-N9-C1'	-5.25	118.25	127.70
67	5	2583	C	C6-N1-C2	-5.25	118.20	120.30
67	5	4991	U	C2-N1-C1'	5.25	124.00	117.70
76	9	876	C	C6-N1-C1'	-5.25	114.50	120.80
76	9	1459	G	C6-C5-N7	-5.25	127.25	130.40
67	5	666	G	N1-C2-N2	5.25	120.92	116.20
67	5	4553	A	C4-N9-C1'	5.25	135.74	126.30
76	9	71	G	C8-N9-C1'	-5.25	120.18	127.00
67	5	4314	C	C6-N1-C2	-5.24	118.20	120.30
67	5	4327	C	N3-C2-O2	-5.24	118.23	121.90
67	5	4375	C	O4'-C1'-N1	5.24	112.39	108.20
76	9	1354	G	N1-C2-N2	-5.24	111.48	116.20
67	5	289	C	C6-N1-C2	-5.24	118.20	120.30
67	5	362	A	C8-N9-C4	5.24	107.90	105.80
67	5	1298	C	C2-N1-C1'	5.24	124.56	118.80
67	5	2820	C	C5-C4-N4	-5.24	116.53	120.20
67	5	4945	G	C4-C5-N7	5.24	112.90	110.80
67	5	15	A	C5-C6-N6	-5.24	119.51	123.70
67	5	756	G	N3-C4-N9	-5.24	122.86	126.00
67	5	1178	G	C8-N9-C4	-5.24	104.30	106.40
67	5	1887	G	C2-N3-C4	-5.24	109.28	111.90
67	5	4259	C	N3-C2-O2	-5.24	118.23	121.90
76	9	547	G	C4-N9-C1'	5.24	133.31	126.50
67	5	1326	A	C8-N9-C4	-5.24	103.71	105.80
67	5	1651	G	C4-C5-N7	5.24	112.89	110.80
67	5	4669	A	C8-N9-C4	-5.24	103.71	105.80
67	5	4989	U	C6-N1-C2	-5.24	117.86	121.00
67	5	313	U	C5-C4-O4	-5.23	122.76	125.90
67	5	1908	A	C5-C6-N6	-5.23	119.51	123.70
67	5	1980	U	P-O3'-C3'	-5.23	113.42	119.70
67	5	2075	G	C4-N9-C1'	5.23	133.30	126.50
67	5	3858	C	C6-N1-C1'	-5.23	114.52	120.80
67	5	4868	G	N3-C4-N9	5.23	129.14	126.00
70	7	93	G	C8-N9-C4	-5.23	104.31	106.40
76	9	1144	A	C5-C6-N6	-5.23	119.51	123.70
44	NN	124	ARG	NE-CZ-NH2	-5.23	117.69	120.30
67	5	1908	A	C5-N7-C8	-5.23	101.28	103.90
67	5	3744	G	N1-C2-N2	-5.23	111.49	116.20
67	5	4279	A	C6-C5-N7	-5.23	128.64	132.30
67	5	4448	G	N1-C6-O6	5.23	123.04	119.90
67	5	4499	G	C8-N9-C1'	-5.23	120.20	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	353	A	C6-C5-N7	-5.23	128.64	132.30
67	5	415	G	C4-N9-C1'	5.23	133.30	126.50
67	5	1658	G	C4-N9-C1'	5.23	133.29	126.50
67	5	4082	G	N3-C4-C5	-5.23	125.99	128.60
67	5	4091	G	C4-N9-C1'	5.23	133.30	126.50
67	5	4164	C	N3-C2-O2	-5.23	118.24	121.90
70	7	82	G	C8-N9-C1'	-5.23	120.20	127.00
76	9	321	C	C5-C4-N4	-5.23	116.54	120.20
67	5	1321	G	C8-N9-C1'	-5.23	120.21	127.00
76	9	1474	A	C5-N7-C8	5.23	106.51	103.90
67	5	401	G	N3-C4-N9	5.22	129.13	126.00
67	5	3671	G	C2-N3-C4	-5.22	109.29	111.90
76	9	1459	G	C4-C5-N7	5.22	112.89	110.80
67	5	1846	G	N1-C2-N2	-5.22	111.50	116.20
67	5	1941	A	N9-C4-C5	5.22	107.89	105.80
67	5	2690	C	C6-N1-C1'	-5.22	114.53	120.80
67	5	2578	G	C4-N9-C1'	5.22	133.29	126.50
67	5	3909	C	C5-C6-N1	-5.22	118.39	121.00
67	5	19	G	C8-N9-C1'	-5.22	120.21	127.00
67	5	1868	A	C6-C5-N7	-5.22	128.65	132.30
67	5	1877	G	N3-C2-N2	5.22	123.55	119.90
67	5	1879	C	N3-C2-O2	-5.22	118.25	121.90
67	5	1938	C	C2-N3-C4	-5.21	117.29	119.90
67	5	2018	C	P-O3'-C3'	5.21	125.96	119.70
67	5	3813	A	C4-N9-C1'	5.21	135.69	126.30
67	5	4394	A	C5-N7-C8	-5.21	101.29	103.90
67	5	4454	G	N3-C2-N2	5.21	123.55	119.90
76	9	810	A	N9-C4-C5	-5.21	103.71	105.80
76	9	1610	G	C6-C5-N7	-5.21	127.27	130.40
67	5	2343	G	C8-N9-C1'	-5.21	120.22	127.00
67	5	3901	A	N1-C6-N6	5.21	121.73	118.60
67	5	1898	C	C6-N1-C2	5.21	122.38	120.30
76	9	1654	G	N9-C4-C5	-5.21	103.31	105.40
67	5	1690	C	N3-C2-O2	-5.21	118.25	121.90
67	5	1723	A	C6-N1-C2	-5.21	115.47	118.60
67	5	666	G	N3-C4-C5	5.21	131.21	128.60
67	5	1911	C	C2-N1-C1'	5.21	124.53	118.80
67	5	4870	G	N1-C2-N2	-5.21	111.51	116.20
73	8	4	C	C2-N1-C1'	5.21	124.53	118.80
67	5	118	C	C6-N1-C1'	-5.21	114.55	120.80
67	5	302	C	C5-C4-N4	-5.21	116.56	120.20
67	5	3783	A	C5-N7-C8	-5.21	101.30	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4279	A	C5-N7-C8	-5.21	101.30	103.90
67	5	4284	C	C2-N1-C1'	5.21	124.53	118.80
67	5	4503	A	C6-N1-C2	-5.21	115.48	118.60
75	Z	12	LEU	CB-CG-CD2	-5.21	102.15	111.00
76	9	1489	A	O4'-C1'-N9	5.21	112.36	108.20
67	5	322	C	C2-N1-C1'	5.21	124.53	118.80
76	9	1014	G	C4-N9-C1'	5.21	133.27	126.50
52	r	20	ARG	CG-CD-NE	5.20	122.73	111.80
67	5	1989	G	N3-C2-N2	5.20	123.54	119.90
67	5	3691	G	O5'-P-OP1	-5.20	101.02	105.70
67	5	4565	C	C2-N1-C1'	5.20	124.52	118.80
67	5	4230	C	N1-C2-O2	5.20	122.02	118.90
67	5	140	G	N1-C6-O6	-5.20	116.78	119.90
67	5	1216	C	N3-C4-C5	5.20	123.98	121.90
67	5	1630	A	N1-C6-N6	-5.20	115.48	118.60
67	5	1632	A	N7-C8-N9	5.20	116.40	113.80
67	5	1786	A	C8-N9-C4	-5.20	103.72	105.80
67	5	3791	C	C5-C4-N4	-5.20	116.56	120.20
67	5	1343	A	C5-C6-N1	5.20	120.30	117.70
67	5	4409	C	N1-C2-O2	5.20	122.02	118.90
76	9	1413	G	C4-N9-C1'	5.20	133.26	126.50
67	5	1648	C	C2-N1-C1'	5.20	124.52	118.80
67	5	2348	G	O4'-C1'-N9	5.20	112.36	108.20
67	5	1543	G	N1-C2-N3	5.20	127.02	123.90
67	5	1554	A	C5-C6-N1	5.20	120.30	117.70
67	5	1653	A	C8-N9-C4	5.20	107.88	105.80
58	t	15	LEU	CB-CG-CD1	-5.19	102.17	111.00
67	5	1998	A	C8-N9-C4	-5.19	103.72	105.80
67	5	2533	C	C5-C4-N4	-5.19	116.56	120.20
67	5	3869	C	N3-C4-C5	5.19	123.98	121.90
67	5	3923	A	C5-C6-N6	-5.19	119.55	123.70
67	5	4164	C	N1-C2-O2	5.19	122.02	118.90
76	9	1146	C	N3-C4-C5	5.19	123.98	121.90
67	5	2280	G	C4-C5-N7	5.19	112.88	110.80
67	5	4603	C	N3-C2-O2	-5.19	118.27	121.90
67	5	112	C	N1-C2-O2	5.19	122.01	118.90
67	5	1538	U	O4'-C1'-N1	5.19	112.35	108.20
67	5	2278	G	C4-N9-C1'	5.19	133.25	126.50
67	5	2699	C	C2-N1-C1'	5.19	124.51	118.80
67	5	2772	C	C6-N1-C1'	-5.19	114.57	120.80
67	5	3619	G	C2-N3-C4	-5.19	109.31	111.90
67	5	4217	G	N3-C2-N2	-5.19	116.27	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4630	G	C8-N9-C4	-5.19	104.32	106.40
76	9	1474	A	N9-C4-C5	5.19	107.88	105.80
22	HH	61	ILE	CG1-CB-CG2	-5.19	99.99	111.40
24	bb	63	LEU	CB-CG-CD1	5.19	119.82	111.00
67	5	2041	A	N9-C4-C5	5.19	107.88	105.80
67	5	3903	A	N9-C4-C5	-5.19	103.72	105.80
76	9	1474	A	C8-N9-C4	-5.19	103.72	105.80
67	5	4253	A	N1-C6-N6	-5.19	115.49	118.60
67	5	4582	C	N1-C2-O2	5.19	122.01	118.90
67	5	1065	G	C2-N3-C4	-5.18	109.31	111.90
67	5	1983	A	N1-C6-N6	-5.18	115.49	118.60
67	5	2438	A	N9-C4-C5	-5.18	103.73	105.80
67	5	2815	A	N3-C4-N9	5.18	131.55	127.40
67	5	4971	A	C6-C5-N7	5.18	135.93	132.30
67	5	1635	C	C5-C4-N4	-5.18	116.57	120.20
67	5	3834	C	C6-N1-C1'	-5.18	114.58	120.80
73	8	88	A	N1-C6-N6	-5.18	115.49	118.60
76	9	1224	G	C8-N9-C1'	5.18	133.74	127.00
67	5	1465	G	N1-C2-N2	-5.18	111.54	116.20
67	5	2458	C	C6-N1-C1'	-5.18	114.58	120.80
67	5	2629	C	C6-N1-C1'	-5.18	114.58	120.80
67	5	2805	C	N1-C2-O2	5.18	122.01	118.90
76	9	419	G	C8-N9-C1'	-5.18	120.27	127.00
67	5	3719	A	C6-C5-N7	-5.18	128.68	132.30
67	5	1358	G	C2-N3-C4	-5.18	109.31	111.90
67	5	2040	A	C8-N9-C1'	-5.18	118.38	127.70
67	5	4184	G	C2-N3-C4	-5.18	109.31	111.90
76	9	223	C	C6-N1-C1'	-5.18	114.59	120.80
76	9	1849	G	N7-C8-N9	5.18	115.69	113.10
67	5	2487	G	C4-N9-C1'	5.17	133.23	126.50
67	5	356	G	C5-C6-N1	-5.17	108.91	111.50
67	5	3653	A	N3-C4-C5	-5.17	123.18	126.80
76	9	1254	C	C6-N1-C2	-5.17	118.23	120.30
67	5	2295	C	N3-C2-O2	-5.17	118.28	121.90
76	9	1538	C	O4'-C1'-N1	5.17	112.34	108.20
67	5	101	A	C4-C5-N7	5.17	113.28	110.70
67	5	417	G	C2-N3-C4	-5.17	109.32	111.90
67	5	1484	G	N1-C2-N2	-5.17	111.55	116.20
67	5	1690	C	C6-N1-C2	-5.17	118.23	120.30
67	5	2349	A	C5-N7-C8	-5.17	101.32	103.90
67	5	2633	U	O4'-C1'-N1	5.17	112.33	108.20
67	5	3659	G	C8-N9-C1'	-5.17	120.28	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4097	G	N3-C4-N9	-5.17	122.90	126.00
76	9	1181	A	C5-N7-C8	-5.17	101.31	103.90
67	5	418	A	C5-N7-C8	-5.17	101.32	103.90
67	5	2449	A	C5-C6-N1	5.17	120.28	117.70
67	5	4688	C	N3-C4-N4	5.17	121.62	118.00
76	9	1329	U	O4'-C1'-N1	-5.17	104.07	108.20
27	II	49	ARG	CB-CG-CD	5.16	125.03	111.60
67	5	1670	G	N9-C4-C5	-5.16	103.33	105.40
67	5	4171	C	N3-C4-C5	5.16	123.97	121.90
67	5	4370	G	C8-N9-C4	-5.16	104.33	106.40
67	5	4687	A	C5-C6-N6	-5.16	119.57	123.70
67	5	1081	C	N3-C4-N4	5.16	121.61	118.00
67	5	4427	G	N3-C2-N2	5.16	123.51	119.90
67	5	4631	G	N3-C4-C5	-5.16	126.02	128.60
76	9	909	G	C6-C5-N7	-5.16	127.30	130.40
67	5	1305	C	C6-N1-C1'	-5.16	114.61	120.80
67	5	1841	C	C2-N1-C1'	5.16	124.47	118.80
67	5	3899	G	N7-C8-N9	5.16	115.68	113.10
67	5	4228	G	N3-C4-C5	-5.16	126.02	128.60
67	5	4878	C	C6-N1-C1'	-5.16	114.61	120.80
67	5	4942	C	C5-C4-N4	5.16	123.81	120.20
73	8	6	C	C6-N1-C2	-5.16	118.24	120.30
76	9	351	G	N3-C2-N2	-5.16	116.29	119.90
76	9	1224	G	C4-N9-C1'	-5.16	119.79	126.50
67	5	1493	G	C4-N9-C1'	5.16	133.20	126.50
70	7	32	A	C5-C6-N1	5.16	120.28	117.70
53	QQ	145	TYR	CA-CB-CG	5.16	123.19	113.40
67	5	2731	C	C2-N1-C1'	5.16	124.47	118.80
67	5	4462	C	N3-C4-C5	5.16	123.96	121.90
67	5	4654	C	C5-C4-N4	-5.16	116.59	120.20
67	5	4694	G	C8-N9-C1'	-5.16	120.30	127.00
76	9	1055	A	C4-N9-C1'	5.16	135.58	126.30
67	5	1929	A	C6-C5-N7	-5.15	128.69	132.30
76	9	533	A	N9-C4-C5	-5.15	103.74	105.80
67	5	4356	G	C8-N9-C4	-5.15	104.34	106.40
67	5	4478	G	C8-N9-C1'	-5.15	120.30	127.00
76	9	1095	U	C6-N1-C2	-5.15	117.91	121.00
67	5	4630	G	N7-C8-N9	5.15	115.67	113.10
67	5	1074	G	C2-N3-C4	-5.15	109.33	111.90
67	5	4195	G	N1-C2-N3	5.15	126.99	123.90
67	5	4978	G	C4-N9-C1'	5.15	133.19	126.50
67	5	5059	C	N3-C2-O2	-5.15	118.30	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	2059	C	C5-C4-N4	-5.15	116.60	120.20
67	5	3864	C	C5-C4-N4	-5.15	116.60	120.20
22	HH	130	LEU	CB-CG-CD2	-5.14	102.25	111.00
67	5	3666	C	C6-N1-C2	-5.14	118.24	120.30
81	B	345	LEU	CB-CG-CD1	-5.14	102.26	111.00
67	5	19	G	C4-N9-C1'	5.14	133.19	126.50
67	5	1657	G	N7-C8-N9	5.14	115.67	113.10
67	5	2081	C	C5-C4-N4	-5.14	116.60	120.20
67	5	2520	C	C6-N1-C2	-5.14	118.24	120.30
67	5	3913	G	N1-C2-N2	-5.14	111.57	116.20
67	5	52	G	C4-N9-C1'	5.14	133.18	126.50
76	9	1532	C	C5-C6-N1	5.14	123.57	121.00
67	5	3623	C	C2-N1-C1'	5.14	124.45	118.80
67	5	2406	G	N7-C8-N9	5.14	115.67	113.10
67	5	3668	C	C2-N1-C1'	5.14	124.45	118.80
67	5	108	A	C8-N9-C1'	-5.14	118.45	127.70
67	5	1884	C	N3-C2-O2	-5.14	118.31	121.90
67	5	1966	C	C6-N1-C2	-5.14	118.25	120.30
67	5	2752	G	C8-N9-C1'	-5.14	120.32	127.00
67	5	3706	C	N3-C2-O2	-5.14	118.31	121.90
67	5	4499	G	C6-C5-N7	-5.14	127.32	130.40
67	5	4525	C	C6-N1-C1'	-5.14	114.64	120.80
67	5	1373	A	C4-N9-C1'	5.13	135.54	126.30
67	5	1729	A	C5-C6-N6	-5.13	119.59	123.70
76	9	909	G	C4-N9-C1'	5.13	133.17	126.50
67	5	47	A	P-O3'-C3'	5.13	125.86	119.70
67	5	4330	G	N1-C6-O6	-5.13	116.82	119.90
76	9	70	G	N3-C2-N2	5.13	123.49	119.90
67	5	1064	G	C6-C5-N7	-5.13	127.32	130.40
67	5	1541	C	C6-N1-C2	-5.13	118.25	120.30
15	F	73	MET	CG-SD-CE	-5.13	92.00	100.20
37	1	49	LEU	CB-CG-CD1	-5.13	102.28	111.00
67	5	83	C	C2-N3-C4	-5.13	117.34	119.90
67	5	1661	C	N1-C2-O2	5.13	121.98	118.90
67	5	2089	G	C8-N9-C1'	-5.13	120.33	127.00
67	5	4391	G	N1-C2-N2	-5.13	111.58	116.20
67	5	4485	C	C6-N1-C1'	-5.13	114.64	120.80
2	C	358	LEU	CB-CG-CD2	-5.13	102.29	111.00
67	5	1836	G	N3-C2-N2	5.13	123.49	119.90
73	8	50	C	N1-C2-O2	5.13	121.98	118.90
67	5	727	C	C2-N1-C1'	5.12	124.44	118.80
67	5	1298	C	N3-C2-O2	-5.12	118.31	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1896	A	C6-C5-N7	-5.12	128.71	132.30
67	5	2468	U	O4'-C1'-N1	5.12	112.30	108.20
67	5	3692	A	C5-C6-N1	5.12	120.26	117.70
67	5	4338	G	N3-C4-C5	5.12	131.16	128.60
23	hh	55	C	O4'-C1'-N1	5.12	112.30	108.20
67	5	44	A	C6-N1-C2	-5.12	115.53	118.60
67	5	63	G	C8-N9-C4	5.12	108.45	106.40
67	5	1329	G	C8-N9-C4	-5.12	104.35	106.40
67	5	4451	G	N1-C2-N3	5.12	126.97	123.90
67	5	1875	C	N3-C4-C5	5.12	123.95	121.90
67	5	409	G	C4-N9-C1'	5.12	133.15	126.50
67	5	1988	G	O4'-C1'-N9	-5.12	104.11	108.20
67	5	4969	C	C2-N1-C1'	5.12	124.43	118.80
76	9	1456	G	O4'-C1'-N9	5.12	112.30	108.20
67	5	241	G	C8-N9-C1'	-5.12	120.35	127.00
67	5	1658	G	C8-N9-C1'	-5.12	120.35	127.00
67	5	1662	C	C5-C4-N4	-5.12	116.62	120.20
67	5	4097	G	O4'-C1'-N9	-5.12	104.11	108.20
67	5	4761	G	N3-C4-N9	-5.12	122.93	126.00
67	5	973	G	C8-N9-C4	5.11	108.44	106.40
67	5	4237	C	N1-C2-O2	5.11	121.97	118.90
76	9	926	A	O4'-C1'-N9	5.11	112.29	108.20
47	OO	27	VAL	CG1-CB-CG2	-5.11	102.72	110.90
67	5	197	A	O4'-C1'-N9	-5.11	104.11	108.20
67	5	2295	C	N1-C2-O2	5.11	121.97	118.90
67	5	2397	G	N1-C2-N3	5.11	126.97	123.90
73	8	44	A	C5-N7-C8	-5.11	101.34	103.90
76	9	561	A	O4'-C1'-N9	-5.11	104.11	108.20
4	DD	96	LEU	CB-CG-CD2	-5.11	102.32	111.00
67	5	2527	A	N9-C4-C5	5.11	107.84	105.80
67	5	3857	G	C6-C5-N7	-5.11	127.34	130.40
67	5	2024	G	C4-N9-C1'	-5.11	119.86	126.50
67	5	2737	C	C6-N1-C1'	-5.11	114.67	120.80
67	5	1727	U	C2-N1-C1'	5.10	123.82	117.70
67	5	4623	G	C4-N9-C1'	5.10	133.13	126.50
23	hh	55	C	C6-N1-C2	-5.10	118.26	120.30
67	5	84	A	N9-C4-C5	-5.10	103.76	105.80
67	5	1330	A	C5-C6-N1	5.10	120.25	117.70
67	5	2290	C	C6-N1-C2	-5.10	118.26	120.30
67	5	3717	A	C5-C6-N6	-5.10	119.62	123.70
67	5	3819	G	N3-C4-C5	-5.10	126.05	128.60
73	8	24	G	N1-C2-N2	-5.10	111.61	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	9	1215	C	O4'-C1'-N1	5.10	112.28	108.20
67	5	50	C	C6-N1-C1'	-5.10	114.68	120.80
67	5	7	C	C2-N1-C1'	5.10	124.41	118.80
67	5	356	G	C6-C5-N7	-5.10	127.34	130.40
67	5	666	G	C8-N9-C1'	5.10	133.63	127.00
67	5	4568	A	C6-N1-C2	-5.10	115.54	118.60
73	8	41	A	C8-N9-C1'	5.10	136.88	127.70
76	9	1409	A	O4'-C1'-N9	5.10	112.28	108.20
19	gg	258	ILE	CG1-CB-CG2	5.10	122.61	111.40
70	7	48	G	N9-C4-C5	-5.10	103.36	105.40
76	9	356	C	C2-N1-C1'	5.10	124.41	118.80
67	5	747	A	C5-N7-C8	-5.10	101.35	103.90
67	5	4631	G	N7-C8-N9	5.10	115.65	113.10
67	5	1607	C	N3-C4-C5	5.09	123.94	121.90
67	5	2840	A	C5-C6-N6	-5.09	119.62	123.70
67	5	2846	G	N3-C4-N9	5.09	129.06	126.00
67	5	3933	G	C2-N3-C4	-5.09	109.35	111.90
67	5	4392	G	C5-C6-O6	5.09	131.66	128.60
73	8	126	C	C6-N1-C1'	5.09	126.91	120.80
76	9	1699	A	N1-C6-N6	5.09	121.66	118.60
67	5	951	G	C2-N3-C4	-5.09	109.35	111.90
67	5	2622	G	C6-C5-N7	-5.09	127.34	130.40
67	5	360	A	N7-C8-N9	5.09	116.35	113.80
67	5	1898	C	C6-N1-C1'	-5.09	114.69	120.80
67	5	3873	G	N3-C4-C5	-5.09	126.05	128.60
76	9	677	G	C8-N9-C1'	-5.09	120.39	127.00
76	9	1164	G	C4-N9-C1'	5.09	133.12	126.50
67	5	1648	C	C6-N1-C1'	-5.09	114.69	120.80
67	5	1885	G	C4-N9-C1'	5.09	133.12	126.50
67	5	26	C	N3-C4-N4	5.09	121.56	118.00
67	5	2003	G	C4-N9-C1'	-5.09	119.89	126.50
67	5	2694	G	C2-N3-C4	-5.09	109.36	111.90
67	5	2724	G	N3-C4-N9	-5.09	122.95	126.00
67	5	4080	C	N3-C2-O2	-5.09	118.34	121.90
67	5	4169	G	N1-C6-O6	5.09	122.95	119.90
67	5	4362	A	N9-C4-C5	5.09	107.83	105.80
67	5	4370	G	C4-N9-C1'	5.09	133.11	126.50
67	5	1929	A	C5-N7-C8	-5.08	101.36	103.90
67	5	2297	G	N3-C4-C5	-5.08	126.06	128.60
67	5	4381	A	C6-N1-C2	-5.08	115.55	118.60
28	ii	88	VAL	N-CA-C	-5.08	97.28	111.00
43	n	8	LYS	CD-CE-NZ	5.08	123.39	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4891	G	N1-C2-N2	-5.08	111.62	116.20
73	8	121	G	N3-C4-C5	5.08	131.14	128.60
76	9	1630	A	N1-C6-N6	5.08	121.65	118.60
67	5	63	G	N1-C6-O6	5.08	122.95	119.90
67	5	2604	C	C5-C4-N4	-5.08	116.64	120.20
67	5	3812	C	C6-N1-C1'	-5.08	114.70	120.80
67	5	3633	C	C5-C4-N4	-5.08	116.64	120.20
67	5	4561	C	N3-C2-O2	-5.08	118.34	121.90
67	5	414	C	C2-N3-C4	-5.08	117.36	119.90
67	5	1235	G	N3-C4-C5	5.08	131.14	128.60
67	5	1363	C	C5-C4-N4	-5.08	116.64	120.20
67	5	1429	C	C6-N1-C2	-5.08	118.27	120.30
67	5	1586	G	O4'-C1'-N9	5.08	112.26	108.20
67	5	1786	A	C5-C6-N1	5.08	120.24	117.70
67	5	4196	G	C8-N9-C4	5.08	108.43	106.40
67	5	4253	A	C5-C6-N6	5.08	127.76	123.70
67	5	4971	A	C8-N9-C1'	5.08	136.84	127.70
73	8	90	C	C6-N1-C1'	-5.08	114.71	120.80
76	9	196	C	N3-C4-C5	-5.08	119.87	121.90
76	9	1584	G	O4'-C1'-N9	-5.08	104.14	108.20
67	5	2284	G	N1-C2-N2	-5.08	111.63	116.20
76	9	845	G	C4-N9-C1'	5.08	133.10	126.50
67	5	343	C	N3-C2-O2	-5.08	118.35	121.90
67	5	1415	G	C8-N9-C4	5.08	108.43	106.40
67	5	3774	A	P-O3'-C3'	5.08	125.79	119.70
76	9	1243	U	C6-N1-C1'	-5.08	114.09	121.20
6	D	212	MET	CA-CB-CG	-5.07	104.68	113.30
67	5	156	G	C2-N3-C4	-5.07	109.36	111.90
67	5	3924	C	C6-N1-C1'	-5.07	114.71	120.80
67	5	4193	C	N3-C4-N4	5.07	121.55	118.00
67	5	4501	U	O4'-C1'-N1	5.07	112.26	108.20
67	5	2275	G	C8-N9-C1'	-5.07	120.41	127.00
67	5	4196	G	C2-N3-C4	-5.07	109.36	111.90
73	8	118	C	N1-C2-O2	5.07	121.94	118.90
67	5	2448	G	N7-C8-N9	5.07	115.63	113.10
67	5	1300	G	C4-N9-C1'	-5.07	119.91	126.50
67	5	1928	C	C2-N3-C4	-5.07	117.37	119.90
67	5	1169	G	N3-C4-C5	5.07	131.13	128.60
67	5	1972	G	P-O3'-C3'	5.07	125.78	119.70
67	5	4980	C	C6-N1-C1'	-5.07	114.72	120.80
67	5	101	A	C6-C5-N7	-5.06	128.75	132.30
67	5	4538	G	C4-C5-N7	5.06	112.83	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	9	931	C	C2-N1-C1'	5.06	124.37	118.80
67	5	2469	C	N3-C4-C5	5.06	123.92	121.90
67	5	2593	C	N1-C2-O2	5.06	121.94	118.90
67	5	4213	A	C8-N9-C1'	-5.06	118.59	127.70
67	5	4945	G	C2-N3-C4	-5.06	109.37	111.90
67	5	678	C	N3-C2-O2	-5.06	118.36	121.90
67	5	1603	C	N3-C2-O2	-5.06	118.36	121.90
25	H	168	LYS	CB-CG-CD	5.06	124.75	111.60
67	5	63	G	N9-C4-C5	-5.06	103.38	105.40
67	5	363	A	C5-C6-N1	5.06	120.23	117.70
67	5	2505	C	C2-N1-C1'	5.06	124.37	118.80
67	5	2655	C	N1-C2-O2	5.06	121.94	118.90
67	5	2860	C	N1-C2-O2	-5.06	115.86	118.90
67	5	3737	A	C6-C5-N7	-5.06	128.76	132.30
67	5	4170	A	N1-C6-N6	-5.06	115.56	118.60
76	9	1109	C	O4'-C1'-N1	5.06	112.25	108.20
76	9	1784	G	C4-N9-C1'	5.06	133.08	126.50
14	ff	146	LEU	CB-CG-CD2	5.06	119.60	111.00
28	ii	188	LEU	CB-CG-CD2	5.06	119.60	111.00
67	5	2280	G	C5-N7-C8	-5.06	101.77	104.30
76	9	213	G	O4'-C1'-N9	5.06	112.25	108.20
76	9	1845	A	C5-C6-N1	5.06	120.23	117.70
2	C	90	GLY	N-CA-C	5.05	125.74	113.10
28	ii	136	LEU	CA-CB-CG	5.05	126.93	115.30
67	5	1846	G	N3-C2-N2	5.05	123.44	119.90
67	5	1859	C	C2-N1-C1'	5.05	124.36	118.80
67	5	2590	G	N3-C2-N2	5.05	123.44	119.90
67	5	3670	C	C5-C4-N4	-5.05	116.66	120.20
67	5	2758	G	N9-C4-C5	-5.05	103.38	105.40
67	5	3877	A	N1-C6-N6	5.05	121.63	118.60
67	5	4942	C	N3-C4-N4	-5.05	114.46	118.00
67	5	342	G	O4'-C1'-N9	5.05	112.24	108.20
67	5	2411	C	N3-C4-N4	5.05	121.54	118.00
67	5	2540	C	C5-C6-N1	5.05	123.53	121.00
67	5	3665	G	C4-N9-C1'	5.05	133.07	126.50
67	5	4259	C	C6-N1-C2	-5.05	118.28	120.30
76	9	1834	A	N1-C2-N3	5.05	131.83	129.30
76	9	1846	G	C8-N9-C4	5.05	108.42	106.40
76	9	1856	C	C2-N1-C1'	5.05	124.36	118.80
67	5	2010	A	C4-N9-C1'	-5.05	117.21	126.30
67	5	4195	G	C8-N9-C1'	-5.05	120.44	127.00
67	5	4217	G	N3-C4-N9	-5.05	122.97	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	4613	C	N3-C4-C5	5.05	123.92	121.90
67	5	4630	G	C5-C6-O6	5.05	131.63	128.60
76	9	1000	C	N3-C4-C5	5.05	123.92	121.90
76	9	84	A	C5-C6-N1	-5.05	115.18	117.70
67	5	108	A	C6-C5-N7	-5.05	128.77	132.30
67	5	375	G	O4'-C1'-N9	5.05	112.24	108.20
67	5	3771	C	N1-C2-O2	5.05	121.93	118.90
67	5	4980	C	C6-N1-C2	5.05	122.32	120.30
67	5	1777	C	C6-N1-C1'	-5.04	114.75	120.80
67	5	2691	U	O4'-C1'-N1	5.04	112.24	108.20
76	9	476	A	C5-C6-N6	-5.04	119.67	123.70
76	9	329	G	N3-C4-C5	-5.04	126.08	128.60
76	9	1280	G	C4-N9-C1'	5.04	133.06	126.50
67	5	2320	G	C4-N9-C1'	5.04	133.05	126.50
76	9	1298	G	O4'-C1'-N9	-5.04	104.17	108.20
67	5	1346	C	C5-C4-N4	-5.04	116.67	120.20
67	5	1998	A	N7-C8-N9	5.04	116.32	113.80
67	5	4669	A	N3-C4-C5	-5.04	123.27	126.80
76	9	1563	G	C2-N3-C4	-5.04	109.38	111.90
76	9	1617	G	N3-C4-N9	-5.04	122.98	126.00
67	5	3652	A	C8-N9-C4	-5.04	103.78	105.80
67	5	4458	C	N3-C4-C5	5.04	123.92	121.90
67	5	1581	G	C4-N9-C1'	5.04	133.05	126.50
67	5	2000	G	P-O3'-C3'	5.04	125.74	119.70
76	9	168	C	C6-N1-C1'	-5.04	114.76	120.80
67	5	3661	G	N3-C2-N2	5.03	123.42	119.90
67	5	3936	A	C6-N1-C2	-5.03	115.58	118.60
67	5	289	C	C6-N1-C1'	-5.03	114.76	120.80
67	5	2072	C	C6-N1-C1'	-5.03	114.76	120.80
67	5	2271	C	C2-N1-C1'	5.03	124.33	118.80
67	5	421	C	C2-N3-C4	-5.03	117.39	119.90
67	5	1853	G	C5-C6-N1	-5.03	108.98	111.50
70	7	95	C	C6-N1-C2	-5.03	118.29	120.30
67	5	2487	G	C8-N9-C1'	-5.03	120.46	127.00
76	9	845	G	C8-N9-C1'	-5.03	120.46	127.00
67	5	343	C	N1-C2-O2	5.03	121.92	118.90
67	5	386	A	C4-N9-C1'	5.03	135.35	126.30
67	5	3936	A	C5-C6-N1	5.03	120.21	117.70
67	5	1581	G	C6-C5-N7	-5.02	127.39	130.40
67	5	4745	G	O4'-C1'-N9	5.02	112.22	108.20
76	9	594	A	N1-C6-N6	-5.02	115.59	118.60
76	9	659	G	C8-N9-C1'	-5.02	120.47	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	1812	C	N3-C2-O2	-5.02	118.39	121.90
67	5	2401	A	C5-C6-N1	5.02	120.21	117.70
67	5	4391	G	N1-C2-N3	5.02	126.91	123.90
67	5	4721	G	C8-N9-C4	-5.02	104.39	106.40
76	9	655	A	N1-C6-N6	5.02	121.61	118.60
82	c	81	LEU	CB-CG-CD2	-5.02	102.47	111.00
67	5	1171	G	C2-N3-C4	-5.02	109.39	111.90
67	5	1330	A	C6-N1-C2	-5.02	115.59	118.60
67	5	1667	A	C5-N7-C8	-5.02	101.39	103.90
67	5	2271	C	C6-N1-C1'	-5.02	114.78	120.80
67	5	1169	G	C4-N9-C1'	-5.02	119.98	126.50
67	5	3751	G	O4'-C1'-N9	5.02	112.21	108.20
76	9	1293	A	O4'-C1'-N9	5.02	112.21	108.20
67	5	711	A	C5-C6-N1	5.01	120.21	117.70
67	5	2046	G	C6-C5-N7	-5.01	127.39	130.40
67	5	3891	A	C6-N1-C2	-5.01	115.59	118.60
73	8	41	A	C8-N9-C4	-5.01	103.79	105.80
76	9	1302	G	N3-C4-N9	-5.01	122.99	126.00
76	9	1573	G	C2-N3-C4	-5.01	109.39	111.90
67	5	1331	C	N3-C2-O2	-5.01	118.39	121.90
67	5	1371	A	C4-C5-N7	5.01	113.21	110.70
67	5	4543	G	C8-N9-C1'	-5.01	120.48	127.00
67	5	5005	G	N3-C4-C5	5.01	131.11	128.60
67	5	1663	C	C6-N1-C1'	-5.01	114.79	120.80
67	5	2532	C	C5-C4-N4	-5.01	116.69	120.20
67	5	2772	C	C2-N1-C1'	5.01	124.31	118.80
67	5	4663	G	C2-N3-C4	-5.01	109.39	111.90
76	9	1826	G	C4-N9-C1'	5.01	133.02	126.50
67	5	1657	G	N1-C2-N2	-5.01	111.69	116.20
67	5	2324	C	C6-N1-C1'	-5.01	114.79	120.80
67	5	2374	A	C5-C6-N1	5.01	120.20	117.70
67	5	3696	C	C6-N1-C1'	-5.01	114.79	120.80
67	5	3854	C	N3-C4-C5	5.01	123.90	121.90
1	A	180	LEU	CB-CG-CD2	-5.01	102.49	111.00
67	5	64	A	C6-C5-N7	-5.01	128.79	132.30
67	5	4399	U	O4'-C1'-N1	5.01	112.21	108.20
67	5	4880	C	N3-C4-N4	-5.01	114.49	118.00
67	5	1574	G	C4-N9-C1'	5.01	133.01	126.50
67	5	1755	C	N1-C1'-C2'	5.01	120.51	114.00
67	5	2694	G	C4-N9-C1'	5.01	133.01	126.50
67	5	2864	A	C5-C6-N6	-5.01	119.69	123.70
76	9	1470	C	C6-N1-C2	-5.00	118.30	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	165	A	C5-C6-N6	-5.00	119.70	123.70
67	5	1585	C	N1-C2-O2	5.00	121.90	118.90
67	5	1893	C	C2-N1-C1'	5.00	124.30	118.80
76	9	18	C	C2-N1-C1'	5.00	124.30	118.80
67	5	2040	A	C4-N9-C1'	5.00	135.30	126.30
67	5	2078	C	N3-C4-N4	5.00	121.50	118.00
67	5	2604	C	N1-C2-O2	5.00	121.90	118.90
67	5	2895	A	N1-C6-N6	5.00	121.60	118.60
67	5	3614	G	O4'-C1'-N9	5.00	112.20	108.20
67	5	3895	G	C8-N9-C4	-5.00	104.40	106.40
67	5	4367	G	N3-C2-N2	5.00	123.40	119.90
76	9	141	A	N1-C6-N6	-5.00	115.60	118.60
76	9	1167	G	C4-N9-C1'	5.00	133.00	126.50

