



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 11:16 am BST

PDB ID : 6YAM
EMDB ID : EMD-10761
Title : Mammalian 48S late-stage translation initiation complex (LS48S+eIF3 IC)
with beta-globin mRNA
Authors : Bochler, A.; Simonetti, A.; Guca, E.; Hashem, Y.
Deposited on : 2020-03-12
Resolution : 3.60 Å(reported)

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

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

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

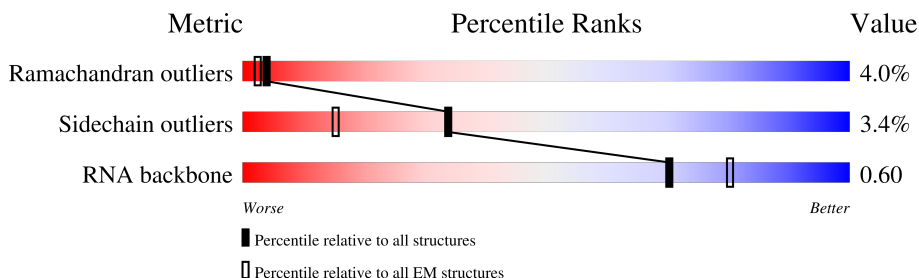
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	75	<div> <div>69%</div> <div> <div>77%</div> <div>16%</div> </div> </div>
2	l	25	<div> <div>28%</div> <div>96%</div> </div>
3	C	208	<div> <div>14%</div> <div>95%</div> <div>5%</div> </div>
4	D	264	<div> <div>22%</div> <div>77%</div> <div>5%</div> <div>19%</div> </div>
5	E	226	<div> <div>14%</div> <div>97%</div> </div>
6	F	227	<div> <div>32%</div> <div>95%</div> <div>5%</div> </div>
7	G	263	<div> <div>17%</div> <div>98%</div> </div>
8	H	191	<div> <div>21%</div> <div>97%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	237	<div>46%</div> <div>96%</div> <div>.</div>
10	J	190	<div>56%</div> <div>94%</div> <div>6%</div>
11	K	206	<div>29%</div> <div>95%</div> <div>.</div>
12	L	182	<div>18%</div> <div>97%</div> <div>..</div>
13	M	98	<div>29%</div> <div>89%</div> <div>9%</div> <div>.</div>
14	N	158	<div>26%</div> <div>94%</div> <div>5%</div> <div>.</div>
15	O	132	<div>85%</div> <div>88%</div> <div>6%</div> <div>6%</div>
16	P	150	<div>21%</div> <div>93%</div> <div>6%</div> <div>.</div>
17	Q	151	<div>18%</div> <div>86%</div> <div>.</div> <div>10%</div>
18	S	141	<div>18%</div> <div>96%</div> <div>.</div>
19	T	135	<div>36%</div> <div>90%</div> <div>.</div> <div>7%</div>
20	V	145	<div>17%</div> <div>95%</div> <div>..</div>
21	W	119	<div>29%</div> <div>87%</div> <div>.</div> <div>13%</div>
22	X	82	<div>17%</div> <div>95%</div> <div>..</div>
23	Y	130	<div>.</div> <div>96%</div> <div>..</div>
24	Z	142	<div>10%</div> <div>96%</div> <div>.</div>
25	a	133	<div>26%</div> <div>83%</div> <div>8%</div> <div>5%</div> <div>5%</div>
26	b	115	<div>7%</div> <div>83%</div> <div>.</div> <div>14%</div>
27	c	84	<div>39%</div> <div>83%</div> <div>14%</div> <div>.</div>
28	d	69	<div>26%</div> <div>91%</div> <div>.</div> <div>7%</div>
29	e	53	<div>36%</div> <div>81%</div> <div>19%</div>
30	f	71	<div>87%</div> <div>86%</div> <div>14%</div>
31	g	313	<div>47%</div> <div>98%</div> <div>.</div>
32	n	75	<div>41%</div> <div>96%</div> <div>.</div>
33	i	59	<div>49%</div> <div>92%</div> <div>7%</div> <div>.</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	2	1863	
35	A	266	
36	B	422	
37	j	144	
38	k	595	
39	U	152	
40	R	145	
41	3	45	
42	m	548	
43	y	1350	
44	v	913	
45	w	445	
46	q	272	
47	r	352	
48	s	218	
49	t	564	
50	u	374	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	C4J	2	1244	X	-	-	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 118536 atoms, of which 0 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 RNA chain called initiator methionylated tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1614	722	299	519	74		

- Molecule 2 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 3 is a protein called 40S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	208	Total	C	N	O	S	0	0
			1643	1045	289	301	8		

- Molecule 4 is a protein called 40S ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1741	1107	309	310	15		

- Molecule 5 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	226	Total	C	N	O	S	0	0
			1743	1127	300	307	9		

- Molecule 6 is a protein called 40S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	227	Total	C	N	O	S	0	0
			1765	1124	317	316	8		

- Molecule 7 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 8 is a protein called 40S ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 9 is a protein called 40S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	237	Total	C	N	O	S	0	0
			1924	1200	387	330	7		

- Molecule 10 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

- Molecule 11 is a protein called 40S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 12 is a protein called 40S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	182	Total	C	N	O	S	0	0
			1499	952	300	245	2		

- Molecule 13 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

- Molecule 14 is a protein called 40S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 15 is a protein called 40S ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 16 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 17 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 18 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 19 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	126	Total	C	N	O	S	0	0
			1019	639	188	187	5		

- Molecule 20 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	141	Total	C	N	O	S	0	0
			1112	701	213	195	3		

- Molecule 21 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 22 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	82	Total	C	N	O	S	0	0
			620	378	117	120	5		

- Molecule 23 is a protein called 40S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 24 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	142	Total	C	N	O	S	0	0
			1107	698	220	185	4		

- Molecule 25 is a protein called 40S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	126	Total	C	N	O	S	0	0
			1021	645	198	173	5		

- Molecule 26 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	99	Total	C	N	O	S	0	0
			789	491	162	130	6		

- Molecule 27 is a protein called 40S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 28 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 29 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 30 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 31 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 32 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	75	Total	C	N	O	S	0	0
			599	382	111	105	1		

- Molecule 33 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	59	Total	C	N	O	S	0	0
			473	293	104	75	1		

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2	1743	Total	C	N	O	P	0	0
			37187	16605	6660	12182	1740		

- Molecule 35 is a protein called eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	266	Total	C	N	O	S	0	0
			2147	1354	376	406	11		

- Molecule 36 is a protein called eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B	422	Total	C	N	O	S	0	0
			3214	2044	561	592	17		

- Molecule 37 is a protein called eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	109	Total	C	N	O	S	0	0
			882	549	168	161	4		

- Molecule 38 is a protein called ATP-binding cassette sub-family E member 1 (ABCE1).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	595	Total	C	N	O	S	0	0
			4693	2995	802	865	31		

- Molecule 39 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	U	145	Total	C	N	O	S	0	0
			1194	747	243	203	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	140	Total	C	N	O	S	0	0
			1154	733	219	195	7		

- Molecule 41 is a RNA chain called beta-globin mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3	45	Total	C	N	O	P	0	0
			960	430	179	306	45		

- Molecule 42 is a protein called eukaryotic translation initiation factor 3 subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	365	Total	C	N	O	S	0	0
			2955	1856	517	564	18		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	603	Total	C	N	O	S	0	0
			4971	3133	897	920	21		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	554	Total	C	N	O	S	0	0
			4508	2830	800	845	33		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	w	419	Total	C	N	O	S	0	0
			3465	2220	586	639	20		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	272	Total	C	N	O	S	0	0
			2111	1330	359	410	12		

- Molecule 47 is a protein called eukaryotic translation initiation factor 3 subunit h.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	215	Total	C	N	O	S	0	0
			1737	1109	285	330	13		

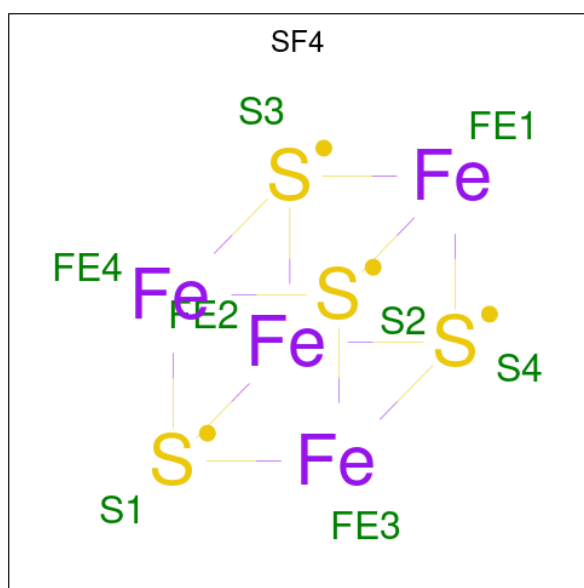
- Molecule 49 is a protein called eukaryotic translation initiation factor 3 subunit l.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	372	Total	C	N	O	S	0	0
			3109	2010	519	563	17		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	365	Total	C	N	O	S	0	0
			2918	1850	493	558	17		

- Molecule 51 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

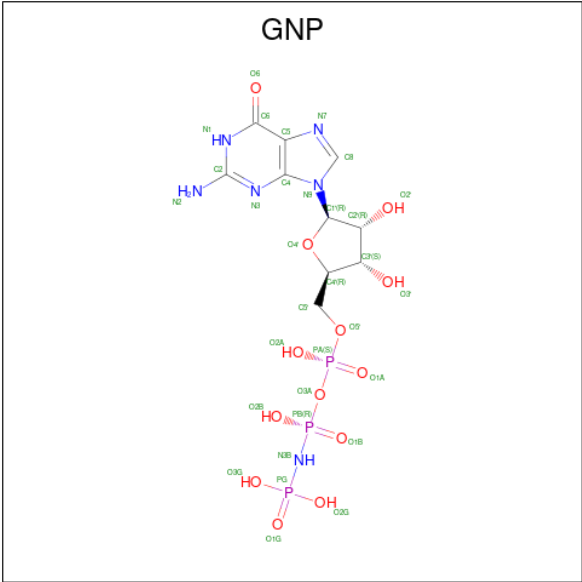


Mol	Chain	Residues	Atoms			AltConf
51	k	1	Total	Fe	S	0
			8	4	4	
51	k	1	Total	Fe	S	0
			8	4	4	

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	k	1	Total	Mg	0
			1	1	

- Molecule 53 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

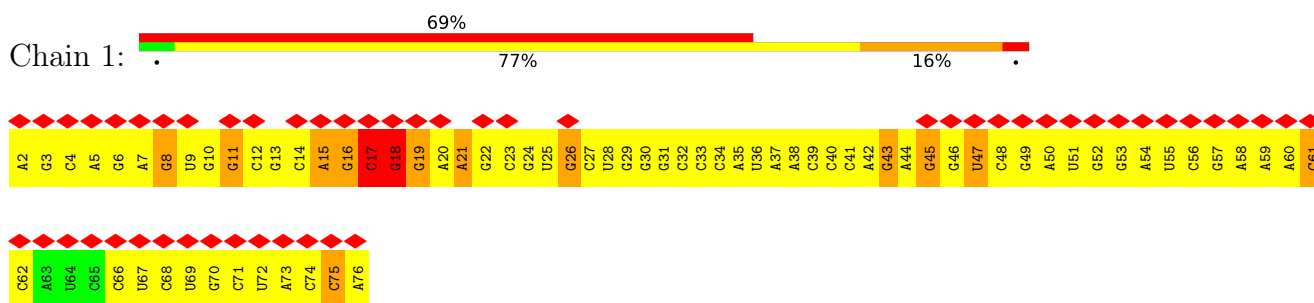


Mol	Chain	Residues	Atoms					AltConf
53	k	1	Total	C	N	O	P	0
			32	10	6	13	3	
53	k	1	Total	C	N	O	P	0
			32	10	6	13	3	

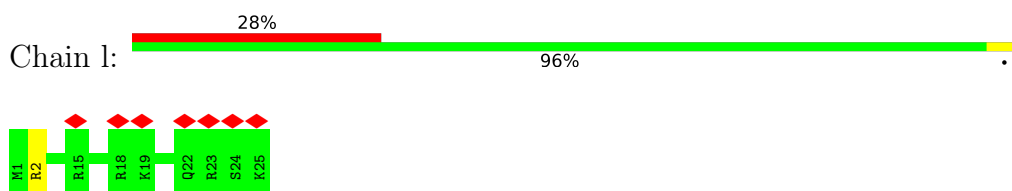
3 Residue-property plots

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

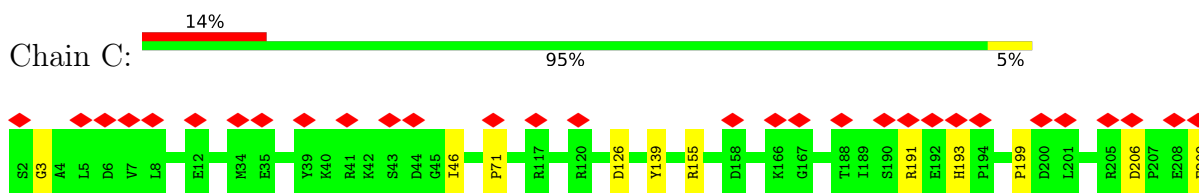
- Molecule 1: initiator methionylated tRNA



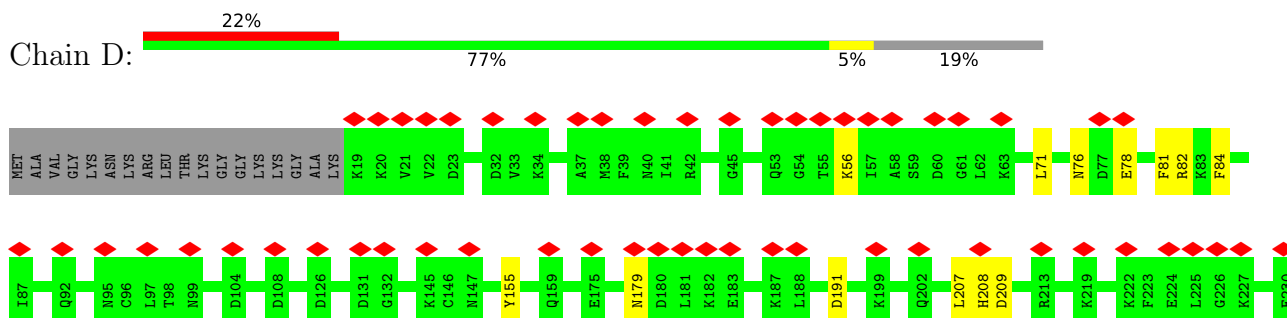
- Molecule 2: 60s ribosomal protein l41

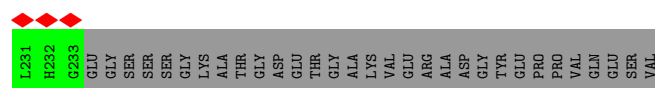


- Molecule 3: 40S ribosomal protein uS2

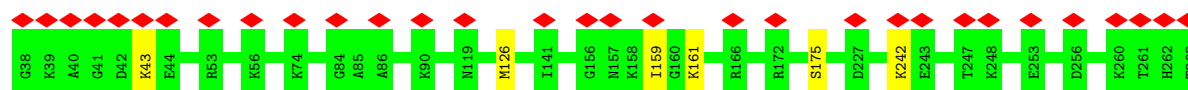


- Molecule 4: 40S ribosomal protein eS1

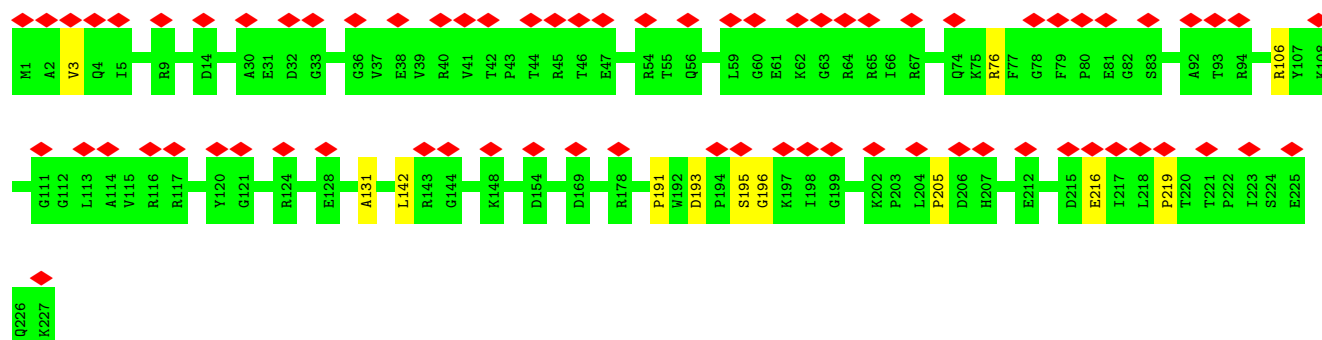




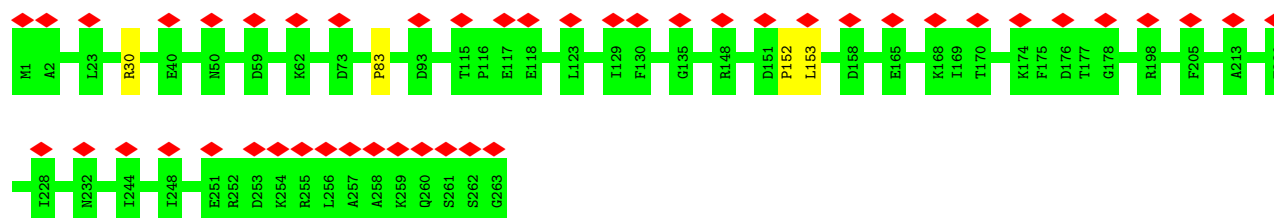
- Molecule 5: 40S ribosomal protein uS5



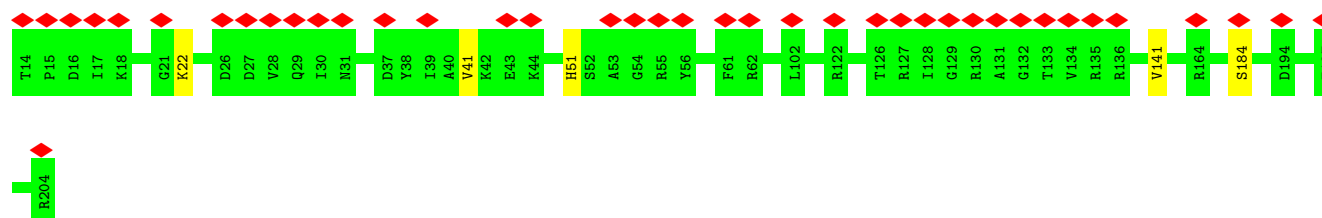
- Molecule 6: 40S ribosomal protein uS3



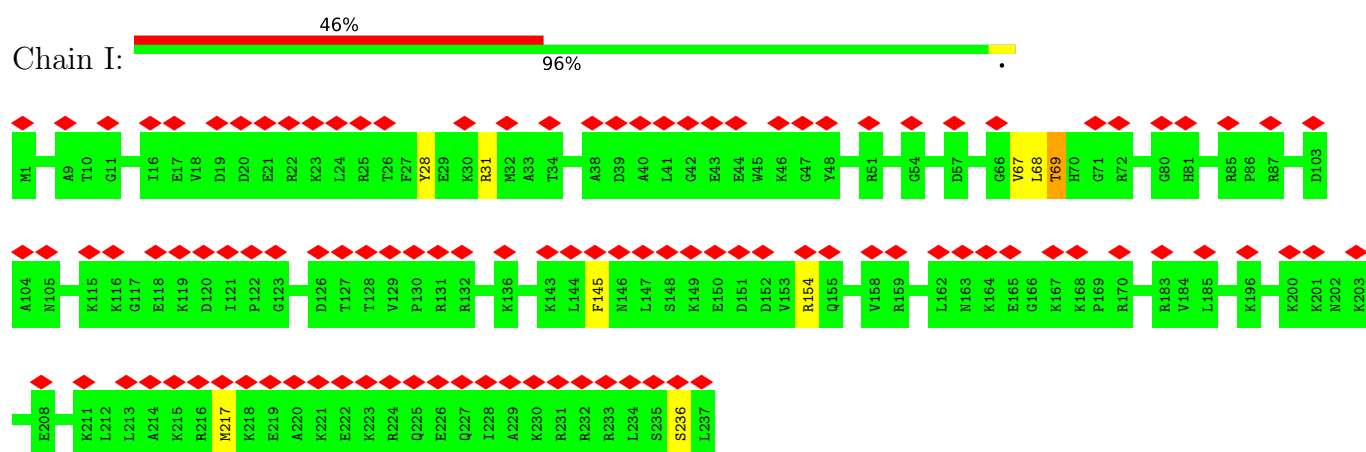
- Molecule 7: 40S ribosomal protein eS4



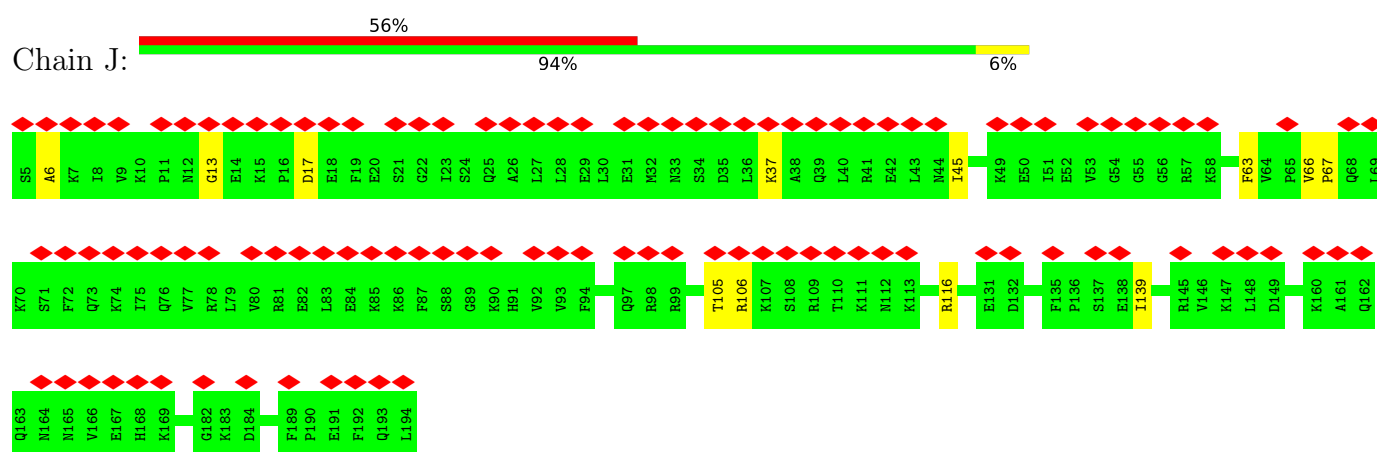
- Molecule 8: 40S ribosomal protein uS7



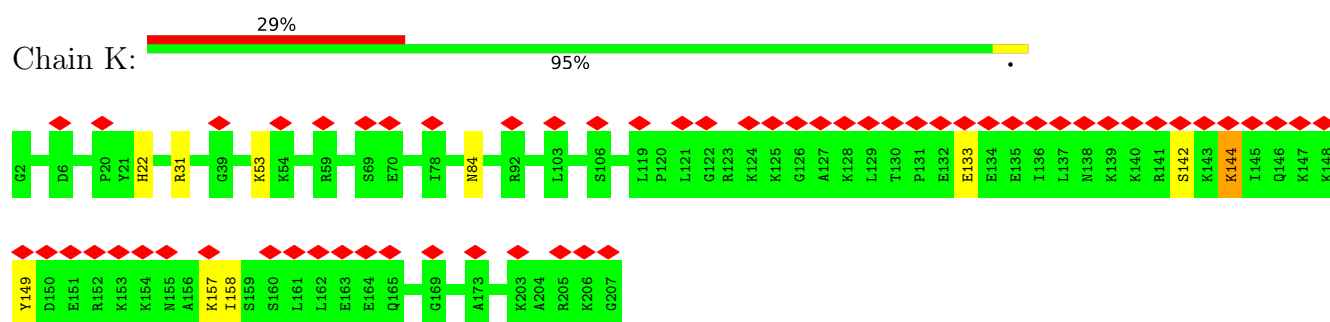
- Molecule 9: 40S ribosomal protein eS6



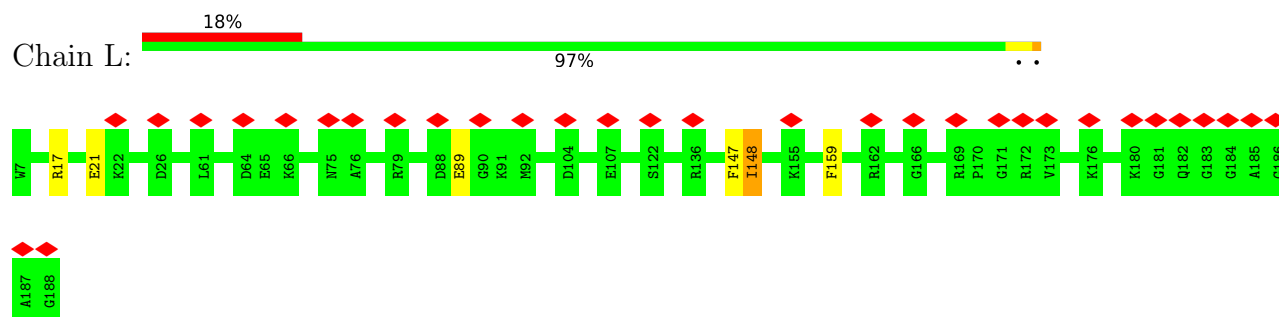
• Molecule 10: ribosomal protein eS7



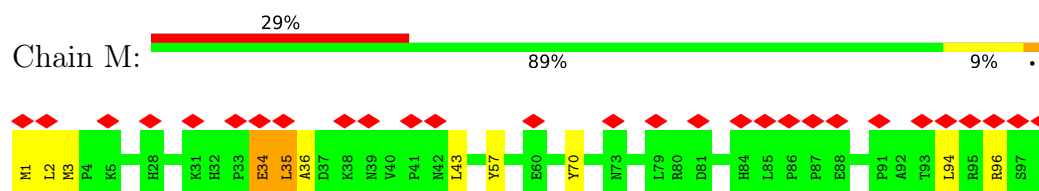
• Molecule 11: 40S ribosomal protein eS8



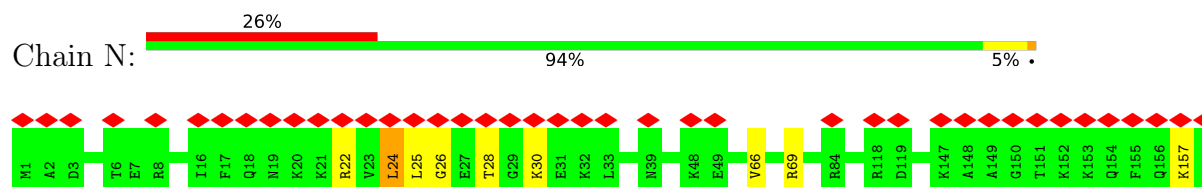
• Molecule 12: 40S ribosomal protein uS4



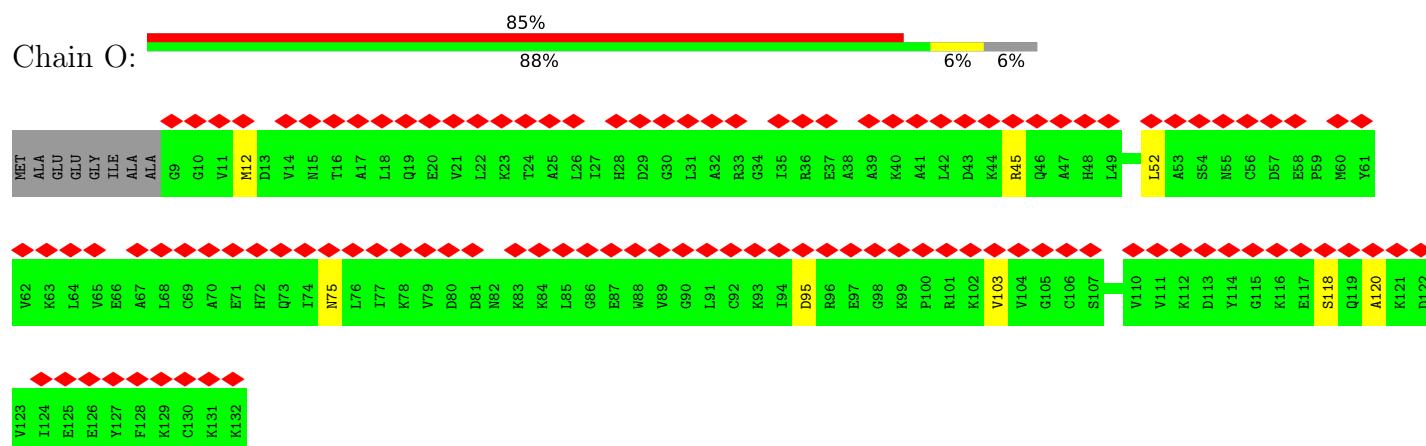
• Molecule 13: 40S ribosomal protein eS10



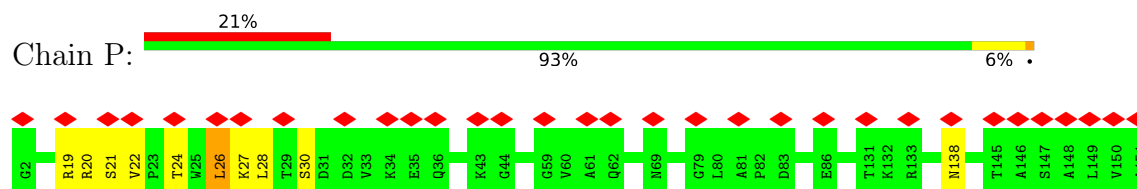
• Molecule 14: 40S ribosomal protein uS17



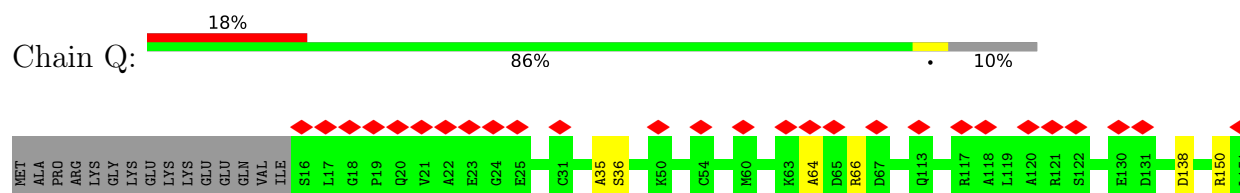
• Molecule 15: 40S ribosomal protein eS12



• Molecule 16: ribosomal protein uS15

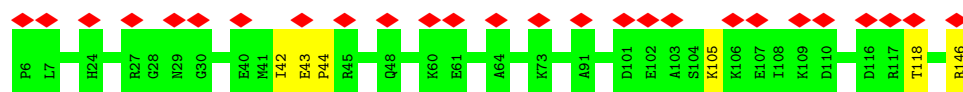


• Molecule 17: 40S ribosomal protein uS11

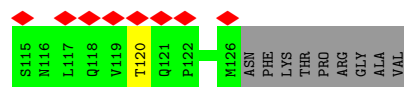
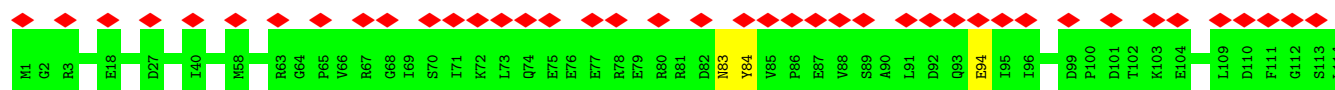
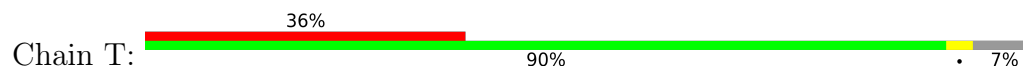


• Molecule 18: 40S ribosomal protein uS9

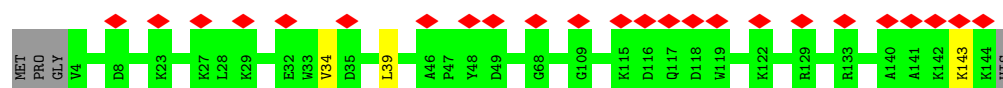




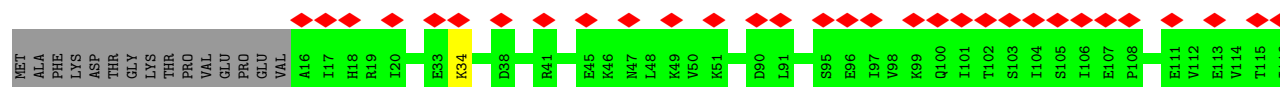
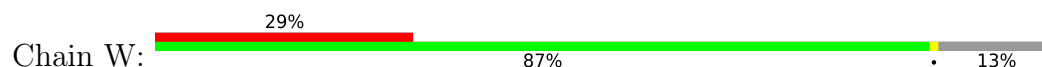
- Molecule 19: 40S ribosomal protein eS17



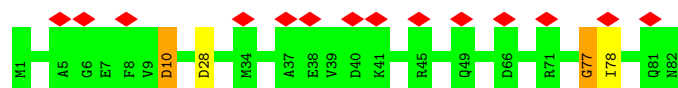
- Molecule 20: 40S ribosomal protein eS19



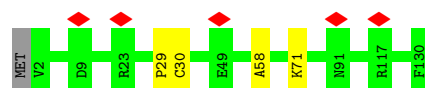
- Molecule 21: 40S ribosomal protein uS10



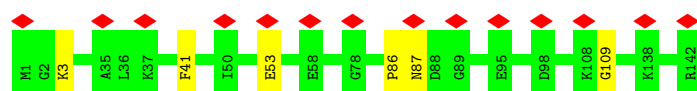
- Molecule 22: 40S ribosomal protein eS21



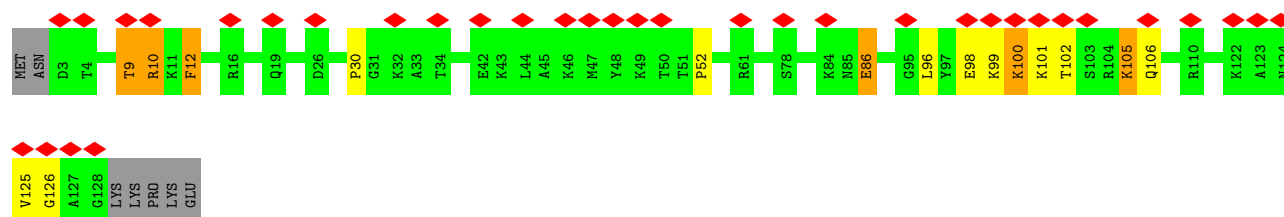
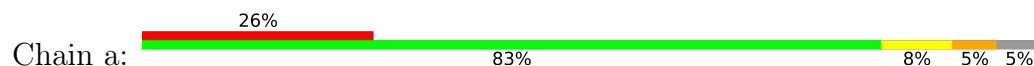
- Molecule 23: 40S ribosomal protein uS8



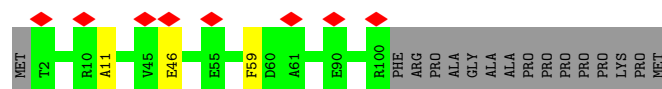
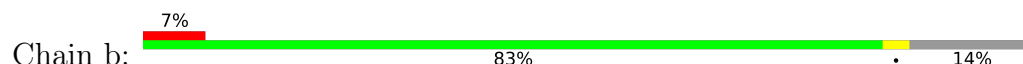
- Molecule 24: 40S ribosomal protein uS12



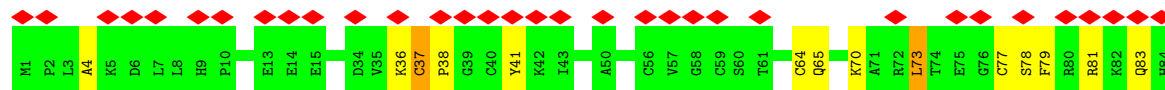
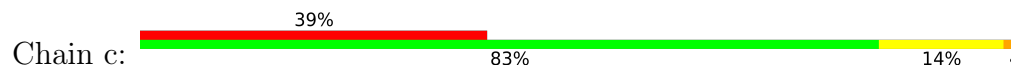
- Molecule 25: 40S ribosomal protein eS24



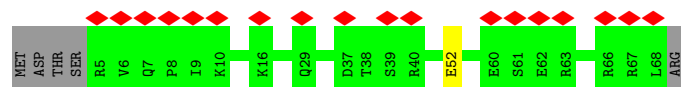
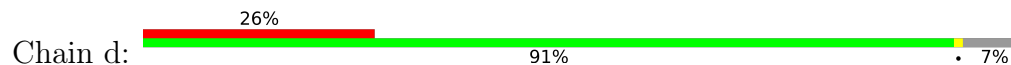
- Molecule 26: 40S ribosomal protein eS26



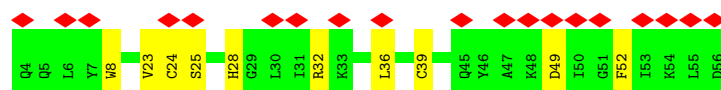
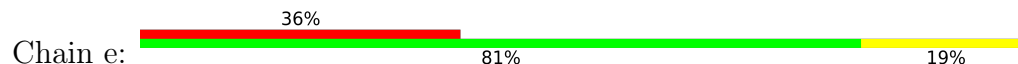
- Molecule 27: 40S ribosomal protein eS27



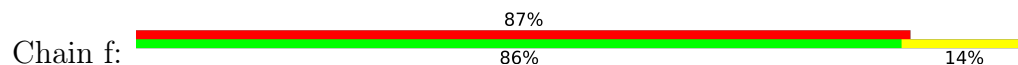
- Molecule 28: 40S ribosomal protein eS28

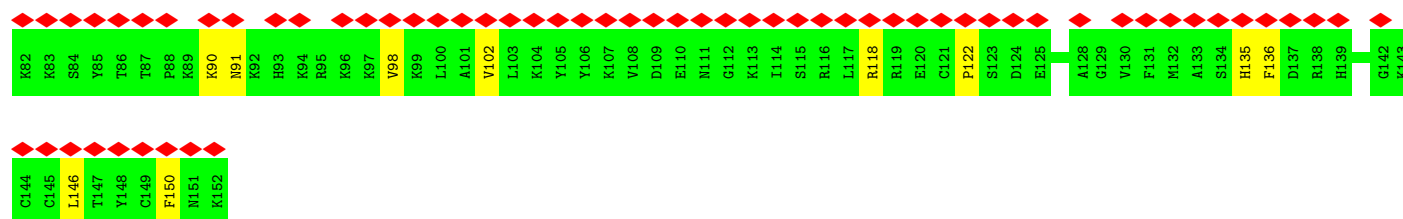


- Molecule 29: ribosomal protein uS14

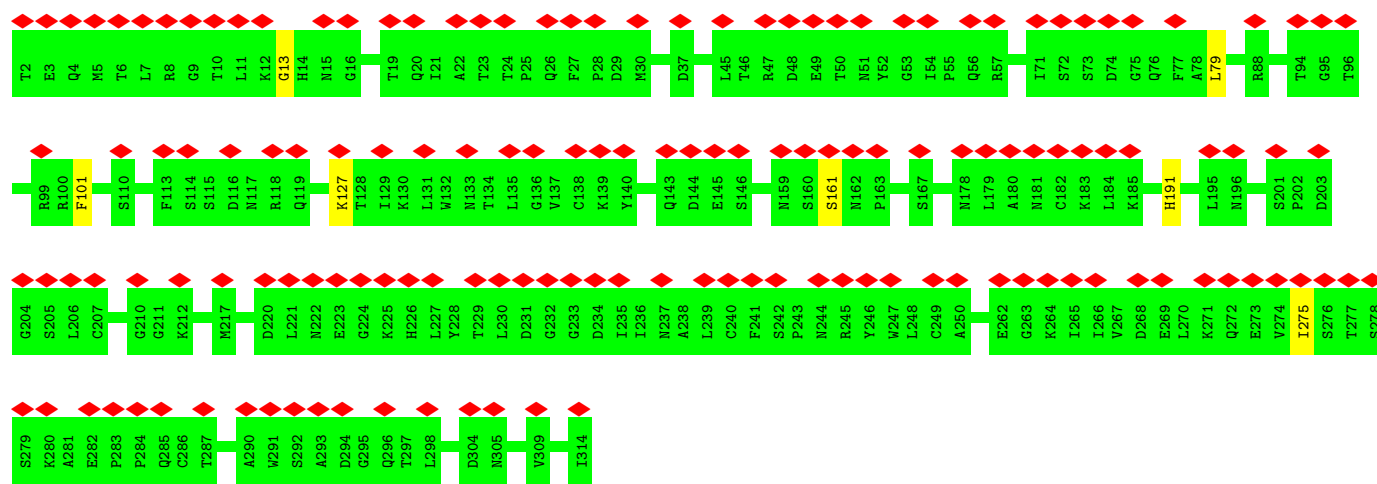


- Molecule 30: ribosomal protein eS31

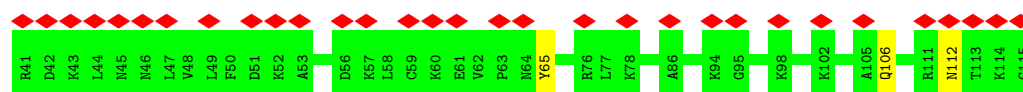
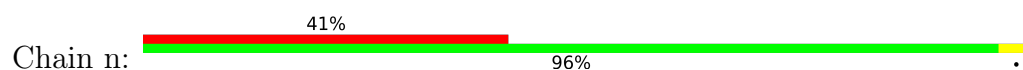




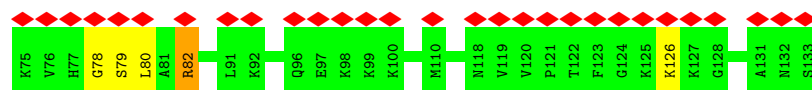
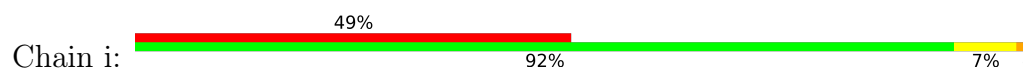
• Molecule 31: ribosomal protein RACK1



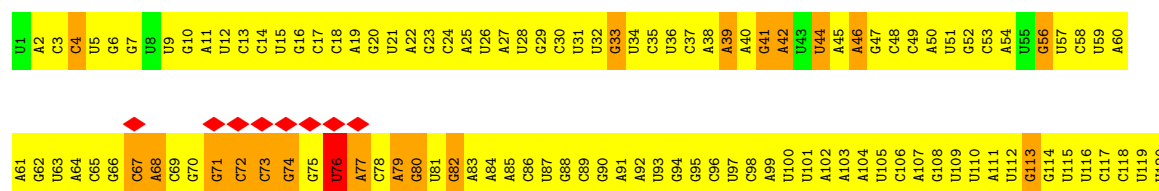
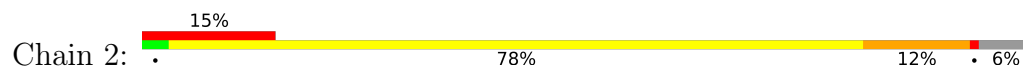
• Molecule 32: ribosomal protein eS25



• Molecule 33: 40S ribosomal protein eS30

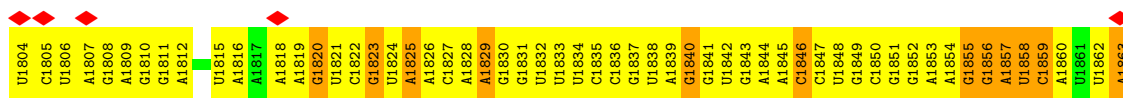


• Molecule 34: 18S ribosomal RNA

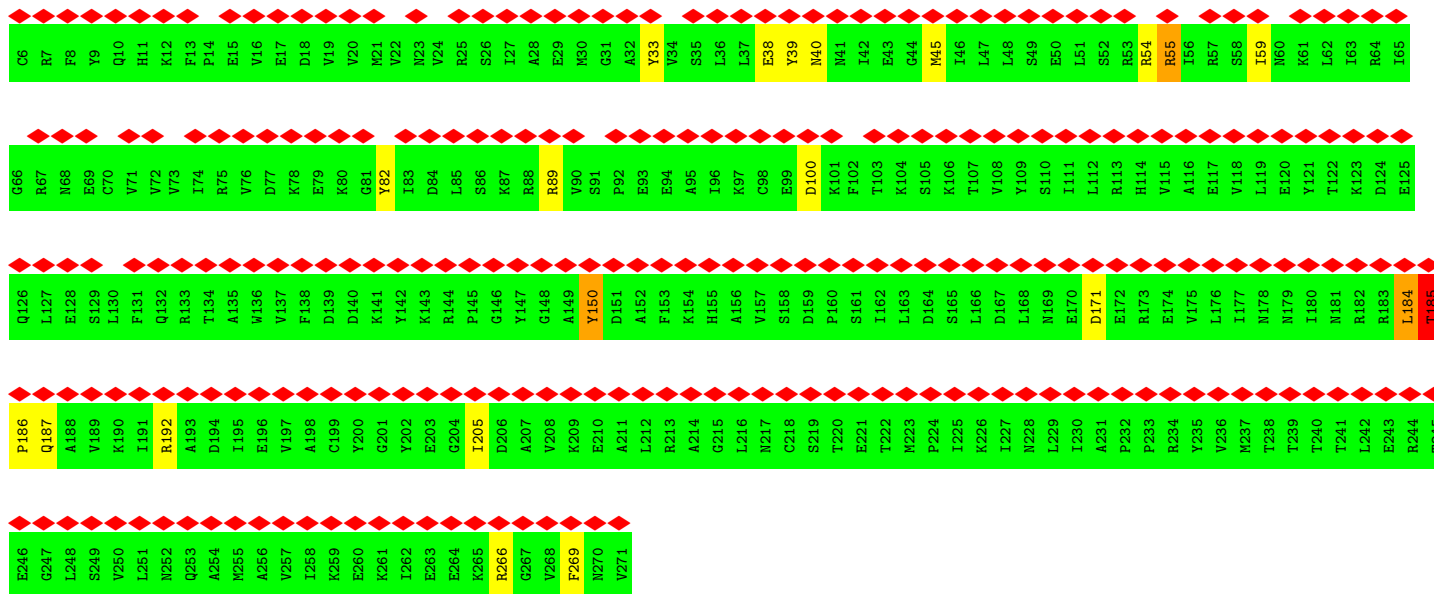
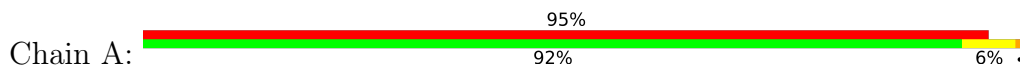




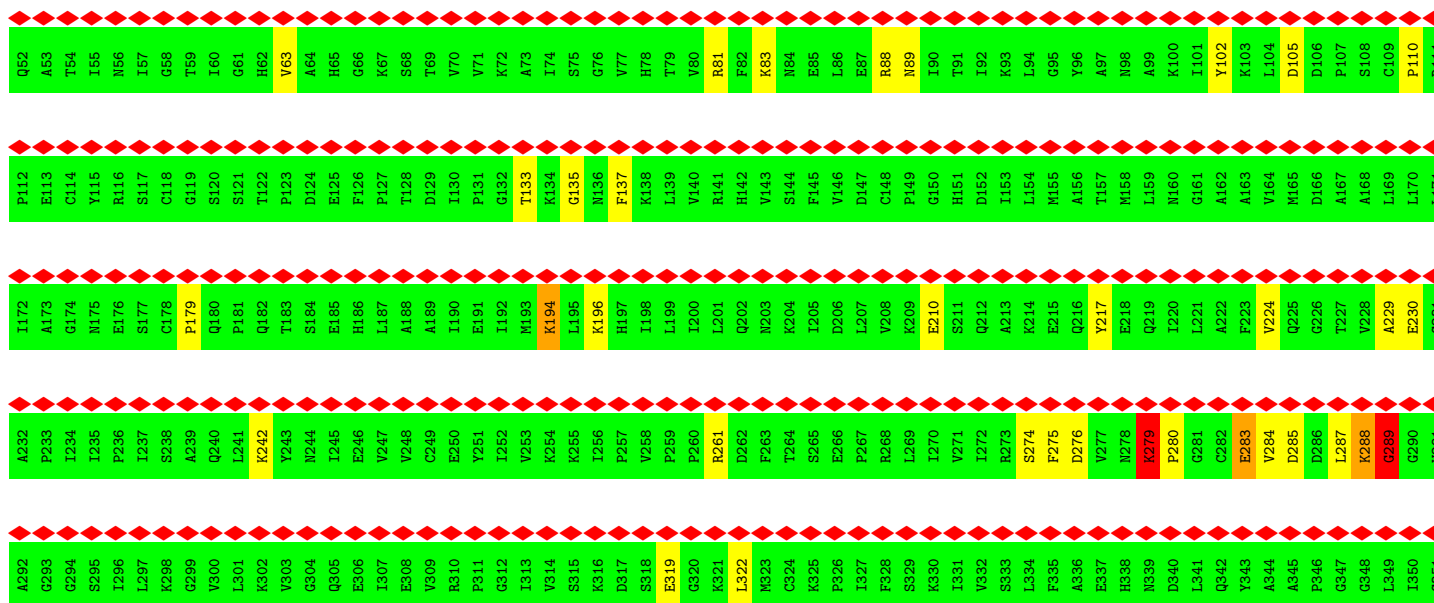
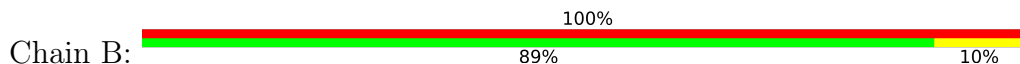




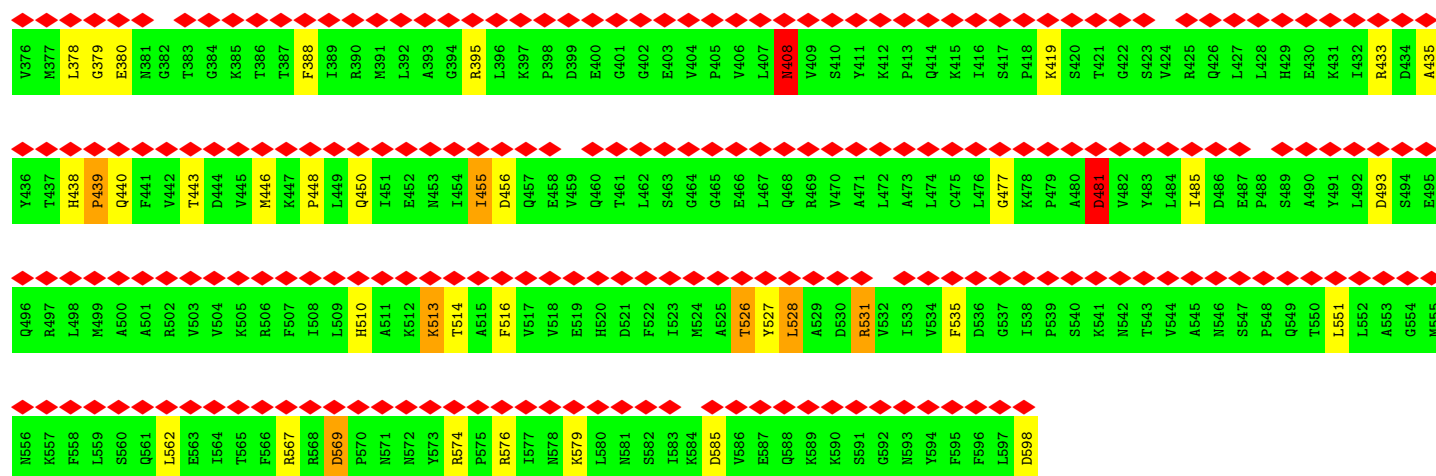
• Molecule 35: eukaryotic translation initiation factor 2 subunit alpha



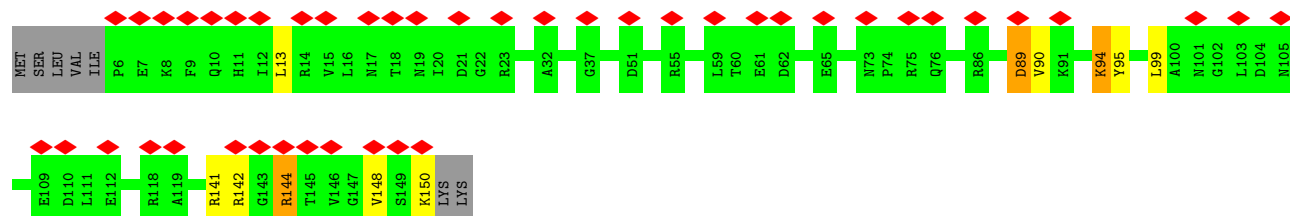
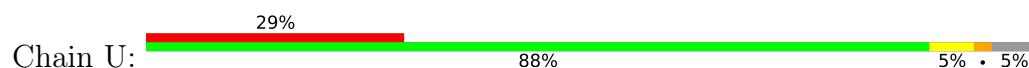
• Molecule 36: eukaryotic translation initiation factor 2 subunit gamma



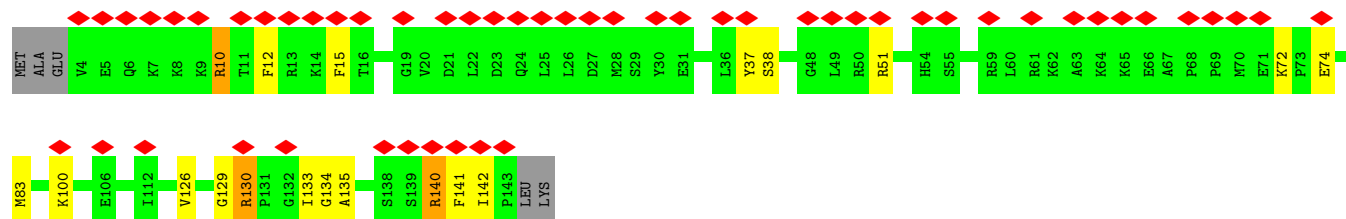
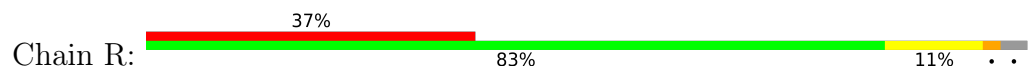




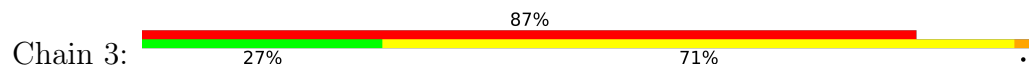
• Molecule 39: 40S ribosomal protein uS13



• Molecule 40: 40S ribosomal protein uS19



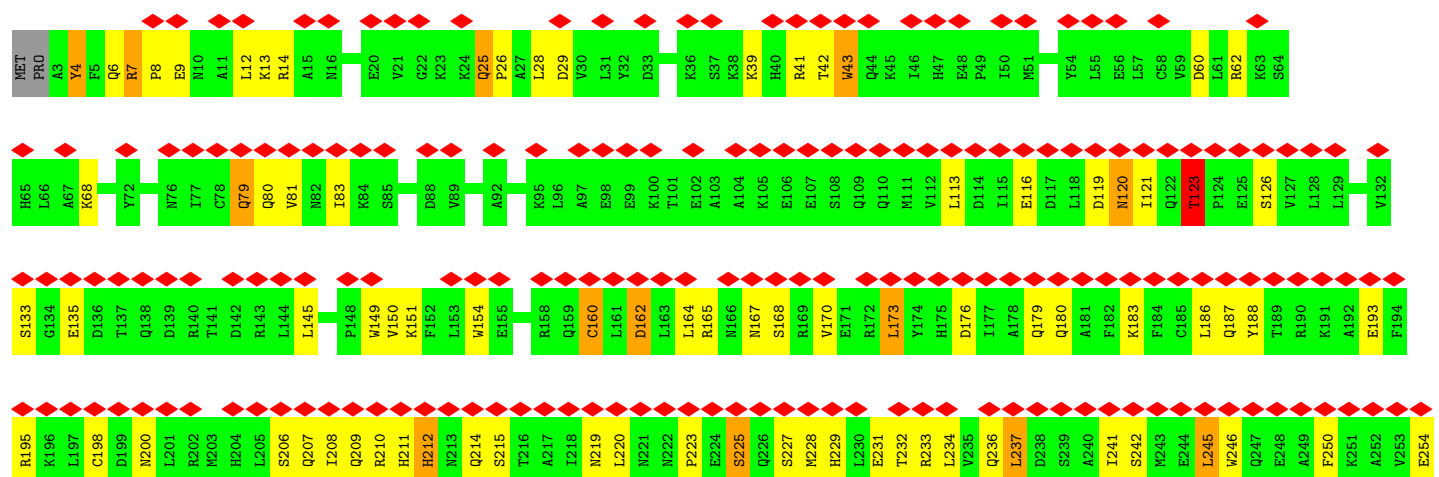
• Molecule 41: beta-globin mRNA



• Molecule 42: eukaryotic translation initiation factor 3 subunit d



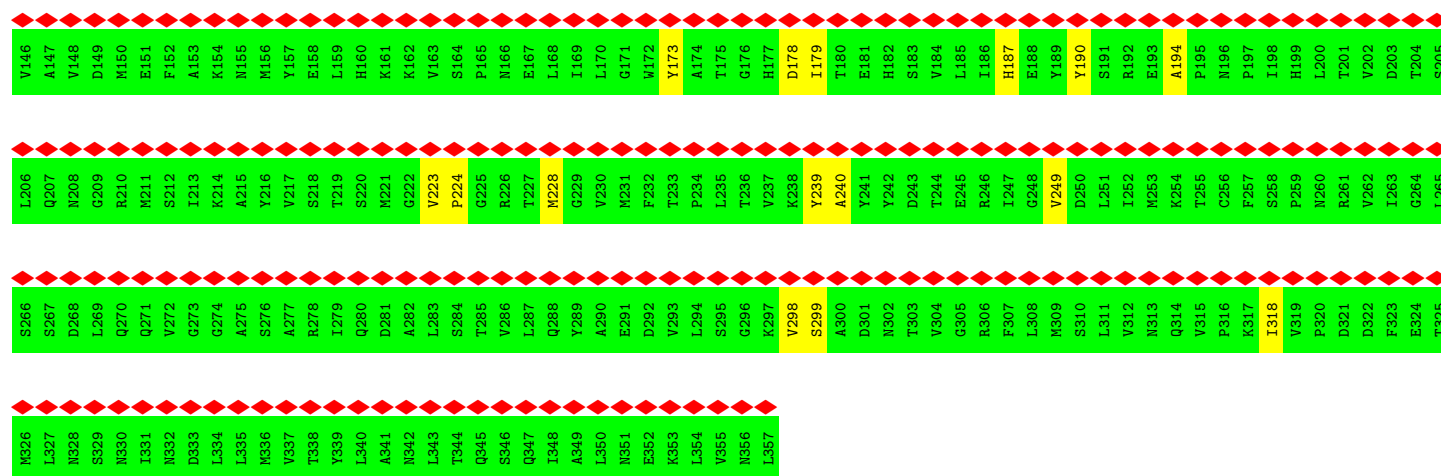
- Molecule 43: Eukaryotic translation initiation factor 3 subunit A



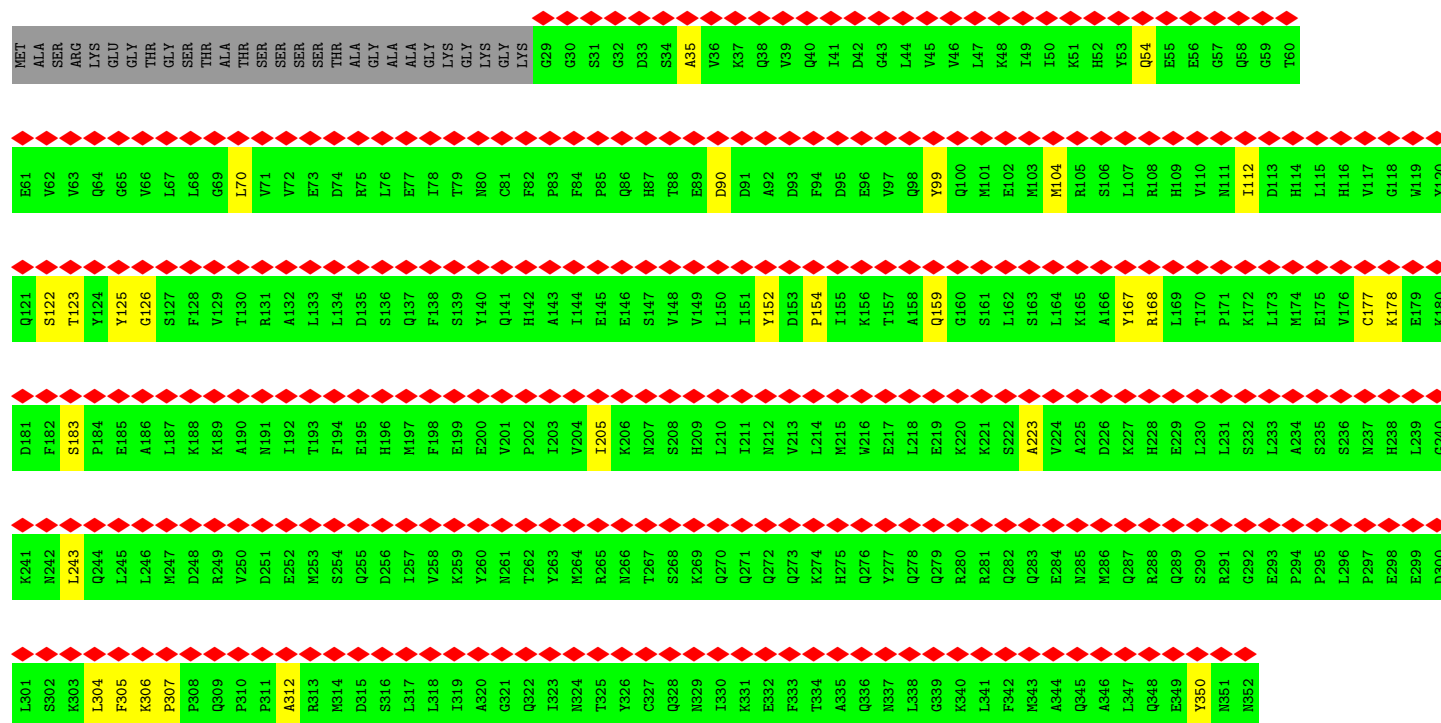
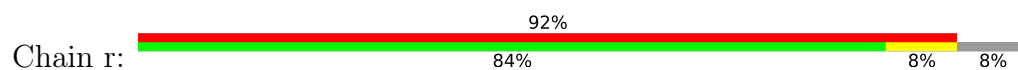


Chain v:

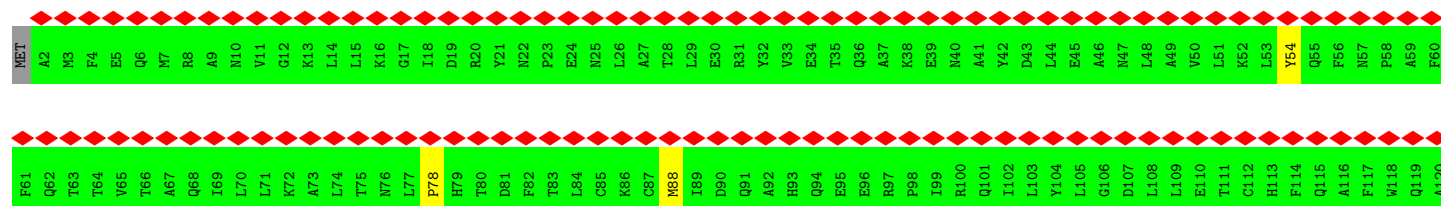




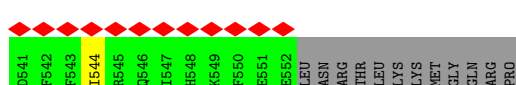
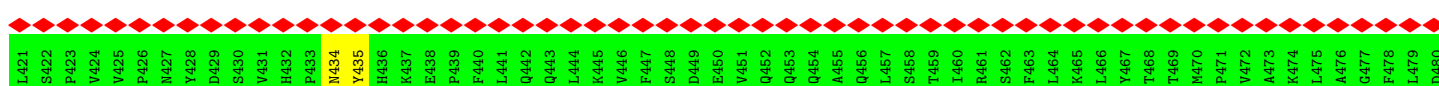
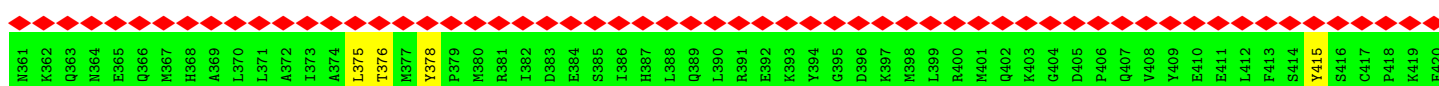
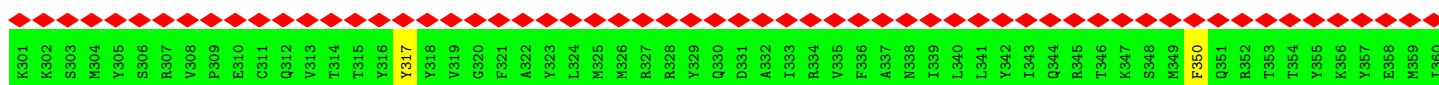
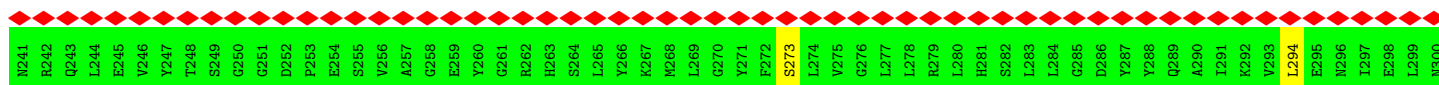
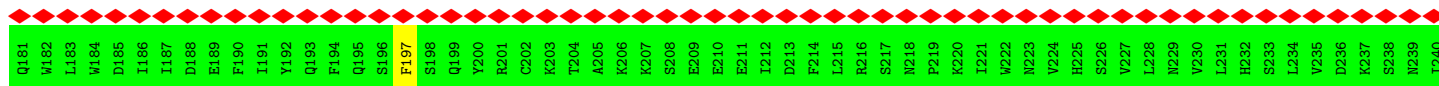
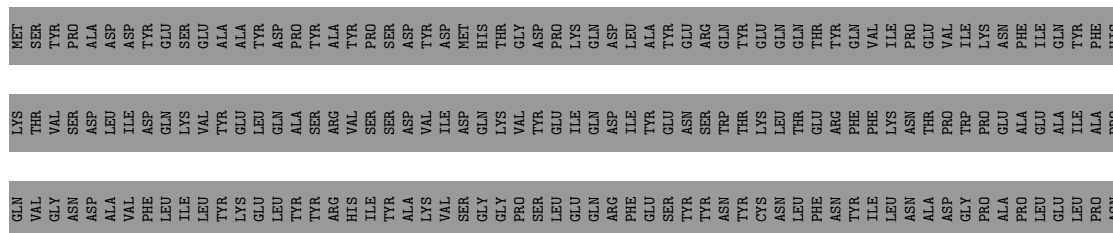
• Molecule 47: eukaryotic translation initiation factor 3 subunit h



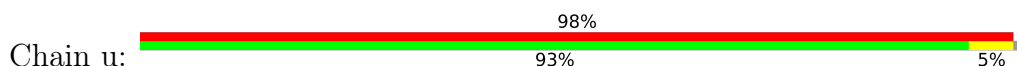
• Molecule 48: Eukaryotic translation initiation factor 3 subunit K



- Molecule 49: eukaryotic translation initiation factor 3 subunit 1



- Molecule 50: Eukaryotic translation initiation factor 3 subunit M



L361	L301	L241	A181	Y121	E61
N362	Q302	T242	S182	T122	S62
K363	I303	I243	K183	Y123	V63
V364	G304	F244	V184	Y124	M64
K365	A305	V245	M185	C125	N65
N366	D306	S246	V186	S126	S66
L367	D307	A247	E187	I127	V67
L368	V308	K248	L188	I128	V68
L369	E309	L249	L189	K129	S69
S370	A310	A250	G190	V130	L70
LEU	F311	S251	S191	A131	L71
SER	V312	Y252	Y192	A132	L72
ASP	I313	V253	T193	S133	I73
THR	D314	K254	E194	C134	L74
	A315	F255	D195	G135	E75
	V316	Y256	N196	A136	P76
	K317	Q257	I197	I137	D77
	T318	N258	S198	Q138	K78
	K319	N259	Q199	Y139	Q79
	K320	K260	A200	I140	E80
	V321	D261	R201	P141	A81
	Y322	F262	V202	T142	L82
	C323	I263	D203	I143	I83
	K324	D264	A204	L144	E84
	I325	S265	H205	D145	S85
	D326	L266	R206	Q146	L86
	Q327	Q267	C207	V147	C87
	T328	L268	T208	R148	E88
	Q329	L269	V209	K149	K89
	R330	H270	R210	W150	L90
	K331	E271	A211	V151	V91
	V332	Q272	L212	S152	K92
	V333	M273	K213	D153	F93
	V334	M274	D214	W154	R94
	S335	A275	P215	N155	E95
	H336	K276	N216	L156	G96
	S337	M277	A217	T157	E97
	T338	R278	F218	T158	R98
	H339	L279	L219	E159	P99
	R340	L280	F220	K160	S100
	T341	T281	D221	K161	L101
	F342	F282	H222	H162	R102
	G343	M283	L223	T163	L103
	K344	Q284	L224	L164	Q104
	Q345	M285	T225	L165	L105
	Q346	A286	L226	R166	L106
	W347	V287	K227	L167	S107
	Q348	E288	P228	L168	N108
	Q349	N289	V229	Y169	L109
	L350	K290	K230	E170	F110
	Y351	E291	F231	A171	H111
	D352	I292	L232	L172	G112
	T353	S293	E233	V173	M113
	L354	F294	Q234	D174	D114
	N355	D295	E235	C175	K115
	A356	T296	L236	K176	N116
	W357	M297	T237	K177	T117
	K358	Q298	H238	S178	P118
	Q359	Q299	D239	D179	V119
	W360	F300	L240	A180	R120

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, T6A, SF4, C4J, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	1.99	11/1770 (0.6%)	2.43	176/2759 (6.4%)
2	l	1.36	0/241	0.93	0/305
3	C	0.97	0/1680	0.97	1/2283 (0.0%)
4	D	0.86	0/1769	0.96	2/2367 (0.1%)
5	E	0.91	0/1779	0.94	1/2399 (0.0%)
6	F	0.97	0/1793	0.98	0/2412
7	G	0.97	0/2125	0.97	0/2856
8	H	0.99	0/1531	0.93	0/2059
9	I	1.01	0/1947	0.98	4/2590 (0.2%)
10	J	0.96	0/1553	1.00	2/2079 (0.1%)
11	K	1.03	0/1709	1.00	3/2278 (0.1%)
12	L	1.07	0/1523	0.91	2/2031 (0.1%)
13	M	0.96	0/852	1.03	4/1147 (0.3%)
14	N	0.97	0/1319	0.95	0/1761
15	O	0.90	0/968	0.95	0/1296
16	P	0.94	0/1232	0.84	0/1656
17	Q	1.03	0/1029	0.98	0/1380
18	S	1.03	0/1142	0.98	0/1528
19	T	0.99	0/1031	0.93	0/1383
20	V	0.99	0/1132	0.91	0/1517
21	W	0.97	0/832	1.00	0/1117
22	X	1.05	1/627 (0.2%)	1.02	3/839 (0.4%)
23	Y	1.00	0/1051	0.96	0/1406
24	Z	0.99	0/1125	0.95	2/1500 (0.1%)
25	a	1.04	1/1038 (0.1%)	1.06	3/1380 (0.2%)
26	b	1.03	0/802	0.94	0/1076
27	c	0.85	0/673	0.89	2/902 (0.2%)
28	d	1.12	0/508	0.95	0/680
29	e	1.11	0/455	1.08	0/603
30	f	0.98	0/594	1.06	2/786 (0.3%)
31	g	0.91	0/2494	1.04	2/3394 (0.1%)
32	n	0.98	0/605	1.01	2/810 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	1.09	0/478	0.98	0/628
34	2	1.58	72/41548 (0.2%)	2.39	4296/64753 (6.6%)
35	A	0.79	1/2178 (0.0%)	1.15	11/2935 (0.4%)
36	B	0.91	2/3267 (0.1%)	1.00	4/4415 (0.1%)
37	j	0.72	1/892 (0.1%)	1.16	7/1186 (0.6%)
38	k	1.53	16/4772 (0.3%)	1.71	58/6428 (0.9%)
39	U	1.04	0/1211	0.95	0/1618
40	R	0.99	0/1177	1.00	3/1571 (0.2%)
41	3	0.54	0/1074	1.03	17/1671 (1.0%)
42	m	0.97	0/3015	0.96	4/4078 (0.1%)
43	y	0.70	1/5059 (0.0%)	0.79	13/6832 (0.2%)
44	v	0.86	2/4585 (0.0%)	1.01	12/6185 (0.2%)
45	w	0.95	0/3538	1.01	15/4786 (0.3%)
46	q	0.91	0/2149	0.97	1/2920 (0.0%)
47	r	0.91	0/2675	0.96	3/3609 (0.1%)
48	s	0.88	0/1772	0.88	4/2396 (0.2%)
49	t	0.95	0/3185	0.95	7/4296 (0.2%)
50	u	0.88	0/2963	0.97	3/3998 (0.1%)
All	All	1.23	108/124467 (0.1%)	1.68	4669/176884 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	3	2
3	C	0	1
4	D	0	1
9	I	0	3
10	J	0	2
11	K	0	2
12	L	0	2
13	M	0	5
17	Q	0	2
18	S	0	2
22	X	0	1
25	a	0	1
26	b	0	1
27	c	0	1
29	e	0	4
30	f	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	i	0	3
34	2	1	46
35	A	0	7
36	B	0	8
37	j	0	12
38	k	0	33
39	U	0	3
43	y	0	8
44	v	0	53
45	w	0	10
46	q	0	6
47	r	0	10
48	s	0	1
49	t	0	5
50	u	0	9
All	All	4	245