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
67	5	1081	C	Sidechain
67	5	1576	G	Sidechain
67	5	1632	A	Sidechain
67	5	3623	C	Sidechain
67	5	3653	A	Sidechain
67	5	39	A	Sidechain
67	5	914	U	Sidechain
76	9	140	U	Sidechain
79	AA	42	LYS	Peptide
53	QQ	140	ARG	Peptide
71	XX	61	GLN	Peptide
3	d	95	ASP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/249 (99%)	219 (89%)	27 (11%)	0	100	100
2	C	360/378 (95%)	335 (93%)	24 (7%)	1 (0%)	41	75
3	d	105/108 (97%)	90 (86%)	13 (12%)	2 (2%)	8	39
4	DD	226/281 (80%)	212 (94%)	13 (6%)	1 (0%)	34	71
5	dd	53/56 (95%)	46 (87%)	7 (13%)	0	100	100
6	D	291/296 (98%)	273 (94%)	18 (6%)	0	100	100
7	e	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
8	EE	260/263 (99%)	244 (94%)	16 (6%)	0	100	100
9	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
10	b	100/226 (44%)	94 (94%)	5 (5%)	1 (1%)	15	52
11	E	208/291 (72%)	189 (91%)	19 (9%)	0	100	100
12	f	107/110 (97%)	98 (92%)	7 (6%)	2 (2%)	8	39
13	FF	181/204 (89%)	164 (91%)	14 (8%)	3 (2%)	9	42
14	ff	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
15	F	223/249 (90%)	213 (96%)	9 (4%)	1 (0%)	34	71
16	g	112/126 (89%)	106 (95%)	6 (5%)	0	100	100
17	BB	211/264 (80%)	193 (92%)	18 (8%)	0	100	100
18	GG	235/263 (89%)	223 (95%)	12 (5%)	0	100	100
19	gg	311/314 (99%)	282 (91%)	27 (9%)	2 (1%)	25	63
20	G	229/242 (95%)	218 (95%)	9 (4%)	2 (1%)	17	54
21	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
22	HH	181/191 (95%)	173 (96%)	8 (4%)	0	100	100
24	bb	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
25	H	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
26	i	100/107 (94%)	94 (94%)	6 (6%)	0	100	100
27	II	204/208 (98%)	188 (92%)	14 (7%)	2 (1%)	15	52
28	ii	417/437 (95%)	389 (93%)	24 (6%)	4 (1%)	15	52
29	I	201/214 (94%)	182 (90%)	19 (10%)	0	100	100
30	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	JJ	183/194 (94%)	177 (97%)	6 (3%)	0	100	100
32	jj	426/428 (100%)	373 (88%)	46 (11%)	7 (2%)	9	43
33	J	168/176 (96%)	160 (95%)	8 (5%)	0	100	100
34	k	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
35	KK	94/151 (62%)	88 (94%)	5 (5%)	1 (1%)	14	50
36	L	208/211 (99%)	192 (92%)	15 (7%)	1 (0%)	29	67
37	l	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
38	LL	139/158 (88%)	133 (96%)	6 (4%)	0	100	100
39	M	136/218 (62%)	123 (90%)	13 (10%)	0	100	100
40	m	50/128 (39%)	46 (92%)	4 (8%)	0	100	100
41	MM	115/123 (94%)	103 (90%)	12 (10%)	0	100	100
42	N	201/204 (98%)	186 (92%)	11 (6%)	4 (2%)	7	39
43	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
44	NN	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	60
45	O	197/203 (97%)	189 (96%)	7 (4%)	1 (0%)	29	67
46	o	102/142 (72%)	98 (96%)	4 (4%)	0	100	100
47	OO	134/156 (86%)	124 (92%)	8 (6%)	2 (2%)	10	44
48	P	151/199 (76%)	143 (95%)	8 (5%)	0	100	100
49	p	89/109 (82%)	82 (92%)	7 (8%)	0	100	100
50	PP	118/145 (81%)	104 (88%)	12 (10%)	2 (2%)	9	42
51	Q	185/188 (98%)	173 (94%)	11 (6%)	1 (0%)	29	67
52	r	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	19	58
53	QQ	140/158 (89%)	133 (95%)	6 (4%)	1 (1%)	22	60
54	R	178/196 (91%)	173 (97%)	5 (3%)	0	100	100
55	s	194/318 (61%)	175 (90%)	17 (9%)	2 (1%)	15	52
56	RR	130/145 (90%)	121 (93%)	9 (7%)	0	100	100
57	S	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	9	42
58	t	151/196 (77%)	134 (89%)	16 (11%)	1 (1%)	22	60
59	SS	142/152 (93%)	137 (96%)	4 (3%)	1 (1%)	22	60
60	T	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
61	TT	139/145 (96%)	131 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	U	97/128 (76%)	89 (92%)	8 (8%)	0	100	100
63	UU	98/118 (83%)	91 (93%)	7 (7%)	0	100	100
64	V	129/132 (98%)	119 (92%)	10 (8%)	0	100	100
65	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
66	W	102/134 (76%)	98 (96%)	4 (4%)	0	100	100
68	WW	127/139 (91%)	118 (93%)	7 (6%)	2 (2%)	9	43
69	X	116/156 (74%)	107 (92%)	9 (8%)	0	100	100
71	XX	139/142 (98%)	125 (90%)	11 (8%)	3 (2%)	6	37
72	Y	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
74	YY	122/146 (84%)	115 (94%)	7 (6%)	0	100	100
75	Z	133/136 (98%)	125 (94%)	6 (4%)	2 (2%)	10	44
77	ZZ	73/122 (60%)	69 (94%)	4 (6%)	0	100	100
78	a	145/147 (99%)	129 (89%)	16 (11%)	0	100	100
79	AA	215/295 (73%)	201 (94%)	13 (6%)	1 (0%)	29	67
80	aa	99/117 (85%)	89 (90%)	9 (9%)	1 (1%)	15	52
81	B	392/402 (98%)	355 (91%)	35 (9%)	2 (0%)	29	67
82	c	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
83	CC	219/259 (85%)	205 (94%)	14 (6%)	0	100	100
84	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
All	All	12362/14087 (88%)	11478 (93%)	823 (7%)	61 (0%)	32	67