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	455	ILE	C-N	-38.75	0.45	1.34
38	k	562	LEU	C-N	-35.45	0.52	1.34
38	k	378	LEU	C-N	34.34	1.94	1.33
1	1	17	C	O3'-P	32.10	1.99	1.61
38	k	408	ASN	C-N	-28.67	0.68	1.34
1	1	17	C	C2'-O2'	-26.02	1.07	1.41
38	k	109	VAL	C-N	25.81	1.79	1.33
38	k	104	GLU	C-N	-25.62	0.75	1.34
38	k	481	ASP	C-N	-23.69	0.79	1.34
38	k	531	ARG	C-N	-22.54	0.82	1.34
38	k	440	GLN	C-N	22.39	1.85	1.34
34	2	80	G	O3'-P	-21.99	1.34	1.61
1	1	18	G	O3'-P	21.71	1.87	1.61
38	k	241	ASP	C-N	-21.56	0.84	1.34
44	v	748	ASP	C-N	20.79	1.81	1.34
34	2	239	U	O3'-P	-20.61	1.36	1.61
34	2	350	A	O3'-P	18.98	1.83	1.61
1	1	18	G	C3'-O3'	-16.69	1.18	1.42
36	B	289	GLY	N-CA	-14.39	1.24	1.46
38	k	150	SER	C-N	-13.59	1.02	1.34
38	k	268	TYR	C-N	-13.58	1.02	1.34
34	2	351	U	O3'-P	-13.55	1.44	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	513	LYS	C-N	13.36	1.64	1.34
1	1	16	G	O3'-P	-12.67	1.46	1.61
38	k	160	LEU	C-N	-12.44	1.05	1.34
25	a	9	THR	C-N	11.66	1.60	1.34
1	1	37	T6A	O3'-P	11.65	1.75	1.61
44	v	762	ASN	C-N	-11.56	1.12	1.33
38	k	493	ASP	C-N	-10.73	1.09	1.34
34	2	1170	U	O3'-P	-10.27	1.48	1.61
35	A	184	LEU	C-N	10.08	1.57	1.34
34	2	1171	G	O3'-P	-9.20	1.50	1.61
22	X	77	GLY	C-N	8.93	1.54	1.34
1	1	18	G	C1'-N9	-7.91	1.35	1.46
37	j	95	TYR	C-N	-7.74	1.16	1.34
34	2	67	C	O3'-P	7.71	1.70	1.61
34	2	1182	U	N3-C4	7.54	1.45	1.38
34	2	1170	U	C2-N3	6.92	1.42	1.37
34	2	1809	A	N7-C5	-6.53	1.35	1.39
43	y	43	TRP	CD2-CE2	-6.53	1.33	1.41
38	k	179	ALA	C-N	6.41	1.48	1.34
34	2	916	A	N7-C5	-6.32	1.35	1.39
34	2	1141	A	N7-C5	-6.26	1.35	1.39
34	2	1023	A	N7-C5	-6.21	1.35	1.39
34	2	822	A	N7-C5	-6.19	1.35	1.39
34	2	1185	A	N7-C5	-6.19	1.35	1.39
34	2	960	A	N7-C5	-6.12	1.35	1.39
34	2	1170	U	C1'-N1	6.10	1.57	1.48
34	2	1584	A	N7-C5	-6.00	1.35	1.39
34	2	1628	A	N7-C5	-5.92	1.35	1.39
34	2	206	A	N7-C5	-5.91	1.35	1.39
34	2	237	G	C2-N3	5.89	1.37	1.32
34	2	437	A	N7-C5	-5.88	1.35	1.39
34	2	1815	U	O3'-P	-5.87	1.54	1.61
34	2	1178	A	N7-C5	-5.75	1.35	1.39
34	2	1192	A	N7-C5	-5.67	1.35	1.39
34	2	1283	A	N7-C5	-5.67	1.35	1.39
34	2	1066	A	N7-C5	-5.66	1.35	1.39
34	2	994	A	N7-C5	-5.64	1.35	1.39
34	2	1045	A	N7-C5	-5.61	1.35	1.39
34	2	1353	A	N7-C5	-5.60	1.35	1.39
1	1	17	C	C3'-O3'	-5.59	1.34	1.42
34	2	190	A	N7-C5	-5.58	1.35	1.39
34	2	102	A	N7-C5	-5.56	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	2	577	A	N7-C5	-5.54	1.35	1.39
34	2	1182	U	N1-C6	5.50	1.43	1.38
34	2	1629	A	N7-C5	-5.47	1.35	1.39
34	2	1186	A	N7-C5	-5.43	1.35	1.39
34	2	1784	A	N7-C5	-5.43	1.35	1.39
34	2	1635	A	N7-C5	-5.42	1.35	1.39
34	2	474	A	N7-C5	-5.42	1.36	1.39
34	2	1714	A	N7-C5	-5.41	1.36	1.39
34	2	318	U	C2-N3	5.41	1.41	1.37
34	2	537	G	C2-N3	5.38	1.37	1.32
34	2	1440	U	C2-N3	5.35	1.41	1.37
34	2	1730	A	N7-C5	-5.35	1.36	1.39
34	2	1615	A	N7-C5	-5.33	1.36	1.39
34	2	1645	A	N7-C5	-5.32	1.36	1.39
34	2	235	C	N3-C4	5.30	1.37	1.33
34	2	554	A	N7-C5	-5.29	1.36	1.39
34	2	1740	A	N7-C5	-5.28	1.36	1.39
34	2	171	A	N7-C5	-5.28	1.36	1.39
34	2	1539	C	N3-C4	5.27	1.37	1.33
34	2	1046	A	N7-C5	-5.26	1.36	1.39
34	2	1182	U	C2-N3	5.26	1.41	1.37
34	2	1170	U	C5-C6	5.20	1.38	1.34
34	2	92	A	N7-C5	-5.19	1.36	1.39
34	2	1170	U	N1-C2	-5.18	1.33	1.38
34	2	80	G	N1-C2	5.17	1.41	1.37
34	2	1767	C	N3-C4	5.15	1.37	1.33
34	2	304	A	N7-C5	-5.13	1.36	1.39
1	1	60	A	N7-C5	-5.12	1.36	1.39
34	2	1747	C	N3-C4	5.12	1.37	1.33
34	2	439	A	N7-C5	-5.12	1.36	1.39
34	2	1772	C	N3-C4	5.11	1.37	1.33
34	2	229	A	N7-C5	-5.11	1.36	1.39
34	2	1746	C	N3-C4	5.08	1.37	1.33
34	2	1774	G	N1-C2	5.08	1.41	1.37
34	2	402	G	C2-N3	5.07	1.36	1.32
34	2	875	C	N3-C4	5.07	1.37	1.33
34	2	1745	C	N3-C4	5.07	1.37	1.33
34	2	827	G	N1-C2	5.06	1.41	1.37
34	2	300	G	N1-C2	5.05	1.41	1.37
1	1	71	C	N3-C4	5.04	1.37	1.33
34	2	1303	U	C2-N3	5.04	1.41	1.37
34	2	82	G	C2-N3	5.03	1.36	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	27	C	N3-C4	5.01	1.37	1.33
36	B	288	LYS	C-N	-5.00	1.24	1.33