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	95	ASP
28	ii	272	THR
32	jj	466	LYS
32	jj	620	GLU
42	N	76	PRO
42	N	77	LYS
50	PP	18	ARG
71	XX	62	PRO
71	XX	86	PRO
27	II	124	LYS
28	ii	181	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	ii	258	TYR
32	jj	224	GLY
32	jj	280	VAL
32	jj	555	HIS
44	NN	108	ASP
45	O	186	GLU
52	r	11	ARG
53	QQ	30	GLY
59	SS	100	ALA
10	b	102	PRO
12	f	107	PRO
28	ii	370	GLU
35	KK	64	TRP
36	L	63	THR
42	N	89	VAL
47	OO	20	GLN
47	OO	30	VAL
55	s	142	GLY
57	S	155	PRO
75	Z	91	LEU
80	aa	99	PRO
13	FF	43	GLU
13	FF	80	GLY
50	PP	80	LEU
57	S	166	ARG
58	t	125	LEU
68	WW	56	HIS
71	XX	61	GLN
75	Z	90	PRO
4	DD	93	THR
12	f	106	TYR
57	S	53	LYS
81	B	17	LEU
81	B	376	HIS
15	F	196	VAL
32	jj	558	ILE
42	N	55	ALA
79	AA	159	ILE
13	FF	21	GLY
19	gg	224	GLY
55	s	25	PRO
68	WW	29	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	d	58	GLY
27	II	3	ILE
19	gg	275	ILE
20	G	216	PRO
51	Q	92	VAL
2	C	83	GLY
20	G	221	VAL
32	jj	464	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/191 (100%)	188 (99%)	2 (1%)	73	84
2	C	302/315 (96%)	301 (100%)	1 (0%)	92	95
3	d	98/99 (99%)	97 (99%)	1 (1%)	76	85
4	DD	190/232 (82%)	185 (97%)	5 (3%)	46	67
5	dd	48/49 (98%)	48 (100%)	0	100	100
6	D	247/249 (99%)	245 (99%)	2 (1%)	81	88
7	e	114/115 (99%)	113 (99%)	1 (1%)	78	87
8	EE	224/225 (100%)	223 (100%)	1 (0%)	91	94
9	ee	46/106 (43%)	46 (100%)	0	100	100
10	b	84/172 (49%)	84 (100%)	0	100	100
11	E	190/251 (76%)	186 (98%)	4 (2%)	53	72
12	f	88/89 (99%)	87 (99%)	1 (1%)	73	84
13	FF	158/170 (93%)	157 (99%)	1 (1%)	86	92
14	ff	61/61 (100%)	59 (97%)	2 (3%)	38	62
15	F	196/218 (90%)	195 (100%)	1 (0%)	88	93
16	g	98/106 (92%)	97 (99%)	1 (1%)	76	85
17	BB	194/229 (85%)	192 (99%)	2 (1%)	76	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	GG	207/228 (91%)	204 (99%)	3 (1%)	67	80
19	gg	272/273 (100%)	270 (99%)	2 (1%)	84	90
20	G	200/207 (97%)	200 (100%)	0	100	100
21	h	109/110 (99%)	108 (99%)	1 (1%)	78	87
22	HH	165/171 (96%)	164 (99%)	1 (1%)	86	92
24	bb	75/76 (99%)	74 (99%)	1 (1%)	69	81
25	H	169/169 (100%)	168 (99%)	1 (1%)	86	92
26	i	86/88 (98%)	86 (100%)	0	100	100
27	II	178/180 (99%)	173 (97%)	5 (3%)	43	65
28	ii	361/376 (96%)	358 (99%)	3 (1%)	81	88
29	I	175/181 (97%)	174 (99%)	1 (1%)	86	92
30	j	73/80 (91%)	72 (99%)	1 (1%)	67	80
31	JJ	161/168 (96%)	159 (99%)	2 (1%)	71	83
32	jj	372/372 (100%)	363 (98%)	9 (2%)	49	69
33	J	143/148 (97%)	141 (99%)	2 (1%)	67	80
34	k	64/65 (98%)	64 (100%)	0	100	100
35	KK	87/127 (68%)	86 (99%)	1 (1%)	73	84
36	L	175/176 (99%)	174 (99%)	1 (1%)	86	92
37	l	47/48 (98%)	46 (98%)	1 (2%)	53	72
38	LL	130/143 (91%)	128 (98%)	2 (2%)	65	79
39	M	117/161 (73%)	112 (96%)	5 (4%)	29	56
40	m	48/116 (41%)	48 (100%)	0	100	100
41	MM	99/104 (95%)	98 (99%)	1 (1%)	76	85
42	N	171/172 (99%)	168 (98%)	3 (2%)	59	77
43	n	24/24 (100%)	24 (100%)	0	100	100
44	NN	130/131 (99%)	127 (98%)	3 (2%)	50	70
45	O	171/173 (99%)	168 (98%)	3 (2%)	59	77
46	o	92/121 (76%)	92 (100%)	0	100	100
47	OO	106/122 (87%)	104 (98%)	2 (2%)	57	75
48	P	134/175 (77%)	133 (99%)	1 (1%)	84	90
49	p	74/87 (85%)	73 (99%)	1 (1%)	67	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	PP	109/130 (84%)	108 (99%)	1 (1%)	78	87
51	Q	164/165 (99%)	163 (99%)	1 (1%)	86	92
52	r	108/121 (89%)	104 (96%)	4 (4%)	34	59
53	QQ	117/130 (90%)	117 (100%)	0	100	100
54	R	159/175 (91%)	157 (99%)	2 (1%)	69	81
55	s	164/258 (64%)	162 (99%)	2 (1%)	71	83
56	RR	119/131 (91%)	117 (98%)	2 (2%)	60	78
57	S	157/157 (100%)	155 (99%)	2 (1%)	69	81
58	t	126/164 (77%)	124 (98%)	2 (2%)	62	78
59	SS	125/132 (95%)	123 (98%)	2 (2%)	62	78
60	T	139/140 (99%)	138 (99%)	1 (1%)	84	90
61	TT	111/115 (96%)	110 (99%)	1 (1%)	78	87
62	U	89/114 (78%)	89 (100%)	0	100	100
63	UU	92/105 (88%)	90 (98%)	2 (2%)	52	71
64	V	101/102 (99%)	97 (96%)	4 (4%)	31	57
65	VV	67/67 (100%)	64 (96%)	3 (4%)	27	54
66	W	86/109 (79%)	84 (98%)	2 (2%)	50	70
68	WW	112/119 (94%)	110 (98%)	2 (2%)	59	77
69	X	106/134 (79%)	106 (100%)	0	100	100
71	XX	113/114 (99%)	112 (99%)	1 (1%)	78	87
72	Y	124/124 (100%)	124 (100%)	0	100	100
74	YY	107/126 (85%)	105 (98%)	2 (2%)	57	75
75	Z	117/118 (99%)	116 (99%)	1 (1%)	78	87
77	ZZ	66/100 (66%)	65 (98%)	1 (2%)	65	79
78	a	119/119 (100%)	119 (100%)	0	100	100
79	AA	180/245 (74%)	177 (98%)	3 (2%)	60	78
80	aa	88/99 (89%)	87 (99%)	1 (1%)	73	84
81	B	342/347 (99%)	340 (99%)	2 (1%)	86	92
82	c	84/98 (86%)	84 (100%)	0	100	100
83	CC	187/208 (90%)	185 (99%)	2 (1%)	73	84
84	cc	55/62 (89%)	54 (98%)	1 (2%)	59	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	10776/11977 (90%)	10648 (99%)	128 (1%)	72	83

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	128	ARG
2	C	188	ARG
3	d	31	LYS
4	DD	76	ARG
4	DD	90	LYS
4	DD	156	LEU
4	DD	167	TYR
4	DD	218	LEU
6	D	37	VAL
6	D	56	THR
7	e	89	LEU
8	EE	49	ARG
11	E	141	ARG
11	E	144	ARG
11	E	242	LYS
11	E	289	LEU
12	f	47	CYS
13	FF	169	ILE
14	ff	99	LYS
14	ff	138	ARG
15	F	30	LYS
16	g	102	ILE
17	BB	38	MET
17	BB	207	LEU
18	GG	103	ASP
18	GG	137	ARG
18	GG	178	ARG
19	gg	289	LEU
19	gg	306	LEU
21	h	28	LEU
22	HH	194	LEU
24	bb	37	CYS
25	H	74	CYS
27	II	12	ARG
27	II	76	THR
27	II	100	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	II	130	THR
27	II	205	ARG
28	ii	63	LYS
28	ii	171	LYS
28	ii	291	PHE
29	I	153	ARG
30	j	58	THR
31	JJ	50	LEU
31	JJ	112	THR
32	jj	249	ARG
32	jj	353	LEU
32	jj	371	ARG
32	jj	384	LYS
32	jj	455	VAL
32	jj	541	LYS
32	jj	551	VAL
32	jj	581	ARG
32	jj	631	LYS
33	J	16	ARG
33	J	58	ARG
35	KK	20	VAL
36	L	10	LEU
37	l	49	LEU
38	LL	33	LEU
38	LL	69	ARG
39	M	5	ARG
39	M	37	LEU
39	M	54	CYS
39	M	57	LEU
39	M	119	ARG
41	MM	31	LEU
42	N	26	ARG
42	N	27	CYS
42	N	162	ARG
44	NN	20	ARG
44	NN	84	LEU
44	NN	107	LYS
45	O	9	LEU
45	O	145	VAL
45	O	156	LEU
47	OO	98	ARG
47	OO	119	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	P	128	ARG
49	p	8	VAL
50	PP	44	ARG
51	Q	97	LYS
52	r	32	LEU
52	r	35	ARG
52	r	80	THR
52	r	103	HIS
54	R	74	ARG
54	R	133	LYS
55	s	95	LEU
55	s	187	LEU
56	RR	30	THR
56	RR	35	CYS
57	S	69	GLU
57	S	174	THR
58	t	90	ARG
58	t	99	LYS
59	SS	52	LEU
59	SS	59	LEU
60	T	146	LYS
61	TT	121	ARG
63	UU	55	ARG
63	UU	88	LEU
64	V	18	LEU
64	V	35	LYS
64	V	48	ARG
64	V	82	ILE
65	VV	11	LEU
65	VV	66	ASP
65	VV	68	SER
66	W	17	HIS
66	W	110	ARG
68	WW	20	ARG
68	WW	104	LEU
71	XX	82	THR
74	YY	79	LEU
74	YY	110	ARG
75	Z	33	THR
77	ZZ	77	LEU
79	AA	58	LEU
79	AA	111	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	AA	163	CYS
80	aa	21	ILE
81	B	248	LEU
81	B	261	ARG
83	CC	78	LEU
83	CC	114	LYS
84	cc	40	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
2	C	212	ASN
2	C	245	HIS
5	dd	3	HIS
5	dd	28	HIS
6	D	175	HIS
6	D	222	GLN
7	e	57	ASN
10	b	12	GLN
11	E	45	HIS
11	E	131	HIS
11	E	214	HIS
11	E	253	GLN
11	E	269	GLN
12	f	24	HIS
12	f	99	HIS
13	FF	31	ASN
13	FF	65	GLN
13	FF	101	HIS
13	FF	107	ASN
13	FF	148	ASN
13	FF	149	GLN
13	FF	203	ASN
14	ff	91	ASN
15	F	57	HIS
15	F	79	ASN
15	F	191	HIS
15	F	199	HIS
16	g	114	GLN
17	BB	118	GLN
17	BB	124	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	BB	186	ASN
18	GG	59	GLN
18	GG	81	HIS
18	GG	146	ASN
19	gg	4	GLN
19	gg	14	HIS
19	gg	147	HIS
19	gg	159	ASN
20	G	82	ASN
20	G	138	GLN
20	G	206	GLN
22	HH	76	GLN
22	HH	97	GLN
22	HH	165	ASN
24	bb	26	GLN
25	H	15	ASN
25	H	78	GLN
25	H	156	ASN
26	i	15	HIS
26	i	20	ASN
27	II	99	ASN
28	ii	132	HIS
28	ii	247	GLN
28	ii	356	HIS
29	I	73	ASN
31	JJ	124	HIS
31	JJ	134	HIS
31	JJ	140	GLN
32	jj	212	HIS
32	jj	214	ASN
32	jj	220	HIS
32	jj	255	ASN
32	jj	410	GLN
32	jj	468	GLN
32	jj	534	GLN
32	jj	540	HIS
35	KK	39	ASN
35	KK	42	ASN
35	KK	61	GLN
35	KK	66	HIS
36	L	87	HIS
37	l	4	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	LL	5	GLN
38	LL	18	GLN
38	LL	39	ASN
38	LL	141	ASN
39	M	131	GLN
40	m	93	ASN
41	MM	28	HIS
41	MM	48	HIS
42	N	15	GLN
42	N	196	ASN
42	N	201	HIS
44	NN	138	ASN
45	O	50	ASN
45	O	72	HIS
45	O	180	GLN
46	o	18	HIS
46	o	36	GLN
47	OO	43	HIS
47	OO	79	GLN
48	P	25	HIS
48	P	28	ASN
48	P	34	GLN
48	P	56	GLN
48	P	75	GLN
48	P	116	HIS
48	P	120	ASN
48	P	133	HIS
48	P	137	ASN
49	p	33	GLN
50	PP	53	GLN
50	PP	114	HIS
51	Q	44	ASN
51	Q	57	ASN
51	Q	151	HIS
52	r	21	ASN
52	r	70	GLN
53	QQ	48	GLN
54	R	36	ASN
54	R	130	ASN
54	R	141	HIS
54	R	158	GLN
55	s	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	s	200	ASN
56	RR	62	GLN
56	RR	83	ASN
57	S	125	GLN
58	t	100	HIS
58	t	118	HIS
59	SS	19	ASN
59	SS	72	GLN
59	SS	97	GLN
59	SS	120	HIS
60	T	95	HIS
60	T	98	HIS
61	TT	12	GLN
61	TT	63	HIS
61	TT	83	GLN
61	TT	126	GLN
61	TT	137	GLN
62	U	95	ASN
64	V	135	ASN
68	WW	5	ASN
69	X	57	GLN
71	XX	46	HIS
72	Y	14	ASN
74	YY	85	ASN
74	YY	94	HIS
74	YY	112	ASN
74	YY	124	ASN
75	Z	132	GLN
77	ZZ	45	ASN
77	ZZ	64	ASN
78	a	14	HIS
78	a	34	ASN
78	a	40	HIS
79	AA	84	GLN
79	AA	215	GLN
81	B	3	HIS
81	B	275	HIS
81	B	315	ASN
81	B	328	ASN
82	c	15	ASN
84	cc	24	GLN
84	cc	26	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	hh	14/15 (93%)	8 (57%)	0
67	5	3516/3705 (94%)	857 (24%)	155 (4%)
70	7	119/120 (99%)	14 (11%)	0
73	8	149/151 (98%)	34 (22%)	5 (3%)
76	9	1679/1779 (94%)	420 (25%)	66 (3%)
All	All	5477/5770 (94%)	1333 (24%)	226 (4%)