All (4669) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	160	LEU	O-C-N	35.04	178.76	122.70
38	k	531	ARG	C-N-CA	-34.40	35.70	121.70
38	k	531	ARG	CA-C-N	-33.55	43.38	117.20
44	v	762	ASN	C-N-CA	-29.30	60.77	122.30
38	k	378	LEU	CA-C-N	-27.37	61.45	116.20
38	k	408	ASN	O-C-N	-25.78	81.45	122.70
44	v	762	ASN	CA-C-N	-25.71	64.77	116.20
38	k	160	LEU	CA-C-N	-25.44	61.23	117.20
38	k	160	LEU	C-N-CA	-25.01	59.17	121.70
44	v	762	ASN	O-C-N	23.61	163.33	123.20
38	k	348	TYR	O-C-N	-21.54	88.23	122.70
38	k	378	LEU	C-N-CA	-21.53	77.09	122.30
34	2	271	G	P-O3'-C3'	21.37	145.34	119.70
38	k	481	ASP	O-C-N	-21.36	88.52	122.70
38	k	531	ARG	O-C-N	20.01	154.72	122.70
38	k	317	VAL	C-N-CD	-18.91	79.01	120.60
34	2	351	U	P-O3'-C3'	18.68	142.11	119.70
38	k	513	LYS	O-C-N	-17.28	95.05	122.70
43	y	7	ARG	C-N-CD	-17.02	83.15	120.60
38	k	493	ASP	O-C-N	16.33	148.82	122.70
1	1	17	C	C4'-C3'-O3'	16.32	145.64	113.00
34	2	1854	A	P-O3'-C3'	15.82	138.69	119.70
38	k	104	GLU	O-C-N	-15.55	97.82	122.70
38	k	455	ILE	O-C-N	-15.54	97.83	122.70
38	k	109	VAL	O-C-N	-14.76	98.10	123.20
25	a	12	PHE	CB-CA-C	14.69	139.78	110.40
34	2	1027	A	N1-C6-N6	14.52	127.31	118.60
34	2	997	A	N1-C6-N6	14.43	127.26	118.60
34	2	1405	A	N1-C6-N6	14.40	127.24	118.60
34	2	1556	A	N1-C6-N6	14.35	127.21	118.60
34	2	1417	A	N1-C6-N6	14.23	127.14	118.60
38	k	481	ASP	C-N-CA	14.19	157.16	121.70
34	2	1032	A	N1-C6-N6	13.99	127.00	118.60
1	1	17	C	O3'-P-O5'	13.88	130.37	104.00
1	1	54	A	N1-C6-N6	13.83	126.90	118.60
34	2	68	A	N1-C6-N6	13.78	126.87	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	519	A	N1-C6-N6	13.76	126.86	118.60
34	2	1007	A	N1-C6-N6	13.70	126.82	118.60
34	2	173	A	N1-C6-N6	13.67	126.81	118.60
34	2	1289	A	N1-C6-N6	13.65	126.79	118.60
34	2	640	A	N1-C6-N6	13.62	126.77	118.60
34	2	1575	A	N1-C6-N6	13.61	126.77	118.60
1	1	60	A	N1-C6-N6	13.60	126.76	118.60
34	2	1190	A	N1-C6-N6	13.60	126.76	118.60
34	2	425	A	N1-C6-N6	13.53	126.72	118.60
34	2	550	A	N1-C6-N6	13.51	126.70	118.60
34	2	834	G	O4'-C1'-N9	13.47	118.97	108.20
34	2	1825	A	N1-C6-N6	13.43	126.66	118.60
1	1	18	G	O3'-P-O5'	13.41	129.49	104.00
34	2	1526	A	N1-C6-N6	13.37	126.62	118.60
34	2	1803	A	N1-C6-N6	13.31	126.59	118.60
34	2	1048	A	N1-C6-N6	13.27	126.56	118.60
34	2	309	A	N1-C6-N6	13.27	126.56	118.60
34	2	545	A	N1-C6-N6	13.22	126.53	118.60
1	1	16	G	O3'-P-O5'	13.21	129.11	104.00
34	2	959	A	N1-C6-N6	13.20	126.52	118.60
34	2	1200	A	N1-C6-N6	13.19	126.52	118.60
34	2	1216	A	N1-C6-N6	13.20	126.52	118.60
34	2	1448	A	N1-C6-N6	13.18	126.51	118.60
34	2	986	A	N1-C6-N6	13.18	126.51	118.60
34	2	1646	A	N1-C6-N6	13.15	126.49	118.60
34	2	940	A	N1-C6-N6	13.14	126.48	118.60
34	2	1609	A	N1-C6-N6	13.08	126.45	118.60
34	2	423	A	N1-C6-N6	13.07	126.44	118.60
34	2	233	A	N1-C6-N6	13.06	126.44	118.60
1	1	21	A	N1-C6-N6	13.04	126.42	118.60
34	2	1853	A	N1-C6-N6	13.03	126.42	118.60
34	2	977	A	N1-C6-N6	13.01	126.41	118.60
34	2	79	A	N1-C6-N6	13.01	126.40	118.60
34	2	904	A	N1-C6-N6	12.99	126.39	118.60
34	2	1141	A	N1-C6-N6	12.99	126.39	118.60
34	2	1800	A	N1-C6-N6	12.99	126.39	118.60
34	2	350	A	N1-C6-N6	12.98	126.39	118.60
34	2	22	A	N1-C6-N6	12.98	126.39	118.60
34	2	1272	A	N1-C6-N6	12.97	126.38	118.60
34	2	1274	A	N1-C6-N6	12.94	126.36	118.60
34	2	988	A	N1-C6-N6	12.92	126.35	118.60
34	2	1596	A	N1-C6-N6	12.89	126.34	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1719	A	N1-C6-N6	12.87	126.32	118.60
34	2	509	A	N1-C6-N6	12.86	126.31	118.60
34	2	64	A	N1-C6-N6	12.85	126.31	118.60
34	2	339	A	N1-C6-N6	12.85	126.31	118.60
34	2	164	A	N1-C6-N6	12.83	126.30	118.60
34	2	589	A	N1-C6-N6	12.83	126.30	118.60
34	2	405	A	N1-C6-N6	12.83	126.30	118.60
34	2	631	A	N1-C6-N6	12.81	126.28	118.60
34	2	1726	A	N1-C6-N6	12.80	126.28	118.60
1	1	38	A	N1-C6-N6	12.78	126.27	118.60
34	2	1854	A	N1-C6-N6	12.78	126.27	118.60
34	2	1179	A	N1-C6-N6	12.78	126.27	118.60
34	2	1465	A	N1-C6-N6	12.77	126.26	118.60
34	2	1016	A	N1-C6-N6	12.76	126.26	118.60
34	2	882	A	N1-C6-N6	12.76	126.25	118.60
38	k	493	ASP	CA-C-N	-12.76	89.13	117.20
1	1	76	A	N1-C6-N6	12.74	126.25	118.60
34	2	630	A	N1-C6-N6	12.69	126.22	118.60
34	2	1242	A	N1-C6-N6	12.69	126.21	118.60
34	2	1375	A	N1-C6-N6	12.67	126.20	118.60
34	2	103	A	N1-C6-N6	12.66	126.20	118.60
34	2	1863	A	N1-C6-N6	12.66	126.20	118.60
34	2	366	A	N1-C6-N6	12.65	126.19	118.60
34	2	535	A	N1-C6-N6	12.65	126.19	118.60
34	2	1177	A	N1-C6-N6	12.64	126.19	118.60
34	2	490	A	N1-C6-N6	12.64	126.19	118.60
34	2	1365	A	N1-C6-N6	12.64	126.19	118.60
34	2	1636	A	N1-C6-N6	12.64	126.18	118.60
34	2	382	A	N1-C6-N6	12.64	126.18	118.60
34	2	398	A	N1-C6-N6	12.63	126.18	118.60
34	2	1349	A	N1-C6-N6	12.64	126.18	118.60
34	2	1378	A	N1-C6-N6	12.63	126.18	118.60
34	2	448	A	N1-C6-N6	12.61	126.17	118.60
34	2	643	A	N1-C6-N6	12.62	126.17	118.60
1	1	58	A	N1-C6-N6	12.61	126.17	118.60
34	2	214	A	N1-C6-N6	12.60	126.16	118.60
34	2	638	A	N1-C6-N6	12.60	126.16	118.60
34	2	388	A	N1-C6-N6	12.59	126.15	118.60
34	2	227	A	N1-C6-N6	12.59	126.15	118.60
34	2	807	A	N1-C6-N6	12.58	126.15	118.60
34	2	1589	A	N1-C6-N6	12.58	126.15	118.60
34	2	510	A	N1-C6-N6	12.58	126.15	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1213	A	N1-C6-N6	12.57	126.14	118.60
34	2	99	A	N1-C6-N6	12.56	126.14	118.60
34	2	518	A	N1-C6-N6	12.56	126.14	118.60
34	2	1659	A	N1-C6-N6	12.56	126.14	118.60
34	2	1470	A	N1-C6-N6	12.56	126.14	118.60
34	2	479	A	N1-C6-N6	12.56	126.13	118.60
34	2	1710	A	N1-C6-N6	12.56	126.14	118.60
34	2	1020	A	N1-C6-N6	12.55	126.13	118.60
34	2	1692	A	N1-C6-N6	12.55	126.13	118.60
34	2	1472	A	N1-C6-N6	12.54	126.12	118.60
34	2	404	A	N1-C6-N6	12.53	126.11	118.60
34	2	1532	A	N1-C6-N6	12.53	126.11	118.60
34	2	953	A	N1-C6-N6	12.51	126.10	118.60
34	2	1145	A	N1-C6-N6	12.50	126.10	118.60
34	2	232	A	N1-C6-N6	12.49	126.09	118.60
41	3	52	A	N1-C6-N6	12.49	126.09	118.60
34	2	1038	A	N1-C6-N6	12.48	126.09	118.60
34	2	976	A	N1-C6-N6	12.47	126.08	118.60
34	2	1564	A	N1-C6-N6	12.47	126.08	118.60
34	2	288	A	N1-C6-N6	12.47	126.08	118.60
34	2	1224	A	N1-C6-N6	12.46	126.08	118.60
34	2	979	A	N1-C6-N6	12.44	126.06	118.60
34	2	1026	A	N1-C6-N6	12.43	126.06	118.60
34	2	565	A	N1-C6-N6	12.42	126.05	118.60
34	2	11	A	N1-C6-N6	12.42	126.05	118.60
34	2	458	A	N1-C6-N6	12.42	126.05	118.60
34	2	584	A	N1-C6-N6	12.41	126.05	118.60
34	2	483	A	N1-C6-N6	12.40	126.04	118.60
34	2	994	A	N1-C6-N6	12.39	126.04	118.60
34	2	107	A	N1-C6-N6	12.39	126.03	118.60
34	2	858	A	N1-C6-N6	12.39	126.03	118.60
34	2	854	A	N1-C6-N6	12.39	126.03	118.60
34	2	958	A	N1-C6-N6	12.38	126.03	118.60
34	2	445	A	N1-C6-N6	12.37	126.02	118.60
34	2	1236	A	N1-C6-N6	12.37	126.02	118.60
34	2	50	A	N1-C6-N6	12.36	126.02	118.60
34	2	1295	A	N1-C6-N6	12.35	126.01	118.60
34	2	85	A	N1-C6-N6	12.35	126.01	118.60
34	2	809	A	N1-C6-N6	12.34	126.01	118.60
34	2	502	A	N1-C6-N6	12.34	126.00	118.60
34	2	1476	A	N1-C6-N6	12.34	126.00	118.60
34	2	1482	A	N1-C6-N6	12.34	126.00	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1401	A	N1-C6-N6	12.34	126.00	118.60
34	2	1005	A	N1-C6-N6	12.32	125.99	118.60
34	2	1280	A	N1-C6-N6	12.31	125.98	118.60
1	1	15	A	N1-C6-N6	12.30	125.98	118.60
34	2	574	A	N1-C6-N6	12.30	125.98	118.60
34	2	455	A	N1-C6-N6	12.29	125.98	118.60
34	2	25	A	N1-C6-N6	12.28	125.97	118.60
34	2	463	A	N1-C6-N6	12.27	125.96	118.60
34	2	512	A	N1-C6-N6	12.27	125.96	118.60
34	2	1844	A	N1-C6-N6	12.27	125.96	118.60
34	2	1019	A	N1-C6-N6	12.27	125.96	118.60
34	2	1328	A	N1-C6-N6	12.26	125.96	118.60
34	2	1366	A	N1-C6-N6	12.26	125.95	118.60
34	2	1382	A	N1-C6-N6	12.25	125.95	118.60
34	2	523	A	N1-C6-N6	12.24	125.94	118.60
34	2	1625	A	N1-C6-N6	12.24	125.94	118.60
34	2	141	A	N1-C6-N6	12.23	125.94	118.60
34	2	354	A	N1-C6-N6	12.23	125.94	118.60
34	2	1089	A	N1-C6-N6	12.23	125.94	118.60
34	2	1031	A	N1-C6-N6	12.23	125.94	118.60
34	2	868	A	N1-C6-N6	12.22	125.94	118.60
34	2	1782	A	N1-C6-N6	12.22	125.93	118.60
34	2	1775	A	N1-C6-N6	12.22	125.93	118.60
34	2	27	A	N1-C6-N6	12.21	125.92	118.60
34	2	1008	A	N1-C6-N6	12.20	125.92	118.60
34	2	1073	A	N1-C6-N6	12.20	125.92	118.60
34	2	1083	A	N1-C6-N6	12.20	125.92	118.60
34	2	1444	A	N1-C6-N6	12.19	125.91	118.60
34	2	573	A	N1-C6-N6	12.19	125.91	118.60
34	2	660	A	N1-C6-N6	12.19	125.91	118.60
34	2	805	A	N1-C6-N6	12.18	125.91	118.60
34	2	1205	A	N1-C6-N6	12.18	125.91	118.60
34	2	40	A	N1-C6-N6	12.18	125.91	118.60
34	2	450	A	N1-C6-N6	12.18	125.91	118.60
34	2	624	A	N1-C6-N6	12.17	125.90	118.60
34	2	1670	A	N1-C6-N6	12.17	125.90	118.60
1	1	59	A	N1-C6-N6	12.17	125.90	118.60
34	2	1204	A	N1-C6-N6	12.16	125.90	118.60
34	2	1451	A	N1-C6-N6	12.16	125.90	118.60
1	1	20	A	N1-C6-N6	12.13	125.88	118.60
34	2	1502	A	N1-C6-N6	12.13	125.88	118.60
34	2	993	A	N1-C6-N6	12.12	125.88	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1860	A	N1-C6-N6	12.13	125.88	118.60
34	2	166	A	N1-C6-N6	12.12	125.87	118.60
1	1	35	A	N1-C6-N6	12.11	125.87	118.60
34	2	1297	A	N1-C6-N6	12.11	125.86	118.60
34	2	223	A	N1-C6-N6	12.09	125.86	118.60
34	2	283	A	N1-C6-N6	12.09	125.86	118.60
34	2	361	A	N1-C6-N6	12.08	125.85	118.60
34	2	983	A	N1-C6-N6	12.08	125.85	118.60
34	2	857	A	N1-C6-N6	12.07	125.84	118.60
34	2	1004	A	N1-C6-N6	12.07	125.84	118.60
34	2	559	A	N1-C6-N6	12.07	125.84	118.60
34	2	812	A	N1-C6-N6	12.06	125.84	118.60
34	2	1690	A	N1-C6-N6	12.06	125.84	118.60
34	2	566	A	N1-C6-N6	12.05	125.83	118.60
34	2	850	A	N1-C6-N6	12.05	125.83	118.60
34	2	1496	G	N1-C6-O6	12.05	127.13	119.90
34	2	1673	A	N1-C6-N6	12.04	125.82	118.60
34	2	1839	A	N1-C6-N6	12.04	125.82	118.60
34	2	544	A	N1-C6-N6	12.04	125.82	118.60
34	2	1674	A	N1-C6-N6	12.03	125.82	118.60
34	2	19	A	N1-C6-N6	12.03	125.82	118.60
1	1	73	A	N1-C6-N6	12.02	125.81	118.60
34	2	429	A	N1-C6-N6	12.02	125.81	118.60
34	2	1080	A	N1-C6-N6	12.02	125.81	118.60
34	2	511	A	N1-C6-N6	12.02	125.81	118.60
34	2	228	A	N1-C6-N6	12.02	125.81	118.60
1	1	44	A	N1-C6-N6	12.01	125.81	118.60
34	2	1574	A	N1-C6-N6	12.01	125.81	118.60
34	2	525	G	N1-C6-O6	12.01	127.11	119.90
34	2	218	A	N1-C6-N6	12.01	125.81	118.60
34	2	516	A	N1-C6-N6	12.01	125.80	118.60
34	2	633	A	N1-C6-N6	12.00	125.80	118.60
34	2	808	A	N1-C6-N6	12.00	125.80	118.60
34	2	476	A	N1-C6-N6	12.00	125.80	118.60
34	2	1379	A	N1-C6-N6	12.00	125.80	118.60
34	2	1340	A	N1-C6-N6	11.99	125.80	118.60
34	2	1195	A	N1-C6-N6	11.98	125.79	118.60
34	2	1076	A	N1-C6-N6	11.97	125.78	118.60
34	2	826	A	N1-C6-N6	11.96	125.78	118.60
34	2	1146	A	N1-C6-N6	11.96	125.78	118.60
34	2	1398	A	N1-C6-N6	11.96	125.78	118.60
34	2	1618	A	N1-C6-N6	11.95	125.77	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	329	A	N1-C6-N6	11.95	125.77	118.60
34	2	619	A	N1-C6-N6	11.94	125.77	118.60
34	2	860	A	N1-C6-N6	11.94	125.77	118.60
34	2	1196	A	N1-C6-N6	11.94	125.77	118.60
34	2	1247	A	N1-C6-N6	11.94	125.76	118.60
34	2	1249	A	N1-C6-N6	11.94	125.76	118.60
34	2	2	A	N1-C6-N6	11.93	125.76	118.60
34	2	644	A	N1-C6-N6	11.93	125.76	118.60
34	2	1353	A	N1-C6-N6	11.93	125.76	118.60
34	2	147	A	N1-C6-N6	11.93	125.76	118.60
34	2	580	A	N1-C6-N6	11.93	125.76	118.60
34	2	326	A	N1-C6-N6	11.93	125.75	118.60
34	2	909	A	N1-C6-N6	11.93	125.75	118.60
34	2	159	A	N1-C6-N6	11.92	125.75	118.60
34	2	861	A	N1-C6-N6	11.91	125.75	118.60
38	k	455	ILE	C-N-CA	-11.91	91.92	121.70
34	2	61	A	N1-C6-N6	11.91	125.75	118.60
34	2	1051	A	N1-C6-N6	11.91	125.74	118.60
34	2	645	A	N1-C6-N6	11.90	125.74	118.60
34	2	1129	A	N1-C6-N6	11.90	125.74	118.60
34	2	609	A	N1-C6-N6	11.89	125.74	118.60
34	2	1384	A	N1-C6-N6	11.89	125.74	118.60
34	2	1551	A	N1-C6-N6	11.89	125.73	118.60
34	2	918	A	N1-C6-N6	11.88	125.73	118.60
34	2	1246	A	N1-C6-N6	11.88	125.73	118.60
34	2	77	A	N1-C6-N6	11.88	125.73	118.60
34	2	1807	A	N1-C6-N6	11.87	125.72	118.60
34	2	1434	A	N1-C6-N6	11.87	125.72	118.60
34	2	887	G	N1-C6-O6	11.87	127.02	119.90
34	2	912	A	N1-C6-N6	11.87	125.72	118.60
34	2	1219	A	N1-C6-N6	11.87	125.72	118.60
34	2	158	A	N1-C6-N6	11.87	125.72	118.60
34	2	662	A	N1-C6-N6	11.87	125.72	118.60
34	2	1054	A	N1-C6-N6	11.86	125.72	118.60
34	2	91	A	N1-C6-N6	11.86	125.72	118.60
34	2	290	A	N1-C6-N6	11.86	125.71	118.60
34	2	293	A	N1-C6-N6	11.86	125.71	118.60
34	2	221	A	N1-C6-N6	11.85	125.71	118.60
34	2	416	A	N1-C6-N6	11.84	125.71	118.60
34	2	871	A	N1-C6-N6	11.84	125.71	118.60
34	2	968	A	N1-C6-N6	11.84	125.71	118.60
34	2	1517	A	N1-C6-N6	11.84	125.71	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	658	A	N1-C6-N6	11.84	125.70	118.60
34	2	1812	A	N1-C6-N6	11.84	125.70	118.60
34	2	1139	A	N1-C6-N6	11.84	125.70	118.60
34	2	1287	A	N1-C6-N6	11.84	125.70	118.60
34	2	1614	A	N1-C6-N6	11.84	125.70	118.60
34	2	654	A	N1-C6-N6	11.83	125.70	118.60
34	2	900	A	N1-C6-N6	11.83	125.70	118.60
34	2	45	A	N1-C6-N6	11.82	125.69	118.60
34	2	1372	A	N1-C6-N6	11.82	125.69	118.60
34	2	899	A	N1-C6-N6	11.82	125.69	118.60
34	2	521	A	N1-C6-N6	11.82	125.69	118.60
34	2	475	A	N1-C6-N6	11.82	125.69	118.60
34	2	379	A	N1-C6-N6	11.81	125.69	118.60
34	2	1096	A	N1-C6-N6	11.81	125.69	118.60
34	2	1291	A	N1-C6-N6	11.80	125.68	118.60
34	2	1787	A	N1-C6-N6	11.81	125.68	118.60
34	2	675	A	N1-C6-N6	11.80	125.68	118.60
34	2	845	A	N1-C6-N6	11.80	125.68	118.60
34	2	866	A	N1-C6-N6	11.80	125.68	118.60
34	2	38	A	N1-C6-N6	11.80	125.68	118.60
34	2	111	A	N1-C6-N6	11.79	125.67	118.60
34	2	618	A	N1-C6-N6	11.79	125.67	118.60
34	2	833	A	N1-C6-N6	11.79	125.67	118.60
34	2	1714	A	N1-C6-N6	11.79	125.67	118.60
34	2	459	A	N1-C6-N6	11.78	125.67	118.60
34	2	1845	A	N1-C6-N6	11.78	125.67	118.60
34	2	865	A	N1-C6-N6	11.77	125.66	118.60
34	2	551	A	N1-C6-N6	11.77	125.66	118.60
34	2	1450	A	N1-C6-N6	11.77	125.66	118.60
34	2	554	A	N1-C6-N6	11.77	125.66	118.60
34	2	226	A	N1-C6-N6	11.76	125.66	118.60
1	1	2	A	N1-C6-N6	11.75	125.65	118.60
34	2	175	A	N1-C6-N6	11.75	125.65	118.60
34	2	1540	A	N1-C6-N6	11.75	125.65	118.60
34	2	595	A	N1-C6-N6	11.75	125.65	118.60
34	2	1494	A	N1-C6-N6	11.74	125.65	118.60
34	2	333	A	N1-C6-N6	11.74	125.64	118.60
34	2	798	A	N1-C6-N6	11.74	125.64	118.60
34	2	1045	A	N1-C6-N6	11.74	125.64	118.60
34	2	54	A	N1-C6-N6	11.73	125.64	118.60
34	2	1184	A	N1-C6-N6	11.73	125.64	118.60
34	2	1485	A	N1-C6-N6	11.72	125.64	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1435	A	N1-C6-N6	11.72	125.63	118.60
34	2	408	A	N1-C6-N6	11.71	125.63	118.60
34	2	1078	A	N1-C6-N6	11.71	125.63	118.60
34	2	513	A	N1-C6-N6	11.70	125.62	118.60
34	2	1826	A	N1-C6-N6	11.69	125.61	118.60
34	2	1795	A	N1-C6-N6	11.69	125.61	118.60
34	2	292	A	N1-C6-N6	11.69	125.61	118.60
34	2	454	A	N1-C6-N6	11.68	125.61	118.60
34	2	337	G	N1-C6-O6	11.67	126.90	119.90
34	2	181	A	N1-C6-N6	11.66	125.60	118.60
34	2	1140	A	N1-C6-N6	11.66	125.60	118.60
34	2	1237	A	N1-C6-N6	11.66	125.60	118.60
34	2	1144	A	N1-C6-N6	11.65	125.59	118.60
34	2	1829	A	N1-C6-N6	11.65	125.59	118.60
34	2	229	A	N1-C6-N6	11.64	125.58	118.60
34	2	806	A	N1-C6-N6	11.64	125.58	118.60
34	2	1410	A	N1-C6-N6	11.64	125.58	118.60
34	2	1483	A	N1-C6-N6	11.64	125.58	118.60
34	2	814	A	N1-C6-N6	11.64	125.58	118.60
34	2	1186	A	N1-C6-N6	11.63	125.58	118.60
34	2	466	A	N1-C6-N6	11.62	125.57	118.60
34	2	553	G	N1-C6-O6	11.62	126.87	119.90
34	2	915	A	N1-C6-N6	11.61	125.57	118.60
34	2	84	A	N1-C6-N6	11.60	125.56	118.60
34	2	661	A	N1-C6-N6	11.59	125.55	118.60
34	2	922	A	N1-C6-N6	11.59	125.55	118.60
34	2	934	A	N1-C6-N6	11.59	125.55	118.60
34	2	1278	A	N1-C6-N6	11.58	125.55	118.60
34	2	1480	A	N1-C6-N6	11.56	125.53	118.60
34	2	659	A	N1-C6-N6	11.55	125.53	118.60
34	2	1694	A	N1-C6-N6	11.55	125.53	118.60
34	2	1583	A	N1-C6-N6	11.54	125.52	118.60
34	2	1632	A	N1-C6-N6	11.53	125.52	118.60
34	2	1740	A	N1-C6-N6	11.51	125.51	118.60
34	2	435	A	N1-C6-N6	11.51	125.51	118.60
34	2	823	A	N1-C6-N6	11.51	125.50	118.60
34	2	338	A	N1-C6-N6	11.50	125.50	118.60
34	2	42	A	N1-C6-N6	11.49	125.50	118.60
34	2	564	A	N1-C6-N6	11.48	125.49	118.60
34	2	1374	A	N1-C6-N6	11.46	125.48	118.60
34	2	1056	A	N1-C6-N6	11.46	125.47	118.60
37	j	29	LYS	O-C-N	-11.46	104.37	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	481	ASP	CA-C-N	11.46	142.40	117.20
34	2	1255	A	N1-C6-N6	11.42	125.45	118.60
34	2	60	A	N1-C6-N6	11.40	125.44	118.60
34	2	1479	A	N1-C6-N6	11.38	125.43	118.60
34	2	1656	A	N1-C6-N6	11.38	125.43	118.60
34	2	804	A	N1-C6-N6	11.34	125.40	118.60
34	2	102	A	N1-C6-N6	11.33	125.40	118.60
34	2	1717	G	N1-C6-O6	11.33	126.70	119.90
34	2	960	A	N1-C6-N6	11.33	125.40	118.60
34	2	992	A	N1-C6-N6	11.33	125.40	118.60
1	1	53	G	N1-C6-O6	11.31	126.69	119.90
34	2	201	G	N1-C6-O6	11.30	126.68	119.90
34	2	1651	G	N1-C6-O6	11.29	126.68	119.90
34	2	1442	A	N1-C6-N6	11.29	125.38	118.60
34	2	1397	A	N1-C6-N6	11.29	125.37	118.60
34	2	821	A	N1-C6-N6	11.29	125.37	118.60
34	2	46	A	N1-C6-N6	11.26	125.36	118.60
34	2	594	A	N1-C6-N6	11.26	125.36	118.60
34	2	204	G	N1-C6-O6	11.25	126.65	119.90
34	2	1461	A	N1-C6-N6	11.25	125.35	118.60
34	2	88	G	N1-C6-O6	11.23	126.64	119.90
34	2	1066	A	N1-C6-N6	11.23	125.34	118.60
34	2	1058	A	N1-C6-N6	11.22	125.33	118.60
34	2	438	A	N1-C6-N6	11.21	125.33	118.60
34	2	1730	A	N1-C6-N6	11.21	125.33	118.60
34	2	1261	A	N1-C6-N6	11.20	125.32	118.60
41	3	64	A	N1-C6-N6	11.19	125.32	118.60
34	2	1857	A	N1-C6-N6	11.18	125.31	118.60
34	2	1605	G	N1-C6-O6	11.15	126.59	119.90
34	2	83	A	N1-C6-N6	11.13	125.28	118.60
34	2	1628	A	N1-C6-N6	11.13	125.28	118.60
34	2	146	G	N1-C6-O6	11.12	126.57	119.90
34	2	300	G	N1-C6-O6	11.12	126.57	119.90
34	2	1178	A	N1-C6-N6	11.11	125.27	118.60
34	2	1635	A	N1-C6-N6	11.09	125.25	118.60
34	2	421	G	N1-C6-O6	11.08	126.55	119.90
1	1	8	G	P-O3'-C3'	11.07	132.98	119.70
34	2	1137	G	N1-C6-O6	11.07	126.54	119.90
44	v	748	ASP	O-C-N	-11.05	105.02	122.70
34	2	1371	G	N1-C6-O6	11.04	126.52	119.90
34	2	1658	A	N1-C6-N6	11.04	125.22	118.60
34	2	951	A	N1-C6-N6	11.03	125.22	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	542	G	N1-C6-O6	11.00	126.50	119.90
34	2	579	G	N1-C6-O6	11.00	126.50	119.90
34	2	1743	G	N1-C6-O6	11.00	126.50	119.90
34	2	208	G	N1-C6-O6	10.99	126.50	119.90
34	2	304	A	N1-C6-N6	10.98	125.19	118.60
34	2	1820	G	N1-C6-O6	10.98	126.49	119.90
1	1	3	G	N1-C6-O6	10.97	126.48	119.90
34	2	1770	G	N1-C6-O6	10.96	126.48	119.90
34	2	663	G	N1-C6-O6	10.95	126.47	119.90
1	1	70	G	N1-C6-O6	10.95	126.47	119.90
38	k	104	GLU	C-N-CA	10.95	149.07	121.70
34	2	1024	A	N1-C6-N6	10.94	125.16	118.60
34	2	526	A	N1-C6-N6	10.92	125.15	118.60
34	2	1809	A	N1-C6-N6	10.92	125.15	118.60
34	2	156	G	N1-C6-O6	10.92	126.45	119.90
37	j	29	LYS	C-N-CA	-10.90	94.44	121.70
34	2	506	A	N1-C6-N6	10.88	125.13	118.60
34	2	437	A	N1-C6-N6	10.86	125.11	118.60
34	2	62	G	N1-C6-O6	10.86	126.41	119.90
34	2	206	A	N1-C6-N6	10.84	125.10	118.60
34	2	7	G	N1-C6-O6	10.83	126.40	119.90
34	2	1732	G	N1-C6-O6	10.82	126.39	119.90
34	2	1424	G	N1-C6-O6	10.81	126.39	119.90
34	2	1799	G	N1-C6-O6	10.79	126.38	119.90
34	2	474	A	N1-C6-N6	10.78	125.07	118.60
34	2	577	A	N1-C6-N6	10.76	125.06	118.60
1	1	43	G	N1-C6-O6	10.75	126.35	119.90
38	k	104	GLU	CA-C-N	10.75	140.85	117.20
34	2	1753	G	N1-C6-O6	10.75	126.35	119.90
34	2	525	G	C5-C6-O6	-10.74	122.16	128.60
34	2	843	A	N1-C6-N6	10.73	125.04	118.60
34	2	1256	A	N1-C6-N6	10.72	125.03	118.60
34	2	104	A	N1-C6-N6	10.71	125.03	118.60
34	2	186	G	N1-C6-O6	10.71	126.33	119.90
34	2	869	G	N1-C6-O6	10.71	126.32	119.90
34	2	401	G	N1-C6-O6	10.70	126.32	119.90
34	2	1752	G	N1-C6-O6	10.69	126.31	119.90
34	2	279	G	N1-C6-O6	10.68	126.31	119.90
34	2	1528	A	N1-C6-N6	10.67	125.00	118.60
34	2	203	G	N1-C6-O6	10.67	126.30	119.90
34	2	1283	A	N1-C6-N6	10.67	125.00	118.60
34	2	1079	A	N1-C6-N6	10.66	125.00	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	80	G	N1-C6-O6	10.66	126.30	119.90
34	2	1455	G	N1-C6-O6	10.64	126.28	119.90
34	2	607	G	N1-C6-O6	10.63	126.28	119.90
34	2	310	G	N1-C6-O6	10.63	126.28	119.90
34	2	170	A	N1-C6-N6	10.62	124.97	118.60
34	2	1774	G	N1-C6-O6	10.62	126.27	119.90
34	2	995	G	N1-C6-O6	10.62	126.27	119.90
34	2	39	A	N1-C6-N6	10.61	124.97	118.60
34	2	1160	G	N1-C6-O6	10.61	126.27	119.90
34	2	606	A	N1-C6-N6	10.61	124.96	118.60
34	2	1202	G	N1-C6-O6	10.59	126.25	119.90
34	2	1266	G	N1-C6-O6	10.58	126.25	119.90
34	2	1688	G	N1-C6-O6	10.58	126.25	119.90
34	2	1392	A	N1-C6-N6	10.58	124.95	118.60
34	2	1784	A	N1-C6-N6	10.57	124.94	118.60
34	2	1185	A	N1-C6-N6	10.56	124.94	118.60
38	k	408	ASN	CA-C-N	10.56	140.43	117.20
34	2	1496	G	C5-C6-O6	-10.55	122.27	128.60
34	2	1776	G	N1-C6-O6	10.55	126.23	119.90
34	2	1748	G	N1-C6-O6	10.54	126.22	119.90
34	2	353	A	N1-C6-N6	10.54	124.92	118.60
34	2	1778	G	N1-C6-O6	10.54	126.22	119.90
34	2	515	A	N1-C6-N6	10.54	124.92	118.60
34	2	1169	A	N1-C6-N6	10.53	124.92	118.60
34	2	1061	G	N1-C6-O6	10.52	126.21	119.90
34	2	1023	A	N1-C6-N6	10.52	124.91	118.60
34	2	52	G	N1-C6-O6	10.51	126.20	119.90
43	y	245	LEU	O-C-N	-10.51	105.89	122.70
34	2	1642	A	N1-C6-N6	10.50	124.90	118.60
34	2	1254	A	N1-C6-N6	10.49	124.89	118.60
34	2	320	G	N1-C6-O6	10.49	126.19	119.90
34	2	1515	G	N1-C6-O6	10.49	126.19	119.90
34	2	1170	U	P-O3'-C3'	10.46	132.25	119.70
34	2	1828	A	N1-C6-N6	10.46	124.88	118.60
34	2	1701	G	N1-C6-O6	10.44	126.16	119.90
34	2	29	G	N1-C6-O6	10.44	126.16	119.90
34	2	384	G	N1-C6-O6	10.43	126.16	119.90
34	2	167	G	N1-C6-O6	10.43	126.16	119.90
34	2	1731	G	N1-C6-O6	10.43	126.16	119.90
34	2	534	G	N1-C6-O6	10.41	126.15	119.90
34	2	500	G	N1-C6-O6	10.41	126.14	119.90
34	2	932	G	N1-C6-O6	10.40	126.14	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1171	G	O3'-P-O5'	10.40	123.76	104.00
34	2	1331	G	N1-C6-O6	10.40	126.14	119.90
34	2	1744	G	N1-C6-O6	10.40	126.14	119.90
34	2	400	G	N1-C6-O6	10.39	126.13	119.90
43	y	245	LEU	C-N-CA	-10.38	95.74	121.70
34	2	1545	G	N1-C6-O6	10.37	126.12	119.90
34	2	1162	G	N1-C6-O6	10.37	126.12	119.90
34	2	1565	G	N1-C6-O6	10.36	126.12	119.90
34	2	92	A	N1-C6-N6	10.35	124.81	118.60
34	2	210	G	N1-C6-O6	10.35	126.11	119.90
34	2	669	A	N1-C6-N6	10.34	124.81	118.60
34	2	1334	G	N1-C6-O6	10.34	126.11	119.90
34	2	1454	G	N1-C6-O6	10.34	126.11	119.90
34	2	41	G	N1-C6-O6	10.34	126.10	119.90
34	2	1348	G	N1-C6-O6	10.34	126.11	119.90
34	2	1823	G	N1-C6-O6	10.34	126.11	119.90
34	2	945	G	N1-C6-O6	10.33	126.10	119.90
34	2	596	G	N1-C6-O6	10.33	126.10	119.90
34	2	1223	G	N1-C6-O6	10.32	126.09	119.90
34	2	1841	G	N1-C6-O6	10.32	126.09	119.90
34	2	1849	G	N1-C6-O6	10.32	126.09	119.90
34	2	670	G	N1-C6-O6	10.31	126.09	119.90
34	2	1100	G	N1-C6-O6	10.31	126.09	119.90
34	2	1046	A	N1-C6-N6	10.30	124.78	118.60
34	2	1208	G	N1-C6-O6	10.30	126.08	119.90
34	2	1361	G	N1-C6-O6	10.30	126.08	119.90
34	2	1794	A	N1-C6-N6	10.30	124.78	118.60
34	2	1781	G	N1-C6-O6	10.30	126.08	119.90
34	2	1605	G	C5-C6-O6	-10.29	122.42	128.60
34	2	1511	G	N1-C6-O6	10.29	126.07	119.90
34	2	1286	G	N1-C6-O6	10.28	126.07	119.90
34	2	323	G	N1-C6-O6	10.27	126.06	119.90
34	2	1324	G	N1-C6-O6	10.27	126.06	119.90
34	2	461	G	N1-C6-O6	10.26	126.06	119.90
34	2	1810	G	N1-C6-O6	10.26	126.05	119.90
34	2	1347	G	N1-C6-O6	10.25	126.05	119.90
34	2	1602	A	N1-C6-N6	10.25	124.75	118.60
34	2	1510	G	N1-C6-O6	10.24	126.05	119.90
34	2	553	G	C5-C6-O6	-10.23	122.46	128.60
34	2	204	G	C5-C6-O6	-10.23	122.46	128.60
34	2	95	G	N1-C6-O6	10.23	126.04	119.90
34	2	920	G	N1-C6-O6	10.23	126.04	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1487	G	N1-C6-O6	10.21	126.03	119.90
34	2	931	G	N1-C6-O6	10.21	126.02	119.90
34	2	123	G	N1-C6-O6	10.20	126.02	119.90
34	2	1519	G	N1-C6-O6	10.20	126.02	119.90
38	k	493	ASP	C-N-CA	-10.19	96.22	121.70
34	2	916	A	N1-C6-N6	10.19	124.72	118.60
34	2	1754	G	N1-C6-O6	10.19	126.01	119.90
34	2	1477	G	N1-C6-O6	10.19	126.01	119.90
34	2	1790	G	N1-C6-O6	10.19	126.01	119.90
34	2	536	G	N1-C6-O6	10.18	126.01	119.90
34	2	1666	G	N1-C6-O6	10.17	126.00	119.90
34	2	524	G	N1-C6-O6	10.17	126.00	119.90
34	2	634	G	N1-C6-O6	10.17	126.00	119.90
34	2	403	G	N1-C6-O6	10.16	125.99	119.90
34	2	1629	A	N1-C6-N6	10.16	124.69	118.60
34	2	190	A	N1-C6-N6	10.15	124.69	118.60
34	2	870	G	N1-C6-O6	10.14	125.99	119.90
34	2	978	G	N1-C6-O6	10.14	125.99	119.90
34	2	1607	G	N1-C6-O6	10.14	125.99	119.90
34	2	1164	G	N1-C6-O6	10.14	125.98	119.90
34	2	1851	G	N1-C6-O6	10.14	125.98	119.90
34	2	822	A	N1-C6-N6	10.13	124.68	118.60
34	2	1037	G	N1-C6-O6	10.13	125.98	119.90
34	2	1606	G	N1-C6-O6	10.14	125.98	119.90
34	2	828	G	N1-C6-O6	10.13	125.98	119.90
34	2	1180	G	N1-C6-O6	10.12	125.97	119.90
34	2	1771	G	N1-C6-O6	10.12	125.97	119.90
34	2	1558	G	N1-C6-O6	10.12	125.97	119.90
34	2	300	G	C5-C6-O6	-10.11	122.53	128.60
34	2	457	G	N1-C6-O6	10.11	125.97	119.90
38	k	348	TYR	CA-C-N	10.11	139.44	117.20
34	2	591	G	N1-C6-O6	10.10	125.96	119.90
34	2	394	G	N1-C6-O6	10.10	125.96	119.90
34	2	1445	G	N1-C6-O6	10.09	125.95	119.90
34	2	23	G	N1-C6-O6	10.09	125.95	119.90
34	2	1837	G	N1-C6-O6	10.08	125.95	119.90
34	2	1265	G	N1-C6-O6	10.08	125.95	119.90
34	2	1067	G	N1-C6-O6	10.07	125.94	119.90
34	2	613	G	N1-C6-O6	10.07	125.94	119.90
34	2	1136	G	N1-C6-O6	10.07	125.94	119.90
34	2	815	G	N1-C6-O6	10.07	125.94	119.90
34	2	1786	G	N1-C6-O6	10.07	125.94	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	208	G	C5-C6-O6	-10.06	122.56	128.60
34	2	385	G	N1-C6-O6	10.05	125.93	119.90
34	2	274	G	N1-C6-O6	10.04	125.93	119.90
34	2	319	G	N1-C6-O6	10.04	125.92	119.90
34	2	1785	A	N1-C6-N6	10.04	124.62	118.60
34	2	1840	G	N1-C6-O6	10.04	125.92	119.90
34	2	1506	G	N1-C6-O6	10.03	125.92	119.90
34	2	1722	G	N1-C6-O6	10.04	125.92	119.90
34	2	212	G	N1-C6-O6	10.03	125.92	119.90
34	2	66	G	N1-C6-O6	10.01	125.91	119.90
34	2	555	G	N1-C6-O6	10.01	125.91	119.90
34	2	948	G	N1-C6-O6	10.01	125.91	119.90
34	2	1509	G	N1-C6-O6	10.01	125.91	119.90
34	2	325	G	N1-C6-O6	10.00	125.90	119.90
34	2	649	G	N1-C6-O6	10.00	125.90	119.90
34	2	1001	G	N1-C6-O6	9.99	125.90	119.90
34	2	542	G	C5-C6-O6	-9.99	122.61	128.60
34	2	1855	G	N1-C6-O6	9.99	125.89	119.90
34	2	1566	G	N1-C6-O6	9.97	125.88	119.90
34	2	393	G	N1-C6-O6	9.96	125.87	119.90
34	2	1718	G	N1-C6-O6	9.96	125.87	119.90
34	2	146	G	C5-C6-O6	-9.95	122.63	128.60
34	2	1036	G	N1-C6-O6	9.95	125.87	119.90
34	2	1092	G	N1-C6-O6	9.95	125.87	119.90
34	2	1229	G	N1-C6-O6	9.95	125.87	119.90
1	1	53	G	C5-C6-O6	-9.95	122.63	128.60
34	2	600	G	N1-C6-O6	9.94	125.86	119.90
34	2	1314	G	N1-C6-O6	9.94	125.87	119.90
34	2	1093	G	N1-C6-O6	9.94	125.86	119.90
34	2	468	G	N1-C6-O6	9.93	125.86	119.90
34	2	289	G	N1-C6-O6	9.92	125.85	119.90
34	2	1452	G	N1-C6-O6	9.92	125.85	119.90
34	2	1220	G	N1-C6-O6	9.92	125.85	119.90
34	2	903	G	N1-C6-O6	9.92	125.85	119.90
34	2	972	G	N1-C6-O6	9.91	125.85	119.90
34	2	6	G	N1-C6-O6	9.91	125.85	119.90
1	1	29	G	N1-C6-O6	9.91	125.85	119.90
34	2	1050	G	N1-C6-O6	9.91	125.85	119.90
34	2	1752	G	C5-C6-O6	-9.91	122.65	128.60
34	2	122	G	N1-C6-O6	9.90	125.84	119.90
34	2	1207	G	N1-C6-O6	9.90	125.84	119.90
34	2	1664	G	N1-C6-O6	9.89	125.83	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	345	G	N1-C6-O6	9.86	125.82	119.90
34	2	827	G	N1-C6-O6	9.86	125.82	119.90
1	1	22	G	N1-C6-O6	9.86	125.82	119.90