All (1333) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
23	hh	42	C
23	hh	43	A
23	hh	45	A
23	hh	46	G
23	hh	49	U
23	hh	52	G
23	hh	54	U
23	hh	55	C
67	5	12	A
67	5	13	U
67	5	15	A
67	5	25	A
67	5	35	U
67	5	39	A
67	5	42	A
67	5	43	U
67	5	48	G
67	5	49	U
67	5	56	A
67	5	58	G
67	5	59	A
67	5	64	A
67	5	65	A
67	5	73	A
67	5	91	G
67	5	93	G
67	5	109	G
67	5	110	C
67	5	118	C
67	5	119	G
67	5	120	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	126	C
67	5	134	G
67	5	135	G
67	5	136	C
67	5	137	G
67	5	143	C
67	5	144	G
67	5	159	C
67	5	172	C
67	5	173	C
67	5	177	G
67	5	179	G
67	5	197	A
67	5	200	U
67	5	201	C
67	5	202	C
67	5	205	C
67	5	209	U
67	5	216	C
67	5	218	A
67	5	220	C
67	5	221	C
67	5	224	U
67	5	226	G
67	5	227	A
67	5	233	U
67	5	234	G
67	5	245	C
67	5	246	G
67	5	253	G
67	5	262	G
67	5	263	G
67	5	266	C
67	5	267	G
67	5	276	C
67	5	279	A
67	5	280	G
67	5	281	U
67	5	297	U
67	5	306	A
67	5	309	C
67	5	310	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	315	G
67	5	316	U
67	5	322	C
67	5	328	A
67	5	334	A
67	5	340	C
67	5	350	C
67	5	357	U
67	5	363	A
67	5	386	A
67	5	387	G
67	5	399	G
67	5	406	C
67	5	407	A
67	5	408	A
67	5	409	G
67	5	410	A
67	5	412	G
67	5	413	G
67	5	414	C
67	5	431	G
67	5	432	U
67	5	446	C
67	5	449	C
67	5	450	G
67	5	452	A
67	5	453	G
67	5	454	U
67	5	457	G
67	5	467	U
67	5	468	U
67	5	469	C
67	5	481	G
67	5	481(A)	C
67	5	482	G
67	5	483	G
67	5	484	U
67	5	485	C
67	5	486	C
67	5	492	U
67	5	493	G
67	5	495	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	497	G
67	5	498	C
67	5	499	G
67	5	505	G
67	5	510	U
67	5	649	A
67	5	654	C
67	5	658	C
67	5	666	G
67	5	667	A
67	5	668	C
67	5	672	C
67	5	683	C
67	5	684	G
67	5	685	C
67	5	687	U
67	5	696	C
67	5	697	G
67	5	704	C
67	5	705	G
67	5	708	G
67	5	719	C
67	5	722	G
67	5	729	G
67	5	730	G
67	5	731	G
67	5	734	G
67	5	738	C
67	5	738(A)	C
67	5	739	G
67	5	747	A
67	5	748	G
67	5	749	G
67	5	750	U
67	5	756	G
67	5	758	G
67	5	911	U
67	5	913	U
67	5	914	U
67	5	916	C
67	5	917	A
67	5	918	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	923	C
67	5	924	C
67	5	925	C
67	5	926	G
67	5	928	C
67	5	929	A
67	5	931	C
67	5	932	A
67	5	933	G
67	5	934	C
67	5	935	A
67	5	935(A)	G
67	5	936	C
67	5	938	C
67	5	939	G
67	5	943	A
67	5	944	A
67	5	945	U
67	5	955	G
67	5	956	A
67	5	957	G
67	5	959	G
67	5	960	A
67	5	961	G
67	5	962	C
67	5	965	G
67	5	966	A
67	5	967	C
67	5	968	C
67	5	969	C
67	5	970	G
67	5	972	C
67	5	973	G
67	5	979	C
67	5	983	C
67	5	990	C
67	5	1072	C
67	5	1073	G
67	5	1075	G
67	5	1076	C
67	5	1078	A
67	5	1079	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	1082	C
67	5	1174	G
67	5	1177	U
67	5	1179	U
67	5	1184	A
67	5	1195	G
67	5	1211	G
67	5	1212	G
67	5	1214	C
67	5	1215	C
67	5	1234	G
67	5	1235	G
67	5	1236	C
67	5	1237	C
67	5	1238	A
67	5	1239	C
67	5	1272	C
67	5	1273	G
67	5	1274	A
67	5	1276	C
67	5	1280	C
67	5	1284	G
67	5	1287	G
67	5	1288	G
67	5	1291	G
67	5	1292	C
67	5	1293	G
67	5	1295	U
67	5	1296	G
67	5	1301	C
67	5	1303	A
67	5	1304	C
67	5	1326	A
67	5	1328	G
67	5	1330	A
67	5	1337	A
67	5	1354	A
67	5	1359	G
67	5	1360	G
67	5	1364	U
67	5	1370	G
67	5	1371	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	1377	G
67	5	1378	C
67	5	1379	C
67	5	1380	G
67	5	1381	U
67	5	1387	A
67	5	1394	G
67	5	1397	A
67	5	1398	A
67	5	1401	C
67	5	1403	G
67	5	1416	G
67	5	1418	C
67	5	1419	G
67	5	1420	A
67	5	1421	G
67	5	1429	C
67	5	1435	G
67	5	1436	C
67	5	1437	C
67	5	1438	U
67	5	1441	C
67	5	1442	C
67	5	1445	U
67	5	1446	C
67	5	1453	G
67	5	1455	G
67	5	1456	C
67	5	1457	G
67	5	1458	C
67	5	1465	G
67	5	1475	G
67	5	1478	C
67	5	1481	C
67	5	1482	G
67	5	1483	C
67	5	1484	G
67	5	1485	C
67	5	1486	C
67	5	1489	G
67	5	1493	G
67	5	1497	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	1498	G
67	5	1502	G
67	5	1514	U
67	5	1516	G
67	5	1518	A
67	5	1523	A
67	5	1525	A
67	5	1534	A
67	5	1535	C
67	5	1547	A
67	5	1554	A
67	5	1563	A
67	5	1564	A
67	5	1566	C
67	5	1574	G
67	5	1578	U
67	5	1586	G
67	5	1591	U
67	5	1596	U
67	5	1601	A
67	5	1602	U
67	5	1612	G
67	5	1613	A
67	5	1624	G
67	5	1625	G
67	5	1626	G
67	5	1631	A
67	5	1633	G
67	5	1634	A
67	5	1654	G
67	5	1656	U
67	5	1661	C
67	5	1670	G
67	5	1676	C
67	5	1677	U
67	5	1679	A
67	5	1691	G
67	5	1724	G
67	5	1726	U
67	5	1734	G
67	5	1735	U
67	5	1740	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	1741	G
67	5	1742	A
67	5	1750	G
67	5	1753	G
67	5	1755	C
67	5	1756	U
67	5	1757	U
67	5	1761	G
67	5	1763	C
67	5	1764	G
67	5	1772	C
67	5	1773	U
67	5	1776	A
67	5	1780	A
67	5	1781	U
67	5	1787	A
67	5	1797	G
67	5	1799	G
67	5	1800	U
67	5	1803	G
67	5	1804	A
67	5	1805	A
67	5	1819	G
67	5	1821	G
67	5	1822	U
67	5	1823	G
67	5	1828	C
67	5	1833	G
67	5	1834	U
67	5	1835	G
67	5	1836	G
67	5	1837	A
67	5	1842	G
67	5	1855	G
67	5	1867	A
67	5	1869	G
67	5	1882	U
67	5	1883	G
67	5	1890	G
67	5	1893	C
67	5	1897	A
67	5	1910	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	1918	U
67	5	1920	C
67	5	1921	C
67	5	1922	G
67	5	1923	A
67	5	1931	C
67	5	1933	G
67	5	1941	A
67	5	1945	G
67	5	1948	G
67	5	1952	G
67	5	1959	U
67	5	1961	G
67	5	1962	A
67	5	1963	C
67	5	1966	C
67	5	1967	A
67	5	1976	G
67	5	1977	C
67	5	1980	U
67	5	1981	G
67	5	1982	G
67	5	1983	A
67	5	1984	A
67	5	1986	U
67	5	1987	C
67	5	1991	A
67	5	1997	U
67	5	2001	G
67	5	2002	A
67	5	2003	G
67	5	2004	U
67	5	2005	G
67	5	2008	U
67	5	2011	C
67	5	2024	G
67	5	2025	A
67	5	2026	A
67	5	2046	G
67	5	2047	A
67	5	2048	U
67	5	2052	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	2055	G
67	5	2056	G
67	5	2062	C
67	5	2064	G
67	5	2069	A
67	5	2070	U
67	5	2084	U
67	5	2085	G
67	5	2089	G
67	5	2090	U
67	5	2092	G
67	5	2093	G
67	5	2094	C
67	5	2095	A
67	5	2097	A
67	5	2098	G
67	5	2100	G
67	5	2101	A
67	5	2102	G
67	5	2104	A
67	5	2106	G
67	5	2107	A
67	5	2108	G
67	5	2110	G
67	5	2259	G
67	5	2260	C
67	5	2262	G
67	5	2266	C
67	5	2267	U
67	5	2268	A
67	5	2269	C
67	5	2270	G
67	5	2275	G
67	5	2278	G
67	5	2279	A
67	5	2288	G
67	5	2289	C
67	5	2295	C
67	5	2300	A
67	5	2301	G
67	5	2313	A
67	5	2314	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	2322	G
67	5	2331	G
67	5	2333	G
67	5	2348	G
67	5	2351	C
67	5	2364	G
67	5	2370	A
67	5	2395	A
67	5	2396	A
67	5	2399	G
67	5	2402	G
67	5	2416	G
67	5	2417	A
67	5	2422	C
67	5	2424	G
67	5	2425	U
67	5	2428	A
67	5	2429	A
67	5	2433	G
67	5	2441	C
67	5	2450	G
67	5	2469	C
67	5	2470	C
67	5	2471	G
67	5	2475	G
67	5	2479	G
67	5	2483	G
67	5	2485	U
67	5	2488	C
67	5	2489	C
67	5	2490	U
67	5	2491	C
67	5	2493	G
67	5	2495	U
67	5	2503	G
67	5	2504	C
67	5	2505	C
67	5	2506	G
67	5	2511	A
67	5	2513	A
67	5	2521	G
67	5	2530	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	2537	A
67	5	2546	G
67	5	2547	G
67	5	2554	U
67	5	2555	G
67	5	2564	G
67	5	2566	G
67	5	2571	C
67	5	2572	C
67	5	2575	U
67	5	2583	C
67	5	2586	G
67	5	2587	A
67	5	2601	A
67	5	2618	G
67	5	2620	G
67	5	2627	C
67	5	2638	G
67	5	2640	G
67	5	2647	A
67	5	2661	U
67	5	2662	G
67	5	2663	G
67	5	2669	C
67	5	2670	C
67	5	2673	G
67	5	2676	A
67	5	2681	G
67	5	2686	G
67	5	2687	U
67	5	2688	G
67	5	2689	C
67	5	2695	A
67	5	2696	A
67	5	2707	U
67	5	2708	U
67	5	2709	C
67	5	2710	C
67	5	2711	G
67	5	2712	G
67	5	2714	G
67	5	2716	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	2719	C
67	5	2721	G
67	5	2725	A
67	5	2726	G
67	5	2740	U
67	5	2743	A
67	5	2744	A
67	5	2754	G
67	5	2760	G
67	5	2761	U
67	5	2763	U
67	5	2764	A
67	5	2769	U
67	5	2772	C
67	5	2787	A
67	5	2788	U
67	5	2789	A
67	5	2790	U
67	5	2794	C
67	5	2795	A
67	5	2796	G
67	5	2798	A
67	5	2806	A
67	5	2807	A
67	5	2808	G
67	5	2814	C
67	5	2826	U
67	5	2827	G
67	5	2828	U
67	5	2829	U
67	5	2835	A
67	5	2838	G
67	5	2839	U
67	5	2842	G
67	5	2845	A
67	5	2855	G
67	5	2864	A
67	5	2875	C
67	5	2884	G
67	5	2896	G
67	5	2897	G
67	5	3598	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	3599	A
67	5	3604	A
67	5	3605	C
67	5	3615	G
67	5	3625	G
67	5	3626	G
67	5	3635	A
67	5	3644	U
67	5	3653	A
67	5	3662	A
67	5	3671	G
67	5	3673	C
67	5	3674	G
67	5	3692	A
67	5	3696	C
67	5	3698	G
67	5	3711	A
67	5	3712	A
67	5	3722	G
67	5	3729	U
67	5	3740	G
67	5	3748	A
67	5	3750	G
67	5	3753	G
67	5	3756	A
67	5	3759	A
67	5	3760	A
67	5	3765	G
67	5	3766	A
67	5	3773	U
67	5	3774	A
67	5	3776	G
67	5	3777	G
67	5	3778	U
67	5	3783	A
67	5	3784	A
67	5	3785	A
67	5	3786	U
67	5	3799	A
67	5	3810	C
67	5	3811	G
67	5	3812	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	3814	U
67	5	3817	A
67	5	3819	G
67	5	3822	U
67	5	3831	U
67	5	3838	U
67	5	3840	U
67	5	3851	U
67	5	3859	G
67	5	3867	A
67	5	3876	A
67	5	3877	A
67	5	3878	C
67	5	3879	G
67	5	3889	G
67	5	3892	U
67	5	3897	G
67	5	3898	G
67	5	3901	A
67	5	3905	A
67	5	3906	A
67	5	3907	G
67	5	3915	U
67	5	3916	G
67	5	3917	A
67	5	3927	U
67	5	3939	G
67	5	3943	A
67	5	3946	G
67	5	4067	U
67	5	4069	U
67	5	4071	U
67	5	4076	G
67	5	4084	G
67	5	4085	A
67	5	4086	G
67	5	4088	C
67	5	4099	G
67	5	4100	C
67	5	4116	C
67	5	4117	U
67	5	4118	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	4119	C
67	5	4120	U
67	5	4121	G
67	5	4122	G
67	5	4125	C
67	5	4127	A
67	5	4150	G
67	5	4158	C
67	5	4162	C
67	5	4163	U
67	5	4164	C
67	5	4166	G
67	5	4171	C
67	5	4183	G
67	5	4184	G
67	5	4190	U
67	5	4191	G
67	5	4203	A
67	5	4212	A
67	5	4213	A
67	5	4218	U
67	5	4219	A
67	5	4225	G
67	5	4229	U
67	5	4232	U
67	5	4233	A
67	5	4249	G
67	5	4251	A
67	5	4255	A
67	5	4257	A
67	5	4258	C
67	5	4265	U
67	5	4268	A
67	5	4271	A
67	5	4273	A
67	5	4281	A
67	5	4291	G
67	5	4297	G
67	5	4304	A
67	5	4305	G
67	5	4306	U
67	5	4314	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	4317	A
67	5	4318	C
67	5	4319	C
67	5	4326	G
67	5	4329	G
67	5	4330	G
67	5	4335	C
67	5	4336	A
67	5	4339	A
67	5	4349	C
67	5	4350	C
67	5	4354	U
67	5	4355	G
67	5	4373	G
67	5	4377	G
67	5	4378	A
67	5	4379	A
67	5	4380	A
67	5	4387	C
67	5	4391	G
67	5	4393	G
67	5	4394	A
67	5	4395	U
67	5	4396	A
67	5	4398	C
67	5	4401	G
67	5	4415	A
67	5	4419	U
67	5	4421	C
67	5	4422	A
67	5	4440	G
67	5	4444	C
67	5	4448	G
67	5	4449	A
67	5	4450	U
67	5	4453	C
67	5	4464	A
67	5	4471	U
67	5	4475	G
67	5	4476	C
67	5	4488	A
67	5	4495	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	4500	U
67	5	4510	A
67	5	4511	A
67	5	4512	U
67	5	4513	A
67	5	4519	C
67	5	4520	G
67	5	4524	G
67	5	4531	U
67	5	4548	A
67	5	4549	G
67	5	4560	C
67	5	4567	G
67	5	4570	G
67	5	4573	G
67	5	4575	G
67	5	4578	G
67	5	4586	G
67	5	4590	A
67	5	4618	G
67	5	4627	U
67	5	4636	U
67	5	4637	G
67	5	4639	G
67	5	4656	A
67	5	4657	U
67	5	4661	G
67	5	4667	C
67	5	4670	C
67	5	4672	A
67	5	4677	U
67	5	4678	G
67	5	4687	A
67	5	4694	G
67	5	4700	A
67	5	4701	A
67	5	4709	U
67	5	4719	G
67	5	4720	C
67	5	4721	G
67	5	4728	U
67	5	4736	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	4737	G
67	5	4745	G
67	5	4751	G
67	5	4754	G
67	5	4755	G
67	5	4756	C
67	5	4757	C
67	5	4759	C
67	5	4761	G
67	5	4765	G
67	5	4771	C
67	5	4772	C
67	5	4868	G
67	5	4870	G
67	5	4871	C
67	5	4872	G
67	5	4873	G
67	5	4874	A
67	5	4875	G
67	5	4876	A
67	5	4877	G
67	5	4882	U
67	5	4883	C
67	5	4885	U
67	5	4887	C
67	5	4891	G
67	5	4895	C
67	5	4897	G
67	5	4910	A
67	5	4912	G
67	5	4914	G
67	5	4915	G
67	5	4918	C
67	5	4919	G
67	5	4921	C
67	5	4924	C
67	5	4925	U
67	5	4926	C
67	5	4928	C
67	5	4931	G
67	5	4935	C
67	5	4937	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	4938	A
67	5	4940	C
67	5	4943	A
67	5	4944	C
67	5	4948	C
67	5	4949	G
67	5	4950	U
67	5	4951	G
67	5	4956	A
67	5	4957	C
67	5	4958	C
67	5	4964	C
67	5	4965	U
67	5	4966	A
67	5	4967	A
67	5	4976	U
67	5	4985	U
67	5	4988	U
67	5	4989	U
67	5	4990	C
67	5	4991	U
67	5	4993	G
67	5	5007	A
67	5	5014	A
67	5	5017	G
67	5	5035	U
67	5	5040	U
67	5	5041	G
67	5	5047	C
67	5	5050	C
67	5	5052	C
67	5	5053	U
67	5	5054	C
67	5	5056	A
67	5	5061	A
67	5	5062	G
70	7	7	G
70	7	11	A
70	7	22	A
70	7	25	G
70	7	33	U
70	7	42	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
70	7	53	U
70	7	54	A
70	7	64	G
70	7	97	G
70	7	100	A
70	7	106	G
70	7	110	G
70	7	120	U
73	8	2	G
73	8	3	A
73	8	32	C
73	8	34	U
73	8	35	C
73	8	49	G
73	8	59	A
73	8	62	A
73	8	63	U
73	8	75	G
73	8	79	G
73	8	86	U
73	8	87	G
73	8	94	G
73	8	95	A
73	8	103	A
73	8	104	A
73	8	105	C
73	8	107	C
73	8	109	C
73	8	110	U
73	8	111	U
73	8	112	G
73	8	114	G
73	8	121	G
73	8	123	U
73	8	124	U
73	8	125	C
73	8	126	C
73	8	127	U
73	8	137	A
73	8	143	G
73	8	150	C
73	8	153	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	2	A
76	9	3	C
76	9	4	C
76	9	17	C
76	9	25	A
76	9	26	U
76	9	33	G
76	9	41	G
76	9	44	U
76	9	45	A
76	9	46	A
76	9	56	G
76	9	58	C
76	9	60	A
76	9	65	C
76	9	67	C
76	9	68	A
76	9	70	G
76	9	71	G
76	9	73	C
76	9	74	G
76	9	75	G
76	9	77	A
76	9	79	A
76	9	99	A
76	9	100	U
76	9	103	A
76	9	104	A
76	9	110	U
76	9	111	A
76	9	113	G
76	9	115	U
76	9	116	U
76	9	124	U
76	9	126	G
76	9	127	C
76	9	129	C
76	9	130	G
76	9	141	A
76	9	143	U
76	9	147	A
76	9	155	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	158	A
76	9	161	U
76	9	162	C
76	9	163	U
76	9	167	G
76	9	168	C
76	9	173	A
76	9	175	A
76	9	182	C
76	9	183	G
76	9	184	G
76	9	188	C
76	9	189	U
76	9	192	C
76	9	200	G
76	9	202	G
76	9	206	G
76	9	213	G
76	9	215	G
76	9	289	G
76	9	292	A
76	9	293	C
76	9	294	U
76	9	302	A
76	9	304	C
76	9	307	G
76	9	308	G
76	9	309	G
76	9	312	G
76	9	314	U
76	9	318	A
76	9	319	C
76	9	322	C
76	9	331	C
76	9	332	G
76	9	335	G
76	9	340	C
76	9	347	G
76	9	351	G
76	9	360	A
76	9	362	C
76	9	364	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	368	U
76	9	370	G
76	9	371	A
76	9	372	U
76	9	381	C
76	9	382	C
76	9	383	G
76	9	384	U
76	9	385	G
76	9	386	C
76	9	400	C
76	9	407	G
76	9	409	C
76	9	417	C
76	9	418	A
76	9	435	A
76	9	438	G
76	9	448	A
76	9	449	A
76	9	450	C
76	9	459	C
76	9	460	A
76	9	462	C
76	9	464	A
76	9	465	A
76	9	466	G
76	9	472	C
76	9	473	A
76	9	474	G
76	9	476	A
76	9	482	G
76	9	487	U
76	9	492	C
76	9	496	C
76	9	507	G
76	9	508	A
76	9	512	A
76	9	516	A
76	9	525	A
76	9	531	A
76	9	532	C
76	9	533	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	544	G
76	9	545	A
76	9	546	G
76	9	548	C
76	9	549	C
76	9	550	C
76	9	551	U
76	9	554	A
76	9	555	A
76	9	556	U
76	9	557	U
76	9	559	G
76	9	563	G
76	9	564	A
76	9	568	C
76	9	576	A
76	9	583	A
76	9	587	A
76	9	588	G
76	9	589	G
76	9	590	A
76	9	591	U
76	9	592	C
76	9	597	G
76	9	598	G
76	9	604	A
76	9	606	G
76	9	607	U
76	9	608	C
76	9	614	C
76	9	620	G
76	9	629	A
76	9	631	U
76	9	637	U
76	9	643	A
76	9	644	G
76	9	655	A
76	9	659	G
76	9	660	C
76	9	663	C
76	9	664	A
76	9	668	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	669	A
76	9	670	A
76	9	671	A
76	9	672	A
76	9	673	G
76	9	684	G
76	9	688	U
76	9	689	U
76	9	732	U
76	9	752	G
76	9	753	C
76	9	754	G
76	9	810	A
76	9	811	A
76	9	812	A
76	9	821	G
76	9	822	U
76	9	830	A
76	9	834	C
76	9	847	A
76	9	861	A
76	9	868	G
76	9	869	A
76	9	870	A
76	9	871	U
76	9	872	A
76	9	873	G
76	9	874	G
76	9	875	A
76	9	877	C
76	9	878	G
76	9	885	U
76	9	887	U
76	9	890	U
76	9	892	U
76	9	913	A
76	9	914	U
76	9	920	A
76	9	922	A
76	9	930	C
76	9	933	G
76	9	934	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	943	U
76	9	955	A
76	9	971	G
76	9	985	G
76	9	990	A
76	9	992	A
76	9	999	G
76	9	1008	A
76	9	1017	U
76	9	1023	A
76	9	1041	G
76	9	1045	U
76	9	1060	A
76	9	1061	U
76	9	1062	A
76	9	1078	C
76	9	1083	A
76	9	1085	C
76	9	1089	G
76	9	1096	G
76	9	1099	G
76	9	1100	A
76	9	1113	A
76	9	1114	U
76	9	1115	U
76	9	1116	C
76	9	1117	C
76	9	1118	C
76	9	1121	G
76	9	1131	G
76	9	1133	A
76	9	1138	C
76	9	1139	C
76	9	1148	A
76	9	1149	A
76	9	1150	A
76	9	1153	C
76	9	1154	U
76	9	1165	G
76	9	1166	G
76	9	1195	A
76	9	1197	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	1207	G
76	9	1208	A
76	9	1211	G
76	9	1213	C
76	9	1215	C
76	9	1216	C
76	9	1221	G
76	9	1223	A
76	9	1224	G
76	9	1240	A
76	9	1242	U
76	9	1251	A
76	9	1253	A
76	9	1254	C
76	9	1256	G
76	9	1257	G
76	9	1259	A
76	9	1260	A
76	9	1265	A
76	9	1271	C
76	9	1274	G
76	9	1275	G
76	9	1281	G
76	9	1284	A
76	9	1285	G
76	9	1286	G
76	9	1287	A
76	9	1289	U
76	9	1293	A
76	9	1298	G
76	9	1299	A
76	9	1300	U
76	9	1301	A
76	9	1302	G
76	9	1307	U
76	9	1308	U
76	9	1313	A
76	9	1314	U
76	9	1316	C
76	9	1330	G
76	9	1331	C
76	9	1342	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	1348	G
76	9	1354	G
76	9	1369	A
76	9	1371	U
76	9	1372	U
76	9	1378	A
76	9	1395	C
76	9	1396	A
76	9	1397	U
76	9	1401	A
76	9	1402	A
76	9	1404	U
76	9	1410	C
76	9	1412	C
76	9	1424	G
76	9	1428	G
76	9	1429	G
76	9	1439	A
76	9	1449	G
76	9	1452	A
76	9	1454	A
76	9	1458	G
76	9	1459	G
76	9	1462	U
76	9	1463	U
76	9	1466	G
76	9	1473	G
76	9	1476	A
76	9	1477	U
76	9	1478	U
76	9	1490	G
76	9	1494	U
76	9	1495	G
76	9	1497	G
76	9	1498	A
76	9	1507	G
76	9	1509	U
76	9	1510	G
76	9	1519	U
76	9	1520	G
76	9	1521	C
76	9	1522	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	1531	A
76	9	1533	A
76	9	1536	G
76	9	1544	C
76	9	1545	A
76	9	1548	G
76	9	1552	G
76	9	1553	C
76	9	1555	U
76	9	1556	A
76	9	1557	C
76	9	1560	U
76	9	1570	G
76	9	1574	C
76	9	1575	G
76	9	1580	A
76	9	1581	C
76	9	1582	C
76	9	1585	U
76	9	1586	U
76	9	1587	G
76	9	1588	A
76	9	1589	A
76	9	1600	G
76	9	1601	A
76	9	1602	U
76	9	1604	G
76	9	1621	U
76	9	1623	A
76	9	1625	U
76	9	1637	A
76	9	1638	G
76	9	1639	G
76	9	1641	A
76	9	1647	A
76	9	1648	G
76	9	1654	G
76	9	1664	A
76	9	1665	G
76	9	1671	G
76	9	1680	G
76	9	1682	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	1683	C
76	9	1686	G
76	9	1689	C
76	9	1695	A
76	9	1698	C
76	9	1699	A
76	9	1700	C
76	9	1703	C
76	9	1715	A
76	9	1721	U
76	9	1722	G
76	9	1726	G
76	9	1728	U
76	9	1729	U
76	9	1730	U
76	9	1737	G
76	9	1753	C
76	9	1756	C
76	9	1758	G
76	9	1760	G
76	9	1772	C
76	9	1783	C
76	9	1785	C
76	9	1800	A
76	9	1823	A
76	9	1825	A
76	9	1826	G
76	9	1829	G
76	9	1831	A
76	9	1835	A
76	9	1836	G
76	9	1838	U
76	9	1849	G
76	9	1851	A
76	9	1861	G
76	9	1862	G
76	9	1863	A
76	9	1865	C
76	9	1866	A
76	9	1867	U
76	9	1868	U
76	9	1869	A

All (226) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
67	5	12	A
67	5	47	A
67	5	48	G
67	5	64	A
67	5	119	G
67	5	125	C
67	5	134	G
67	5	143	C
67	5	159	C
67	5	217	C
67	5	226	G
67	5	234	G
67	5	245	C
67	5	265	C
67	5	275	C
67	5	278	G
67	5	385	A
67	5	387	G
67	5	406	C
67	5	408	A
67	5	409	G
67	5	449	C
67	5	480	C
67	5	481(A)	C
67	5	482	G
67	5	484	U
67	5	485	C
67	5	492	U
67	5	497	G
67	5	498	C
67	5	504	G
67	5	696	C
67	5	729	G
67	5	738(A)	C
67	5	747	A
67	5	748	G
67	5	915	A
67	5	916	C
67	5	930	G
67	5	935(A)	G
67	5	955	G
67	5	956	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	959	G
67	5	965	G
67	5	966	A
67	5	969	C
67	5	971(A)	G
67	5	1071	C
67	5	1072	C
67	5	1211	G
67	5	1214	C
67	5	1236	C
67	5	1238	A
67	5	1287	G
67	5	1291	G
67	5	1295	U
67	5	1329	G
67	5	1354	A
67	5	1358	G
67	5	1359	G
67	5	1370	G
67	5	1378	C
67	5	1380	G
67	5	1420	A
67	5	1440	U
67	5	1445	U
67	5	1455	G
67	5	1477	C
67	5	1481	C
67	5	1484	G
67	5	1485	C
67	5	1497	A
67	5	1502	G
67	5	1563	A
67	5	1633	G
67	5	1733	G
67	5	1734	G
67	5	1740	C
67	5	1804	A
67	5	1815	G
67	5	1818	G
67	5	1833	G
67	5	1834	U
67	5	1835	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	1836	G
67	5	1881	C
67	5	1892	A
67	5	1921	C
67	5	1935	C
67	5	1979	A
67	5	1983	A
67	5	2046	G
67	5	2068	C
67	5	2088	A
67	5	2089	G
67	5	2100	G
67	5	2265	G
67	5	2266	C
67	5	2278	G
67	5	2313	A
67	5	2398	U
67	5	2428	A
67	5	2467	U
67	5	2468	U
67	5	2474	G
67	5	2475	G
67	5	2490	U
67	5	2502	A
67	5	2546	G
67	5	2587	A
67	5	2661	U
67	5	2695	A
67	5	2754	G
67	5	2794	C
67	5	2806	A
67	5	3625	G
67	5	3673	C
67	5	3697	U
67	5	3710	G
67	5	3765	G
67	5	3809	G
67	5	3876	A
67	5	3888	G
67	5	3904	G
67	5	4075	U
67	5	4076	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
67	5	4084	G
67	5	4119	C
67	5	4121	G
67	5	4124	G
67	5	4162	C
67	5	4170	A
67	5	4232	U
67	5	4254	G
67	5	4266	G
67	5	4378	A
67	5	4395	U
67	5	4448	G
67	5	4449	A
67	5	4510	A
67	5	4527	G
67	5	4626	A
67	5	4694	G
67	5	4699	U
67	5	4719	G
67	5	4871	C
67	5	4872	G
67	5	4876	A
67	5	4884	G
67	5	4925	U
67	5	4936	G
67	5	4942	C
67	5	4947	U
67	5	4965	U
67	5	4966	A
73	8	2	G
73	8	86	U
73	8	94	G
73	8	110	U
73	8	124	U
76	9	2	A
76	9	72	C
76	9	110	U
76	9	126	G
76	9	160	U
76	9	182	C
76	9	293	C
76	9	308	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	369	C
76	9	370	G
76	9	434	G
76	9	448	A
76	9	465	A
76	9	473	A
76	9	487	U
76	9	532	C
76	9	550	C
76	9	553	U
76	9	555	A
76	9	563	G
76	9	591	U
76	9	606	G
76	9	620	G
76	9	642	U
76	9	670	A
76	9	688	U
76	9	752	G
76	9	821	G
76	9	869	A
76	9	870	A
76	9	872	A
76	9	874	G
76	9	1016	U
76	9	1114	U
76	9	1115	U
76	9	1120	U
76	9	1137	U
76	9	1165	G
76	9	1215	C
76	9	1253	A
76	9	1264	C
76	9	1284	A
76	9	1286	G
76	9	1313	A
76	9	1330	G
76	9	1394	G
76	9	1395	C
76	9	1396	A
76	9	1489	A
76	9	1493	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	9	1519	U
76	9	1520	G
76	9	1535	U
76	9	1585	U
76	9	1637	A
76	9	1638	G
76	9	1646	C
76	9	1664	A
76	9	1665	G
76	9	1679	A
76	9	1721	U
76	9	1744	G
76	9	1824	A
76	9	1835	A
76	9	1867	U
76	9	1868	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 289 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	GCP	jj	700	-	27,34,34	4.66	10 (37%)	34,54,54	1.74	8 (23%)
88	BLS	5	5122	67	28,31,31	3.73	14 (50%)	28,43,43	2.06	10 (35%)

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
87	GCP	jj	700	-	-	5/15/38/38	0/3/3/3
88	BLS	5	5122	67	-	8/21/38/38	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	jj	700	GCP	O4'-C1'	15.21	1.62	1.41
87	jj	700	GCP	C2'-C1'	-14.43	1.31	1.53
88	5	5122	BLS	O5'-C5'	-11.48	1.24	1.43
88	5	5122	BLS	C3'-C2'	7.36	1.55	1.33
88	5	5122	BLS	C4'-C5'	7.17	1.69	1.53
87	jj	700	GCP	O4'-C4'	-6.12	1.31	1.45
87	jj	700	GCP	PB-O3A	5.67	1.64	1.58
88	5	5122	BLS	C7-N6	5.45	1.45	1.34
87	jj	700	GCP	C2-N2	5.28	1.44	1.33
88	5	5122	BLS	C14-N12	4.76	1.45	1.35
88	5	5122	BLS	C14-N15	4.52	1.44	1.34
88	5	5122	BLS	C1'-C2'	-3.91	1.40	1.49
88	5	5122	BLS	C4-N4	3.52	1.45	1.35
87	jj	700	GCP	O3'-C3'	-3.05	1.35	1.43
87	jj	700	GCP	O2'-C2'	2.88	1.49	1.43
88	5	5122	BLS	C1'-N1	-2.75	1.41	1.49
87	jj	700	GCP	C5-C4	-2.68	1.33	1.40
88	5	5122	BLS	C4'-C3'	-2.52	1.40	1.49
88	5	5122	BLS	C5-C4	-2.48	1.35	1.41
88	5	5122	BLS	O7-C7	-2.45	1.18	1.23
88	5	5122	BLS	C6-N1	-2.42	1.32	1.35
87	jj	700	GCP	PB-O2B	-2.33	1.50	1.56
88	5	5122	BLS	C5'-C6'	2.27	1.57	1.53
87	jj	700	GCP	O6-C6	-2.08	1.19	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	5122	BLS	C8-C7-N6	4.97	122.84	116.33
87	jj	700	GCP	N3-C2-N1	-4.76	120.88	127.22
87	jj	700	GCP	C2-N3-C4	4.62	120.63	115.36
88	5	5122	BLS	C4-N3-C2	3.71	120.10	116.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	jj	700	GCP	PB-O3A-PA	-3.32	122.04	132.56
88	5	5122	BLS	C11-C10-C9	-3.21	108.49	114.52
88	5	5122	BLS	C4'-N6-C7	-3.15	119.76	123.13
88	5	5122	BLS	O5'-C1'-C2'	-3.09	111.46	113.13
88	5	5122	BLS	N4-C4-N3	3.06	121.33	116.49
88	5	5122	BLS	O7-C7-C8	-2.93	117.21	121.50
87	jj	700	GCP	C5-C6-N1	-2.61	119.86	123.43
87	jj	700	GCP	C4-C5-N7	-2.55	106.74	109.40
87	jj	700	GCP	N2-C2-N1	2.51	121.15	117.25
87	jj	700	GCP	C2'-C3'-C4'	-2.46	97.86	102.64
87	jj	700	GCP	C3'-C2'-C1'	2.42	104.61	100.98
88	5	5122	BLS	C1'-C2'-C3'	-2.35	119.44	122.52
88	5	5122	BLS	O4-C6'-O3	-2.15	119.20	124.09
88	5	5122	BLS	C3'-C4'-N6	-2.12	106.70	110.60

There are no chirality outliers.

All (13) torsion outliers are listed below:

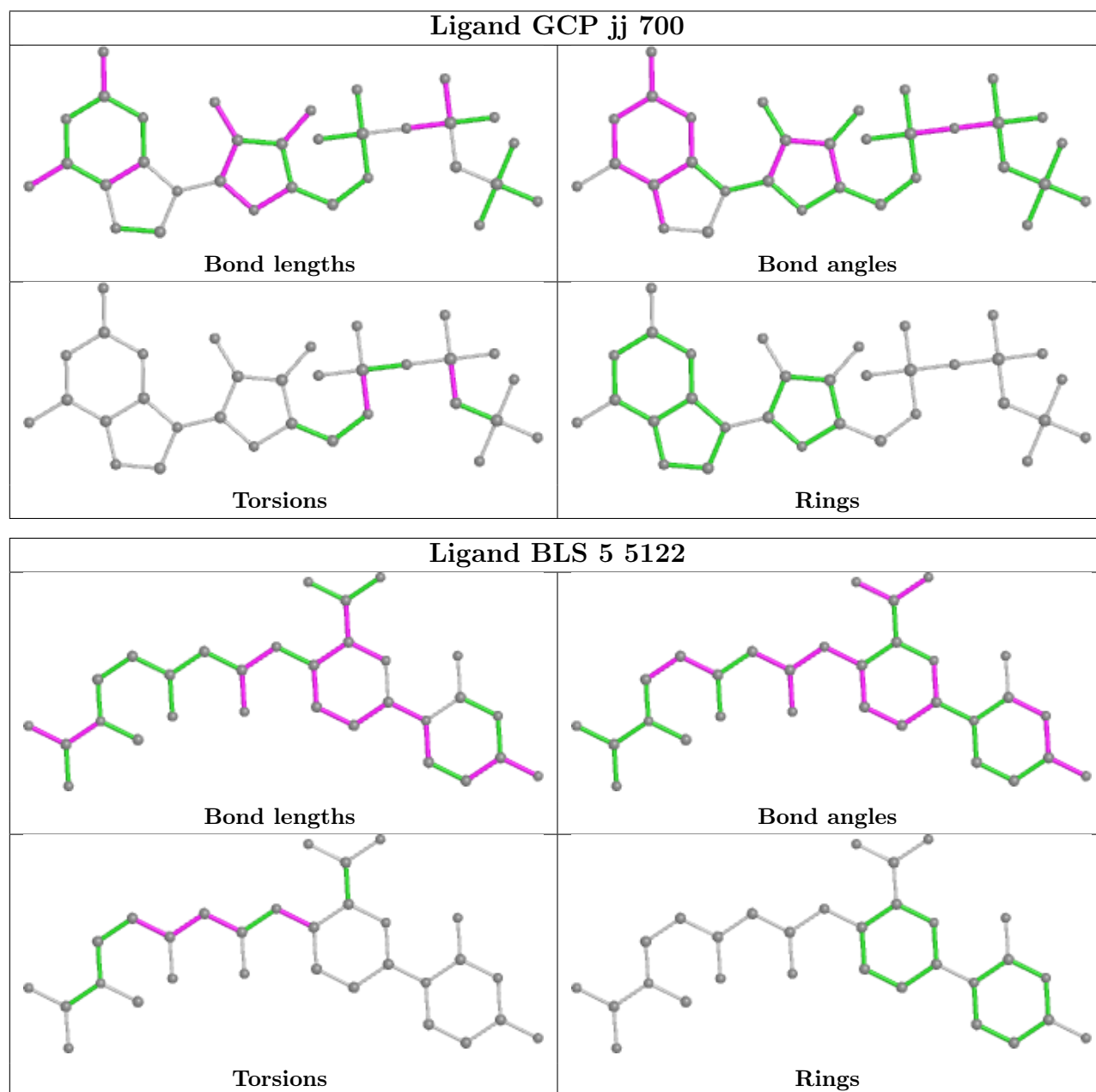
Mol	Chain	Res	Type	Atoms
87	jj	700	GCP	PG-C3B-PB-O1B
87	jj	700	GCP	PG-C3B-PB-O2B
87	jj	700	GCP	PG-C3B-PB-O3A
87	jj	700	GCP	C5'-O5'-PA-O3A
88	5	5122	BLS	C3'-C4'-N6-C7
88	5	5122	BLS	C7-C8-C9-N9
88	5	5122	BLS	C11-C10-C9-C8
88	5	5122	BLS	C11-C10-C9-N9
88	5	5122	BLS	N6-C7-C8-C9
88	5	5122	BLS	O7-C7-C8-C9
87	jj	700	GCP	C5'-O5'-PA-O2A
88	5	5122	BLS	C7-C8-C9-C10
88	5	5122	BLS	C5'-C4'-N6-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
67	5	7
76	9	7
73	8	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	990:C	O3'	1064:G	P	17.61
1	5	1406(C):G	O3'	1411:C	P	17.48
1	8	79:G	O3'	85:U	P	15.70
1	5	4138:C	O3'	4146:G	P	15.08
1	9	322:C	O3'	323:C	P	9.57
1	9	798:G	O3'	799:U	P	5.28
1	5	1438:U	O3'	1440:U	P	4.98
1	9	1295:A	O3'	1296:U	P	4.76
1	5	5020:G	O3'	5021:C	P	4.72
1	9	304:C	O3'	305:U	P	4.39
1	5	170:C	O3'	171:U	P	4.32
1	5	751:G	O3'	752:G	P	3.76
1	9	902:G	O3'	903:A	P	3.75
1	9	309:G	O3'	310:C	P	3.57
1	9	903:A	O3'	904:A	P	3.28

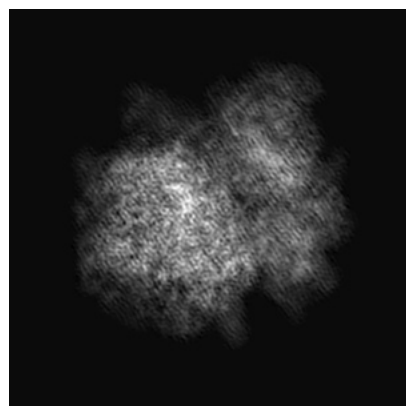
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12632. These allow visual inspection of the internal detail of the map and identification of artifacts.

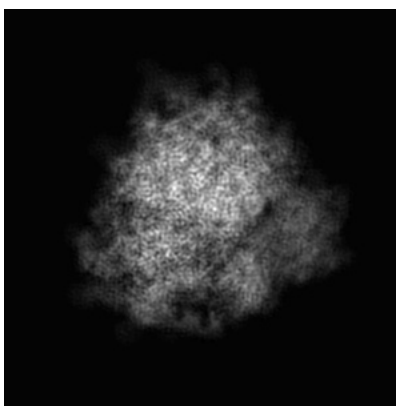
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

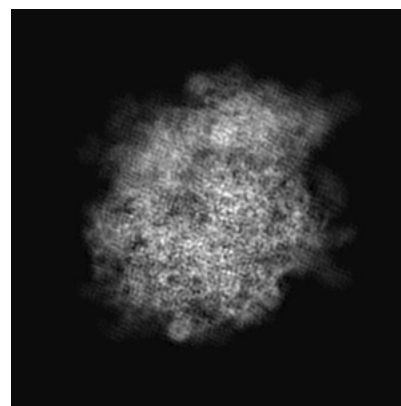
6.1.1 Primary map



X

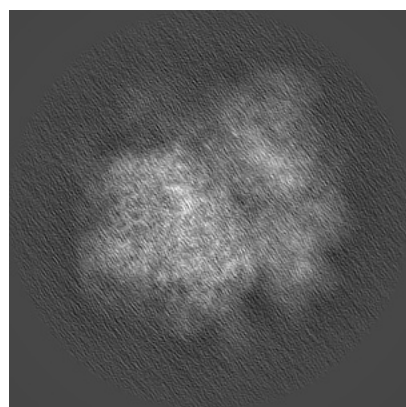


Y

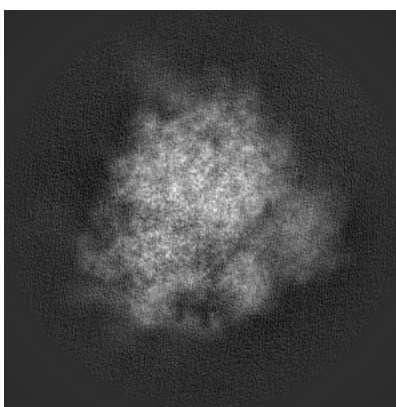


Z

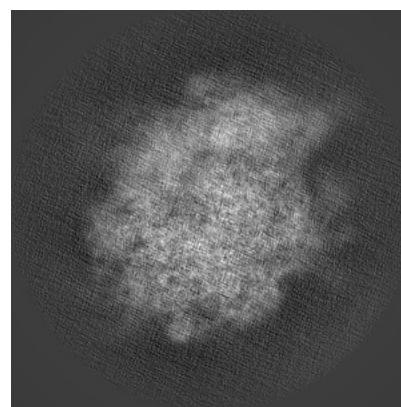
6.1.2 Raw map



X



Y

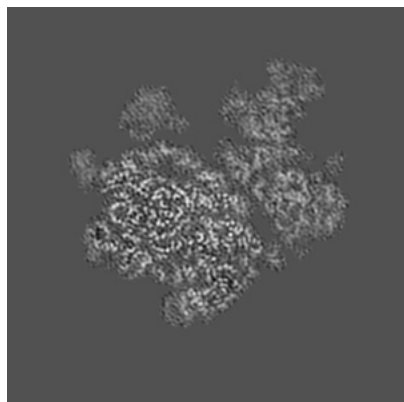


Z

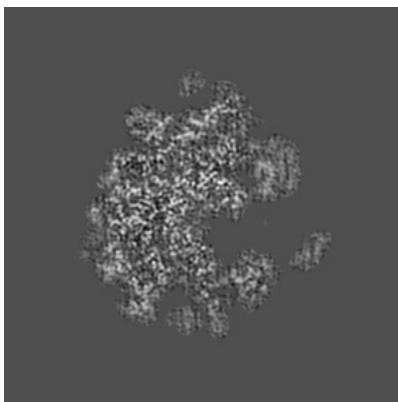
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

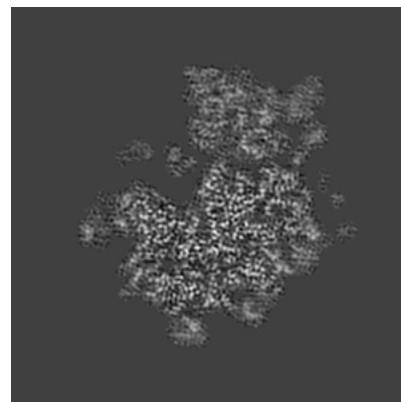
6.2.1 Primary map



X Index: 150

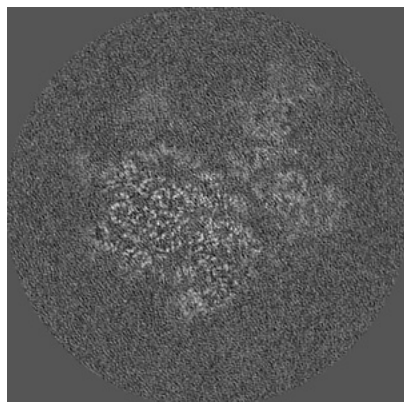


Y Index: 150

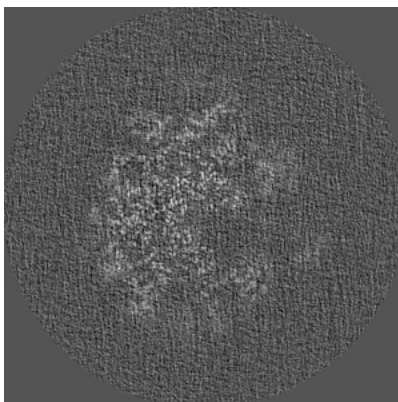


Z Index: 150

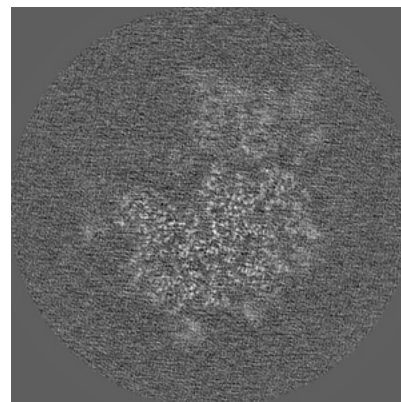
6.2.2 Raw map



X Index: 150



Y Index: 150

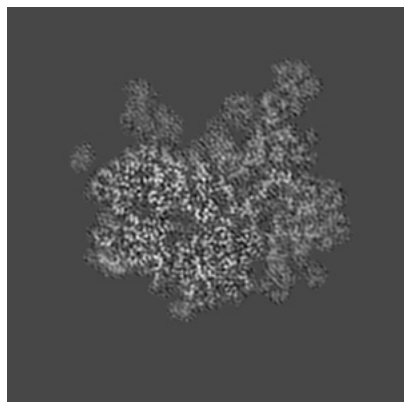


Z Index: 150

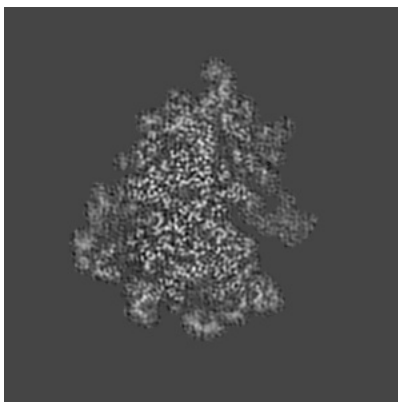
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