34	2	1323	G	N1-C6-O6	9.86	125.82	119.90
34	2	201	G	C5-C6-O6	-9.86	122.69	128.60
34	2	601	G	N1-C6-O6	9.85	125.81	119.90
34	2	1443	G	N1-C6-O6	9.84	125.81	119.90
34	2	307	G	N1-C6-O6	9.84	125.80	119.90
1	1	3	G	C5-C6-O6	-9.84	122.70	128.60
34	2	1316	G	N1-C6-O6	9.84	125.80	119.90
34	2	1778	G	C5-C6-O6	-9.84	122.70	128.60
34	2	1101	G	N1-C6-O6	9.83	125.80	119.90
34	2	274	G	C5-C6-O6	-9.83	122.70	128.60
34	2	1320	G	N1-C6-O6	9.83	125.80	119.90
34	2	625	G	N1-C6-O6	9.81	125.79	119.90
34	2	1584	A	N1-C6-N6	9.81	124.48	118.60
34	2	1571	G	N1-C6-O6	9.80	125.78	119.90
34	2	1649	G	N1-C6-O6	9.80	125.78	119.90
34	2	411	G	N1-C6-O6	9.80	125.78	119.90
34	2	1572	G	N1-C6-O6	9.80	125.78	119.90
34	2	803	G	N1-C6-O6	9.80	125.78	119.90
34	2	47	G	N1-C6-O6	9.79	125.77	119.90
34	2	1025	G	N1-C6-O6	9.79	125.77	119.90
34	2	919	G	N1-C6-O6	9.78	125.77	119.90
34	2	1675	G	N1-C6-O6	9.79	125.77	119.90
34	2	1006	G	N1-C6-O6	9.78	125.77	119.90
34	2	1568	G	N1-C6-O6	9.78	125.77	119.90
34	2	1615	A	N1-C6-N6	9.78	124.47	118.60
34	2	1669	G	N1-C6-O6	9.77	125.76	119.90
34	2	1341	G	N1-C6-O6	9.77	125.76	119.90
34	2	303	G	N1-C6-O6	9.76	125.76	119.90
1	1	11	G	N1-C6-O6	9.76	125.76	119.90
34	2	981	G	N1-C6-O6	9.76	125.75	119.90
34	2	1122	G	N1-C6-O6	9.75	125.75	119.90
34	2	1653	G	N1-C6-O6	9.75	125.75	119.90
34	2	1072	G	N1-C6-O6	9.74	125.75	119.90
34	2	464	G	N1-C6-O6	9.74	125.74	119.90
34	2	943	G	N1-C6-O6	9.74	125.74	119.90
34	2	1232	G	N1-C6-O6	9.73	125.74	119.90
34	2	855	G	N1-C6-O6	9.73	125.74	119.90
34	2	1561	G	N1-C6-O6	9.73	125.74	119.90
34	2	636	G	N1-C6-O6	9.73	125.74	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1130	G	N1-C6-O6	9.73	125.74	119.90
34	2	156	G	C5-C6-O6	-9.73	122.76	128.60
34	2	409	G	N1-C6-O6	9.72	125.73	119.90
34	2	898	G	N1-C6-O6	9.72	125.73	119.90
34	2	974	G	N1-C6-O6	9.72	125.73	119.90
34	2	434	G	N1-C6-O6	9.71	125.73	119.90
34	2	1125	G	N1-C6-O6	9.71	125.73	119.90
34	2	56	G	N1-C6-O6	9.69	125.71	119.90
34	2	1137	G	C5-C6-O6	-9.69	122.79	128.60
34	2	1774	G	C5-C6-O6	-9.68	122.79	128.60
34	2	1047	G	N1-C6-O6	9.68	125.71	119.90
1	1	52	G	N1-C6-O6	9.68	125.71	119.90
34	2	149	A	N1-C6-N6	9.68	124.41	118.60
34	2	1362	G	N1-C6-O6	9.67	125.70	119.90
34	2	1033	G	N1-C6-O6	9.67	125.70	119.90
34	2	856	G	N1-C6-O6	9.66	125.70	119.90
34	2	1416	G	N1-C6-O6	9.66	125.70	119.90
34	2	1446	G	N1-C6-O6	9.66	125.70	119.90
1	1	57	G	N1-C6-O6	9.66	125.69	119.90
34	2	460	G	N1-C6-O6	9.65	125.69	119.90
34	2	890	G	N1-C6-O6	9.65	125.69	119.90
34	2	897	G	N1-C6-O6	9.64	125.69	119.90
34	2	1462	G	N1-C6-O6	9.64	125.69	119.90
34	2	1599	G	N1-C6-O6	9.64	125.69	119.90
34	2	952	G	N1-C6-O6	9.64	125.68	119.90
34	2	1748	G	C5-C6-O6	-9.64	122.82	128.60
34	2	427	G	N1-C6-O6	9.63	125.68	119.90
34	2	1218	G	N1-C6-O6	9.63	125.68	119.90
34	2	1183	G	N1-C6-O6	9.63	125.68	119.90
34	2	271	G	N1-C6-O6	9.62	125.67	119.90
34	2	906	G	N1-C6-O6	9.61	125.67	119.90
34	2	1645	A	N1-C6-N6	9.61	124.36	118.60
1	1	70	G	C5-C6-O6	-9.59	122.84	128.60
34	2	1753	G	C5-C6-O6	-9.59	122.85	128.60
34	2	1727	G	N1-C6-O6	9.58	125.65	119.90
34	2	891	G	N1-C6-O6	9.58	125.65	119.90
34	2	1608	G	N1-C6-O6	9.57	125.64	119.90
34	2	1225	G	N1-C6-O6	9.57	125.64	119.90
34	2	499	G	N1-C6-O6	9.57	125.64	119.90
34	2	1085	G	N1-C6-O6	9.57	125.64	119.90
34	2	1721	G	N1-C6-O6	9.57	125.64	119.90
34	2	113	G	N1-C6-O6	9.56	125.64	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1697	G	N1-C6-O6	9.56	125.64	119.90
34	2	1776	G	C5-C6-O6	-9.56	122.86	128.60
34	2	360	G	N1-C6-O6	9.56	125.63	119.90
34	2	337	G	C5-C6-O6	-9.55	122.87	128.60
34	2	971	G	N1-C6-O6	9.54	125.63	119.90
34	2	1321	G	N1-C6-O6	9.54	125.62	119.90
1	1	30	G	N1-C6-O6	9.53	125.62	119.90
34	2	1523	G	N1-C6-O6	9.52	125.61	119.90
1	1	18	G	O4'-C1'-N9	9.52	115.82	108.20
1	1	43	G	C5-C6-O6	-9.52	122.89	128.60
34	2	20	G	N1-C6-O6	9.51	125.61	119.90
34	2	1098	G	N1-C6-O6	9.51	125.61	119.90
34	2	1475	G	N1-C6-O6	9.51	125.61	119.90
34	2	1163	G	N1-C6-O6	9.51	125.60	119.90
34	2	186	G	C5-C6-O6	-9.50	122.90	128.60
34	2	1789	G	N1-C6-O6	9.50	125.60	119.90
38	k	510	HIS	O-C-N	-9.50	107.50	122.70
34	2	495	G	N1-C6-O6	9.50	125.60	119.90
34	2	587	G	N1-C6-O6	9.50	125.60	119.90
34	2	29	G	C5-C6-O6	-9.49	122.91	128.60
34	2	1570	G	N1-C6-O6	9.48	125.59	119.90
34	2	1231	G	N1-C6-O6	9.48	125.59	119.90
34	2	1394	G	N1-C6-O6	9.48	125.59	119.90
34	2	395	G	N1-C6-O6	9.48	125.59	119.90
34	2	1633	G	N1-C6-O6	9.47	125.58	119.90
34	2	456	G	N1-C6-O6	9.47	125.58	119.90
34	2	590	G	N1-C6-O6	9.47	125.58	119.90
34	2	930	G	N1-C6-O6	9.47	125.58	119.90
34	2	1535	G	N1-C6-O6	9.47	125.58	119.90
34	2	1598	G	N1-C6-O6	9.46	125.58	119.90
34	2	1770	G	C5-C6-O6	-9.46	122.92	128.60
34	2	367	G	N1-C6-O6	9.46	125.57	119.90
34	2	1471	G	N1-C6-O6	9.45	125.57	119.90
34	2	887	G	C5-C6-O6	-9.45	122.93	128.60
34	2	1521	G	N1-C6-O6	9.45	125.57	119.90
1	1	8	G	N1-C6-O6	9.44	125.56	119.90
34	2	375	G	N1-C6-O6	9.43	125.56	119.90
34	2	1309	A	N1-C6-N6	9.43	124.26	118.60
38	k	268	TYR	O-C-N	-9.43	107.61	122.70
34	2	1241	G	N1-C6-O6	9.43	125.56	119.90
34	2	320	G	C5-C6-O6	-9.42	122.95	128.60
38	k	150	SER	CA-C-N	-9.42	96.48	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	508	G	N1-C6-O6	9.41	125.55	119.90
34	2	1455	G	C5-C6-O6	-9.41	122.95	128.60
34	2	1811	G	N1-C6-O6	9.41	125.55	119.90
34	2	62	G	C5-C6-O6	-9.41	122.95	128.60
34	2	1427	G	N1-C6-O6	9.41	125.54	119.90
34	2	421	G	C5-C6-O6	-9.40	122.96	128.60
34	2	1486	G	N1-C6-O6	9.40	125.54	119.90
34	2	145	G	N1-C6-O6	9.39	125.53	119.90
34	2	1852	G	N1-C6-O6	9.38	125.53	119.90
38	k	272	VAL	CA-C-N	-9.38	96.56	117.20
34	2	1277	G	N1-C6-O6	9.38	125.53	119.90
34	2	430	G	N1-C6-O6	9.38	125.53	119.90
34	2	1418	G	N1-C6-O6	9.38	125.53	119.90
34	2	1830	G	N1-C6-O6	9.37	125.52	119.90
34	2	1206	G	N1-C6-O6	9.37	125.52	119.90
34	2	1290	G	N1-C6-O6	9.36	125.52	119.90
1	1	16	G	N1-C6-O6	9.36	125.52	119.90
34	2	938	G	N1-C6-O6	9.36	125.52	119.90
34	2	108	G	N1-C6-O6	9.35	125.51	119.90
34	2	183	G	N1-C6-O6	9.35	125.51	119.90
34	2	422	G	N1-C6-O6	9.35	125.51	119.90
34	2	1579	G	N1-C6-O6	9.34	125.51	119.90
34	2	1744	G	C5-C6-O6	-9.33	123.00	128.60
34	2	494	G	N1-C6-O6	9.33	125.50	119.90
34	2	995	G	C5-C6-O6	-9.32	123.01	128.60
34	2	813	G	N1-C6-O6	9.32	125.49	119.90
34	2	351	U	OP1-P-O3'	-9.31	84.71	105.20
34	2	1308	G	N1-C6-O6	9.31	125.49	119.90
34	2	1565	G	C5-C6-O6	-9.31	123.01	128.60
34	2	579	G	C5-C6-O6	-9.30	123.02	128.60
34	2	1147	G	N1-C6-O6	9.30	125.48	119.90
34	2	80	G	C5-C6-O6	-9.30	123.02	128.60
34	2	534	G	C5-C6-O6	-9.29	123.02	128.60
34	2	1536	G	N1-C6-O6	9.29	125.47	119.90
34	2	1841	G	C5-C6-O6	-9.29	123.03	128.60
34	2	1531	G	N1-C6-O6	9.27	125.46	119.90
34	2	1593	G	N1-C6-O6	9.27	125.46	119.90
1	1	13	G	N1-C6-O6	9.26	125.45	119.90
34	2	279	G	C5-C6-O6	-9.25	123.05	128.60
34	2	1126	G	N1-C6-O6	9.25	125.45	119.90
34	2	503	G	N1-C6-O6	9.24	125.44	119.90
34	2	1172	G	N1-C6-O6	9.24	125.44	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	155	G	N1-C6-O6	9.22	125.43	119.90
34	2	1294	G	N1-C6-O6	9.22	125.43	119.90
34	2	1160	G	C5-C6-O6	-9.21	123.07	128.60
34	2	7	G	C5-C6-O6	-9.21	123.07	128.60
34	2	1371	G	C5-C6-O6	-9.21	123.07	128.60
37	j	82	ARG	NE-CZ-NH1	9.20	124.90	120.30
34	2	1061	G	C5-C6-O6	-9.20	123.08	128.60
34	2	1671	U	P-O3'-C3'	9.20	130.74	119.70
34	2	498	A	N1-C6-N6	9.19	124.11	118.60
34	2	1416	G	C5-C6-O6	-9.19	123.09	128.60
34	2	496	G	N1-C6-O6	9.18	125.41	119.90
34	2	1010	G	N1-C6-O6	9.18	125.41	119.90
34	2	199	G	N1-C6-O6	9.18	125.41	119.90
34	2	426	G	N1-C6-O6	9.18	125.41	119.90
34	2	1781	G	C5-C6-O6	-9.17	123.10	128.60
34	2	1044	G	N1-C6-O6	9.17	125.40	119.90
34	2	1631	G	N1-C6-O6	9.16	125.40	119.90
34	2	1447	G	N1-C6-O6	9.16	125.40	119.90
34	2	578	G	N1-C6-O6	9.16	125.39	119.90
34	2	1171	G	N1-C6-O6	9.15	125.39	119.90
34	2	401	G	C5-C6-O6	-9.13	123.12	128.60
34	2	385	G	C5-C6-O6	-9.12	123.13	128.60
34	2	500	G	C5-C6-O6	-9.12	123.13	128.60
34	2	989	G	N1-C6-O6	9.12	125.38	119.90
34	2	604	G	N1-C6-O6	9.12	125.37	119.90
34	2	1681	G	N1-C6-O6	9.12	125.37	119.90
34	2	1192	A	N1-C6-N6	9.12	124.07	118.60
34	2	400	G	C5-C6-O6	-9.12	123.13	128.60
34	2	663	G	C5-C6-O6	-9.11	123.13	128.60
34	2	1251	G	N1-C6-O6	9.11	125.36	119.90
34	2	238	G	N1-C6-O6	9.11	125.36	119.90
34	2	237	G	C5-C6-O6	-9.10	123.14	128.60
34	2	212	G	C5-C6-O6	-9.09	123.14	128.60
34	2	1271	G	N1-C6-O6	9.09	125.35	119.90
34	2	1731	G	C5-C6-O6	-9.08	123.15	128.60
34	2	350	A	O3'-P-O5'	-9.07	86.76	104.00
34	2	555	G	C5-C6-O6	-9.07	123.16	128.60
34	2	588	G	N1-C6-O6	9.07	125.34	119.90
34	2	592	G	N1-C6-O6	9.07	125.34	119.90
34	2	1064	G	N1-C6-O6	9.07	125.34	119.90
34	2	655	G	N1-C6-O6	9.06	125.34	119.90
34	2	1344	G	N1-C6-O6	9.06	125.34	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	167	G	C5-C6-O6	-9.06	123.17	128.60
34	2	955	G	N1-C6-O6	9.05	125.33	119.90
34	2	1383	G	N1-C6-O6	9.05	125.33	119.90
34	2	1100	G	C5-C6-O6	-9.04	123.18	128.60
34	2	967	G	N1-C6-O6	9.04	125.32	119.90
34	2	1651	G	C5-C6-O6	-9.04	123.18	128.60
34	2	1030	A	N1-C6-N6	9.03	124.02	118.60
34	2	945	G	C5-C6-O6	-9.03	123.18	128.60
34	2	441	G	N1-C6-O6	9.02	125.31	119.90
34	2	1040	G	N1-C6-O6	9.02	125.31	119.90
34	2	1454	G	C5-C6-O6	-9.01	123.19	128.60
34	2	1751	G	N1-C6-O6	9.01	125.31	119.90
34	2	114	G	N1-C6-O6	9.01	125.30	119.90
34	2	1425	G	N1-C6-O6	9.01	125.30	119.90
34	2	1222	G	N1-C6-O6	9.00	125.30	119.90
34	2	1634	G	N1-C6-O6	9.00	125.30	119.90
34	2	1199	G	N1-C6-O6	8.99	125.30	119.90
34	2	1647	G	N1-C6-O6	8.99	125.30	119.90
34	2	457	G	C5-C6-O6	-8.99	123.21	128.60
34	2	966	G	N1-C6-O6	8.99	125.30	119.90
34	2	874	G	N1-C6-O6	8.99	125.29	119.90
34	2	123	G	C5-C6-O6	-8.98	123.21	128.60
34	2	1469	G	N1-C6-O6	8.98	125.29	119.90
34	2	824	G	N1-C6-O6	8.98	125.29	119.90
34	2	1519	G	C5-C6-O6	-8.98	123.21	128.60
34	2	1055	G	N1-C6-O6	8.97	125.28	119.90
34	2	1136	G	C5-C6-O6	-8.97	123.22	128.60
34	2	403	G	C5-C6-O6	-8.97	123.22	128.60
34	2	1515	G	C5-C6-O6	-8.97	123.22	128.60
34	2	932	G	C5-C6-O6	-8.96	123.22	128.60
34	2	153	G	N1-C6-O6	8.96	125.28	119.90
34	2	1402	G	N1-C6-O6	8.96	125.28	119.90
34	2	928	G	N1-C6-O6	8.95	125.27	119.90
34	2	1717	G	C5-C6-O6	-8.95	123.23	128.60
34	2	828	G	C5-C6-O6	-8.95	123.23	128.60
34	2	273	G	N1-C6-O6	8.94	125.26	119.90
34	2	1334	G	C5-C6-O6	-8.93	123.24	128.60
35	A	184	LEU	C-N-CA	8.93	144.03	121.70
34	2	925	G	N1-C6-O6	8.93	125.25	119.90
34	2	1193	G	N1-C6-O6	8.93	125.25	119.90
34	2	41	G	C5-C6-O6	-8.92	123.25	128.60
34	2	817	G	N1-C6-O6	8.91	125.25	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	607	G	C5-C6-O6	-8.91	123.25	128.60
34	2	1612	G	N1-C6-O6	8.91	125.24	119.90
34	2	1512	G	N1-C6-O6	8.90	125.24	119.90
34	2	1607	G	C5-C6-O6	-8.90	123.26	128.60
34	2	842	G	N1-C6-O6	8.90	125.24	119.90
34	2	1229	G	C5-C6-O6	-8.90	123.26	128.60
34	2	634	G	C5-C6-O6	-8.89	123.27	128.60
34	2	1786	G	C5-C6-O6	-8.89	123.27	128.60
34	2	982	G	N1-C6-O6	8.89	125.23	119.90
34	2	310	G	C5-C6-O6	-8.88	123.27	128.60
34	2	472	G	N1-C6-O6	8.88	125.23	119.90
34	2	1208	G	C5-C6-O6	-8.88	123.27	128.60
34	2	1773	G	N1-C6-O6	8.88	125.23	119.90
34	2	576	G	N1-C6-O6	8.87	125.22	119.90
34	2	827	G	C5-C6-O6	-8.87	123.28	128.60
34	2	646	G	N1-C6-O6	8.87	125.22	119.90
34	2	16	G	N1-C6-O6	8.86	125.22	119.90
34	2	126	G	N1-C6-O6	8.86	125.22	119.90
34	2	954	G	N1-C6-O6	8.86	125.22	119.90
34	2	1754	G	C5-C6-O6	-8.86	123.28	128.60
34	2	1155	G	N1-C6-O6	8.86	125.21	119.90
34	2	88	G	C5-C6-O6	-8.85	123.29	128.60
34	2	270	G	N1-C6-O6	8.85	125.21	119.90
34	2	1739	G	N1-C6-O6	8.85	125.21	119.90
34	2	322	G	N1-C6-O6	8.84	125.21	119.90
34	2	1324	G	C5-C6-O6	-8.84	123.29	128.60
34	2	1361	G	C5-C6-O6	-8.84	123.29	128.60
34	2	987	G	N1-C6-O6	8.84	125.20	119.90
34	2	424	G	N1-C6-O6	8.84	125.20	119.90
34	2	903	G	C5-C6-O6	-8.84	123.30	128.60
34	2	1286	G	C5-C6-O6	-8.84	123.30	128.60
1	1	16	G	OP2-P-O3'	-8.83	85.78	105.20
38	k	241	ASP	CA-C-N	-8.83	97.78	117.20
34	2	837	G	N1-C6-O6	8.82	125.19	119.90
34	2	222	G	N1-C6-O6	8.82	125.19	119.90
34	2	1627	G	N1-C6-O6	8.82	125.19	119.90
34	2	1729	G	N1-C6-O6	8.82	125.19	119.90
34	2	1820	G	C5-C6-O6	-8.82	123.31	128.60
34	2	1424	G	C5-C6-O6	-8.82	123.31	128.60
34	2	1082	G	N1-C6-O6	8.82	125.19	119.90
34	2	1281	G	N1-C6-O6	8.82	125.19	119.90
34	2	319	G	C5-C6-O6	-8.81	123.31	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1194	G	N1-C6-O6	8.81	125.19	119.90
36	B	288	LYS	C-N-CA	8.81	140.81	122.30
34	2	1127	G	N1-C6-O6	8.81	125.19	119.90
34	2	1831	G	N1-C6-O6	8.81	125.18	119.90
34	2	75	G	N1-C6-O6	8.80	125.18	119.90
34	2	1037	G	C5-C6-O6	-8.81	123.32	128.60
34	2	341	G	N1-C6-O6	8.80	125.18	119.90
34	2	1732	G	C5-C6-O6	-8.80	123.32	128.60
34	2	177	G	N1-C6-O6	8.80	125.18	119.90
34	2	323	G	C5-C6-O6	-8.80	123.32	128.60
34	2	613	G	C5-C6-O6	-8.79	123.33	128.60
34	2	1381	G	N1-C6-O6	8.79	125.17	119.90
34	2	1606	G	C5-C6-O6	-8.79	123.33	128.60
1	1	24	G	N1-C6-O6	8.78	125.17	119.90
34	2	1649	G	C5-C6-O6	-8.78	123.33	128.60
34	2	1510	G	C5-C6-O6	-8.78	123.33	128.60
34	2	1771	G	C5-C6-O6	-8.77	123.34	128.60
34	2	1154	G	N1-C6-O6	8.77	125.16	119.90
34	2	1217	G	N1-C6-O6	8.76	125.16	119.90
34	2	187	C	O4'-C1'-N1	8.76	115.21	108.20
1	1	46	G	N1-C6-O6	8.76	125.16	119.90
34	2	536	G	C5-C6-O6	-8.76	123.34	128.60
34	2	1345	G	N1-C6-O6	8.76	125.16	119.90
34	2	864	G	N1-C6-O6	8.76	125.15	119.90
34	2	1318	G	N1-C6-O6	8.76	125.15	119.90
34	2	1547	G	N1-C6-O6	8.76	125.15	119.90
34	2	1566	G	C5-C6-O6	-8.75	123.35	128.60
34	2	373	G	N1-C6-O6	8.75	125.15	119.90
34	2	497	G	N1-C6-O6	8.75	125.15	119.90
34	2	863	G	N1-C6-O6	8.75	125.15	119.90
34	2	1390	G	N1-C6-O6	8.74	125.15	119.90
34	2	1487	G	C5-C6-O6	-8.74	123.35	128.60
34	2	1562	G	N1-C6-O6	8.74	125.14	119.90
34	2	1029	G	N1-C6-O6	8.74	125.14	119.90
34	2	1317	G	N1-C6-O6	8.73	125.14	119.90
34	2	1409	G	N1-C6-O6	8.73	125.14	119.90
34	2	1601	G	N1-C6-O6	8.73	125.14	119.90
34	2	467	G	N1-C6-O6	8.73	125.14	119.90
34	2	877	G	N1-C6-O6	8.73	125.14	119.90
34	2	1493	G	N1-C6-O6	8.73	125.14	119.90
34	2	870	G	C5-C6-O6	-8.73	123.36	128.60
34	2	298	G	N1-C6-O6	8.72	125.13	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1377	G	N1-C6-O6	8.72	125.13	119.90
34	2	1175	G	N1-C6-O6	8.72	125.13	119.90
34	2	71	G	N1-C6-O6	8.71	125.13	119.90
34	2	184	G	N1-C6-O6	8.71	125.13	119.90
34	2	1701	G	C5-C6-O6	-8.71	123.37	128.60
34	2	1153	G	N1-C6-O6	8.70	125.12	119.90
34	2	1808	G	N1-C6-O6	8.70	125.12	119.90
34	2	1276	G	N1-C6-O6	8.70	125.12	119.90
34	2	1001	G	C5-C6-O6	-8.70	123.38	128.60
34	2	205	G	N1-C6-O6	8.69	125.11	119.90
34	2	1326	G	N1-C6-O6	8.69	125.11	119.90
34	2	1793	G	N1-C6-O6	8.69	125.11	119.90
34	2	1743	G	C5-C6-O6	-8.69	123.39	128.60
34	2	47	G	C5-C6-O6	-8.69	123.39	128.60
34	2	924	G	N1-C6-O6	8.69	125.11	119.90
34	2	1125	G	C5-C6-O6	-8.69	123.39	128.60
34	2	1783	G	N1-C6-O6	8.68	125.11	119.90
34	2	1203	G	N1-C6-O6	8.68	125.11	119.90
34	2	1509	G	C5-C6-O6	-8.68	123.39	128.60
34	2	815	G	C5-C6-O6	-8.67	123.40	128.60
34	2	470	G	N1-C6-O6	8.66	125.10	119.90
34	2	543	U	O4'-C1'-N1	8.66	115.13	108.20
34	2	591	G	C5-C6-O6	-8.66	123.40	128.60
34	2	74	G	N1-C6-O6	8.66	125.10	119.90
34	2	667	G	N1-C6-O6	8.66	125.10	119.90
34	2	1572	G	C5-C6-O6	-8.66	123.40	128.60
34	2	921	G	N1-C6-O6	8.65	125.09	119.90
34	2	1138	G	N1-C6-O6	8.65	125.09	119.90
34	2	1704	G	N1-C6-O6	8.64	125.09	119.90
34	2	991	G	N1-C6-O6	8.64	125.08	119.90
34	2	442	G	N1-C6-O6	8.64	125.08	119.90
34	2	1164	G	C5-C6-O6	-8.64	123.42	128.60
34	2	1095	G	N1-C6-O6	8.63	125.08	119.90
34	2	1851	G	C5-C6-O6	-8.63	123.42	128.60
34	2	1619	U	O4'-C1'-N1	8.63	115.10	108.20
34	2	6	G	C5-C6-O6	-8.62	123.43	128.60
34	2	94	G	N1-C6-O6	8.62	125.07	119.90
34	2	1191	A	N1-C6-N6	8.62	123.77	118.60
34	2	1477	G	C5-C6-O6	-8.62	123.43	128.60
34	2	370	G	N1-C6-O6	8.62	125.07	119.90
34	2	1503	G	N1-C6-O6	8.62	125.07	119.90
34	2	394	G	C5-C6-O6	-8.61	123.43	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	397	G	N1-C6-O6	8.61	125.07	119.90
34	2	1039	G	N1-C6-O6	8.61	125.07	119.90
34	2	616	G	N1-C6-O6	8.60	125.06	119.90
34	2	841	G	N1-C6-O6	8.60	125.06	119.90
34	2	596	G	C5-C6-O6	-8.60	123.44	128.60
34	2	1389	G	N1-C6-O6	8.60	125.06	119.90
34	2	1738	G	N1-C6-O6	8.59	125.06	119.90
34	2	906	G	C5-C6-O6	-8.59	123.44	128.60
34	2	150	A	N1-C6-N6	8.59	123.75	118.60
34	2	625	G	C5-C6-O6	-8.59	123.45	128.60
34	2	1506	G	C5-C6-O6	-8.59	123.45	128.60
34	2	832	G	N1-C6-O6	8.59	125.05	119.90
34	2	1253	G	N1-C6-O6	8.58	125.05	119.90
34	2	911	G	N1-C6-O6	8.58	125.05	119.90
34	2	1810	G	C5-C6-O6	-8.58	123.45	128.60
34	2	1420	G	N1-C6-O6	8.58	125.05	119.90
34	2	1511	G	C5-C6-O6	-8.57	123.46	128.60
34	2	70	G	N1-C6-O6	8.56	125.04	119.90
34	2	1036	G	C5-C6-O6	-8.56	123.46	128.60
34	2	1545	G	C5-C6-O6	-8.56	123.46	128.60
34	2	410	G	N1-C6-O6	8.56	125.03	119.90
34	2	415	G	N1-C6-O6	8.56	125.03	119.90
1	1	29	G	C5-C6-O6	-8.55	123.47	128.60
34	2	289	G	C5-C6-O6	-8.55	123.47	128.60
34	2	957	G	N1-C6-O6	8.55	125.03	119.90
34	2	1165	G	N1-C6-O6	8.55	125.03	119.90
34	2	1457	G	N1-C6-O6	8.55	125.03	119.90
34	2	1722	G	C5-C6-O6	-8.54	123.47	128.60
1	1	26	G	N1-C6-O6	8.54	125.02	119.90
34	2	972	G	C5-C6-O6	-8.54	123.48	128.60
38	k	513	LYS	C-N-CA	8.54	143.04	121.70
34	2	436	G	N1-C6-O6	8.53	125.02	119.90
34	2	943	G	C5-C6-O6	-8.53	123.48	128.60
34	2	1282	G	N1-C6-O6	8.53	125.02	119.90
34	2	1655	C	C2-N1-C1'	8.53	128.19	118.80
34	2	931	G	C5-C6-O6	-8.53	123.48	128.60
34	2	929	G	N1-C6-O6	8.53	125.02	119.90
34	2	1765	G	N1-C6-O6	8.53	125.02	119.90
1	1	17	C	P-O3'-C3'	8.52	129.93	119.70
34	2	375	G	C5-C6-O6	-8.52	123.49	128.60
34	2	402	G	N1-C6-O6	8.52	125.01	119.90
34	2	1360	U	O4'-C1'-N1	8.51	115.01	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	674	G	N1-C6-O6	8.51	125.01	119.90
34	2	1202	G	C5-C6-O6	-8.51	123.50	128.60
34	2	328	G	N1-C6-O6	8.50	125.00	119.90
34	2	673	G	N1-C6-O6	8.50	125.00	119.90
34	2	615	G	N1-C6-O6	8.50	125.00	119.90
34	2	1167	G	N1-C6-O6	8.49	125.00	119.90
34	2	1504	A	N1-C6-N6	8.49	123.70	118.60
34	2	280	G	N1-C6-O6	8.49	124.99	119.90
34	2	1643	G	N1-C6-O6	8.49	124.99	119.90
34	2	1600	G	N1-C6-O6	8.49	124.99	119.90
34	2	848	G	N1-C6-O6	8.48	124.99	119.90
34	2	1266	G	C5-C6-O6	-8.48	123.51	128.60
34	2	1823	G	C5-C6-O6	-8.48	123.51	128.60
34	2	524	G	C5-C6-O6	-8.48	123.51	128.60
34	2	1790	G	C5-C6-O6	-8.48	123.51	128.60
34	2	1265	G	C5-C6-O6	-8.47	123.52	128.60
34	2	1541	G	N1-C6-O6	8.47	124.98	119.90
34	2	1232	G	C5-C6-O6	-8.47	123.52	128.60
34	2	1047	G	C5-C6-O6	-8.47	123.52	128.60
34	2	307	G	C5-C6-O6	-8.46	123.52	128.60
38	k	241	ASP	O-C-N	8.45	136.22	122.70
34	2	1718	G	C5-C6-O6	-8.45	123.53	128.60
34	2	917	G	N1-C6-O6	8.44	124.96	119.90
34	2	1207	G	C5-C6-O6	-8.44	123.54	128.60
34	2	189	G	N1-C6-O6	8.44	124.96	119.90
34	2	1571	G	C5-C6-O6	-8.44	123.54	128.60
1	1	19	G	N1-C6-O6	8.43	124.96	119.90
34	2	601	G	C5-C6-O6	-8.43	123.54	128.60
34	2	317	G	N1-C6-O6	8.43	124.95	119.90
34	2	1270	G	N1-C6-O6	8.43	124.95	119.90
34	2	52	G	C5-C6-O6	-8.42	123.55	128.60
34	2	325	G	C5-C6-O6	-8.42	123.55	128.60
34	2	1314	G	C5-C6-O6	-8.41	123.55	128.60
45	w	134	TYR	CB-CG-CD2	-8.41	115.95	121.00
34	2	952	G	C5-C6-O6	-8.41	123.55	128.60
34	2	1350	G	N1-C6-O6	8.41	124.95	119.90
34	2	1298	G	N1-C6-O6	8.41	124.95	119.90
34	2	180	G	N1-C6-O6	8.40	124.94	119.90
34	2	345	G	C5-C6-O6	-8.40	123.56	128.60
34	2	387	G	N1-C6-O6	8.40	124.94	119.90
34	2	505	G	N1-C6-O6	8.40	124.94	119.90
34	2	1407	G	N1-C6-O6	8.40	124.94	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1446	G	C5-C6-O6	-8.40	123.56	128.60
34	2	1837	G	C5-C6-O6	-8.40	123.56	128.60
34	2	1652	G	N1-C6-O6	8.39	124.94	119.90
34	2	10	G	N1-C6-O6	8.39	124.94	119.90
34	2	548	G	N1-C6-O6	8.39	124.94	119.90
34	2	549	G	N1-C6-O6	8.39	124.93	119.90
34	2	1452	G	C5-C6-O6	-8.38	123.57	128.60
34	2	427	G	C5-C6-O6	-8.38	123.57	128.60
34	2	1025	G	C5-C6-O6	-8.38	123.57	128.60
34	2	237	G	N1-C6-O6	8.38	124.92	119.90
34	2	537	G	N1-C6-O6	8.38	124.93	119.90
34	2	1088	G	N1-C6-O6	8.38	124.92	119.90
34	2	1252	G	N1-C6-O6	8.37	124.92	119.90
34	2	981	G	C5-C6-O6	-8.36	123.58	128.60
1	1	10	G	N1-C6-O6	8.36	124.92	119.90
34	2	1713	G	N1-C6-O6	8.36	124.92	119.90
34	2	56	G	C5-C6-O6	-8.36	123.59	128.60
34	2	1568	G	C5-C6-O6	-8.35	123.59	128.60
34	2	1006	G	C5-C6-O6	-8.35	123.59	128.60
34	2	1362	G	C5-C6-O6	-8.35	123.59	128.60
34	2	90	G	N1-C6-O6	8.34	124.91	119.90
34	2	282	G	N1-C6-O6	8.34	124.90	119.90
34	2	82	G	N1-C6-O6	8.34	124.90	119.90
34	2	1130	G	C5-C6-O6	-8.34	123.60	128.60
34	2	1443	G	C5-C6-O6	-8.34	123.60	128.60
34	2	851	G	N1-C6-O6	8.33	124.90	119.90
34	2	1093	G	C5-C6-O6	-8.33	123.60	128.60
35	A	184	LEU	O-C-N	8.33	136.03	122.70
34	2	1475	G	C5-C6-O6	-8.33	123.60	128.60
34	2	1414	C	C2-N1-C1'	8.33	127.96	118.80
34	2	1357	G	N1-C6-O6	8.32	124.89	119.90
34	2	803	G	C5-C6-O6	-8.32	123.61	128.60
34	2	1323	G	C5-C6-O6	-8.32	123.61	128.60
34	2	1835	C	O4'-C1'-N1	8.31	114.85	108.20
34	2	1352	G	N1-C6-O6	8.30	124.88	119.90
34	2	33	G	N1-C6-O6	8.29	124.88	119.90
34	2	1166	A	N1-C6-N6	8.29	123.58	118.60
34	2	1231	G	C5-C6-O6	-8.29	123.62	128.60
34	2	1341	G	C5-C6-O6	-8.29	123.62	128.60
34	2	1830	G	C5-C6-O6	-8.29	123.62	128.60
34	2	1445	G	C5-C6-O6	-8.28	123.63	128.60
34	2	1688	G	C5-C6-O6	-8.27	123.64	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1543	G	N1-C6-O6	8.27	124.86	119.90
34	2	1135	C	C2-N1-C1'	8.27	127.89	118.80
34	2	905	G	N1-C6-O6	8.26	124.86	119.90
34	2	670	G	C5-C6-O6	-8.25	123.65	128.60
34	2	898	G	C5-C6-O6	-8.25	123.65	128.60
34	2	428	G	N1-C6-O6	8.24	124.84	119.90
34	2	66	G	C5-C6-O6	-8.24	123.66	128.60
34	2	649	G	C5-C6-O6	-8.24	123.66	128.60
34	2	948	G	C5-C6-O6	-8.23	123.66	128.60
34	2	1119	C	O4'-C1'-N1	8.23	114.78	108.20
34	2	1535	G	C5-C6-O6	-8.23	123.67	128.60
1	1	7	A	O4'-C1'-N9	8.22	114.78	108.20
34	2	468	G	C5-C6-O6	-8.22	123.67	128.60
34	2	122	G	C5-C6-O6	-8.22	123.67	128.60
34	2	1666	G	C5-C6-O6	-8.21	123.67	128.60
1	1	52	G	C5-C6-O6	-8.21	123.67	128.60
34	2	1347	G	C5-C6-O6	-8.21	123.68	128.60
34	2	360	G	C5-C6-O6	-8.21	123.68	128.60
34	2	381	C	O4'-C1'-N1	8.20	114.76	108.20
34	2	384	G	C5-C6-O6	-8.20	123.68	128.60
34	2	1101	G	C5-C6-O6	-8.19	123.69	128.60
34	2	834	G	N1-C6-O6	8.19	124.81	119.90
34	2	1697	G	C5-C6-O6	-8.18	123.69	128.60
1	1	30	G	C5-C6-O6	-8.17	123.70	128.60
34	2	1072	G	C5-C6-O6	-8.17	123.70	128.60
34	2	165	G	N1-C6-O6	8.15	124.79	119.90
34	2	1050	G	C5-C6-O6	-8.15	123.71	128.60
34	2	1582	G	N1-C6-O6	8.14	124.78	119.90
34	2	74	G	O4'-C1'-N9	8.13	114.71	108.20
34	2	879	U	O4'-C1'-N1	8.13	114.70	108.20
34	2	937	C	O4'-C1'-N1	8.13	114.70	108.20
34	2	422	G	C5-C6-O6	-8.13	123.72	128.60
34	2	351	U	O3'-P-O5'	8.12	119.43	104.00
34	2	876	G	N1-C6-O6	8.12	124.77	119.90
34	2	1856	G	N1-C6-O6	8.12	124.77	119.90
1	1	11	G	C5-C6-O6	-8.11	123.73	128.60
1	1	66	C	O4'-C1'-N1	8.11	114.69	108.20
34	2	1147	G	C5-C6-O6	-8.11	123.73	128.60
22	X	78	ILE	N-CA-C	8.11	132.89	111.00
34	2	849	C	C2-N1-C1'	8.11	127.72	118.80
34	2	95	G	C5-C6-O6	-8.10	123.74	128.60
34	2	140	U	O4'-C1'-N1	8.10	114.68	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	303	G	C5-C6-O6	-8.09	123.74	128.60
34	2	1218	G	C5-C6-O6	-8.09	123.75	128.60
34	2	1843	G	N1-C6-O6	8.08	124.75	119.90
34	2	600	G	C5-C6-O6	-8.08	123.75	128.60
34	2	974	G	C5-C6-O6	-8.07	123.75	128.60
34	2	1660	G	N1-C6-O6	8.07	124.74	119.90
34	2	1849	G	C5-C6-O6	-8.07	123.76	128.60
34	2	1348	G	C5-C6-O6	-8.07	123.76	128.60
34	2	352	C	O4'-C1'-N1	8.06	114.65	108.20
34	2	461	G	C5-C6-O6	-8.06	123.76	128.60
34	2	880	C	O4'-C1'-N1	8.06	114.65	108.20
34	2	1427	G	C5-C6-O6	-8.06	123.77	128.60
34	2	1241	G	C5-C6-O6	-8.05	123.77	128.60
34	2	1595	G	N1-C6-O6	8.05	124.73	119.90
34	2	729	C	O4'-C1'-N1	8.05	114.64	108.20
38	k	272	VAL	O-C-N	8.04	135.56	122.70
34	2	508	G	C5-C6-O6	-8.03	123.78	128.60
34	2	1267	C	O4'-C1'-N1	8.03	114.62	108.20
34	2	1675	G	C5-C6-O6	-8.03	123.78	128.60
34	2	322	G	O4'-C1'-N9	8.03	114.62	108.20
34	2	848	G	P-O3'-C3'	8.03	129.33	119.70
50	u	139	TYR	CB-CG-CD2	-8.03	116.19	121.00
34	2	1094	C	O4'-C1'-N1	8.02	114.62	108.20
34	2	1664	G	C5-C6-O6	-8.01	123.79	128.60
34	2	989	G	C5-C6-O6	-8.01	123.80	128.60
34	2	395	G	C5-C6-O6	-8.01	123.80	128.60
34	2	1727	G	C5-C6-O6	-8.00	123.80	128.60
34	2	494	G	C5-C6-O6	-8.00	123.80	128.60
34	2	1806	U	O4'-C1'-N1	7.99	114.59	108.20
34	2	499	G	C5-C6-O6	-7.98	123.81	128.60
34	2	1290	G	C5-C6-O6	-7.98	123.81	128.60
34	2	1608	G	C5-C6-O6	-7.98	123.81	128.60
34	2	568	C	O4'-C1'-N1	7.98	114.58	108.20
1	1	25	U	O4'-C1'-N1	7.97	114.58	108.20
34	2	1053	C	O4'-C1'-N1	7.97	114.58	108.20
34	2	409	G	C5-C6-O6	-7.97	123.82	128.60
34	2	495	G	C5-C6-O6	-7.97	123.82	128.60
34	2	587	G	C5-C6-O6	-7.97	123.82	128.60
34	2	891	G	C5-C6-O6	-7.96	123.82	128.60
34	2	1669	G	C5-C6-O6	-7.96	123.82	128.60
34	2	856	G	C5-C6-O6	-7.96	123.82	128.60
34	2	430	G	C5-C6-O6	-7.96	123.82	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1099	C	O4'-C1'-N1	7.96	114.57	108.20
34	2	1486	G	C5-C6-O6	-7.96	123.83	128.60
34	2	1789	G	C5-C6-O6	-7.96	123.83	128.60
34	2	1206	G	C5-C6-O6	-7.95	123.83	128.60
34	2	1779	C	O4'-C1'-N1	7.94	114.55	108.20
34	2	1210	A	N1-C6-N6	7.93	123.36	118.60
34	2	1201	C	O4'-C1'-N1	7.93	114.55	108.20
34	2	1847	C	O4'-C1'-N1	7.93	114.55	108.20
34	2	439	A	N1-C6-N6	7.93	123.36	118.60
34	2	37	C	O4'-C1'-N1	7.93	114.54	108.20
34	2	1162	G	C5-C6-O6	-7.93	123.84	128.60
34	2	1855	G	C5-C6-O6	-7.93	123.84	128.60
34	2	481	C	O4'-C1'-N1	7.92	114.54	108.20
34	2	460	G	C5-C6-O6	-7.92	123.85	128.60
34	2	1471	G	C5-C6-O6	-7.92	123.85	128.60
34	2	1331	G	C5-C6-O6	-7.91	123.85	128.60
34	2	1598	G	C5-C6-O6	-7.91	123.86	128.60
1	1	62	C	O4'-C1'-N1	7.91	114.53	108.20
34	2	590	G	C5-C6-O6	-7.88	123.87	128.60
34	2	869	G	C5-C6-O6	-7.88	123.87	128.60
34	2	431	C	O4'-C1'-N1	7.88	114.51	108.20
34	2	376	C	O4'-C1'-N1	7.88	114.50	108.20
34	2	1225	G	C5-C6-O6	-7.87	123.88	128.60
34	2	235	C	O4'-C1'-N1	7.87	114.49	108.20
34	2	837	G	C5-C6-O6	-7.87	123.88	128.60
34	2	1067	G	C5-C6-O6	-7.87	123.88	128.60
34	2	1852	G	C5-C6-O6	-7.87	123.88	128.60
1	1	8	G	C5-C6-O6	-7.86	123.88	128.60
34	2	113	G	C5-C6-O6	-7.86	123.89	128.60
34	2	1840	G	C5-C6-O6	-7.86	123.89	128.60
34	2	923	C	O4'-C1'-N1	7.85	114.48	108.20
34	2	939	U	O4'-C1'-N1	7.85	114.48	108.20
34	2	1220	G	C5-C6-O6	-7.85	123.89	128.60
34	2	1599	G	C5-C6-O6	-7.84	123.89	128.60
34	2	496	G	C5-C6-O6	-7.84	123.90	128.60
34	2	1223	G	C5-C6-O6	-7.83	123.90	128.60
34	2	1135	C	O4'-C1'-N1	7.83	114.47	108.20
38	k	272	VAL	C-N-CA	-7.83	102.13	121.70
1	1	6	G	O4'-C1'-N9	7.81	114.45	108.20
34	2	975	C	O4'-C1'-N1	7.81	114.45	108.20
34	2	1187	C	O4'-C1'-N1	7.81	114.44	108.20
34	2	653	C	O4'-C1'-N1	7.80	114.44	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1421	G	N1-C6-O6	7.80	124.58	119.90
34	2	299	G	N1-C6-O6	7.79	124.58	119.90
34	2	550	A	O4'-C1'-N9	7.79	114.44	108.20
34	2	1811	G	C5-C6-O6	-7.79	123.92	128.60
34	2	489	G	N1-C6-O6	7.79	124.57	119.90
34	2	1561	G	C5-C6-O6	-7.79	123.93	128.60
34	2	464	G	C5-C6-O6	-7.78	123.93	128.60