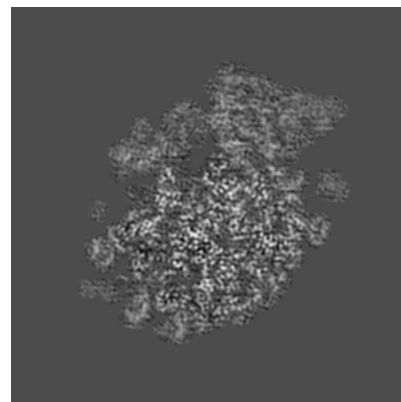
6.3.1 Primary map



X Index: 158

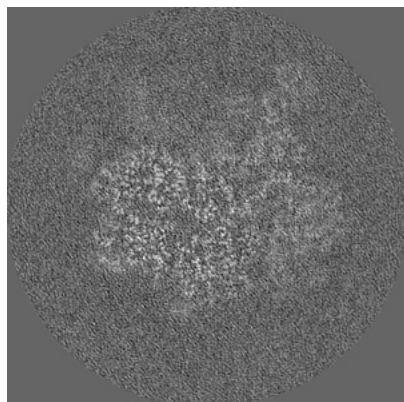


Y Index: 130

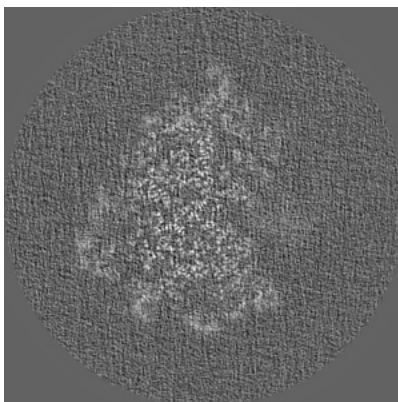


Z Index: 128

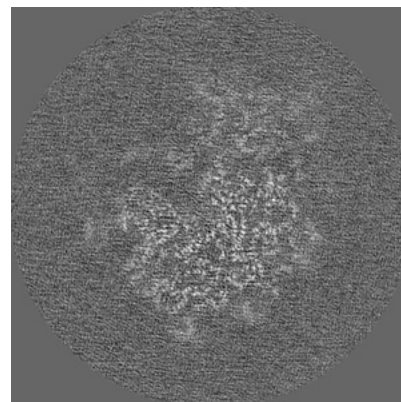
6.3.2 Raw map



X Index: 158



Y Index: 130

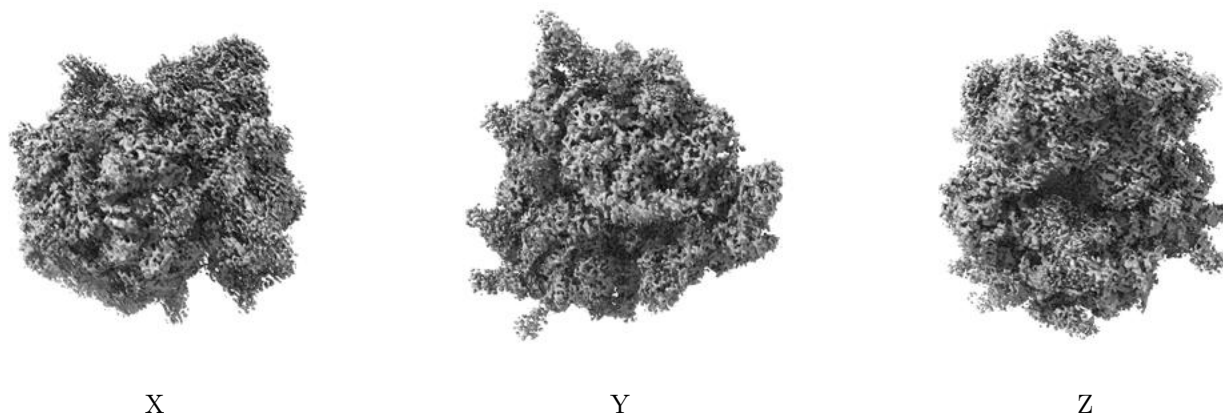


Z Index: 148

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

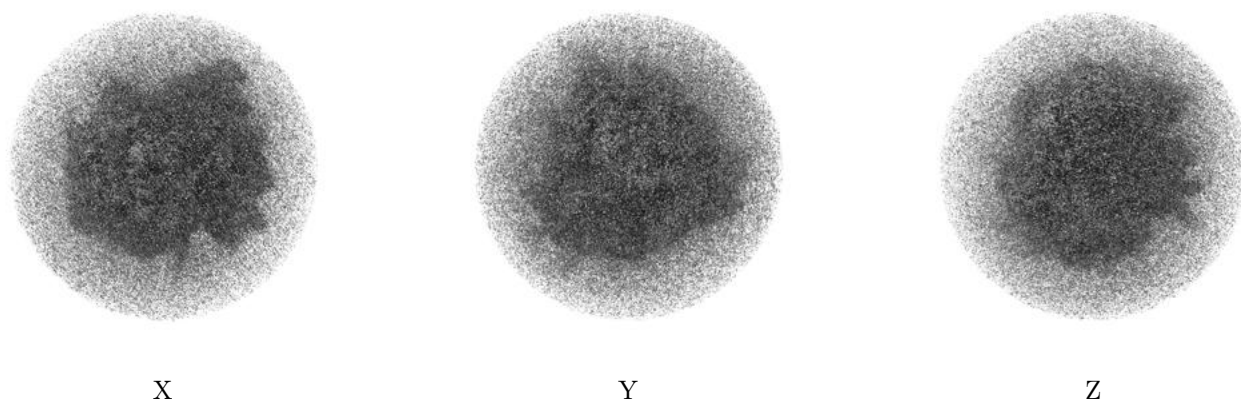
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

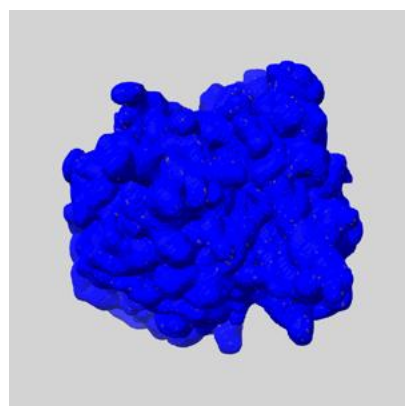
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

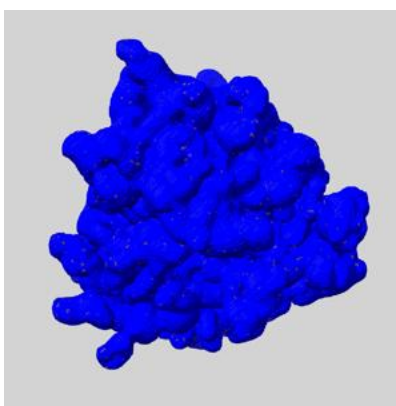
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

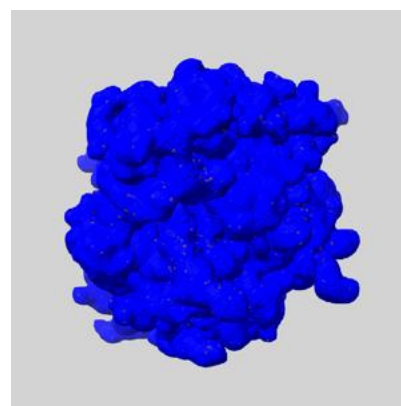
6.5.1 emd_12632_msk_1.map [i](#)



X



Y

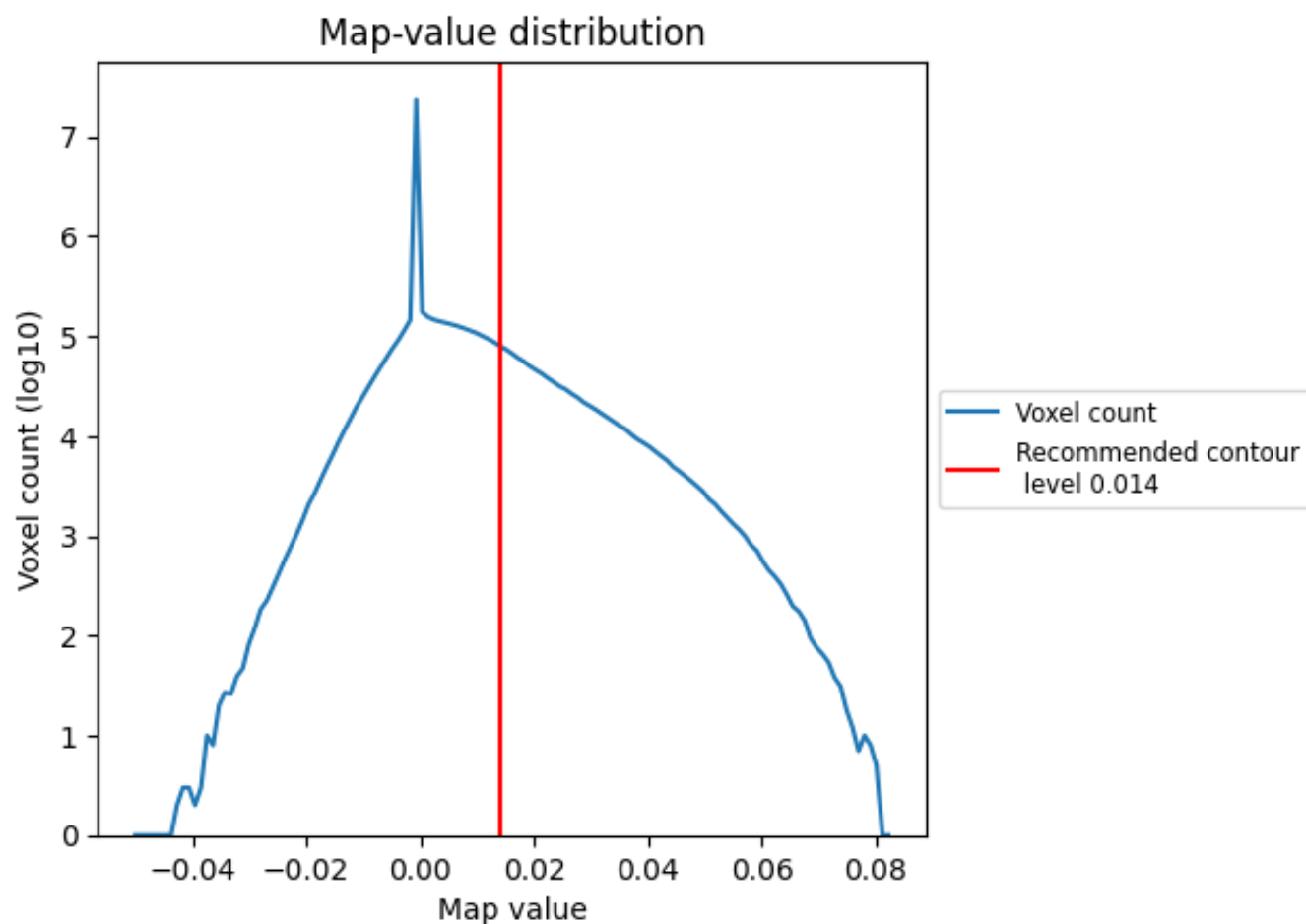


Z

7 Map analysis [i](#)

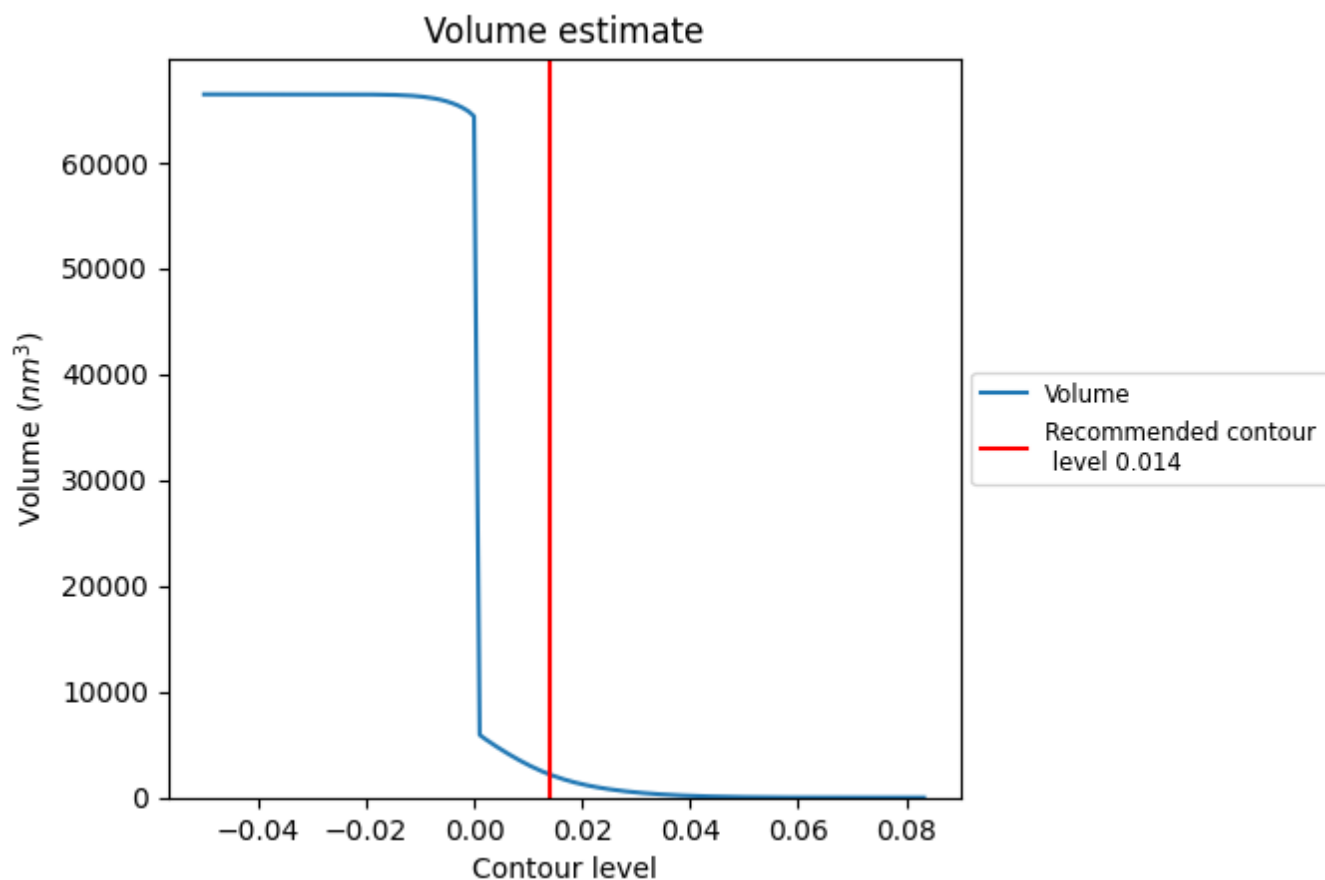
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