34	2	118	C	O4'-C1'-N1	7.78	114.42	108.20
34	2	1102	C	O4'-C1'-N1	7.77	114.42	108.20
34	2	919	G	C5-C6-O6	-7.77	123.94	128.60
34	2	1558	G	C5-C6-O6	-7.77	123.94	128.60
34	2	469	C	O4'-C1'-N1	7.76	114.41	108.20
34	2	1033	G	C5-C6-O6	-7.76	123.94	128.60
34	2	446	C	O4'-C1'-N1	7.76	114.41	108.20
34	2	1405	A	C5-C6-N6	-7.76	117.49	123.70
34	2	69	C	O4'-C1'-N1	7.76	114.41	108.20
34	2	380	C	O4'-C1'-N1	7.76	114.41	108.20
50	u	139	TYR	CB-CG-CD1	7.75	125.65	121.00
34	2	1120	C	O4'-C1'-N1	7.75	114.40	108.20
34	2	635	C	O4'-C1'-N1	7.75	114.40	108.20
34	2	1316	G	C5-C6-O6	-7.74	123.95	128.60
34	2	106	C	O4'-C1'-N1	7.74	114.39	108.20
34	2	890	G	C5-C6-O6	-7.73	123.96	128.60
34	2	1639	C	O4'-C1'-N1	7.73	114.39	108.20
34	2	830	C	O4'-C1'-N1	7.73	114.38	108.20
34	2	820	C	O4'-C1'-N1	7.72	114.38	108.20
34	2	179	C	O4'-C1'-N1	7.72	114.38	108.20
34	2	1633	G	C5-C6-O6	-7.72	123.97	128.60
34	2	183	G	C5-C6-O6	-7.72	123.97	128.60
34	2	1182	U	O4'-C1'-N1	7.71	114.37	108.20
34	2	560	C	O4'-C1'-N1	7.71	114.37	108.20
34	2	1407	G	P-O3'-C3'	7.71	128.95	119.70
34	2	1411	C	O4'-C1'-N1	7.71	114.37	108.20
34	2	1653	G	C5-C6-O6	-7.71	123.97	128.60
34	2	312	C	O4'-C1'-N1	7.71	114.36	108.20
34	2	920	G	C5-C6-O6	-7.70	123.98	128.60
34	2	875	C	O4'-C1'-N1	7.70	114.36	108.20
34	2	203	G	C5-C6-O6	-7.70	123.98	128.60
34	2	1122	G	C5-C6-O6	-7.70	123.98	128.60
34	2	876	G	O4'-C1'-N9	7.69	114.35	108.20
34	2	1745	C	N3-C4-N4	7.69	123.38	118.00
34	2	1681	G	C5-C6-O6	-7.69	123.99	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1028	C	O4'-C1'-N1	7.69	114.35	108.20
1	1	13	G	C5-C6-O6	-7.68	123.99	128.60
34	2	197	U	O4'-C1'-N1	7.67	114.34	108.20
34	2	210	G	C5-C6-O6	-7.67	124.00	128.60
34	2	1121	C	O4'-C1'-N1	7.67	114.34	108.20
34	2	306	C	O4'-C1'-N1	7.67	114.33	108.20
34	2	367	G	C5-C6-O6	-7.67	124.00	128.60
34	2	1417	A	C5-C6-N6	-7.67	117.56	123.70
34	2	1556	A	C5-C6-N6	-7.67	117.57	123.70
1	1	51	U	O4'-C1'-N1	7.67	114.33	108.20
34	2	946	C	O4'-C1'-N1	7.67	114.33	108.20
25	a	125	VAL	C-N-CA	-7.66	106.21	122.30
34	2	933	C	O4'-C1'-N1	7.66	114.33	108.20
34	2	1043	C	O4'-C1'-N1	7.66	114.33	108.20
34	2	35	C	O4'-C1'-N1	7.66	114.32	108.20
34	2	332	C	O4'-C1'-N1	7.64	114.31	108.20
1	1	22	G	C5-C6-O6	-7.64	124.02	128.60
34	2	1268	C	O4'-C1'-N1	7.63	114.31	108.20
34	2	522	C	O4'-C1'-N1	7.63	114.31	108.20
34	2	1862	U	O4'-C1'-N1	7.63	114.31	108.20
34	2	1741	U	O4'-C1'-N1	7.63	114.30	108.20
34	2	30	C	O4'-C1'-N1	7.63	114.30	108.20
34	2	930	G	C5-C6-O6	-7.63	124.02	128.60
34	2	1709	U	O4'-C1'-N1	7.62	114.30	108.20
34	2	1517	A	O4'-C1'-N9	7.62	114.30	108.20
34	2	434	G	C5-C6-O6	-7.62	124.03	128.60
34	2	971	G	C5-C6-O6	-7.61	124.03	128.60
34	2	456	G	C5-C6-O6	-7.61	124.03	128.60
34	2	1733	C	O4'-C1'-N1	7.61	114.29	108.20
34	2	926	C	O4'-C1'-N1	7.61	114.29	108.20
34	2	1053	C	C2-N1-C1'	7.60	127.16	118.80
34	2	369	C	O4'-C1'-N1	7.60	114.28	108.20
34	2	1123	C	O4'-C1'-N1	7.59	114.28	108.20
34	2	231	C	O4'-C1'-N1	7.59	114.27	108.20
34	2	901	C	O4'-C1'-N1	7.59	114.27	108.20
1	1	57	G	C5-C6-O6	-7.59	124.05	128.60
34	2	626	C	O4'-C1'-N1	7.59	114.27	108.20
34	2	1799	G	C5-C6-O6	-7.59	124.05	128.60
1	1	61	C	O4'-C1'-N1	7.58	114.27	108.20
34	2	411	G	C5-C6-O6	-7.58	124.05	128.60
34	2	1333	C	O4'-C1'-N1	7.58	114.27	108.20
34	2	48	C	O4'-C1'-N1	7.58	114.26	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	839	C	O4'-C1'-N1	7.58	114.26	108.20
34	2	1002	C	O4'-C1'-N1	7.58	114.26	108.20
34	2	1090	C	O4'-C1'-N1	7.57	114.26	108.20
34	2	1468	C	O4'-C1'-N1	7.57	114.25	108.20
34	2	352	C	N3-C4-C5	-7.57	118.87	121.90
34	2	628	C	O4'-C1'-N1	7.57	114.25	108.20
34	2	96	C	O4'-C1'-N1	7.56	114.25	108.20
34	2	1536	G	C5-C6-O6	-7.56	124.06	128.60
34	2	916	A	C4-C5-C6	7.56	120.78	117.00
34	2	1497	C	O4'-C1'-N1	7.56	114.25	108.20
34	2	1227	C	O4'-C1'-N1	7.55	114.24	108.20
34	2	1805	C	O4'-C1'-N1	7.55	114.24	108.20
34	2	348	C	O4'-C1'-N1	7.55	114.24	108.20
34	2	414	C	O4'-C1'-N1	7.55	114.24	108.20
34	2	20	G	C5-C6-O6	-7.55	124.07	128.60
34	2	1275	C	O4'-C1'-N1	7.55	114.24	108.20
34	2	896	C	O4'-C1'-N1	7.54	114.24	108.20
38	k	241	ASP	C-N-CA	-7.54	102.84	121.70
34	2	23	G	C5-C6-O6	-7.54	124.08	128.60
34	2	997	A	C5-C6-N6	-7.54	117.67	123.70
34	2	731	C	O4'-C1'-N1	7.54	114.23	108.20
34	2	878	U	O4'-C1'-N1	7.54	114.23	108.20
34	2	272	C	N3-C4-N4	7.54	123.27	118.00
34	2	558	C	O4'-C1'-N1	7.52	114.22	108.20
34	2	1180	G	C5-C6-O6	-7.52	124.09	128.60
34	2	374	U	O4'-C1'-N1	7.52	114.21	108.20
34	2	848	G	O4'-C1'-N9	7.52	114.22	108.20
34	2	1801	C	O4'-C1'-N1	7.51	114.21	108.20
34	2	1092	G	C5-C6-O6	-7.51	124.09	128.60
34	2	393	G	C5-C6-O6	-7.50	124.10	128.60
34	2	1163	G	C5-C6-O6	-7.50	124.10	128.60
34	2	1678	C	O4'-C1'-N1	7.50	114.20	108.20
34	2	1735	C	O4'-C1'-N1	7.50	114.20	108.20
34	2	1604	C	O4'-C1'-N1	7.50	114.20	108.20
34	2	79	A	C5-C6-N6	-7.49	117.70	123.70
34	2	236	C	O4'-C1'-N1	7.49	114.19	108.20
34	2	1683	C	O4'-C1'-N1	7.49	114.19	108.20
34	2	1013	U	O4'-C1'-N1	7.49	114.19	108.20
34	2	273	G	C5-C6-O6	-7.49	124.11	128.60
1	1	32	C	O4'-C1'-N1	7.49	114.19	108.20
34	2	980	C	O4'-C1'-N1	7.49	114.19	108.20
34	2	873	C	O4'-C1'-N1	7.48	114.19	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1684	C	O4'-C1'-N1	7.48	114.18	108.20
34	2	1321	G	C5-C6-O6	-7.48	124.11	128.60
34	2	728	U	O4'-C1'-N1	7.48	114.18	108.20
34	2	1010	G	C5-C6-O6	-7.47	124.12	128.60
34	2	239	U	O4'-C1'-N1	7.47	114.17	108.20
34	2	1294	G	C5-C6-O6	-7.46	124.12	128.60
34	2	978	G	C5-C6-O6	-7.46	124.12	128.60
34	2	1705	C	O4'-C1'-N1	7.46	114.17	108.20
34	2	1063	C	O4'-C1'-N1	7.46	114.17	108.20
34	2	235	C	N3-C4-N4	7.45	123.22	118.00
34	2	881	U	O4'-C1'-N1	7.45	114.16	108.20
34	2	426	G	C5-C6-O6	-7.45	124.13	128.60
34	2	220	C	O4'-C1'-N1	7.45	114.16	108.20
44	v	748	ASP	CA-C-N	7.45	133.59	117.20
34	2	944	C	O4'-C1'-N1	7.45	114.16	108.20
34	2	1746	C	N3-C4-N4	7.45	123.21	118.00
1	1	71	C	O4'-C1'-N1	7.44	114.16	108.20
34	2	206	A	C4-C5-C6	7.44	120.72	117.00
34	2	629	C	O4'-C1'-N1	7.44	114.16	108.20
34	2	1466	C	O4'-C1'-N1	7.44	114.15	108.20
34	2	1299	C	C2-N1-C1'	7.43	126.97	118.80
34	2	1539	C	N3-C4-N4	7.43	123.20	118.00
34	2	538	C	N3-C4-N4	7.43	123.20	118.00
34	2	1788	C	O4'-C1'-N1	7.43	114.14	108.20
34	2	1425	G	C5-C6-O6	-7.42	124.15	128.60
34	2	36	U	O4'-C1'-N1	7.42	114.14	108.20
34	2	969	C	O4'-C1'-N1	7.42	114.14	108.20
34	2	1370	C	O4'-C1'-N1	7.42	114.14	108.20
43	y	245	LEU	CA-C-N	-7.42	100.88	117.20
34	2	165	G	O4'-C1'-N9	7.42	114.13	108.20
34	2	145	G	C5-C6-O6	-7.41	124.15	128.60
34	2	1553	C	O4'-C1'-N1	7.41	114.13	108.20
34	2	517	C	O4'-C1'-N1	7.41	114.12	108.20
34	2	849	C	C6-N1-C1'	-7.41	111.91	120.80
34	2	327	C	O4'-C1'-N1	7.40	114.12	108.20
34	2	1749	C	O4'-C1'-N1	7.40	114.12	108.20
34	2	927	C	O4'-C1'-N1	7.39	114.11	108.20
34	2	1624	C	O4'-C1'-N1	7.39	114.11	108.20
34	2	1846	C	O4'-C1'-N1	7.39	114.11	108.20
34	2	1436	C	O4'-C1'-N1	7.39	114.11	108.20
34	2	73	C	P-O3'-C3'	7.39	128.56	119.70
34	2	1087	C	O4'-C1'-N1	7.39	114.11	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1142	C	N3-C4-N4	7.39	123.17	118.00
38	k	150	SER	O-C-N	7.39	134.52	122.70
34	2	86	C	O4'-C1'-N1	7.38	114.11	108.20
34	2	1749	C	N3-C4-N4	7.38	123.17	118.00
34	2	484	C	O4'-C1'-N1	7.38	114.11	108.20
34	2	570	U	O4'-C1'-N1	7.38	114.11	108.20
34	2	1523	G	C5-C6-O6	-7.38	124.17	128.60
34	2	305	U	O4'-C1'-N1	7.38	114.10	108.20
34	2	324	C	O4'-C1'-N1	7.38	114.10	108.20
34	2	538	C	O4'-C1'-N1	7.37	114.10	108.20
34	2	1394	G	C5-C6-O6	-7.37	124.18	128.60
34	2	1772	C	O4'-C1'-N1	7.37	114.10	108.20
34	2	533	C	O4'-C1'-N1	7.37	114.09	108.20
34	2	954	G	O4'-C1'-N9	7.37	114.09	108.20
34	2	1226	C	O4'-C1'-N1	7.37	114.09	108.20
34	2	1209	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	1414	C	C6-N1-C1'	-7.36	111.96	120.80
34	2	443	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	1131	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	1387	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	1522	C	O4'-C1'-N1	7.36	114.09	108.20
1	1	14	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	1622	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	608	C	O4'-C1'-N1	7.35	114.08	108.20
34	2	1768	C	O4'-C1'-N1	7.35	114.08	108.20
34	2	270	G	C5-C6-O6	-7.35	124.19	128.60
34	2	507	C	O4'-C1'-N1	7.35	114.08	108.20
34	2	154	U	O4'-C1'-N1	7.35	114.08	108.20
34	2	359	C	O4'-C1'-N1	7.35	114.08	108.20
34	2	1183	G	C5-C6-O6	-7.35	124.19	128.60
1	1	12	C	O4'-C1'-N1	7.35	114.08	108.20
34	2	1277	G	C5-C6-O6	-7.35	124.19	128.60
34	2	1456	C	O4'-C1'-N1	7.34	114.08	108.20
34	2	271	G	C5-C6-O6	-7.34	124.19	128.60
34	2	1343	U	O4'-C1'-N1	7.34	114.07	108.20
34	2	1768	C	N3-C4-N4	7.34	123.14	118.00
34	2	278	U	O4'-C1'-N1	7.33	114.07	108.20
34	2	552	U	O4'-C1'-N1	7.33	114.06	108.20
34	2	1214	C	O4'-C1'-N1	7.33	114.06	108.20
34	2	1742	C	O4'-C1'-N1	7.33	114.06	108.20
34	2	108	G	C5-C6-O6	-7.33	124.20	128.60
34	2	1178	A	C4-C5-C6	7.33	120.66	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1330	G	N1-C6-O6	7.33	124.30	119.90
34	2	1655	C	C6-N1-C1'	-7.33	112.01	120.80
34	2	1310	U	O4'-C1'-N1	7.32	114.06	108.20
1	1	4	C	O4'-C1'-N1	7.32	114.06	108.20
34	2	668	U	O4'-C1'-N1	7.32	114.06	108.20
34	2	178	C	O4'-C1'-N1	7.32	114.06	108.20
34	2	1531	G	C5-C6-O6	-7.32	124.21	128.60
34	2	199	G	C5-C6-O6	-7.32	124.21	128.60
34	2	1176	C	O4'-C1'-N1	7.32	114.06	108.20
34	2	1402	G	C5-C6-O6	-7.32	124.21	128.60
34	2	432	C	O4'-C1'-N1	7.32	114.05	108.20
34	2	1085	G	C5-C6-O6	-7.32	124.21	128.60
34	2	162	C	O4'-C1'-N1	7.32	114.05	108.20
34	2	1734	C	O4'-C1'-N1	7.32	114.05	108.20
34	2	1320	G	C5-C6-O6	-7.31	124.21	128.60
34	2	1537	C	O4'-C1'-N1	7.31	114.05	108.20
34	2	193	C	O4'-C1'-N1	7.31	114.05	108.20
34	2	1850	C	O4'-C1'-N1	7.31	114.05	108.20
34	2	1802	U	O4'-C1'-N1	7.31	114.05	108.20
34	2	1156	U	O4'-C1'-N1	7.31	114.05	108.20
34	2	1181	C	O4'-C1'-N1	7.31	114.05	108.20
34	2	1041	U	O4'-C1'-N1	7.30	114.04	108.20
34	2	331	C	O4'-C1'-N1	7.30	114.04	108.20
34	2	1836	C	O4'-C1'-N1	7.30	114.04	108.20
34	2	1415	C	O4'-C1'-N1	7.30	114.04	108.20
34	2	1311	U	O4'-C1'-N1	7.30	114.04	108.20
34	2	1624	C	N3-C4-N4	7.29	123.11	118.00
34	2	1498	C	O4'-C1'-N1	7.29	114.03	108.20
34	2	1007	A	C5-C6-N6	-7.29	117.87	123.70
34	2	420	C	O4'-C1'-N1	7.29	114.03	108.20
34	2	1332	C	O4'-C1'-N1	7.29	114.03	108.20
34	2	1200	A	C5-C6-N6	-7.29	117.87	123.70
34	2	949	C	O4'-C1'-N1	7.28	114.03	108.20
34	2	1252	G	C5-C6-O6	-7.28	124.23	128.60
1	1	60	A	C4-C5-C6	7.28	120.64	117.00
34	2	413	U	O4'-C1'-N1	7.28	114.02	108.20
34	2	1128	C	O4'-C1'-N1	7.28	114.02	108.20
34	2	1173	U	O4'-C1'-N1	7.28	114.02	108.20
34	2	1322	U	O4'-C1'-N1	7.27	114.02	108.20
34	2	1273	C	O4'-C1'-N1	7.27	114.01	108.20
34	2	1027	A	C5-C6-N6	-7.26	117.89	123.70
1	1	27	C	N3-C4-N4	7.26	123.08	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1736	U	O4'-C1'-N1	7.26	114.01	108.20
34	2	1023	A	C4-C5-C6	7.26	120.63	117.00
34	2	928	G	C5-C6-O6	-7.26	124.25	128.60
34	2	987	G	C5-C6-O6	-7.26	124.25	128.60
34	2	567	U	O4'-C1'-N1	7.25	114.00	108.20
34	2	1385	C	O4'-C1'-N1	7.25	114.00	108.20
34	2	641	U	O4'-C1'-N1	7.25	114.00	108.20
34	2	1563	C	O4'-C1'-N1	7.25	114.00	108.20
34	2	1570	G	C5-C6-O6	-7.25	124.25	128.60
34	2	424	G	C5-C6-O6	-7.25	124.25	128.60
34	2	53	C	O4'-C1'-N1	7.24	114.00	108.20
34	2	632	U	O4'-C1'-N1	7.24	113.99	108.20
1	1	23	C	O4'-C1'-N1	7.24	113.99	108.20
34	2	407	C	O4'-C1'-N1	7.24	113.99	108.20
34	2	1124	C	O4'-C1'-N1	7.24	113.99	108.20
34	2	368	U	O4'-C1'-N1	7.23	113.98	108.20
34	2	1032	A	C5-C6-N6	-7.23	117.92	123.70
34	2	1409	G	C5-C6-O6	-7.23	124.26	128.60
34	2	1676	U	O4'-C1'-N1	7.23	113.98	108.20
34	2	219	U	O4'-C1'-N1	7.22	113.98	108.20
34	2	813	G	C5-C6-O6	-7.22	124.27	128.60
34	2	844	U	O4'-C1'-N1	7.22	113.98	108.20
34	2	1028	C	N3-C4-N4	7.22	123.06	118.00
34	2	1593	G	C5-C6-O6	-7.22	124.27	128.60
34	2	1631	G	C5-C6-O6	-7.22	124.27	128.60
34	2	1772	C	N3-C4-N4	7.22	123.06	118.00
34	2	1042	U	O4'-C1'-N1	7.22	113.97	108.20
38	k	109	VAL	CA-C-N	7.22	130.64	116.20
34	2	1520	C	O4'-C1'-N1	7.22	113.97	108.20
34	2	1426	C	O4'-C1'-N1	7.21	113.97	108.20
34	2	392	C	O4'-C1'-N1	7.21	113.97	108.20
34	2	173	A	C5-C6-N6	-7.21	117.93	123.70
34	2	217	U	O4'-C1'-N1	7.21	113.97	108.20
34	2	671	U	O4'-C1'-N1	7.21	113.96	108.20
34	2	847	C	O4'-C1'-N1	7.21	113.96	108.20
34	2	1045	A	C4-C5-C6	7.21	120.60	117.00
34	2	1447	G	C5-C6-O6	-7.20	124.28	128.60
34	2	1077	U	O4'-C1'-N1	7.20	113.96	108.20
34	2	1158	C	O4'-C1'-N1	7.20	113.96	108.20
34	2	480	C	O4'-C1'-N1	7.20	113.96	108.20
34	2	1185	A	C4-C5-C6	7.20	120.60	117.00
34	2	1796	C	O4'-C1'-N1	7.20	113.96	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1345	G	C5-C6-O6	-7.19	124.28	128.60
1	1	49	G	O4'-C1'-N9	7.19	113.95	108.20
34	2	1671	U	O4'-C1'-N1	7.19	113.95	108.20
34	2	227	A	C4-C5-C6	7.19	120.59	117.00
34	2	1848	U	O4'-C1'-N1	7.19	113.95	108.20
34	2	355	C	O4'-C1'-N1	7.18	113.95	108.20
34	2	406	U	O4'-C1'-N1	7.18	113.95	108.20
34	2	627	U	O4'-C1'-N1	7.18	113.95	108.20
34	2	162	C	N3-C4-N4	7.18	123.03	118.00
34	2	532	U	O4'-C1'-N1	7.18	113.94	108.20
34	2	1562	G	O4'-C1'-N9	7.18	113.94	108.20
34	2	1054	A	O4'-C1'-N9	7.18	113.94	108.20
34	2	441	G	C5-C6-O6	-7.17	124.30	128.60
34	2	1248	C	O4'-C1'-N1	7.17	113.94	108.20
34	2	1143	C	O4'-C1'-N1	7.17	113.94	108.20
34	2	1547	G	C5-C6-O6	-7.17	124.30	128.60
34	2	213	C	N3-C4-N4	7.17	123.02	118.00
34	2	153	G	C5-C6-O6	-7.17	124.30	128.60
34	2	17	C	O4'-C1'-N1	7.17	113.93	108.20
34	2	191	C	N3-C4-N4	7.17	123.02	118.00
1	1	46	G	C5-C6-O6	-7.16	124.30	128.60
34	2	192	U	O4'-C1'-N1	7.16	113.93	108.20
34	2	309	A	C5-C6-N6	-7.16	117.97	123.70
34	2	1592	C	O4'-C1'-N1	7.16	113.93	108.20
34	2	344	U	O4'-C1'-N1	7.16	113.93	108.20
34	2	377	C	O4'-C1'-N1	7.16	113.93	108.20
34	2	432	C	N3-C4-N4	7.16	123.01	118.00
34	2	588	G	C5-C6-O6	-7.16	124.30	128.60
34	2	28	U	O4'-C1'-N1	7.16	113.93	108.20
34	2	605	C	O4'-C1'-N1	7.16	113.92	108.20
34	2	855	G	C5-C6-O6	-7.15	124.31	128.60
34	2	1319	U	O4'-C1'-N1	7.15	113.92	108.20
34	2	1499	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	89	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	286	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	569	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	846	C	O4'-C1'-N1	7.15	113.92	108.20
35	A	184	LEU	CA-C-N	-7.15	101.46	117.20
34	2	437	A	C4-C5-C6	7.15	120.58	117.00
34	2	1512	G	C5-C6-O6	-7.15	124.31	128.60
34	2	947	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	954	G	C5-C6-O6	-7.15	124.31	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1423	C	N3-C4-N4	7.15	123.00	118.00
1	1	75	C	O4'-C1'-N1	7.14	113.91	108.20
34	2	1650	C	O4'-C1'-N1	7.14	113.91	108.20
1	1	72	U	O4'-C1'-N1	7.14	113.91	108.20
34	2	503	G	C5-C6-O6	-7.14	124.32	128.60
34	2	1040	G	C5-C6-O6	-7.13	124.32	128.60
34	2	447	C	O4'-C1'-N1	7.13	113.90	108.20
34	2	970	C	O4'-C1'-N1	7.13	113.90	108.20
1	1	71	C	N3-C4-N4	7.13	122.99	118.00
34	2	86	C	N3-C4-N4	7.13	122.99	118.00
34	2	24	C	O4'-C1'-N1	7.12	113.90	108.20
34	2	117	C	O4'-C1'-N1	7.12	113.90	108.20
34	2	1543	G	C5-C6-O6	-7.12	124.33	128.60
34	2	1559	C	O4'-C1'-N1	7.12	113.90	108.20
34	2	462	C	O4'-C1'-N1	7.12	113.90	108.20
1	1	4	C	N3-C4-N4	7.12	122.98	118.00
34	2	364	G	N1-C6-O6	7.12	124.17	119.90
34	2	655	G	C5-C6-O6	-7.12	124.33	128.60
34	2	1804	U	O4'-C1'-N1	7.12	113.89	108.20
34	2	1822	C	O4'-C1'-N1	7.12	113.89	108.20
34	2	1586	C	O4'-C1'-N1	7.12	113.89	108.20
34	2	1301	C	O4'-C1'-N1	7.12	113.89	108.20
34	2	1750	C	O4'-C1'-N1	7.12	113.89	108.20
34	2	838	C	O4'-C1'-N1	7.11	113.89	108.20
34	2	519	A	C5-C6-N6	-7.11	118.01	123.70
34	2	961	U	O4'-C1'-N1	7.11	113.89	108.20
34	2	213	C	O4'-C1'-N1	7.11	113.89	108.20
34	2	1000	U	O4'-C1'-N1	7.11	113.89	108.20
34	2	1430	C	O4'-C1'-N1	7.11	113.89	108.20
34	2	1567	C	O4'-C1'-N1	7.11	113.89	108.20
1	1	16	G	C5-C6-O6	-7.11	124.33	128.60
34	2	730	C	O4'-C1'-N1	7.11	113.89	108.20
34	2	1359	C	N3-C4-N4	7.11	122.97	118.00
34	2	15	U	O4'-C1'-N1	7.10	113.88	108.20
34	2	412	U	O4'-C1'-N1	7.10	113.88	108.20
22	X	78	ILE	N-CA-CB	-7.10	94.47	110.80
34	2	527	C	O4'-C1'-N1	7.10	113.88	108.20
34	2	347	C	O4'-C1'-N1	7.10	113.88	108.20
34	2	1418	G	C5-C6-O6	-7.10	124.34	128.60
34	2	1555	U	O4'-C1'-N1	7.10	113.88	108.20
34	2	1634	G	C5-C6-O6	-7.10	124.34	128.60
34	2	1682	C	O4'-C1'-N1	7.10	113.88	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	114	G	C5-C6-O6	-7.10	124.34	128.60
34	2	1055	G	C5-C6-O6	-7.09	124.34	128.60
34	2	1467	C	O4'-C1'-N1	7.09	113.88	108.20
34	2	1585	C	O4'-C1'-N1	7.09	113.87	108.20
1	1	27	C	O4'-C1'-N1	7.09	113.87	108.20
34	2	529	C	O4'-C1'-N1	7.09	113.87	108.20
34	2	913	U	O4'-C1'-N1	7.09	113.87	108.20
34	2	1172	G	C5-C6-O6	-7.09	124.35	128.60
34	2	1521	G	C5-C6-O6	-7.09	124.35	128.60
34	2	1621	C	O4'-C1'-N1	7.09	113.87	108.20
34	2	636	G	C5-C6-O6	-7.08	124.35	128.60
34	2	1670	A	O4'-C1'-N9	7.08	113.87	108.20
34	2	1769	U	O4'-C1'-N1	7.08	113.87	108.20
34	2	1560	C	O4'-C1'-N1	7.08	113.86	108.20
34	2	1584	A	C4-C5-C6	7.08	120.54	117.00
34	2	1312	C	O4'-C1'-N1	7.08	113.86	108.20
34	2	1720	U	O4'-C1'-N1	7.08	113.86	108.20
34	2	18	C	N3-C4-N4	7.08	122.95	118.00
34	2	598	C	O4'-C1'-N1	7.07	113.86	108.20
34	2	18	C	O4'-C1'-N1	7.07	113.86	108.20
34	2	581	U	O4'-C1'-N1	7.07	113.86	108.20
41	3	51	C	O4'-C1'-N1	7.07	113.86	108.20
34	2	994	A	C4-C5-C6	7.07	120.53	117.00
34	2	187	C	N3-C4-N4	7.07	122.95	118.00
45	w	134	TYR	CB-CG-CD1	7.07	125.24	121.00
34	2	578	G	C5-C6-O6	-7.07	124.36	128.60
34	2	1647	G	C5-C6-O6	-7.07	124.36	128.60
1	1	54	A	C5-C6-N6	-7.07	118.05	123.70
34	2	1623	C	N3-C4-N4	7.07	122.95	118.00
34	2	1809	A	C4-C5-C6	7.06	120.53	117.00
34	2	938	G	C5-C6-O6	-7.06	124.36	128.60
34	2	173	A	C4-C5-C6	7.06	120.53	117.00
34	2	1524	C	O4'-C1'-N1	7.06	113.85	108.20
34	2	1711	C	O4'-C1'-N1	7.06	113.85	108.20
34	2	1747	C	N3-C4-N4	7.06	122.94	118.00
34	2	1153	G	C5-C6-O6	-7.06	124.36	128.60
34	2	151	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	487	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	1170	U	O4'-C1'-N1	7.05	113.84	108.20
34	2	1699	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	1478	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	1184	A	C4-C5-C6	7.05	120.53	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1200	A	C4-C5-C6	7.05	120.53	117.00
34	2	1353	A	C4-C5-C6	7.05	120.52	117.00
34	2	1665	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	1065	U	O4'-C1'-N1	7.04	113.84	108.20
34	2	336	C	N3-C4-N4	7.04	122.93	118.00
34	2	17	C	N3-C4-N4	7.04	122.93	118.00
34	2	611	C	O4'-C1'-N1	7.04	113.83	108.20
34	2	1009	U	O4'-C1'-N1	7.04	113.83	108.20
34	2	200	U	O4'-C1'-N1	7.04	113.83	108.20
34	2	1003	C	O4'-C1'-N1	7.03	113.83	108.20
34	2	1257	C	O4'-C1'-N1	7.03	113.83	108.20
41	3	50	C	O4'-C1'-N1	7.03	113.83	108.20
34	2	799	C	O4'-C1'-N1	7.03	113.83	108.20
34	2	664	C	O4'-C1'-N1	7.03	113.82	108.20
34	2	1527	C	O4'-C1'-N1	7.03	113.82	108.20
34	2	885	U	O4'-C1'-N1	7.03	113.82	108.20
34	2	486	C	O4'-C1'-N1	7.02	113.82	108.20
34	2	1673	A	O4'-C1'-N9	7.02	113.82	108.20
34	2	1021	U	O4'-C1'-N1	7.02	113.82	108.20
34	2	635	C	N3-C4-N4	7.01	122.91	118.00
34	2	990	C	O4'-C1'-N1	7.01	113.81	108.20
34	2	1500	U	O4'-C1'-N1	7.01	113.81	108.20
34	2	209	C	N3-C4-N4	7.01	122.91	118.00
34	2	1433	C	O4'-C1'-N1	7.01	113.81	108.20
34	2	639	U	O4'-C1'-N1	7.01	113.81	108.20
34	2	1773	G	C5-C6-O6	-7.01	124.39	128.60
34	2	233	A	C5-C6-N6	-7.00	118.10	123.70
34	2	198	U	O4'-C1'-N1	7.00	113.80	108.20
34	2	973	C	O4'-C1'-N1	7.00	113.80	108.20
38	k	388	PHE	CB-CG-CD2	-7.00	115.90	120.80
34	2	1661	C	O4'-C1'-N1	7.00	113.80	108.20
1	1	40	C	O4'-C1'-N1	7.00	113.80	108.20
34	2	194	C	N3-C4-N4	6.99	122.90	118.00
34	2	1779	C	N3-C4-N4	6.99	122.90	118.00
34	2	330	C	O4'-C1'-N1	6.99	113.79	108.20
34	2	1380	C	O4'-C1'-N1	6.99	113.79	108.20
34	2	93	U	O4'-C1'-N1	6.99	113.79	108.20
34	2	963	C	O4'-C1'-N1	6.99	113.79	108.20
34	2	1082	G	C5-C6-O6	-6.99	124.41	128.60
34	2	1308	G	C5-C6-O6	-6.99	124.41	128.60
34	2	174	C	O4'-C1'-N1	6.99	113.79	108.20
34	2	222	G	C5-C6-O6	-6.99	124.41	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1326	G	C5-C6-O6	-6.99	124.41	128.60
34	2	38	A	O4'-C1'-N9	6.98	113.79	108.20
1	1	31	G	O4'-C1'-N9	6.98	113.79	108.20
34	2	602	U	O4'-C1'-N1	6.98	113.78	108.20
34	2	321	C	O4'-C1'-N1	6.98	113.78	108.20
34	2	185	C	O4'-C1'-N1	6.98	113.78	108.20
34	2	666	C	O4'-C1'-N1	6.98	113.78	108.20
34	2	817	G	C5-C6-O6	-6.97	124.42	128.60
34	2	1360	U	C2-N1-C1'	6.97	126.07	117.70
34	2	1489	C	N3-C4-N4	6.97	122.88	118.00
34	2	491	C	O4'-C1'-N1	6.97	113.78	108.20
34	2	612	C	O4'-C1'-N1	6.97	113.78	108.20
34	2	81	U	O4'-C1'-N1	6.97	113.77	108.20
34	2	452	C	N3-C4-N4	6.97	122.88	118.00
34	2	1258	C	O4'-C1'-N1	6.97	113.77	108.20
34	2	236	C	N3-C4-N4	6.96	122.88	118.00
34	2	730	C	N3-C4-N4	6.96	122.88	118.00
34	2	822	A	C4-C5-C6	6.96	120.48	117.00
34	2	1376	C	O4'-C1'-N1	6.96	113.77	108.20
34	2	163	U	O4'-C1'-N1	6.96	113.77	108.20
34	2	1698	C	O4'-C1'-N1	6.96	113.77	108.20
34	2	1271	G	C5-C6-O6	-6.96	124.43	128.60
34	2	842	G	C5-C6-O6	-6.95	124.43	128.60
34	2	1233	C	N3-C4-N4	6.95	122.87	118.00
34	2	837	G	O4'-C1'-N9	6.95	113.76	108.20
34	2	1283	A	C4-C5-C6	6.95	120.48	117.00
1	1	24	G	C5-C6-O6	-6.95	124.43	128.60
34	2	1035	C	O4'-C1'-N1	6.95	113.76	108.20
34	2	1281	G	C5-C6-O6	-6.95	124.43	128.60
34	2	1425	G	O4'-C1'-N9	6.95	113.76	108.20
34	2	1155	G	C5-C6-O6	-6.95	124.43	128.60
34	2	1472	A	C4-C5-C6	6.95	120.47	117.00
34	2	990	C	N3-C4-N4	6.95	122.86	118.00
34	2	1217	G	C5-C6-O6	-6.95	124.43	128.60
34	2	471	C	O4'-C1'-N1	6.94	113.75	108.20
34	2	1395	C	O4'-C1'-N1	6.94	113.75	108.20
34	2	1071	C	O4'-C1'-N1	6.94	113.75	108.20
34	2	1745	C	O4'-C1'-N1	6.94	113.75	108.20
34	2	906	G	O4'-C1'-N9	6.94	113.75	108.20
34	2	982	G	C5-C6-O6	-6.93	124.44	128.60
34	2	548	G	C5-C6-O6	-6.93	124.44	128.60
34	2	1751	G	C5-C6-O6	-6.93	124.44	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	378	U	O4'-C1'-N1	6.93	113.75	108.20
34	2	1383	G	C5-C6-O6	-6.93	124.44	128.60
34	2	544	A	O4'-C1'-N9	6.93	113.74	108.20
34	2	470	G	C5-C6-O6	-6.93	124.44	128.60
34	2	30	C	N3-C4-N4	6.93	122.85	118.00
34	2	824	G	C5-C6-O6	-6.93	124.44	128.60
34	2	1714	A	C4-C5-C6	6.93	120.46	117.00
34	2	1640	C	O4'-C1'-N1	6.92	113.74	108.20
34	2	124	U	O4'-C1'-N1	6.92	113.74	108.20
34	2	1186	A	C4-C5-C6	6.92	120.46	117.00
34	2	1390	G	C5-C6-O6	-6.92	124.45	128.60
34	2	452	C	O4'-C1'-N1	6.92	113.74	108.20
34	2	1429	C	O4'-C1'-N1	6.92	113.74	108.20
34	2	1766	C	O3'-P-O5'	6.92	117.15	104.00
34	2	1376	C	N3-C4-N4	6.92	122.84	118.00
34	2	1091	U	O4'-C1'-N1	6.92	113.73	108.20
34	2	1737	C	O4'-C1'-N1	6.92	113.73	108.20
34	2	301	C	O4'-C1'-N1	6.91	113.73	108.20
34	2	396	U	O4'-C1'-N1	6.91	113.73	108.20
34	2	556	U	O4'-C1'-N1	6.91	113.73	108.20
34	2	955	G	C5-C6-O6	-6.91	124.45	128.60
34	2	1098	G	C5-C6-O6	-6.91	124.45	128.60
34	2	1462	G	C5-C6-O6	-6.91	124.45	128.60
34	2	1712	C	O4'-C1'-N1	6.91	113.73	108.20
34	2	1766	C	O4'-C1'-N1	6.91	113.73	108.20
1	1	60	A	C5-C6-N6	-6.91	118.17	123.70
34	2	941	U	O4'-C1'-N1	6.91	113.72	108.20
34	2	1412	C	O4'-C1'-N1	6.90	113.72	108.20
1	1	18	G	P-O3'-C3'	6.90	127.98	119.70
34	2	197	U	C2-N1-C1'	6.90	125.98	117.70
34	2	1230	C	O4'-C1'-N1	6.90	113.72	108.20
34	2	1628	A	C4-C5-C6	6.90	120.45	117.00
34	2	802	U	O4'-C1'-N1	6.90	113.72	108.20
34	2	71	G	O4'-C1'-N9	6.89	113.72	108.20
34	2	557	C	O4'-C1'-N1	6.89	113.72	108.20
34	2	806	A	O4'-C1'-N9	6.89	113.72	108.20
35	A	269	PHE	CB-CG-CD2	-6.89	115.97	120.80
34	2	1039	G	C5-C6-O6	-6.89	124.47	128.60
34	2	1335	U	O4'-C1'-N1	6.89	113.71	108.20
1	1	41	C	O4'-C1'-N1	6.89	113.71	108.20
34	2	1253	G	C5-C6-O6	-6.89	124.47	128.60
34	2	646	G	C5-C6-O6	-6.88	124.47	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1539	C	O4'-C1'-N1	6.88	113.71	108.20
34	2	585	U	O4'-C1'-N1	6.88	113.70	108.20
34	2	650	C	O4'-C1'-N1	6.88	113.70	108.20
34	2	935	U	O4'-C1'-N1	6.88	113.70	108.20
1	1	18	G	OP1-P-O3'	-6.88	90.07	105.20
34	2	1167	G	C5-C6-O6	-6.88	124.47	128.60
34	2	1679	C	O4'-C1'-N1	6.88	113.70	108.20
34	2	123	G	O4'-C1'-N9	6.87	113.70	108.20
34	2	465	C	O4'-C1'-N1	6.87	113.70	108.20
34	2	895	U	O4'-C1'-N1	6.87	113.70	108.20
34	2	1381	G	C5-C6-O6	-6.87	124.48	128.60
34	2	399	C	O4'-C1'-N1	6.87	113.69	108.20
34	2	864	G	C5-C6-O6	-6.87	124.48	128.60
34	2	1297	A	C4-C5-C6	6.87	120.43	117.00
34	2	1825	A	C5-C6-N6	-6.87	118.21	123.70
34	2	336	C	O4'-C1'-N1	6.87	113.69	108.20
34	2	451	U	O4'-C1'-N1	6.86	113.69	108.20
34	2	1002	C	N3-C4-N4	6.86	122.80	118.00
34	2	1154	G	C5-C6-O6	-6.86	124.48	128.60
34	2	449	C	O4'-C1'-N1	6.86	113.69	108.20
34	2	343	C	O4'-C1'-N1	6.86	113.69	108.20
34	2	349	U	O4'-C1'-N1	6.86	113.69	108.20
34	2	147	A	C4-C5-C6	6.86	120.43	117.00
34	2	1747	C	O4'-C1'-N1	6.85	113.68	108.20
34	2	286	C	N3-C4-N4	6.85	122.80	118.00
34	2	1703	C	O4'-C1'-N1	6.85	113.68	108.20
34	2	68	A	C5-C6-N6	-6.85	118.22	123.70
34	2	586	U	O4'-C1'-N1	6.85	113.68	108.20
25	a	86	GLU	N-CA-CB	6.85	122.92	110.60
34	2	94	G	C5-C6-O6	-6.85	124.49	128.60
34	2	1833	U	O4'-C1'-N1	6.85	113.68	108.20
34	2	1473	U	O4'-C1'-N1	6.85	113.68	108.20
34	2	1730	A	C4-C5-C6	6.85	120.42	117.00
34	2	925	G	C5-C6-O6	-6.84	124.49	128.60
34	2	875	C	N3-C4-N4	6.84	122.79	118.00
34	2	1315	U	O4'-C1'-N1	6.84	113.67	108.20
34	2	1834	U	O4'-C1'-N1	6.84	113.67	108.20
34	2	1493	G	C5-C6-O6	-6.84	124.50	128.60
34	2	322	G	C5-C6-O6	-6.84	124.50	128.60
34	2	911	G	O4'-C1'-N9	6.84	113.67	108.20
34	2	672	U	O4'-C1'-N1	6.83	113.67	108.20
34	2	936	U	O4'-C1'-N1	6.83	113.67	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1838	U	O4'-C1'-N1	6.83	113.67	108.20
1	1	12	C	N3-C4-N4	6.83	122.78	118.00
1	1	34	C	N3-C4-N4	6.83	122.78	118.00
34	2	561	U	O4'-C1'-N1	6.83	113.67	108.20
34	2	966	G	C5-C6-O6	-6.83	124.50	128.60
34	2	1750	C	N3-C4-N4	6.83	122.78	118.00
34	2	1318	G	C5-C6-O6	-6.83	124.50	128.60
34	2	1423	C	O4'-C1'-N1	6.83	113.66	108.20
34	2	592	G	C5-C6-O6	-6.83	124.50	128.60
38	k	510	HIS	C-N-CA	6.83	138.77	121.70
34	2	334	U	O4'-C1'-N1	6.83	113.66	108.20
34	2	810	U	O4'-C1'-N1	6.83	113.66	108.20
34	2	1728	U	O4'-C1'-N1	6.83	113.66	108.20
34	2	358	U	O4'-C1'-N1	6.82	113.66	108.20
34	2	1141	A	C4-C5-C6	6.82	120.41	117.00
34	2	1463	C	O4'-C1'-N1	6.82	113.66	108.20
34	2	929	G	C5-C6-O6	-6.82	124.51	128.60
34	2	1294	G	O4'-C1'-N9	6.82	113.66	108.20
34	2	604	G	C5-C6-O6	-6.82	124.51	128.60
34	2	14	C	O4'-C1'-N1	6.82	113.65	108.20
34	2	1389	G	C5-C6-O6	-6.82	124.51	128.60
34	2	1562	G	C5-C6-O6	-6.82	124.51	128.60
34	2	1203	G	C5-C6-O6	-6.81	124.51	128.60
1	1	21	A	C5-C6-N6	-6.81	118.25	123.70
34	2	209	C	O4'-C1'-N1	6.81	113.65	108.20
34	2	1159	C	O4'-C1'-N1	6.81	113.65	108.20
34	2	373	G	C5-C6-O6	-6.81	124.52	128.60
34	2	1215	C	O4'-C1'-N1	6.80	113.64	108.20
34	2	1623	C	O4'-C1'-N1	6.80	113.64	108.20
34	2	863	G	C5-C6-O6	-6.80	124.52	128.60
34	2	1239	U	O4'-C1'-N1	6.79	113.64	108.20
34	2	504	U	O4'-C1'-N1	6.79	113.63	108.20
34	2	1554	C	O4'-C1'-N1	6.79	113.63	108.20
34	2	97	U	O4'-C1'-N1	6.79	113.63	108.20