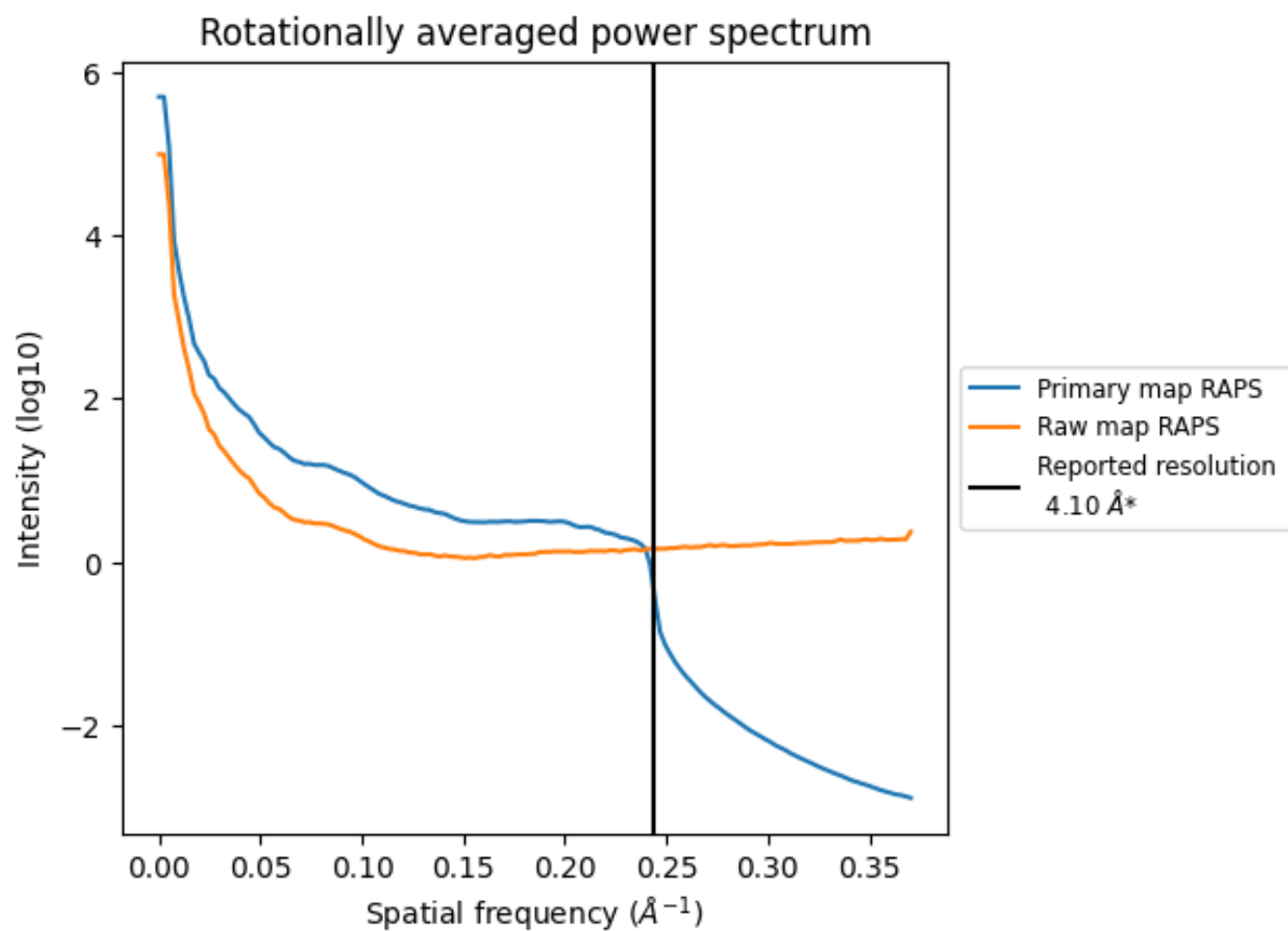
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2180 nm^3 ; this corresponds to an approximate mass of 1970 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

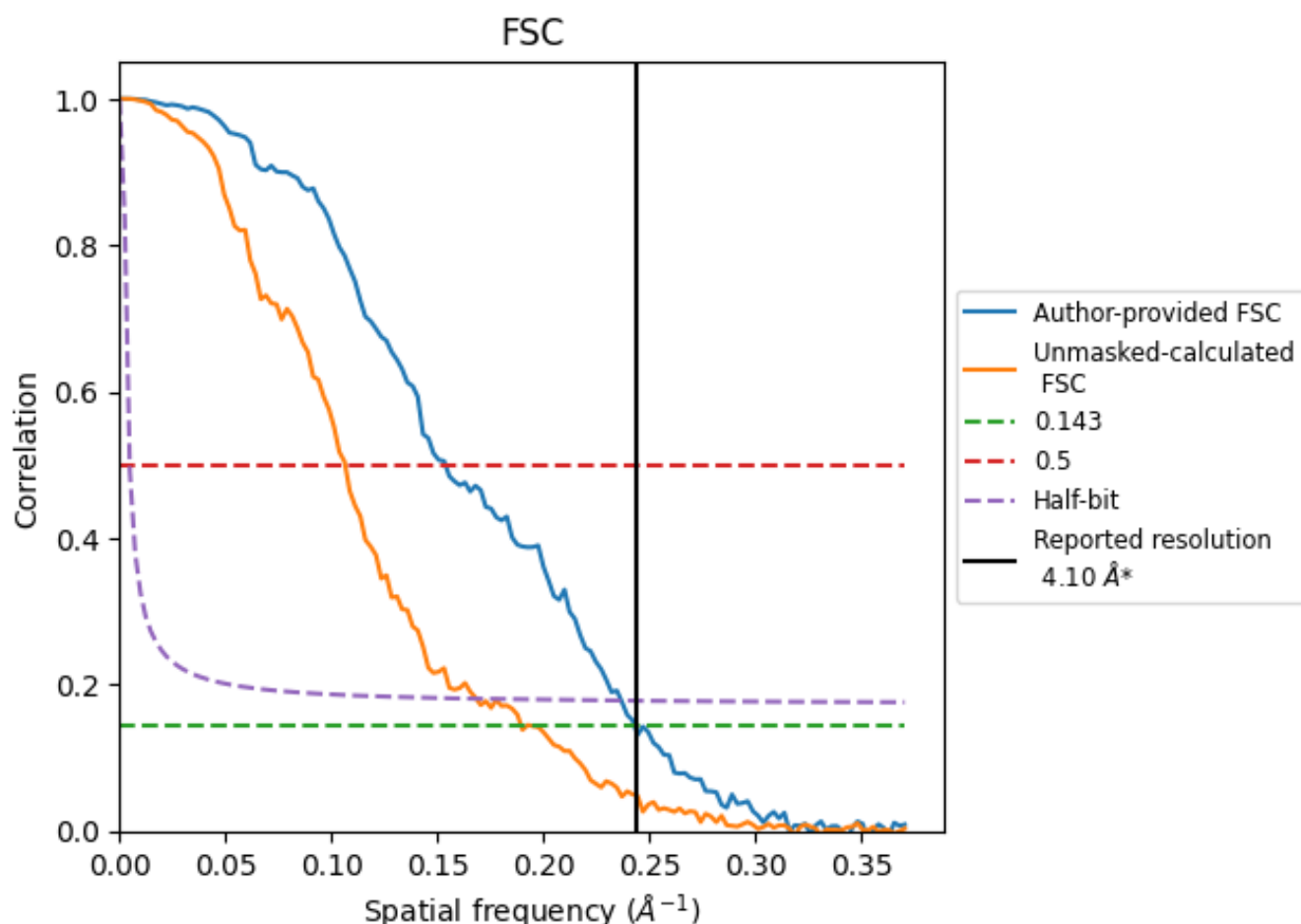


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

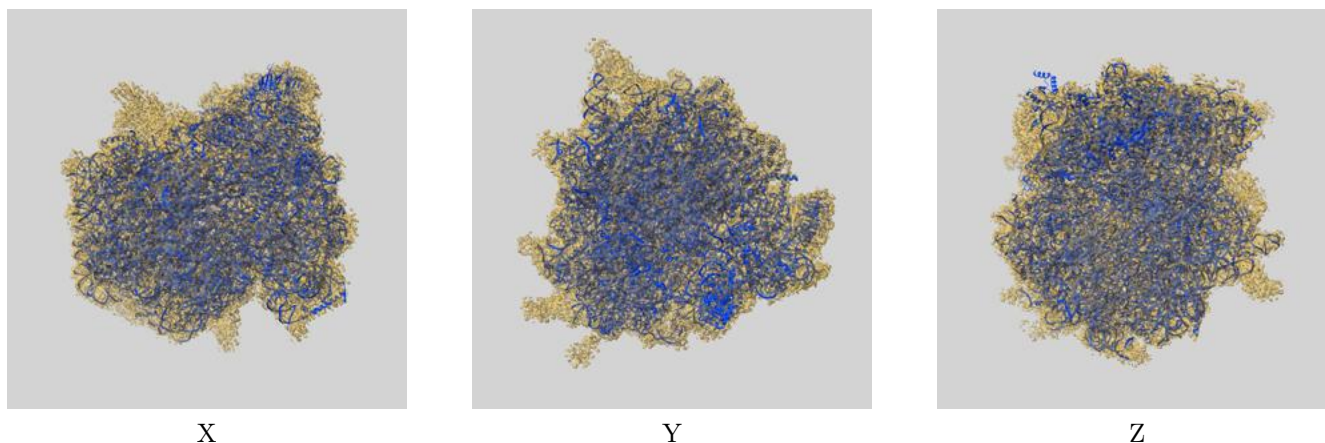
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	6.51	4.22
Unmasked-calculated*	5.28	9.40	5.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.28 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

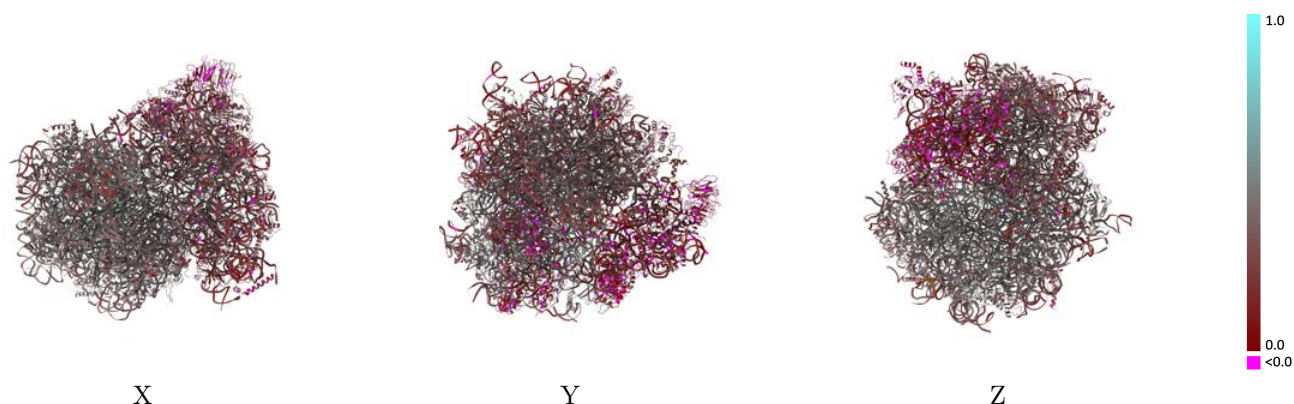
This section contains information regarding the fit between EMDB map EMD-12632 and PDB model 7NWH. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



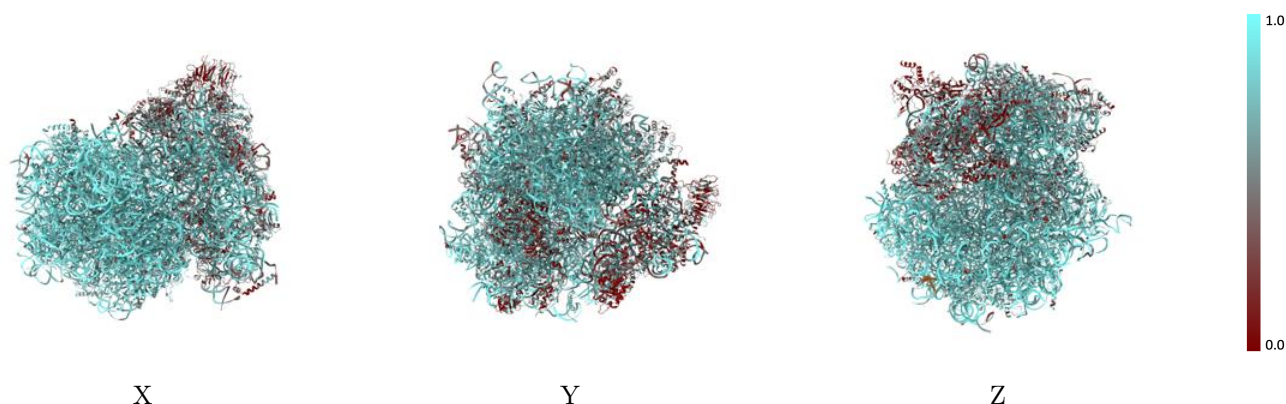
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



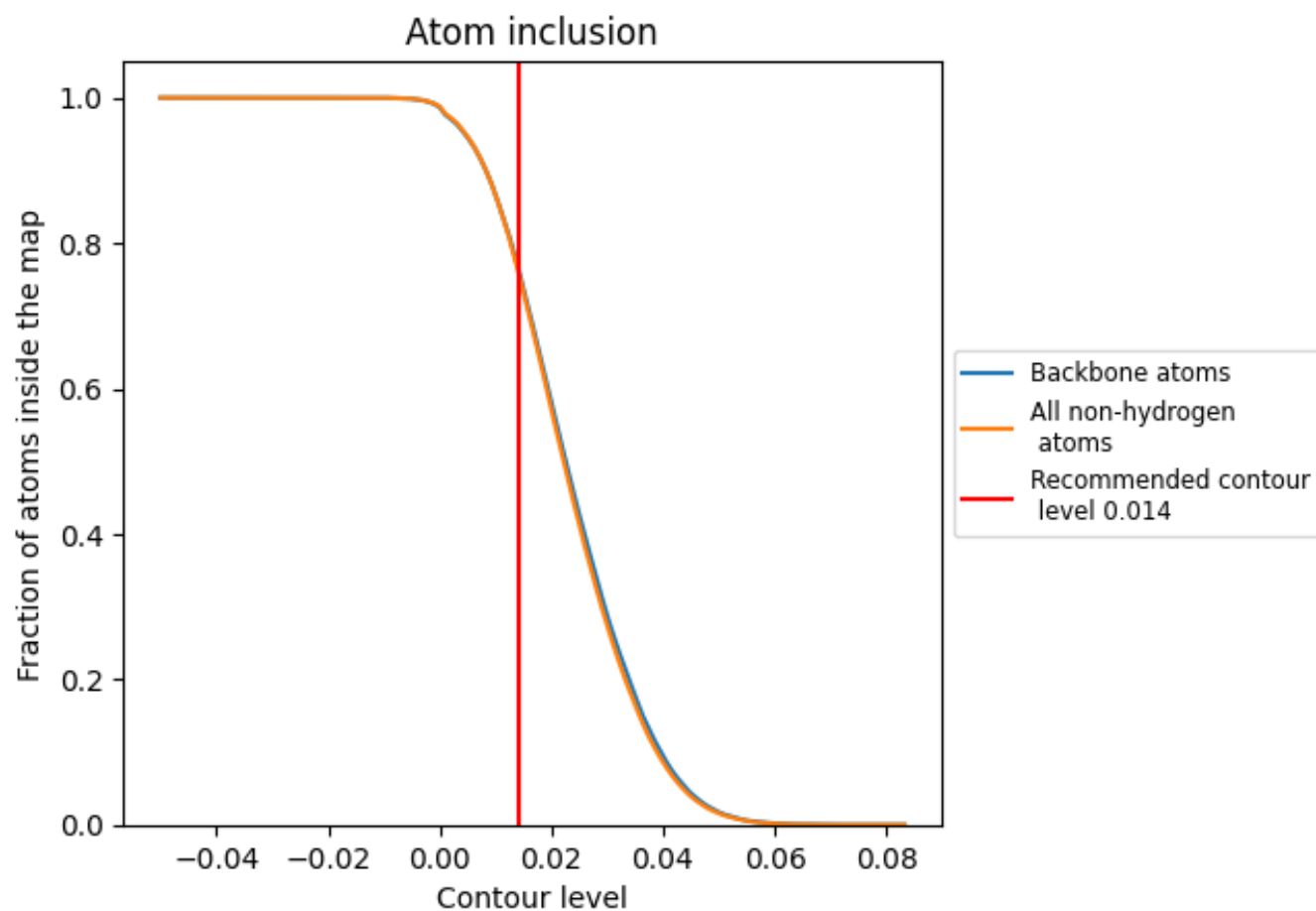
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7638	 0.3480
5	 0.9284	 0.3970
7	 0.9629	 0.4130
8	 0.9481	 0.4100
9	 0.7792	 0.2790
A	 0.8125	 0.4540
AA	 0.6058	 0.3260
B	 0.8007	 0.4370
BB	 0.5574	 0.2980
C	 0.8136	 0.4440
CC	 0.6568	 0.3580
D	 0.7991	 0.3880
DD	 0.3699	 0.2000
E	 0.8023	 0.4100
EE	 0.6000	 0.3260
F	 0.8010	 0.4240
FF	 0.3401	 0.1590
G	 0.7540	 0.3880
GG	 0.5024	 0.2420
H	 0.7740	 0.4150
HH	 0.4887	 0.2780
I	 0.8055	 0.4320
II	 0.5821	 0.3030
J	 0.7540	 0.3480
JJ	 0.6526	 0.3220
KK	 0.3987	 0.1850
L	 0.7748	 0.4060
LL	 0.6596	 0.3600
M	 0.8089	 0.4130
MM	 0.0805	 0.0870
N	 0.8451	 0.4470
NN	 0.6132	 0.3210
O	 0.8186	 0.4320
OO	 0.5512	 0.2680
P	 0.8260	 0.4440



















Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
PP	 0.4933	 0.1590
Q	 0.8021	 0.4370
QQ	 0.4359	 0.1810
R	 0.7495	 0.3910
RR	 0.3998	 0.2170
S	 0.8210	 0.4420
SS	 0.4812	 0.1830
T	 0.7981	 0.4440
TT	 0.4499	 0.1640
U	 0.7383	 0.3510
UU	 0.4083	 0.1710
V	 0.7724	 0.4530
VV	 0.5997	 0.3340
W	 0.5704	 0.3100
WW	 0.6485	 0.3580
X	 0.8064	 0.4180
XX	 0.7283	 0.3910
Y	 0.8089	 0.4200
YY	 0.5403	 0.2790
Z	 0.7931	 0.3830
ZZ	 0.3688	 0.1690
a	 0.8220	 0.4490
aa	 0.6624	 0.3430
b	 0.7215	 0.3870
bb	 0.5540	 0.3160
c	 0.6935	 0.3420
cc	 0.2745	 0.1690
d	 0.7783	 0.4200
dd	 0.4502	 0.1990
e	 0.8269	 0.4580
ee	 0.5915	 0.3220
f	 0.8468	 0.4600
ff	 0.3457	 0.2120
g	 0.7805	 0.4170
gg	 0.2727	 0.1370
h	 0.8018	 0.3970
hh	 0.2132	 0.1730
i	 0.7714	 0.3880
ii	 0.2776	 0.1660
j	 0.8739	 0.4480
jj	 0.2419	 0.1590
k	 0.7397	 0.3890

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
l	 0.8361	 0.4370
m	 0.8149	 0.4180
n	 0.6284	 0.3300
o	 0.7787	 0.4390
p	 0.7939	 0.4420
r	 0.8025	 0.4280
s	 0.3246	 0.1490
t	 0.3155	 0.1860