34	2	321	C	N3-C4-N4	6.79	122.75	118.00
34	2	874	G	C5-C6-O6	-6.79	124.53	128.60
34	2	1803	A	C5-C6-N6	-6.79	118.27	123.70
13	M	57	TYR	CB-CG-CD2	-6.79	116.93	121.00
34	2	317	G	P-O3'-C3'	6.79	127.84	119.70
34	2	1793	G	C5-C6-O6	-6.79	124.53	128.60
41	3	40	C	OP2-P-O3'	-6.79	90.27	105.20
34	2	622	C	N3-C4-N4	6.78	122.75	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	849	C	O4'-C1'-N1	6.78	113.63	108.20
34	2	960	A	C4-C5-C6	6.78	120.39	117.00
34	2	1086	C	O4'-C1'-N1	6.78	113.62	108.20
34	2	488	C	O4'-C1'-N1	6.78	113.62	108.20
34	2	598	C	N3-C4-N4	6.78	122.74	118.00
34	2	1827	C	O4'-C1'-N1	6.78	113.62	108.20
34	2	100	U	O4'-C1'-N1	6.78	113.62	108.20
34	2	1325	U	O4'-C1'-N1	6.78	113.62	108.20
34	2	540	C	N3-C4-N4	6.77	122.74	118.00
34	2	615	G	C5-C6-O6	-6.77	124.54	128.60
34	2	832	G	C5-C6-O6	-6.77	124.54	128.60
34	2	1251	G	C5-C6-O6	-6.77	124.54	128.60
34	2	1662	U	O4'-C1'-N1	6.77	113.62	108.20
34	2	155	G	C5-C6-O6	-6.77	124.54	128.60
34	2	216	U	O4'-C1'-N1	6.77	113.62	108.20
34	2	1508	C	O4'-C1'-N1	6.77	113.62	108.20
34	2	1655	C	O4'-C1'-N1	6.77	113.61	108.20
34	2	1263	C	O4'-C1'-N1	6.76	113.61	108.20
34	2	597	U	O4'-C1'-N1	6.76	113.61	108.20
34	2	34	U	O4'-C1'-N1	6.76	113.61	108.20
34	2	1233	C	O4'-C1'-N1	6.76	113.61	108.20
34	2	1843	G	O4'-C1'-N9	6.76	113.61	108.20
34	2	1070	C	O4'-C1'-N1	6.76	113.61	108.20
34	2	1740	A	C4-C5-C6	6.75	120.38	117.00
34	2	480	C	N3-C4-N4	6.75	122.73	118.00
34	2	531	U	O4'-C1'-N1	6.75	113.60	108.20
34	2	611	C	N3-C4-N4	6.75	122.73	118.00
34	2	1464	C	O4'-C1'-N1	6.75	113.60	108.20
34	2	415	G	C5-C6-O6	-6.75	124.55	128.60
34	2	144	U	O4'-C1'-N1	6.75	113.60	108.20
34	2	1615	A	C4-C5-C6	6.75	120.37	117.00
34	2	1808	G	C5-C6-O6	-6.75	124.55	128.60
45	w	13	PHE	CB-CG-CD1	6.75	125.52	120.80
34	2	418	U	O4'-C1'-N1	6.75	113.60	108.20
34	2	1497	C	N3-C4-N4	6.75	122.72	118.00
34	2	1637	U	O4'-C1'-N1	6.75	113.60	108.20
34	2	311	C	N3-C4-N4	6.74	122.72	118.00
34	2	1122	G	O4'-C1'-N9	6.74	113.59	108.20
34	2	1831	G	C5-C6-O6	-6.74	124.55	128.60
49	t	435	TYR	CB-CG-CD2	-6.74	116.96	121.00
34	2	1292	U	O4'-C1'-N1	6.74	113.59	108.20
34	2	1305	C	O4'-C1'-N1	6.74	113.59	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	36	U	O4'-C1'-N1	6.74	113.59	108.20
34	2	16	G	C5-C6-O6	-6.74	124.56	128.60
34	2	1354	U	O4'-C1'-N1	6.74	113.59	108.20
34	2	1559	C	N3-C4-N4	6.74	122.72	118.00
34	2	1595	G	C5-C6-O6	-6.74	124.56	128.60
34	2	5	U	O4'-C1'-N1	6.73	113.59	108.20
34	2	797	U	O4'-C1'-N1	6.73	113.59	108.20
34	2	911	G	C5-C6-O6	-6.73	124.56	128.60
34	2	1070	C	N3-C4-N4	6.73	122.71	118.00
34	2	1135	C	C6-N1-C1'	-6.73	112.72	120.80
34	2	294	C	O4'-C1'-N1	6.73	113.58	108.20
34	2	350	A	C5-C6-N6	-6.73	118.32	123.70
34	2	363	G	N1-C6-O6	6.73	123.94	119.90
34	2	539	C	N3-C4-N4	6.73	122.71	118.00
34	2	1143	C	N3-C4-N4	6.73	122.71	118.00
34	2	1725	U	O4'-C1'-N1	6.73	113.58	108.20
34	2	397	G	C5-C6-O6	-6.72	124.56	128.60
34	2	471	C	N3-C4-N4	6.72	122.71	118.00
34	2	626	C	N3-C4-N4	6.72	122.71	118.00
34	2	1199	G	C5-C6-O6	-6.72	124.56	128.60
34	2	1588	C	O4'-C1'-N1	6.72	113.58	108.20
9	I	145	PHE	CB-CG-CD1	6.72	125.50	120.80
34	2	852	C	O4'-C1'-N1	6.72	113.58	108.20
34	2	1404	U	O4'-C1'-N1	6.72	113.58	108.20
34	2	1420	G	C5-C6-O6	-6.72	124.57	128.60
34	2	1542	C	O4'-C1'-N1	6.72	113.58	108.20
34	2	665	U	O4'-C1'-N1	6.72	113.58	108.20
34	2	674	G	C5-C6-O6	-6.72	124.57	128.60
34	2	1351	C	O4'-C1'-N1	6.72	113.58	108.20
34	2	1579	G	C5-C6-O6	-6.72	124.57	128.60
34	2	1575	A	C5-C6-N6	-6.72	118.33	123.70
34	2	75	G	O4'-C1'-N9	6.71	113.57	108.20
34	2	472	G	C5-C6-O6	-6.71	124.57	128.60
34	2	1171	G	C5-C6-O6	-6.71	124.57	128.60
34	2	520	U	O4'-C1'-N1	6.71	113.57	108.20
34	2	973	C	N3-C4-N4	6.71	122.70	118.00
34	2	1591	U	O4'-C1'-N1	6.71	113.57	108.20
34	2	1858	U	O4'-C1'-N1	6.71	113.57	108.20
34	2	594	A	C4-C5-C6	6.71	120.35	117.00
34	2	1503	G	C5-C6-O6	-6.71	124.58	128.60
34	2	233	A	C4-C5-C6	6.71	120.35	117.00
34	2	67	C	OP2-P-O3'	6.71	119.95	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	575	C	O4'-C1'-N1	6.71	113.56	108.20
34	2	33	G	C5-C6-O6	-6.70	124.58	128.60
34	2	1463	C	N3-C4-N4	6.70	122.69	118.00
34	2	571	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	917	G	C5-C6-O6	-6.70	124.58	128.60
34	2	69	C	N3-C4-N4	6.70	122.69	118.00
34	2	291	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	523	A	C5-C6-N1	-6.70	114.35	117.70
34	2	550	A	C5-C6-N6	-6.70	118.34	123.70
34	2	642	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	942	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	194	C	O4'-C1'-N1	6.70	113.56	108.20
34	2	473	C	O4'-C1'-N1	6.70	113.56	108.20
34	2	1263	C	N3-C4-N4	6.70	122.69	118.00
34	2	1066	A	C4-C5-C6	6.70	120.35	117.00
34	2	1484	C	N3-C4-N4	6.70	122.69	118.00
38	k	513	LYS	CA-C-N	6.70	131.93	117.20
34	2	115	U	O4'-C1'-N1	6.69	113.55	108.20
34	2	48	C	N3-C4-N4	6.69	122.68	118.00
34	2	468	G	O4'-C1'-N9	6.69	113.55	108.20
34	2	1853	A	C5-C6-N6	-6.69	118.35	123.70
34	2	872	C	N3-C4-N4	6.69	122.68	118.00
34	2	977	A	C5-C6-N6	-6.69	118.35	123.70
34	2	177	G	C5-C6-O6	-6.69	124.59	128.60
34	2	1289	A	C5-C6-N6	-6.69	118.35	123.70
34	2	301	C	N3-C4-N4	6.69	122.68	118.00
34	2	1127	G	C5-C6-O6	-6.69	124.59	128.60
34	2	841	G	C5-C6-O6	-6.68	124.59	128.60
34	2	465	C	N3-C4-N4	6.68	122.68	118.00
34	2	1299	C	O4'-C1'-N1	6.68	113.55	108.20
34	2	420	C	N3-C4-N4	6.68	122.68	118.00
34	2	402	G	N3-C2-N2	6.68	124.58	119.90
34	2	529	C	N3-C4-N4	6.68	122.68	118.00
34	2	1355	U	O4'-C1'-N1	6.68	113.54	108.20
34	2	362	U	O4'-C1'-N1	6.68	113.54	108.20
34	2	105	U	O4'-C1'-N1	6.68	113.54	108.20
34	2	126	G	C5-C6-O6	-6.67	124.60	128.60
34	2	168	C	O4'-C1'-N1	6.67	113.54	108.20
34	2	1201	C	N3-C4-N4	6.67	122.67	118.00
1	1	58	A	C4-C5-C6	6.67	120.33	117.00
34	2	87	U	O4'-C1'-N1	6.67	113.53	108.20
34	2	1044	G	C5-C6-O6	-6.67	124.60	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1787	A	C5-C6-N1	-6.67	114.37	117.70
11	K	149	TYR	CB-CG-CD2	-6.67	117.00	121.00
34	2	1612	G	C5-C6-O6	-6.67	124.60	128.60
34	2	1062	U	O4'-C1'-N1	6.66	113.53	108.20
34	2	1377	G	C5-C6-O6	-6.66	124.60	128.60
34	2	1638	U	O4'-C1'-N1	6.66	113.53	108.20
34	2	229	A	C4-C5-C6	6.66	120.33	117.00
34	2	957	G	C5-C6-O6	-6.66	124.61	128.60
34	2	1029	G	C5-C6-O6	-6.66	124.61	128.60
34	2	1700	C	O4'-C1'-N1	6.66	113.53	108.20
34	2	1767	C	O4'-C1'-N1	6.66	113.53	108.20
34	2	298	G	C5-C6-O6	-6.66	124.61	128.60
34	2	442	G	C5-C6-O6	-6.66	124.61	128.60
34	2	1767	C	N3-C4-N4	6.65	122.66	118.00
34	2	193	C	N3-C4-N4	6.65	122.66	118.00
34	2	640	A	C5-C6-N6	-6.65	118.38	123.70
34	2	854	A	C5-C6-N1	-6.65	114.37	117.70
34	2	808	A	C5-C6-N6	-6.65	118.38	123.70
34	2	1800	A	C5-C6-N6	-6.65	118.38	123.70
34	2	317	G	C5-C6-O6	-6.65	124.61	128.60
34	2	1618	A	O4'-C1'-N9	6.64	113.52	108.20
34	2	57	U	O4'-C1'-N1	6.64	113.51	108.20
34	2	238	G	C5-C6-O6	-6.64	124.61	128.60
34	2	1095	G	C5-C6-O6	-6.64	124.61	128.60
34	2	355	C	N3-C4-N4	6.64	122.65	118.00
34	2	549	G	C5-C6-O6	-6.64	124.61	128.60
34	2	1175	G	C5-C6-O6	-6.64	124.61	128.60
34	2	573	A	C5-C6-N6	-6.64	118.39	123.70
34	2	838	C	N3-C4-N4	6.64	122.65	118.00
34	2	991	G	C5-C6-O6	-6.64	124.62	128.60
34	2	1192	A	C4-C5-C6	6.64	120.32	117.00
34	2	619	A	C4-C5-C6	6.64	120.32	117.00
34	2	999	U	O4'-C1'-N1	6.64	113.51	108.20
34	2	101	U	O4'-C1'-N1	6.63	113.51	108.20
34	2	924	G	C5-C6-O6	-6.63	124.62	128.60
34	2	1842	U	O4'-C1'-N1	6.63	113.51	108.20
34	2	391	A	N1-C6-N6	6.63	122.58	118.60
34	2	1685	U	O4'-C1'-N1	6.63	113.51	108.20
34	2	1738	G	C5-C6-O6	-6.63	124.62	128.60
34	2	425	A	C5-C6-N6	-6.63	118.39	123.70
34	2	1288	C	O4'-C1'-N1	6.63	113.50	108.20
34	2	1822	C	N3-C4-N4	6.63	122.64	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	19	G	C5-C6-O6	-6.63	124.62	128.60
34	2	1262	C	O4'-C1'-N1	6.63	113.50	108.20
34	2	328	G	C5-C6-O6	-6.63	124.62	128.60
34	2	1074	C	O4'-C1'-N1	6.63	113.50	108.20
34	2	1188	U	O4'-C1'-N1	6.63	113.50	108.20
34	2	1279	C	O4'-C1'-N1	6.63	113.50	108.20
41	3	64	A	C4-C5-C6	6.63	120.31	117.00
34	2	1272	A	C5-C6-N6	-6.63	118.40	123.70
34	2	455	A	C4-C5-C6	6.62	120.31	117.00
34	2	1682	C	N3-C4-N4	6.62	122.64	118.00
1	1	34	C	O4'-C1'-N1	6.62	113.50	108.20
34	2	230	C	O4'-C1'-N1	6.62	113.50	108.20
34	2	1403	U	O4'-C1'-N1	6.62	113.50	108.20
34	2	1556	A	C4-C5-C6	6.62	120.31	117.00
34	2	282	G	C5-C6-O6	-6.62	124.63	128.60
34	2	164	A	C5-C6-N6	-6.62	118.41	123.70
34	2	1357	G	C5-C6-O6	-6.62	124.63	128.60
34	2	1609	A	C5-C6-N6	-6.62	118.41	123.70
34	2	1713	G	N3-C2-N2	6.62	124.53	119.90
34	2	1613	C	O4'-C1'-N1	6.62	113.49	108.20
34	2	876	G	C5-C6-O6	-6.62	124.63	128.60
34	2	1346	U	O4'-C1'-N1	6.62	113.49	108.20
34	2	1440	U	O4'-C1'-N1	6.62	113.49	108.20
34	2	1766	C	N3-C4-N4	6.62	122.63	118.00
11	K	142	SER	C-N-CA	6.61	138.23	121.70
34	2	576	G	C5-C6-O6	-6.61	124.63	128.60
34	2	1048	A	C5-C6-N6	-6.61	118.41	123.70
34	2	1449	C	C2-N1-C1'	6.61	126.07	118.80
34	2	1846	C	N3-C4-N4	6.61	122.63	118.00
34	2	575	C	N3-C4-N4	6.61	122.62	118.00
34	2	1142	C	O4'-C1'-N1	6.61	113.49	108.20
34	2	1457	G	C5-C6-O6	-6.60	124.64	128.60
34	2	102	A	C4-C5-C6	6.60	120.30	117.00
34	2	308	C	O4'-C1'-N1	6.60	113.48	108.20
34	2	428	G	O4'-C1'-N9	6.60	113.48	108.20
34	2	1469	G	C5-C6-O6	-6.60	124.64	128.60
34	2	1518	C	N3-C4-N4	6.59	122.61	118.00
34	2	71	G	C5-C6-O6	-6.59	124.64	128.60
34	2	1533	C	O4'-C1'-N1	6.59	113.47	108.20
1	1	23	C	N3-C4-N4	6.59	122.61	118.00
34	2	851	G	C5-C6-O6	-6.59	124.64	128.60
34	2	1088	G	C5-C6-O6	-6.59	124.65	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1643	G	C5-C6-O6	-6.59	124.64	128.60
34	2	446	C	N3-C4-N4	6.59	122.61	118.00
34	2	1216	A	C5-C6-N6	-6.59	118.43	123.70
34	2	1331	G	N3-C2-N2	6.59	124.51	119.90
34	2	341	G	O4'-C1'-N9	6.59	113.47	108.20
34	2	577	A	C4-C5-C6	6.58	120.29	117.00
34	2	1099	C	N3-C4-N4	6.58	122.61	118.00
34	2	1365	A	C4-C5-C6	6.58	120.29	117.00
34	2	1646	A	C5-C6-N6	-6.58	118.43	123.70
34	2	497	G	C5-C6-O6	-6.58	124.65	128.60
34	2	1419	C	O4'-C1'-N1	6.58	113.47	108.20
34	2	616	G	C5-C6-O6	-6.58	124.65	128.60
34	2	877	G	C5-C6-O6	-6.58	124.65	128.60
34	2	968	A	C4-C5-C6	6.58	120.29	117.00
34	2	1417	A	C4-C5-C6	6.58	120.29	117.00
34	2	1428	U	O4'-C1'-N1	6.58	113.46	108.20
34	2	280	G	C5-C6-O6	-6.58	124.65	128.60
34	2	889	U	O4'-C1'-N1	6.58	113.46	108.20
34	2	1240	U	O4'-C1'-N1	6.58	113.46	108.20
34	2	1448	A	C5-C6-N6	-6.58	118.44	123.70
34	2	313	C	N3-C4-N4	6.58	122.60	118.00
34	2	1788	C	N3-C4-N4	6.58	122.60	118.00
34	2	276	U	O4'-C1'-N1	6.57	113.46	108.20
34	2	1700	C	N3-C4-N4	6.57	122.60	118.00
34	2	12	U	O4'-C1'-N1	6.57	113.46	108.20
34	2	33	G	O4'-C1'-N9	6.57	113.46	108.20
34	2	419	C	O4'-C1'-N1	6.57	113.46	108.20
34	2	1739	G	C5-C6-O6	-6.57	124.66	128.60
34	2	104	A	C4-C5-C6	6.57	120.29	117.00
34	2	186	G	O4'-C1'-N9	6.57	113.46	108.20
34	2	1439	C	O4'-C1'-N1	6.57	113.46	108.20
34	2	387	G	C5-C6-O6	-6.57	124.66	128.60
34	2	402	G	C5-C6-O6	-6.57	124.66	128.60
34	2	539	C	O4'-C1'-N1	6.57	113.45	108.20
34	2	1836	C	N3-C4-N4	6.57	122.60	118.00
34	2	653	C	N3-C4-N4	6.57	122.60	118.00
34	2	80	G	P-O3'-C3'	6.56	127.58	119.70
34	2	1765	G	C5-C6-O6	-6.56	124.66	128.60
34	2	806	A	C4-C5-C6	6.56	120.28	117.00
34	2	1126	G	C5-C6-O6	-6.56	124.66	128.60
34	2	1721	G	C5-C6-O6	-6.56	124.66	128.60
34	2	281	U	O4'-C1'-N1	6.56	113.45	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	370	G	C5-C6-O6	-6.56	124.66	128.60
34	2	647	U	O4'-C1'-N1	6.56	113.45	108.20
34	2	1627	G	C5-C6-O6	-6.56	124.66	128.60
47	r	223	ALA	N-CA-CB	6.56	119.28	110.10
34	2	1677	C	N3-C4-N4	6.56	122.59	118.00
34	2	811	U	O4'-C1'-N1	6.56	113.44	108.20
34	2	74	G	C5-C6-O6	-6.55	124.67	128.60
34	2	1332	C	N3-C4-N4	6.55	122.59	118.00
34	2	419	C	N3-C4-N4	6.55	122.59	118.00
13	M	57	TYR	CB-CG-CD1	6.55	124.93	121.00
34	2	1293	U	O4'-C1'-N1	6.55	113.44	108.20
34	2	1168	U	O4'-C1'-N1	6.55	113.44	108.20
34	2	1219	A	P-O3'-C3'	-6.55	111.84	119.70
34	2	1303	U	O4'-C1'-N1	6.55	113.44	108.20
34	2	1270	G	C5-C6-O6	-6.55	124.67	128.60
34	2	1525	U	O4'-C1'-N1	6.55	113.44	108.20
34	2	1197	U	O4'-C1'-N1	6.54	113.44	108.20
34	2	1228	U	O4'-C1'-N1	6.54	113.44	108.20
34	2	1408	C	N3-C4-N4	6.54	122.58	118.00
34	2	1049	C	N3-C4-N4	6.54	122.58	118.00
34	2	184	G	C5-C6-O6	-6.54	124.67	128.60
34	2	1464	C	N3-C4-N4	6.54	122.58	118.00
34	2	1797	U	O4'-C1'-N1	6.54	113.43	108.20
34	2	1732	G	O4'-C1'-N9	6.54	113.43	108.20
34	2	589	A	C5-C6-N6	-6.54	118.47	123.70
34	2	907	C	N3-C4-N4	6.54	122.58	118.00
34	2	1262	C	N3-C4-N4	6.54	122.58	118.00
34	2	1854	A	C5-C6-N6	-6.54	118.47	123.70
34	2	933	C	N3-C4-N4	6.54	122.58	118.00
34	2	1250	C	O4'-C1'-N1	6.54	113.43	108.20
34	2	1796	C	N3-C4-N4	6.54	122.57	118.00
38	k	408	ASN	C-N-CA	6.54	138.04	121.70
34	2	872	C	O4'-C1'-N1	6.53	113.43	108.20
36	B	289	GLY	N-CA-C	6.53	129.44	113.10
34	2	1577	C	N3-C4-N4	6.53	122.57	118.00
34	2	1635	A	C4-C5-C6	6.53	120.27	117.00
34	2	1729	G	C5-C6-O6	-6.53	124.68	128.60
34	2	4	C	O4'-C1'-N1	6.53	113.42	108.20
34	2	469	C	N3-C4-N4	6.53	122.57	118.00
34	2	1054	A	C4-C5-C6	6.53	120.27	117.00
34	2	1570	G	O4'-C1'-N9	6.53	113.42	108.20
37	j	21	SER	N-CA-CB	6.53	120.30	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	75	G	C5-C6-O6	-6.53	124.68	128.60
34	2	170	A	C4-C5-C6	6.53	120.26	117.00
34	2	537	G	C5-C6-O6	-6.53	124.68	128.60
34	2	1382	A	C4-C5-C6	6.53	120.26	117.00
34	2	182	C	O4'-C1'-N1	6.53	113.42	108.20
34	2	1451	A	C5-C6-N1	-6.53	114.44	117.70
34	2	70	G	C5-C6-O6	-6.52	124.69	128.60
34	2	1305	C	N3-C4-N4	6.52	122.57	118.00
34	2	884	U	O4'-C1'-N1	6.52	113.42	108.20
34	2	527	C	N3-C4-N4	6.52	122.56	118.00
34	2	1193	G	C5-C6-O6	-6.52	124.69	128.60
34	2	1856	G	C5-C6-O6	-6.52	124.69	128.60
34	2	1317	G	C5-C6-O6	-6.52	124.69	128.60
34	2	1481	U	O4'-C1'-N1	6.51	113.41	108.20
34	2	1733	C	N3-C4-N4	6.51	122.56	118.00
40	R	37	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	1	47	U	O4'-C1'-N1	6.51	113.41	108.20
34	2	31	U	O4'-C1'-N1	6.51	113.41	108.20
34	2	151	C	N3-C4-N4	6.51	122.56	118.00
34	2	1230	C	N3-C4-N4	6.51	122.56	118.00
34	2	1801	C	N3-C4-N4	6.51	122.56	118.00
34	2	637	U	O4'-C1'-N1	6.51	113.41	108.20
34	2	1165	G	C5-C6-O6	-6.51	124.69	128.60
34	2	1569	C	O4'-C1'-N1	6.51	113.41	108.20
34	2	1600	G	C5-C6-O6	-6.51	124.69	128.60
34	2	190	A	C4-C5-C6	6.51	120.25	117.00
34	2	1174	U	O4'-C1'-N1	6.51	113.41	108.20
34	2	1274	A	C5-C6-N6	-6.51	118.49	123.70
34	2	959	A	C5-C6-N6	-6.50	118.50	123.70
34	2	1075	C	O4'-C1'-N1	6.50	113.40	108.20
34	2	1414	C	O4'-C1'-N1	6.50	113.40	108.20
34	2	894	U	O4'-C1'-N1	6.50	113.40	108.20
34	2	1177	A	C5-C6-N6	-6.50	118.50	123.70
34	2	90	G	C5-C6-O6	-6.50	124.70	128.60
34	2	1329	U	O4'-C1'-N1	6.50	113.40	108.20
34	2	1704	G	C5-C6-O6	-6.50	124.70	128.60
34	2	92	A	C4-C5-C6	6.50	120.25	117.00
34	2	275	C	C2-N1-C1'	6.50	125.95	118.80
34	2	1622	C	N3-C4-N4	6.50	122.55	118.00
34	2	1798	U	O4'-C1'-N1	6.50	113.40	108.20
1	1	56	C	O4'-C1'-N1	6.50	113.40	108.20
34	2	673	G	C5-C6-O6	-6.50	124.70	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	840	U	O4'-C1'-N1	6.49	113.39	108.20
34	2	1139	A	C4-C5-C6	6.49	120.25	117.00
34	2	1273	C	N3-C4-N4	6.49	122.55	118.00
34	2	1344	G	C5-C6-O6	-6.49	124.70	128.60
34	2	1268	C	N3-C4-N4	6.49	122.54	118.00
34	2	1517	A	C4-C5-C6	6.49	120.25	117.00
34	2	308	C	N3-C4-N4	6.49	122.54	118.00
34	2	1515	G	C4-N9-C1'	6.49	134.94	126.50
34	2	324	C	N3-C4-N4	6.49	122.54	118.00
34	2	410	G	C5-C6-O6	-6.49	124.71	128.60
34	2	180	G	C5-C6-O6	-6.48	124.71	128.60
34	2	231	C	N3-C4-N4	6.48	122.54	118.00
34	2	988	A	C4-C5-C6	6.48	120.24	117.00
34	2	1843	G	C5-C6-O6	-6.48	124.71	128.60
34	2	623	C	N3-C4-N4	6.48	122.54	118.00
34	2	1278	A	C4-C5-C6	6.48	120.24	117.00
34	2	386	U	O4'-C1'-N1	6.48	113.38	108.20
34	2	466	A	C5-C6-N6	-6.48	118.52	123.70
34	2	501	U	O4'-C1'-N1	6.48	113.38	108.20
34	2	800	U	O4'-C1'-N1	6.48	113.38	108.20
34	2	1272	A	C4-C5-C6	6.48	120.24	117.00
34	2	1742	C	N3-C4-N4	6.48	122.53	118.00
34	2	1520	C	N3-C4-N4	6.47	122.53	118.00
38	k	567	ARG	NE-CZ-NH2	6.47	123.54	120.30
34	2	512	A	C4-C5-C6	6.47	120.24	117.00
34	2	608	C	N3-C4-N4	6.47	122.53	118.00
34	2	1805	C	N3-C4-N4	6.47	122.53	118.00
1	1	54	A	C4-C5-C6	6.47	120.23	117.00
34	2	339	A	C5-C6-N6	-6.47	118.52	123.70
34	2	1222	G	C5-C6-O6	-6.47	124.72	128.60
34	2	1755	U	O4'-C1'-N1	6.47	113.38	108.20
34	2	1784	A	C4-C5-C6	6.47	120.23	117.00
34	2	51	U	O4'-C1'-N1	6.47	113.37	108.20
34	2	839	C	N3-C4-N4	6.47	122.53	118.00
34	2	1297	A	O4'-C1'-N9	6.47	113.37	108.20
34	2	549	G	O4'-C1'-N9	6.46	113.37	108.20
34	2	1532	A	C4-C5-C6	6.46	120.23	117.00
41	3	52	A	C5-C6-N6	-6.46	118.53	123.70
34	2	996	C	O4'-C1'-N1	6.46	113.37	108.20
34	2	1526	A	C5-C6-N1	-6.46	114.47	117.70
34	2	1187	C	N3-C4-N4	6.46	122.52	118.00
34	2	1219	A	C4-C5-C6	6.46	120.23	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	287	U	O4'-C1'-N1	6.46	113.37	108.20
34	2	1275	C	N3-C4-N4	6.46	122.52	118.00
34	2	1560	C	N3-C4-N4	6.46	122.52	118.00
34	2	1792	C	O4'-C1'-N1	6.46	113.37	108.20
34	2	119	U	O4'-C1'-N1	6.45	113.36	108.20
34	2	1172	G	O4'-C1'-N9	6.45	113.36	108.20
34	2	1285	U	O4'-C1'-N1	6.45	113.36	108.20
34	2	1724	U	O4'-C1'-N1	6.45	113.36	108.20
34	2	474	A	C4-C5-C6	6.45	120.22	117.00
34	2	1131	C	N3-C4-N4	6.45	122.52	118.00
34	2	1375	A	C4-C5-C6	6.45	120.22	117.00
34	2	103	A	C5-C6-N6	-6.45	118.54	123.70
34	2	348	C	N3-C4-N4	6.45	122.51	118.00
34	2	622	C	O4'-C1'-N1	6.45	113.36	108.20
34	2	1342	U	O4'-C1'-N1	6.45	113.36	108.20
34	2	1610	U	O4'-C1'-N1	6.45	113.36	108.20
34	2	1618	A	C4-C5-C6	6.45	120.22	117.00
34	2	1620	U	O4'-C1'-N1	6.45	113.36	108.20
1	1	26	G	C5-C6-O6	-6.45	124.73	128.60
34	2	211	U	O4'-C1'-N1	6.45	113.36	108.20
34	2	1128	C	N3-C4-N4	6.45	122.51	118.00
34	2	1198	U	O4'-C1'-N1	6.45	113.36	108.20
34	2	1859	C	O4'-C1'-N1	6.45	113.36	108.20
9	I	145	PHE	CB-CG-CD2	-6.44	116.29	120.80
34	2	1068	U	O4'-C1'-N1	6.44	113.35	108.20
34	2	1702	U	O4'-C1'-N1	6.44	113.35	108.20
34	2	829	C	N3-C4-N4	6.44	122.51	118.00
34	2	1060	C	N3-C4-N4	6.44	122.51	118.00
35	A	269	PHE	CB-CG-CD1	6.44	125.31	120.80
34	2	1208	G	O4'-C1'-N9	6.44	113.35	108.20
34	2	227	A	C5-C6-N6	-6.43	118.55	123.70
34	2	666	C	N3-C4-N4	6.43	122.50	118.00
34	2	1661	C	N3-C4-N4	6.43	122.50	118.00
34	2	436	G	C5-C6-O6	-6.43	124.74	128.60
34	2	530	U	O4'-C1'-N1	6.43	113.34	108.20
34	2	902	U	O4'-C1'-N1	6.43	113.34	108.20
34	2	1138	G	C5-C6-O6	-6.43	124.74	128.60
34	2	1492	U	O4'-C1'-N1	6.43	113.34	108.20
11	K	149	TYR	CB-CG-CD1	6.43	124.86	121.00
34	2	977	A	C4-C5-C6	6.43	120.21	117.00
34	2	1548	C	O4'-C1'-N1	6.43	113.34	108.20
34	2	1264	C	N3-C4-N4	6.43	122.50	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	558	C	N3-C4-N4	6.42	122.50	118.00
34	2	862	U	O4'-C1'-N1	6.42	113.34	108.20
34	2	1015	C	O4'-C1'-N1	6.42	113.34	108.20
34	2	868	A	C4-C5-C6	6.42	120.21	117.00
34	2	1210	A	C4-C5-C6	6.42	120.21	117.00
34	2	1370	C	N3-C4-N4	6.42	122.50	118.00
34	2	1665	C	N3-C4-N4	6.42	122.50	118.00
34	2	488	C	N3-C4-N4	6.42	122.49	118.00
34	2	1587	C	O4'-C1'-N1	6.42	113.34	108.20
34	2	521	A	C5-C6-N1	-6.42	114.49	117.70
34	2	1308	G	N3-C2-N2	6.42	124.39	119.90
34	2	1369	C	O4'-C1'-N1	6.42	113.33	108.20
34	2	214	A	C4-C5-C6	6.42	120.21	117.00
34	2	342	U	O4'-C1'-N1	6.42	113.33	108.20
34	2	962	U	O4'-C1'-N1	6.42	113.33	108.20
34	2	1349	A	C5-C6-N6	-6.42	118.57	123.70
34	2	416	A	C4-C5-C6	6.41	120.21	117.00
34	2	1467	C	N3-C4-N4	6.41	122.49	118.00
38	k	455	ILE	CA-C-N	-6.41	103.09	117.20
34	2	50	A	C4-C5-C6	6.41	120.20	117.00
34	2	460	G	O4'-C1'-N9	6.41	113.33	108.20
34	2	907	C	O4'-C1'-N1	6.41	113.33	108.20
34	2	937	C	N3-C4-N4	6.41	122.48	118.00
34	2	1630	C	N3-C4-N4	6.41	122.49	118.00
34	2	505	G	C5-C6-O6	-6.41	124.76	128.60
34	2	1276	G	C5-C6-O6	-6.41	124.76	128.60
34	2	148	U	O4'-C1'-N1	6.41	113.32	108.20
34	2	175	A	O4'-C1'-N9	6.41	113.33	108.20
34	2	848	G	C5-C6-O6	-6.41	124.76	128.60
34	2	1298	G	C5-C6-O6	-6.41	124.76	128.60
34	2	816	U	O4'-C1'-N1	6.40	113.32	108.20
34	2	1474	U	O4'-C1'-N1	6.40	113.32	108.20
34	2	1564	A	C4-C5-C6	6.40	120.20	117.00
34	2	1648	U	O4'-C1'-N1	6.40	113.32	108.20
34	2	312	C	N3-C4-N4	6.40	122.48	118.00
34	2	834	G	C5-C6-O6	-6.40	124.76	128.60
34	2	1552	C	O4'-C1'-N1	6.40	113.32	108.20
1	1	14	C	N3-C4-N4	6.39	122.48	118.00
34	2	1034	U	O4'-C1'-N1	6.39	113.31	108.20
38	k	481	ASP	CB-CG-OD1	6.39	124.05	118.30
1	1	45	G	O4'-C1'-N9	6.39	113.31	108.20
34	2	544	A	C4-C5-C6	6.39	120.19	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1024	A	C4-C5-C6	6.39	120.19	117.00
34	2	1373	U	O4'-C1'-N1	6.39	113.31	108.20
34	2	380	C	N3-C4-N4	6.39	122.47	118.00
34	2	331	C	N3-C4-N4	6.38	122.47	118.00
34	2	1680	U	O4'-C1'-N1	6.38	113.31	108.20
34	2	524	G	O4'-C1'-N9	6.38	113.31	108.20
34	2	925	G	O4'-C1'-N9	6.38	113.31	108.20
34	2	1630	C	O4'-C1'-N1	6.38	113.31	108.20
1	1	40	C	N3-C4-N4	6.38	122.47	118.00
34	2	405	A	C5-C6-N6	-6.38	118.60	123.70
1	1	38	A	C5-C6-N6	-6.38	118.60	123.70
34	2	1601	G	C5-C6-O6	-6.38	124.77	128.60
34	2	831	C	O4'-C1'-N1	6.38	113.30	108.20
34	2	1046	A	O4'-C1'-N9	6.38	113.30	108.20
34	2	623	C	O4'-C1'-N1	6.37	113.30	108.20
34	2	1652	G	C5-C6-O6	-6.37	124.78	128.60
34	2	64	A	C5-C6-N6	-6.37	118.60	123.70
34	2	350	A	C4-C5-C6	6.37	120.19	117.00
34	2	1060	C	O4'-C1'-N1	6.37	113.30	108.20
34	2	417	U	O4'-C1'-N1	6.37	113.29	108.20
34	2	1213	A	C4-C5-C6	6.37	120.18	117.00
34	2	1386	U	O4'-C1'-N1	6.37	113.29	108.20
34	2	341	G	C5-C6-O6	-6.36	124.78	128.60
34	2	657	U	O4'-C1'-N1	6.36	113.29	108.20
34	2	1352	G	C5-C6-O6	-6.36	124.78	128.60
34	2	1494	A	C4-C5-C6	6.36	120.18	117.00
34	2	1850	C	N3-C4-N4	6.36	122.45	118.00
34	2	1071	C	N3-C4-N4	6.36	122.45	118.00
34	2	392	C	N3-C4-N4	6.36	122.45	118.00
48	s	54	TYR	CB-CG-CD2	-6.36	117.18	121.00
34	2	1064	G	C5-C6-O6	-6.36	124.78	128.60
34	2	112	U	O4'-C1'-N1	6.36	113.29	108.20
34	2	522	C	N3-C4-N4	6.36	122.45	118.00
34	2	799	C	N3-C4-N4	6.36	122.45	118.00
34	2	46	A	C4-C5-C6	6.36	120.18	117.00
34	2	1681	G	O4'-C1'-N9	6.36	113.28	108.20
34	2	13	C	O4'-C1'-N1	6.35	113.28	108.20
34	2	109	U	O4'-C1'-N1	6.35	113.28	108.20
34	2	365	U	O4'-C1'-N1	6.35	113.28	108.20
34	2	1049	C	O4'-C1'-N1	6.35	113.28	108.20
34	2	1261	A	C4-C5-C6	6.35	120.18	117.00
34	2	408	A	C4-C5-C6	6.35	120.18	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1190	A	C5-C6-N1	-6.35	114.52	117.70
34	2	1557	C	O4'-C1'-N1	6.35	113.28	108.20
1	1	17	C	OP2-P-O3'	-6.35	91.23	105.20
34	2	428	G	C5-C6-O6	-6.35	124.79	128.60
34	2	551	A	C4-C5-C6	6.35	120.17	117.00
34	2	1014	U	O4'-C1'-N1	6.35	113.28	108.20
34	2	1044	G	N3-C2-N2	6.35	124.34	119.90
34	2	569	C	N3-C4-N4	6.34	122.44	118.00
34	2	1787	A	C4-C5-C6	6.34	120.17	117.00
34	2	1645	A	C4-C5-C6	6.34	120.17	117.00
1	1	10	G	C5-C6-O6	-6.34	124.80	128.60
34	2	606	A	C4-C5-C6	6.34	120.17	117.00
34	2	984	C	N3-C4-N4	6.34	122.44	118.00
34	2	1384	A	C4-C5-C6	6.34	120.17	117.00
34	2	1683	C	N3-C4-N4	6.34	122.44	118.00
45	w	268	ARG	C-N-CA	6.34	137.54	121.70
34	2	583	C	O4'-C1'-N1	6.33	113.27	108.20
34	2	822	A	C5-C6-N1	-6.33	114.53	117.70
34	2	893	U	O4'-C1'-N1	6.33	113.27	108.20
34	2	996	C	N3-C4-N4	6.33	122.43	118.00
34	2	1827	C	N3-C4-N4	6.33	122.43	118.00
34	2	892	U	O4'-C1'-N1	6.33	113.27	108.20
34	2	970	C	N3-C4-N4	6.33	122.43	118.00
34	2	1791	U	O4'-C1'-N1	6.33	113.27	108.20
34	2	78	C	O4'-C1'-N1	6.33	113.26	108.20
34	2	1589	A	C4-C5-C6	6.33	120.17	117.00
34	2	1853	A	C4-C5-C6	6.33	120.17	117.00
34	2	171	A	N1-C6-N6	6.33	122.40	118.60
34	2	189	G	C5-C6-O6	-6.33	124.80	128.60
34	2	1577	C	O4'-C1'-N1	6.33	113.26	108.20
34	2	306	C	N3-C4-N4	6.33	122.43	118.00
34	2	618	A	C4-C5-C6	6.33	120.16	117.00
34	2	1295	A	C4-C5-C6	6.33	120.16	117.00
34	2	82	G	C5-C6-O6	-6.32	124.81	128.60
34	2	106	C	N3-C4-N4	6.32	122.43	118.00
34	2	858	A	C4-C5-C6	6.32	120.16	117.00
34	2	905	G	C5-C6-O6	-6.32	124.81	128.60
34	2	1073	A	C4-C5-C6	6.32	120.16	117.00
34	2	1541	G	C5-C6-O6	-6.32	124.81	128.60
34	2	1603	U	O4'-C1'-N1	6.32	113.26	108.20
34	2	40	A	C4-C5-C6	6.32	120.16	117.00
34	2	829	C	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(°)
34	2	299	G	C5-C6-O6	-6.32	124.81	128.60
34	2	563	U	O4'-C1'-N1	6.32	113.25	108.20
34	2	1140	A	C4-C5-C6	6.32	120.16	117.00
34	2	352	C	N3-C4-N4	6.32	122.42	118.00
34	2	565	A	C4-C5-C6	6.32	120.16	117.00
34	2	883	U	O4'-C1'-N1	6.32	113.25	108.20
34	2	988	A	C5-C6-N6	-6.32	118.65	123.70
34	2	1516	C	N3-C4-N4	6.32	122.42	118.00
1	1	13	G	O4'-C1'-N9	6.32	113.25	108.20
34	2	116	U	O4'-C1'-N1	6.32	113.25	108.20
34	2	599	U	O4'-C1'-N1	6.32	113.25	108.20
34	2	843	A	C4-C5-C6	6.32	120.16	117.00
34	2	912	A	P-O3'-C3'	6.32	127.28	119.70
34	2	1825	A	C4-C5-C6	6.32	120.16	117.00
34	2	1282	G	C5-C6-O6	-6.31	124.81	128.60
34	2	467	G	O4'-C1'-N9	6.31	113.25	108.20
34	2	659	A	C4-C5-C6	6.31	120.16	117.00
34	2	964	U	O4'-C1'-N1	6.31	113.25	108.20
34	2	67	C	O3'-P-O5'	-6.31	92.01	104.00
34	2	366	A	C5-C6-N6	-6.31	118.65	123.70
34	2	580	A	C4-C5-C6	6.31	120.16	117.00
34	2	825	C	N3-C4-N4	6.31	122.42	118.00
34	2	888	U	O4'-C1'-N1	6.31	113.25	108.20
34	2	1686	U	O4'-C1'-N1	6.31	113.25	108.20
45	w	323	PHE	CB-CG-CD1	6.31	125.22	120.80
1	1	21	A	C4-C5-C6	6.31	120.15	117.00
34	2	84	A	C4-C5-C6	6.31	120.15	117.00
34	2	361	A	C4-C5-C6	6.31	120.15	117.00
34	2	140	U	P-O3'-C3'	6.31	127.27	119.70
34	2	1080	A	C4-C5-C6	6.31	120.15	117.00
34	2	1148	U	O4'-C1'-N1	6.31	113.24	108.20
34	2	120	U	O4'-C1'-N1	6.30	113.24	108.20
34	2	89	C	N3-C4-N4	6.30	122.41	118.00
34	2	479	A	C5-C6-N6	-6.30	118.66	123.70
34	2	234	C	O4'-C1'-N1	6.30	113.24	108.20
34	2	614	C	O4'-C1'-N1	6.30	113.24	108.20
34	2	979	A	C4-C5-C6	6.30	120.15	117.00
34	2	1022	C	N3-C4-N4	6.30	122.41	118.00
34	2	1089	A	C4-C5-C6	6.30	120.15	117.00
34	2	1307	C	O4'-C1'-N1	6.30	113.24	108.20
34	2	444	U	O4'-C1'-N1	6.30	113.24	108.20
34	2	918	A	C4-C5-C6	6.30	120.15	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1023	A	C5-C6-N1	-6.30	114.55	117.70
34	2	1465	A	C5-C6-N6	-6.30	118.66	123.70
34	2	433	U	O4'-C1'-N1	6.29	113.24	108.20
34	2	447	C	N3-C4-N4	6.29	122.41	118.00
34	2	614	C	N3-C4-N4	6.29	122.41	118.00
34	2	914	U	O4'-C1'-N1	6.29	113.23	108.20
34	2	1245	C	O4'-C1'-N1	6.29	113.23	108.20
34	2	1372	A	C4-C5-C6	6.29	120.15	117.00
34	2	675	A	O4'-C1'-N9	6.29	113.23	108.20
34	2	11	A	C4-C5-C6	6.29	120.14	117.00
34	2	676	U	O4'-C1'-N1	6.29	113.23	108.20
34	2	230	C	N3-C4-N4	6.29	122.40	118.00
34	2	1003	C	N3-C4-N4	6.29	122.40	118.00
34	2	1527	C	N3-C4-N4	6.29	122.40	118.00
34	2	1626	U	O4'-C1'-N1	6.29	113.23	108.20
34	2	398	A	C4-C5-C6	6.29	120.14	117.00
34	2	1213	A	C5-C6-N6	-6.29	118.67	123.70
34	2	1157	U	O4'-C1'-N1	6.28	113.23	108.20
34	2	645	A	C4-C5-C6	6.28	120.14	117.00
34	2	1828	A	C4-C5-C6	6.28	120.14	117.00
34	2	1508	C	N3-C4-N4	6.28	122.39	118.00
34	2	1058	A	C4-C5-C6	6.28	120.14	117.00
34	2	1340	A	C4-C5-C6	6.28	120.14	117.00
34	2	329	A	C4-C5-C6	6.28	120.14	117.00
34	2	927	C	N3-C4-N4	6.28	122.39	118.00
34	2	1046	A	C4-C5-C6	6.28	120.14	117.00
34	2	1181	C	N3-C4-N4	6.28	122.39	118.00
34	2	1450	A	C4-C5-C6	6.28	120.14	117.00
34	2	1052	U	O4'-C1'-N1	6.27	113.22	108.20
34	2	1713	G	C5-C6-O6	-6.27	124.84	128.60
40	R	37	TYR	CB-CG-CD1	6.27	124.76	121.00
34	2	1737	C	N3-C4-N4	6.27	122.39	118.00
34	2	509	A	C5-C6-N1	-6.27	114.57	117.70
34	2	1726	A	C5-C6-N6	-6.27	118.69	123.70
34	2	83	A	C4-C5-C6	6.26	120.13	117.00
34	2	392	C	N3-C4-C5	-6.26	119.39	121.90
34	2	998	U	O4'-C1'-N1	6.26	113.21	108.20
34	2	1043	C	N3-C4-N4	6.26	122.39	118.00
34	2	1453	U	O4'-C1'-N1	6.26	113.21	108.20
34	2	414	C	N3-C4-N4	6.26	122.38	118.00
34	2	1169	A	C4-C5-C6	6.26	120.13	117.00
34	2	164	A	C4-C5-C6	6.26	120.13	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1621	C	N3-C4-N4	6.26	122.38	118.00
34	2	1646	A	C4-C5-C6	6.26	120.13	117.00
1	1	50	A	O4'-C1'-N9	6.26	113.21	108.20
34	2	506	A	C4-C5-C6	6.26	120.13	117.00
34	2	1032	A	C4-C5-C6	6.26	120.13	117.00
34	2	1242	A	C4-C5-C6	6.26	120.13	117.00
34	2	177	G	N3-C2-N2	6.26	124.28	119.90
34	2	372	C	O4'-C1'-N1	6.26	113.21	108.20
34	2	729	C	N3-C4-N4	6.26	122.38	118.00
34	2	1532	A	C5-C6-N6	-6.26	118.69	123.70
34	2	10	G	C5-C6-O6	-6.26	124.85	128.60
34	2	1660	G	C5-C6-O6	-6.26	124.85	128.60
34	2	1369	C	N3-C4-N4	6.25	122.38	118.00
34	2	1517	A	C5-C6-N1	-6.25	114.57	117.70
34	2	1712	C	N3-C4-N4	6.25	122.38	118.00
34	2	545	A	C5-C6-N6	-6.25	118.70	123.70
34	2	987	G	C4-N9-C1'	6.25	134.63	126.50
34	2	1444	A	C4-C5-C6	6.25	120.13	117.00
34	2	1826	A	C4-C5-C6	6.25	120.13	117.00
38	k	150	SER	C-N-CA	-6.25	106.07	121.70
34	2	366	A	C4-C5-C6	6.25	120.13	117.00
34	2	1388	U	O4'-C1'-N1	6.25	113.20	108.20
34	2	388	A	C5-C6-N6	-6.25	118.70	123.70
34	2	541	U	O4'-C1'-N1	6.25	113.20	108.20
34	2	1030	A	C4-C5-C6	6.25	120.12	117.00
34	2	1636	A	C5-C6-N6	-6.25	118.70	123.70
34	2	1513	C	C2-N1-C1'	6.25	125.67	118.80
34	2	630	A	C4-C5-C6	6.24	120.12	117.00
34	2	467	G	C5-C6-O6	-6.24	124.86	128.60
1	1	62	C	N3-C4-N4	6.24	122.37	118.00
34	2	21	U	O4'-C1'-N1	6.24	113.19	108.20
34	2	479	A	C4-C5-C6	6.24	120.12	117.00
34	2	485	U	O4'-C1'-N1	6.24	113.19	108.20
34	2	1170	U	OP1-P-O3'	6.24	118.93	105.20
34	2	946	C	N3-C4-N4	6.24	122.37	118.00
34	2	1726	A	C4-C5-C6	6.24	120.12	117.00
34	2	1069	U	O4'-C1'-N1	6.23	113.19	108.20
34	2	1190	A	C5-C6-N6	-6.23	118.71	123.70
38	k	510	HIS	CA-C-N	6.23	130.91	117.20
34	2	382	A	C5-C6-N6	-6.23	118.72	123.70
34	2	1632	A	C4-C5-C6	6.23	120.11	117.00
34	2	439	A	C4-C5-C6	6.23	120.11	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	921	G	C5-C6-O6	-6.23	124.86	128.60
34	2	958	A	C4-C5-C6	6.23	120.11	117.00
34	2	975	C	N3-C4-N4	6.23	122.36	118.00
34	2	1625	A	C5-C6-N1	-6.23	114.59	117.70
34	2	443	C	N3-C4-N4	6.23	122.36	118.00
34	2	826	A	C4-C5-C6	6.23	120.11	117.00
34	2	1313	U	O4'-C1'-N1	6.22	113.18	108.20
34	2	582	C	O4'-C1'-N1	6.22	113.18	108.20
34	2	1020	A	C4-C5-C6	6.22	120.11	117.00
34	2	288	A	C4-C5-C6	6.22	120.11	117.00
34	2	967	G	C5-C6-O6	-6.22	124.87	128.60
34	2	1089	A	C5-C6-N1	-6.22	114.59	117.70
34	2	1513	C	N3-C4-C5	-6.22	119.41	121.90
34	2	1613	C	N3-C4-N4	6.22	122.35	118.00
34	2	1792	C	N3-C4-N4	6.22	122.35	118.00
34	2	518	A	C5-C6-N6	-6.21	118.73	123.70
34	2	667	G	C5-C6-O6	-6.21	124.87	128.60
34	2	986	A	C5-C6-N6	-6.21	118.73	123.70
34	2	1020	A	C5-C6-N6	-6.21	118.73	123.70
34	2	1097	U	O4'-C1'-N1	6.21	113.17	108.20
34	2	1224	A	C5-C6-N6	-6.21	118.73	123.70
34	2	1328	A	C5-C6-N6	-6.21	118.73	123.70
34	2	1663	U	O4'-C1'-N1	6.21	113.17	108.20
34	2	228	A	C4-C5-C6	6.21	120.11	117.00
34	2	338	A	C4-C5-C6	6.21	120.11	117.00
34	2	1656	A	C4-C5-C6	6.21	120.11	117.00
34	2	1301	C	N3-C4-N4	6.21	122.35	118.00
34	2	99	A	C5-C6-N6	-6.21	118.73	123.70
34	2	304	A	C4-C5-C6	6.21	120.10	117.00
34	2	511	A	C4-C5-C6	6.21	120.11	117.00
34	2	283	A	C4-C5-C6	6.21	120.10	117.00
34	2	1302	U	O4'-C1'-N1	6.21	113.17	108.20
34	2	1363	U	O4'-C1'-N1	6.21	113.17	108.20
34	2	1479	A	O4'-C1'-N9	6.21	113.17	108.20
45	w	256	TYR	CB-CG-CD2	-6.21	117.28	121.00
9	I	28	TYR	CB-CG-CD2	-6.21	117.28	121.00
34	2	513	A	C4-C5-C6	6.21	120.10	117.00
34	2	1602	A	C4-C5-C6	6.21	120.10	117.00
34	2	1689	U	O4'-C1'-N1	6.21	113.16	108.20
1	1	33	C	O4'-C1'-N1	6.20	113.16	108.20
34	2	1375	A	C5-C6-N6	-6.20	118.74	123.70
34	2	1398	A	C5-C6-N6	-6.20	118.74	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1431	C	O4'-C1'-N1	6.20	113.16	108.20
34	2	1596	A	C5-C6-N6	-6.20	118.74	123.70
34	2	1666	G	N3-C2-N2	6.20	124.24	119.90
34	2	644	A	C4-C5-C6	6.20	120.10	117.00
34	2	1480	A	C4-C5-C6	6.20	120.10	117.00
34	2	1498	C	N3-C4-N4	6.20	122.34	118.00
34	2	195	C	O4'-C1'-N1	6.20	113.16	108.20
34	2	1379	A	C4-C5-C6	6.20	120.10	117.00
45	w	256	TYR	CB-CG-CD1	6.20	124.72	121.00
34	2	32	U	O4'-C1'-N1	6.20	113.16	108.20
34	2	1588	C	N3-C4-N4	6.20	122.34	118.00
41	3	52	A	C4-C5-C6	6.20	120.10	117.00
34	2	882	A	C5-C6-N6	-6.20	118.74	123.70
1	1	2	A	O4'-C1'-N9	6.20	113.16	108.20
34	2	4	C	N3-C4-N4	6.20	122.34	118.00
34	2	929	G	O4'-C1'-N9	6.20	113.16	108.20
34	2	1385	C	N3-C4-N4	6.20	122.34	118.00
34	2	554	A	C4-C5-C6	6.19	120.10	117.00
34	2	963	C	N3-C4-N4	6.19	122.34	118.00
1	1	66	C	N3-C4-N4	6.19	122.33	118.00
34	2	1839	A	C4-C5-C6	6.19	120.10	117.00
34	2	1860	A	C4-C5-C6	6.19	120.10	117.00
34	2	487	C	N3-C4-N4	6.19	122.33	118.00
34	2	674	G	O4'-C1'-N9	6.19	113.15	108.20
34	2	1006	G	O4'-C1'-N9	6.19	113.15	108.20
34	2	1673	A	C4-C5-C6	6.19	120.09	117.00
34	2	1005	A	C5-C6-N6	-6.19	118.75	123.70
34	2	1794	A	C4-C5-C6	6.19	120.09	117.00
1	1	76	A	C5-C6-N6	-6.19	118.75	123.70
34	2	377	C	N3-C4-N4	6.19	122.33	118.00
34	2	566	A	C4-C5-C6	6.19	120.09	117.00
34	2	1078	A	C4-C5-C6	6.18	120.09	117.00
34	2	1614	A	C4-C5-C6	6.18	120.09	117.00
34	2	1783	G	C5-C6-O6	-6.18	124.89	128.60
34	2	77	A	C4-C5-C6	6.18	120.09	117.00
34	2	886	U	O4'-C1'-N1	6.18	113.15	108.20
34	2	1380	C	N3-C4-N4	6.18	122.33	118.00
34	2	1413	C	N3-C4-N4	6.18	122.33	118.00
34	2	1694	A	C4-C5-C6	6.18	120.09	117.00
34	2	330	C	N3-C4-N4	6.18	122.33	118.00
34	2	595	A	C4-C5-C6	6.18	120.09	117.00
34	2	1145	A	C5-C6-N6	-6.18	118.75	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1479	A	C4-C5-C6	6.18	120.09	117.00
34	2	1501	U	O4'-C1'-N1	6.18	113.14	108.20
34	2	1604	C	N3-C4-C5	-6.18	119.43	121.90
34	2	1395	C	N3-C4-N4	6.18	122.33	118.00
34	2	1518	C	O4'-C1'-N1	6.18	113.14	108.20
34	2	1668	U	O4'-C1'-N1	6.18	113.14	108.20
34	2	1236	A	C5-C6-N6	-6.18	118.76	123.70
34	2	195	C	N3-C4-C5	-6.18	119.43	121.90
34	2	825	C	O4'-C1'-N1	6.18	113.14	108.20
34	2	1378	A	C4-C5-C6	6.18	120.09	117.00
34	2	1719	A	C4-C5-C6	6.18	120.09	117.00
34	2	168	C	N3-C4-N4	6.17	122.32	118.00
34	2	232	A	C4-C5-C6	6.17	120.09	117.00
34	2	310	G	O4'-C1'-N9	6.17	113.14	108.20
34	2	535	A	C5-C6-N6	-6.17	118.76	123.70
34	2	584	A	C4-C5-C6	6.17	120.09	117.00
34	2	1378	A	C5-C6-N6	-6.17	118.76	123.70
34	2	1502	A	C4-C5-C6	6.17	120.09	117.00
34	2	859	U	O4'-C1'-N1	6.17	113.14	108.20
34	2	1236	A	C4-C5-C6	6.17	120.09	117.00
34	2	1124	C	N3-C4-N4	6.17	122.32	118.00
34	2	1629	A	C4-C5-C6	6.17	120.09	117.00
34	2	1715	U	O4'-C1'-N1	6.17	113.14	108.20
34	2	1255	A	C4-C5-C6	6.17	120.08	117.00
34	2	1353	A	C5-C6-N1	-6.17	114.62	117.70
34	2	1391	C	O4'-C1'-N1	6.17	113.14	108.20
34	2	1687	U	O4'-C1'-N1	6.17	113.13	108.20
34	2	220	C	N3-C4-N4	6.17	122.32	118.00
34	2	944	C	N3-C4-N4	6.17	122.32	118.00
34	2	1132	U	O4'-C1'-N1	6.17	113.13	108.20
1	1	41	C	N3-C4-N4	6.16	122.31	118.00
34	2	91	A	C4-C5-C6	6.16	120.08	117.00
34	2	983	A	C4-C5-C6	6.16	120.08	117.00
34	2	1844	A	C5-C6-N1	-6.16	114.62	117.70
34	2	852	C	N3-C4-N4	6.16	122.31	118.00
34	2	1775	A	C5-C6-N6	-6.16	118.77	123.70
34	2	915	A	C4-C5-C6	6.16	120.08	117.00
34	2	1854	A	C4-C5-C6	6.16	120.08	117.00
34	2	1280	A	C5-C6-N6	-6.16	118.78	123.70
34	2	1775	A	C4-C5-C6	6.16	120.08	117.00
34	2	1299	C	C6-N1-C1'	-6.16	113.41	120.80
34	2	1672	U	O4'-C1'-N1	6.16	113.12	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	483	A	C5-C6-N6	-6.15	118.78	123.70
34	2	662	A	C4-C5-C6	6.15	120.08	117.00
34	2	854	A	C4-C5-C6	6.15	120.08	117.00
34	2	1436	C	N3-C4-N4	6.15	122.31	118.00
34	2	238	G	O4'-C1'-N9	6.15	113.12	108.20
34	2	807	A	C5-C6-N1	-6.15	114.62	117.70
34	2	1083	A	C4-C5-C6	6.15	120.08	117.00
34	2	35	C	N3-C4-N4	6.15	122.31	118.00
34	2	861	A	C4-C5-C6	6.15	120.08	117.00
34	2	1349	A	C4-C5-C6	6.15	120.08	117.00
34	2	1578	C	O4'-C1'-N1	6.15	113.12	108.20
34	2	22	A	C5-C6-N6	-6.15	118.78	123.70
34	2	1391	C	N3-C4-N4	6.15	122.30	118.00
34	2	1409	G	O4'-C1'-N9	6.15	113.12	108.20
34	2	1470	A	C5-C6-N6	-6.15	118.78	123.70
34	2	1703	C	N3-C4-C5	-6.15	119.44	121.90
34	2	1145	A	C4-C5-C6	6.15	120.07	117.00
34	2	1585	C	N3-C4-N4	6.15	122.30	118.00
34	2	486	C	N3-C4-N4	6.15	122.30	118.00
34	2	489	G	C5-C6-O6	-6.15	124.91	128.60
34	2	215	U	O4'-C1'-N1	6.14	113.11	108.20
34	2	1401	A	C5-C6-N6	-6.14	118.78	123.70
34	2	1650	C	N3-C4-N4	6.14	122.30	118.00
34	2	1845	A	C4-C5-C6	6.14	120.07	117.00
34	2	388	A	C4-C5-C6	6.14	120.07	117.00
34	2	1234	U	O4'-C1'-N1	6.14	113.11	108.20
34	2	26	U	O4'-C1'-N1	6.14	113.11	108.20
34	2	165	G	C5-C6-O6	-6.14	124.92	128.60
34	2	394	G	O4'-C1'-N9	6.14	113.11	108.20
34	2	1102	C	N3-C4-N4	6.14	122.30	118.00
34	2	1312	C	N3-C4-N4	6.14	122.30	118.00
34	2	1524	C	N3-C4-N4	6.14	122.30	118.00
34	2	1829	A	C4-C5-C6	6.14	120.07	117.00
34	2	809	A	C4-C5-C6	6.14	120.07	117.00
34	2	1222	G	N3-C2-N2	6.14	124.20	119.90
24	Z	41	PHE	CB-CG-CD1	6.14	125.10	120.80
34	2	458	A	C4-C5-C6	6.14	120.07	117.00
34	2	638	A	C4-C5-C6	6.14	120.07	117.00
34	2	858	A	C5-C6-N6	-6.14	118.79	123.70
34	2	1407	G	C5-C6-O6	-6.14	124.92	128.60
34	2	1596	A	C4-C5-C6	6.14	120.07	117.00
1	1	76	A	C4-C5-C6	6.13	120.07	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	398	A	C5-C6-N6	-6.13	118.79	123.70
34	2	1209	C	N3-C4-N4	6.13	122.29	118.00
34	2	1401	A	C4-C5-C6	6.13	120.07	117.00
45	w	13	PHE	CB-CG-CD2	-6.13	116.51	120.80
34	2	490	A	C4-C5-C6	6.13	120.07	117.00
34	2	1063	C	N3-C4-N4	6.13	122.29	118.00
1	1	24	G	O4'-C1'-N9	6.13	113.11	108.20
1	1	59	A	C4-C5-C6	6.13	120.06	117.00
34	2	121	U	O4'-C1'-N1	6.13	113.10	108.20
34	2	340	C	N3-C4-N4	6.13	122.29	118.00
34	2	347	C	N3-C4-N4	6.13	122.29	118.00
34	2	1557	C	N3-C4-N4	6.13	122.29	118.00
34	2	214	A	C5-C6-N6	-6.13	118.80	123.70
34	2	565	A	C5-C6-N6	-6.13	118.80	123.70
34	2	1366	A	C5-C6-N6	-6.13	118.80	123.70
34	2	1466	C	N3-C4-N4	6.13	122.29	118.00
34	2	240	C	O4'-C1'-N1	6.12	113.10	108.20
34	2	425	A	C4-C5-C6	6.12	120.06	117.00
34	2	545	A	C4-C5-C6	6.12	120.06	117.00
34	2	823	A	C4-C5-C6	6.12	120.06	117.00
34	2	992	A	C4-C5-C6	6.12	120.06	117.00
34	2	643	A	C4-C5-C6	6.12	120.06	117.00
34	2	1554	C	N3-C4-N4	6.12	122.28	118.00
34	2	181	A	C4-C5-C6	6.12	120.06	117.00
34	2	1739	G	N3-C2-N2	6.12	124.18	119.90
34	2	518	A	C4-C5-C6	6.12	120.06	117.00
34	2	1038	A	C5-C6-N6	-6.12	118.81	123.70
34	2	1226	C	N3-C4-N4	6.12	122.28	118.00
34	2	1711	C	N3-C4-N4	6.12	122.28	118.00
34	2	1863	A	C5-C6-N6	-6.12	118.81	123.70
34	2	1237	A	C4-C5-C6	6.11	120.06	117.00
34	2	1589	A	C5-C6-N6	-6.11	118.81	123.70
34	2	53	C	N3-C4-N4	6.11	122.28	118.00
34	2	1659	A	C4-C5-C6	6.11	120.06	117.00
34	2	835	C	C2-N1-C1'	6.11	125.52	118.80
34	2	1120	C	N3-C4-N4	6.11	122.28	118.00
34	2	1807	A	C4-C5-C6	6.11	120.06	117.00
34	2	73	C	O4'-C1'-N1	6.11	113.08	108.20
34	2	141	A	C5-C6-N6	-6.11	118.81	123.70
34	2	833	A	C4-C5-C6	6.11	120.05	117.00
34	2	1611	U	O4'-C1'-N1	6.11	113.09	108.20
34	2	1644	U	O4'-C1'-N1	6.11	113.09	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	574	A	C5-C6-N6	-6.11	118.81	123.70
34	2	953	A	C4-C5-C6	6.11	120.05	117.00
34	2	1189	U	O4'-C1'-N1	6.11	113.08	108.20
34	2	332	C	N3-C4-N4	6.10	122.27	118.00
34	2	1242	A	C5-C6-N6	-6.10	118.82	123.70
34	2	731	C	N3-C4-N4	6.10	122.27	118.00
34	2	99	A	C4-C5-C6	6.10	120.05	117.00
34	2	218	A	C4-C5-C6	6.10	120.05	117.00
34	2	326	A	C4-C5-C6	6.10	120.05	117.00
34	2	404	A	C5-C6-N6	-6.10	118.82	123.70
34	2	490	A	C5-C6-N6	-6.10	118.82	123.70
34	2	994	A	C5-C6-N1	-6.10	114.65	117.70
34	2	1123	C	N3-C4-N4	6.10	122.27	118.00
34	2	1141	A	C5-C6-N6	-6.10	118.82	123.70
34	2	1495	U	O4'-C1'-N1	6.10	113.08	108.20
34	2	1540	A	O4'-C1'-N9	6.10	113.08	108.20
1	1	69	U	O4'-C1'-N1	6.10	113.08	108.20
34	2	445	A	C4-C5-C6	6.10	120.05	117.00
34	2	98	C	N3-C4-N4	6.09	122.27	118.00
34	2	149	A	O4'-C1'-N9	6.09	113.08	108.20
34	2	361	A	C5-C6-N6	-6.09	118.82	123.70
34	2	1161	G	O4'-C1'-N9	6.09	113.08	108.20
34	2	912	A	C4-C5-C6	6.09	120.05	117.00
34	2	1045	A	C5-C6-N1	-6.09	114.65	117.70
34	2	1636	A	C4-C5-C6	6.09	120.05	117.00
49	t	486	PHE	C-N-CA	6.09	136.93	121.70
34	2	63	U	O4'-C1'-N1	6.09	113.07	108.20
34	2	1277	G	O4'-C1'-N9	6.09	113.07	108.20
34	2	225	C	O4'-C1'-N1	6.09	113.07	108.20
34	2	640	A	C4-C5-C6	6.09	120.04	117.00
34	2	1538	U	O4'-C1'-N1	6.09	113.07	108.20
34	2	232	A	C5-C6-N6	-6.08	118.83	123.70
34	2	354	A	C5-C6-N1	-6.08	114.66	117.70
34	2	1803	A	C4-C5-C6	6.08	120.04	117.00
34	2	850	A	C4-C5-C6	6.08	120.04	117.00
34	2	1716	U	O4'-C1'-N1	6.08	113.07	108.20
34	2	343	C	N3-C4-N4	6.08	122.26	118.00
34	2	405	A	C4-C5-C6	6.08	120.04	117.00
34	2	1863	A	C4-C5-C6	6.08	120.04	117.00
34	2	85	A	C5-C6-N1	-6.08	114.66	117.70
34	2	1176	C	N3-C4-N4	6.08	122.26	118.00
34	2	459	A	C4-C5-C6	6.08	120.04	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	516	A	O4'-C1'-N9	6.08	113.06	108.20
34	2	1693	C	N3-C4-N4	6.08	122.25	118.00
34	2	1719	A	C5-C6-N6	-6.08	118.84	123.70
12	L	159	PHE	CB-CG-CD1	6.08	125.05	120.80
34	2	536	G	P-O3'-C3'	6.08	126.99	119.70
34	2	317	G	O4'-C1'-N9	6.07	113.06	108.20
34	2	1178	A	C5-C6-N1	-6.07	114.66	117.70
34	2	1540	A	C4-C5-C6	6.07	120.04	117.00
34	2	1551	A	C4-C5-C6	6.07	120.04	117.00
34	2	1690	A	C4-C5-C6	6.07	120.04	117.00
37	j	95	TYR	CB-CG-CD2	-6.07	117.36	121.00
34	2	1076	A	C4-C5-C6	6.07	120.04	117.00
38	k	440	GLN	O-C-N	-6.07	112.98	122.70
34	2	940	A	C5-C6-N1	-6.07	114.67	117.70
34	2	1079	A	C4-C5-C6	6.07	120.03	117.00
34	2	1333	C	N3-C4-N4	6.07	122.25	118.00
34	2	1625	A	C4-C5-C6	6.07	120.03	117.00
34	2	845	A	C4-C5-C6	6.07	120.03	117.00
34	2	182	C	N3-C4-N4	6.07	122.25	118.00
34	2	42	A	C4-C5-C6	6.07	120.03	117.00
34	2	152	U	O4'-C1'-N1	6.07	113.05	108.20
34	2	449	C	N3-C4-N4	6.07	122.25	118.00
34	2	450	A	C4-C5-C6	6.06	120.03	117.00
34	2	1214	C	N3-C4-N4	6.06	122.24	118.00
34	2	922	A	C4-C5-C6	6.06	120.03	117.00
34	2	940	A	C5-C6-N6	-6.06	118.85	123.70
34	2	1073	A	C5-C6-N6	-6.06	118.85	123.70
34	2	1056	A	O4'-C1'-N9	6.06	113.05	108.20
34	2	1136	G	O4'-C1'-N9	6.06	113.05	108.20
34	2	1227	C	N3-C4-N4	6.06	122.24	118.00
34	2	1247	A	C4-C5-C6	6.06	120.03	117.00
34	2	1306	U	O4'-C1'-N1	6.06	113.05	108.20
34	2	1609	A	C4-C5-C6	6.06	120.03	117.00
34	2	395	G	O4'-C1'-N9	6.06	113.05	108.20
34	2	904	A	C5-C6-N6	-6.06	118.85	123.70
34	2	1583	A	C4-C5-C6	6.06	120.03	117.00
34	2	624	A	C4-C5-C6	6.06	120.03	117.00
34	2	1337	C	N3-C4-N4	6.06	122.24	118.00
34	2	476	A	C4-C5-C6	6.05	120.03	117.00
34	2	1392	A	C4-C5-C6	6.05	120.03	117.00
34	2	1684	C	N3-C4-N4	6.05	122.24	118.00
34	2	127	C	O4'-C1'-N1	6.05	113.04	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	959	A	C4-C5-C6	6.05	120.03	117.00
34	2	1431	C	N3-C4-N4	6.05	122.24	118.00
34	2	643	A	C5-C6-N6	-6.05	118.86	123.70
34	2	1350	G	C5-C6-O6	-6.05	124.97	128.60
34	2	1422	U	O4'-C1'-N1	6.05	113.04	108.20
34	2	1835	C	N3-C4-N4	6.05	122.23	118.00
34	2	453	C	O4'-C1'-N1	6.05	113.04	108.20
34	2	589	A	C4-C5-C6	6.05	120.02	117.00
34	2	960	A	O4'-C1'-N9	6.05	113.04	108.20
34	2	1426	C	N3-C4-N4	6.05	122.23	118.00
34	2	1482	A	C4-C5-C6	6.05	120.02	117.00
34	2	1582	G	C5-C6-O6	-6.05	124.97	128.60
34	2	207	U	O4'-C1'-N1	6.05	113.04	108.20
34	2	554	A	O4'-C1'-N9	6.05	113.04	108.20
34	2	909	A	C4-C5-C6	6.05	120.02	117.00
34	2	1669	G	N3-C2-N2	6.05	124.13	119.90
34	2	1249	A	C4-C5-C6	6.04	120.02	117.00
34	2	205	G	C5-C6-O6	-6.04	124.97	128.60
34	2	850	A	C5-C6-N1	-6.04	114.68	117.70
34	2	1470	A	C4-C5-C6	6.04	120.02	117.00
34	2	1695	C	N3-C4-N4	6.04	122.23	118.00
34	2	195	C	N3-C4-N4	6.04	122.23	118.00
34	2	303	G	O4'-C1'-N9	6.04	113.03	108.20
34	2	327	C	N3-C4-N4	6.04	122.23	118.00
34	2	798	A	C4-C5-C6	6.04	120.02	117.00
34	2	900	A	C5-C6-N1	-6.04	114.68	117.70
34	2	1007	A	C4-C5-C6	6.04	120.02	117.00
34	2	1029	G	N3-C2-N2	6.04	124.13	119.90
34	2	1179	A	C5-C6-N6	-6.04	118.87	123.70
34	2	1639	C	N3-C4-N4	6.04	122.23	118.00
34	2	1862	U	C2-N1-C1'	6.04	124.95	117.70
34	2	514	U	O4'-C1'-N1	6.04	113.03	108.20
34	2	1269	C	N3-C4-N4	6.04	122.23	118.00
34	2	175	A	C4-C5-C6	6.04	120.02	117.00
34	2	423	A	C5-C6-N6	-6.04	118.87	123.70
34	2	951	A	C4-C5-C6	6.04	120.02	117.00
34	2	1494	A	C5-C6-N1	-6.04	114.68	117.70
34	2	1567	C	N3-C4-C5	-6.04	119.48	121.90
34	2	423	A	C5-C6-N1	-6.04	114.68	117.70
34	2	141	A	C4-C5-C6	6.04	120.02	117.00
34	2	297	C	O4'-C1'-N1	6.04	113.03	108.20
34	2	516	A	C4-C5-C6	6.04	120.02	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1008	A	C4-C5-C6	6.04	120.02	117.00
34	2	1274	A	C4-C5-C6	6.04	120.02	117.00
34	2	1780	U	O4'-C1'-N1	6.04	113.03	108.20
34	2	223	A	C4-C5-C6	6.03	120.02	117.00
34	2	916	A	C5-C6-N1	-6.03	114.68	117.70
34	2	1053	C	C6-N1-C1'	-6.03	113.56	120.80
34	2	1368	U	O4'-C1'-N1	6.03	113.03	108.20
34	2	1460	C	O4'-C1'-N1	6.03	113.03	108.20
34	2	1667	U	O4'-C1'-N1	6.03	113.03	108.20
34	2	1734	C	N3-C4-N4	6.03	122.22	118.00
34	2	107	A	C4-C5-C6	6.03	120.02	117.00
34	2	559	A	C4-C5-C6	6.03	120.02	117.00
34	2	1295	A	C5-C6-N6	-6.03	118.87	123.70
42	m	278	PHE	CB-CG-CD1	6.03	125.02	120.80
1	1	58	A	C5-C6-N6	-6.03	118.88	123.70
34	2	1144	A	C4-C5-C6	6.03	120.02	117.00
34	2	1476	A	C4-C5-C6	6.03	120.02	117.00
34	2	107	A	C5-C6-N6	-6.03	118.88	123.70
34	2	169	U	O4'-C1'-N1	6.03	113.02	108.20
34	2	1287	A	C4-C5-C6	6.03	120.01	117.00
34	2	1473	U	C2-N1-C1'	6.03	124.94	117.70
34	2	1710	A	C4-C5-C6	6.03	120.02	117.00
34	2	346	C	N3-C4-N4	6.03	122.22	118.00
34	2	540	C	O4'-C1'-N1	6.03	113.02	108.20
34	2	1365	A	C5-C6-N6	-6.03	118.88	123.70
34	2	442	G	O4'-C1'-N9	6.03	113.02	108.20
34	2	1094	C	N3-C4-N4	6.03	122.22	118.00
34	2	1031	A	C4-C5-C6	6.02	120.01	117.00
34	2	1398	A	C4-C5-C6	6.02	120.01	117.00
34	2	171	A	C4-C5-C6	6.02	120.01	117.00
34	2	346	C	O4'-C1'-N1	6.02	113.02	108.20
34	2	1081	C	N3-C4-C5	-6.02	119.49	121.90
34	2	1590	U	O4'-C1'-N1	6.02	113.02	108.20
34	2	1785	A	C4-C5-C6	6.02	120.01	117.00
34	2	629	C	N3-C4-N4	6.02	122.22	118.00
34	2	20	G	O4'-C1'-N9	6.02	113.02	108.20
34	2	445	A	C5-C6-N1	-6.02	114.69	117.70
34	2	976	A	C5-C6-N6	-6.02	118.88	123.70
34	2	153	G	O4'-C1'-N9	6.02	113.01	108.20
34	2	225	C	N3-C4-N4	6.02	122.21	118.00
34	2	968	A	C5-C6-N1	-6.02	114.69	117.70
34	2	1019	A	C4-C5-C6	6.02	120.01	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1194	G	C5-C6-O6	-6.02	124.99	128.60
34	2	521	A	C4-C5-C6	6.01	120.01	117.00
34	2	1289	A	C4-C5-C6	6.01	120.01	117.00
34	2	24	C	N3-C4-C5	-6.01	119.50	121.90
34	2	805	A	C4-C5-C6	6.01	120.01	117.00
34	2	1574	A	C5-C6-N6	-6.01	118.89	123.70
34	2	1693	C	O4'-C1'-N1	6.01	113.01	108.20
34	2	1001	G	O4'-C1'-N9	6.01	113.01	108.20
34	2	1146	A	C4-C5-C6	6.01	120.01	117.00
34	2	206	A	C5-C6-N1	-6.01	114.70	117.70
34	2	984	C	O4'-C1'-N1	6.01	113.01	108.20
34	2	1405	A	C4-C5-C6	6.01	120.00	117.00
34	2	898	G	O4'-C1'-N9	6.01	113.01	108.20
34	2	1119	C	N3-C4-N4	6.01	122.21	118.00
1	1	35	A	C4-C5-C6	6.01	120.00	117.00
34	2	234	C	N3-C4-C5	-6.00	119.50	121.90
34	2	333	A	C4-C5-C6	6.00	120.00	117.00
34	2	976	A	C4-C5-C6	6.00	120.00	117.00
34	2	1754	G	O4'-C1'-N9	6.00	113.00	108.20
34	2	882	A	C4-C5-C6	6.00	120.00	117.00
34	2	630	A	C5-C6-N6	-6.00	118.90	123.70
34	2	1800	A	C4-C5-C6	6.00	120.00	117.00
34	2	340	C	O4'-C1'-N1	6.00	113.00	108.20
34	2	860	A	C4-C5-C6	6.00	120.00	117.00
34	2	1374	A	C4-C5-C6	6.00	120.00	117.00
34	2	1774	G	O4'-C1'-N9	6.00	113.00	108.20
34	2	1026	A	C4-C5-C6	6.00	120.00	117.00
34	2	1245	C	N3-C4-N4	6.00	122.20	118.00
1	1	67	U	O4'-C1'-N1	5.99	113.00	108.20
34	2	448	A	C5-C6-N6	-5.99	118.91	123.70
34	2	664	C	N3-C4-C5	-5.99	119.50	121.90
34	2	1432	C	N3-C4-N4	5.99	122.19	118.00
34	2	1553	C	N3-C4-N4	5.99	122.19	118.00
37	j	19	ASN	C-N-CA	5.99	136.68	121.70
34	2	979	A	C5-C6-N6	-5.99	118.91	123.70
34	2	1451	A	C4-C5-C6	5.99	120.00	117.00
34	2	528	U	O4'-C1'-N1	5.99	112.99	108.20
34	2	1212	C	O4'-C1'-N1	5.99	112.99	108.20
34	2	1005	A	O4'-C1'-N9	5.99	112.99	108.20
34	2	1659	A	C5-C6-N6	-5.99	118.91	123.70
34	2	339	A	C4-C5-C6	5.99	119.99	117.00
34	2	1264	C	O4'-C1'-N1	5.99	112.99	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1526	A	C5-C6-N6	-5.99	118.91	123.70
34	2	14	C	N3-C4-C5	-5.98	119.51	121.90
34	2	564	A	C4-C5-C6	5.98	119.99	117.00
34	2	1067	G	O4'-C1'-N9	5.98	112.99	108.20
34	2	45	A	C4-C5-C6	5.98	119.99	117.00
34	2	49	C	O4'-C1'-N1	5.98	112.98	108.20
34	2	435	A	C4-C5-C6	5.98	119.99	117.00
34	2	1011	U	O4'-C1'-N1	5.98	112.98	108.20
34	2	166	A	C4-C5-C6	5.98	119.99	117.00
34	2	880	C	N3-C4-N4	5.98	122.19	118.00
34	2	972	G	O4'-C1'-N9	5.98	112.98	108.20
34	2	1067	G	P-O3'-C3'	5.98	126.88	119.70
34	2	1196	A	C4-C5-C6	5.98	119.99	117.00
34	2	1465	A	C4-C5-C6	5.98	119.99	117.00
34	2	1587	C	N3-C4-N4	5.98	122.18	118.00
34	2	1782	A	C4-C5-C6	5.98	119.99	117.00
34	2	404	A	C4-C5-C6	5.98	119.99	117.00
34	2	463	A	C4-C5-C6	5.98	119.99	117.00
34	2	463	A	C5-C6-N6	-5.98	118.92	123.70
34	2	58	C	N3-C4-N4	5.97	122.18	118.00
34	2	502	A	C4-C5-C6	5.97	119.99	117.00
34	2	1607	G	O4'-C1'-N9	5.97	112.98	108.20
34	2	631	A	C4-C5-C6	5.97	119.99	117.00
34	2	943	G	O4'-C1'-N9	5.97	112.98	108.20
34	2	1016	A	C5-C6-N6	-5.97	118.92	123.70
34	2	1616	U	O4'-C1'-N1	5.97	112.98	108.20
1	1	73	A	C4-C5-C6	5.97	119.99	117.00
34	2	293	A	C5-C6-N1	-5.97	114.71	117.70
34	2	517	C	N3-C4-N4	5.97	122.18	118.00
34	2	1735	C	N3-C4-C5	-5.97	119.51	121.90
34	2	1291	A	C5-C6-N1	-5.97	114.72	117.70
34	2	9	U	O4'-C1'-N1	5.97	112.97	108.20
34	2	897	G	C5-C6-O6	-5.97	125.02	128.60
34	2	857	A	C4-C5-C6	5.97	119.98	117.00
34	2	1443	G	O4'-C1'-N9	5.97	112.97	108.20
34	2	1534	U	O4'-C1'-N1	5.97	112.97	108.20
34	2	1691	C	O4'-C1'-N1	5.96	112.97	108.20
35	A	33	TYR	CB-CG-CD1	5.96	124.58	121.00
34	2	381	C	N3-C4-N4	5.96	122.17	118.00
34	2	1224	A	C4-C5-C6	5.96	119.98	117.00
34	2	1307	C	N3-C4-N4	5.96	122.17	118.00
34	2	72	C	N3-C4-N4	5.96	122.17	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	t	435	TYR	CB-CG-CD1	5.96	124.58	121.00
34	2	559	A	C5-C6-N6	-5.96	118.93	123.70
34	2	638	A	C5-C6-N6	-5.96	118.93	123.70
34	2	953	A	C5-C6-N1	-5.96	114.72	117.70
34	2	1472	A	C5-C6-N6	-5.96	118.93	123.70
34	2	1597	U	O4'-C1'-N1	5.96	112.97	108.20
1	1	26	G	O4'-C1'-N9	5.96	112.97	108.20
34	2	812	A	C4-C5-C6	5.96	119.98	117.00
34	2	1005	A	C4-C5-C6	5.96	119.98	117.00
34	2	1101	G	O4'-C1'-N9	5.96	112.96	108.20
34	2	326	A	C5-C6-N1	-5.95	114.72	117.70
34	2	918	A	C5-C6-N6	-5.95	118.94	123.70
34	2	475	A	C4-C5-C6	5.95	119.98	117.00
34	2	1171	G	O4'-C1'-N9	5.95	112.96	108.20
34	2	493	C	N3-C4-N4	5.95	122.16	118.00
34	2	900	A	C4-C5-C6	5.95	119.97	117.00
34	2	1670	A	C5-C6-N6	-5.95	118.94	123.70
34	2	1826	A	C5-C6-N1	-5.95	114.73	117.70
34	2	1090	C	N3-C4-N4	5.95	122.16	118.00
34	2	379	A	C5-C6-N6	-5.95	118.94	123.70
34	2	934	A	C4-C5-C6	5.95	119.97	117.00
34	2	1177	A	C4-C5-C6	5.95	119.97	117.00
34	2	430	G	O4'-C1'-N9	5.94	112.95	108.20
1	1	44	A	C4-C5-C6	5.94	119.97	117.00
34	2	2	A	C4-C5-C6	5.94	119.97	117.00
34	2	288	A	C5-C6-N6	-5.94	118.95	123.70
34	2	423	A	C4-C5-C6	5.94	119.97	117.00
34	2	1243	C	O4'-C1'-N1	5.94	112.95	108.20
34	2	1600	G	N3-C2-N2	5.94	124.06	119.90
34	2	1195	A	C4-C5-C6	5.94	119.97	117.00
34	2	1482	A	C5-C6-N6	-5.94	118.95	123.70
34	2	482	C	O4'-C1'-N1	5.94	112.95	108.20
34	2	1211	C	N3-C4-N4	5.94	122.16	118.00
34	2	1218	G	O4'-C1'-N9	5.94	112.95	108.20
34	2	1441	U	O4'-C1'-N1	5.94	112.95	108.20
34	2	54	A	C4-C5-C6	5.94	119.97	117.00
34	2	188	U	O4'-C1'-N1	5.94	112.95	108.20
34	2	511	A	C5-C6-N1	-5.94	114.73	117.70
34	2	1081	C	N3-C4-N4	5.94	122.16	118.00
34	2	226	A	C4-C5-C6	5.93	119.97	117.00
34	2	474	A	C5-C6-N1	-5.93	114.73	117.70
34	2	510	A	C5-C6-N6	-5.93	118.95	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	523	A	C4-C5-C6	5.93	119.97	117.00
34	2	631	A	C5-C6-N6	-5.93	118.95	123.70
34	2	1250	C	N3-C4-N4	5.93	122.15	118.00
34	2	1657	U	O4'-C1'-N1	5.93	112.95	108.20
34	2	1048	A	C4-C5-C6	5.93	119.97	117.00
34	2	1406	C	N3-C4-N4	5.93	122.15	118.00
34	2	1218	G	O3'-P-O5'	-5.93	92.73	104.00
34	2	1642	A	C4-C5-C6	5.93	119.97	117.00
34	2	1161	G	N1-C6-O6	5.93	123.46	119.90
34	2	1781	G	O4'-C1'-N9	5.93	112.94	108.20
34	2	103	A	C4-C5-C6	5.92	119.96	117.00
34	2	335	U	O4'-C1'-N1	5.92	112.94	108.20
34	2	525	G	O4'-C1'-N9	5.92	112.94	108.20
34	2	1256	A	C4-C5-C6	5.92	119.96	117.00
34	2	1249	A	C5-C6-N6	-5.92	118.96	123.70
34	2	979	A	O4'-C1'-N9	5.92	112.94	108.20
34	2	1004	A	C4-C5-C6	5.92	119.96	117.00
34	2	39	A	C4-C5-C6	5.92	119.96	117.00
34	2	904	A	C5-C6-N1	-5.92	114.74	117.70
34	2	1472	A	P-O3'-C3'	5.92	126.80	119.70
34	2	1812	A	C4-C5-C6	5.92	119.96	117.00
34	2	582	C	N3-C4-N4	5.91	122.14	118.00
1	1	74	C	N3-C4-N4	5.91	122.14	118.00
34	2	1408	C	O4'-C1'-N1	5.91	112.93	108.20
34	2	19	A	C4-C5-C6	5.91	119.95	117.00
34	2	809	A	C5-C6-N6	-5.90	118.98	123.70
34	2	853	U	O4'-C1'-N1	5.90	112.92	108.20
34	2	1127	G	O4'-C1'-N9	5.90	112.92	108.20
34	2	1434	A	C5-C6-N6	-5.90	118.98	123.70
34	2	1461	A	C4-C5-C6	5.90	119.95	117.00
34	2	1584	A	C5-C6-N1	-5.90	114.75	117.70
34	2	899	A	C4-C5-C6	5.90	119.95	117.00
34	2	1533	C	N3-C4-C5	-5.90	119.54	121.90
34	2	1721	G	O4'-C1'-N9	5.90	112.92	108.20
34	2	1255	A	C5-C6-N6	-5.90	118.98	123.70
1	1	42	A	O4'-C1'-N9	5.90	112.92	108.20
34	2	376	C	N3-C4-N4	5.90	122.13	118.00
34	2	821	A	C4-C5-C6	5.90	119.95	117.00
34	2	1038	A	C4-C5-C6	5.90	119.95	117.00
1	1	15	A	C5-C6-N6	-5.89	118.98	123.70
34	2	513	A	O4'-C1'-N9	5.89	112.92	108.20
34	2	1291	A	C4-C5-C6	5.89	119.95	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	509	A	C4-C5-C6	5.89	119.95	117.00
34	2	1139	A	C5-C6-N6	-5.89	118.99	123.70
34	2	1844	A	C4-C5-C6	5.89	119.95	117.00
34	2	27	A	C5-C6-N6	-5.89	118.99	123.70
1	1	30	G	O4'-C1'-N9	5.89	112.91	108.20
34	2	272	C	O4'-C1'-N1	5.89	112.91	108.20
34	2	357	U	O4'-C1'-N1	5.89	112.91	108.20
34	2	1219	A	C5-C6-N6	-5.89	118.99	123.70
34	2	1746	C	O4'-C1'-N1	5.89	112.91	108.20
34	2	498	A	C4-C5-C6	5.89	119.94	117.00
34	2	865	A	C4-C5-C6	5.89	119.94	117.00
34	2	1435	A	C4-C5-C6	5.89	119.94	117.00
34	2	1661	C	N3-C4-C5	-5.89	119.55	121.90
34	2	631	A	C5-C6-N1	-5.88	114.76	117.70
34	2	1641	C	N3-C4-N4	5.88	122.12	118.00
34	2	40	A	C5-C6-N6	-5.88	119.00	123.70
34	2	516	A	C5-C6-N1	-5.88	114.76	117.70
34	2	61	A	C4-C5-C6	5.88	119.94	117.00
34	2	1336	U	O4'-C1'-N1	5.88	112.90	108.20
34	2	1004	A	C5-C6-N6	-5.88	119.00	123.70
34	2	1008	A	C5-C6-N6	-5.88	119.00	123.70
42	m	278	PHE	CB-CG-CD2	-5.88	116.69	120.80
34	2	147	A	C5-C6-N6	-5.88	119.00	123.70
34	2	292	A	C4-C5-C6	5.88	119.94	117.00
34	2	1204	A	C4-C5-C6	5.88	119.94	117.00
34	2	804	A	C4-C5-C6	5.88	119.94	117.00
1	1	59	A	C5-C6-N1	-5.87	114.76	117.70
34	2	814	A	C4-C5-C6	5.87	119.94	117.00
34	2	986	A	C5-C6-N1	-5.87	114.76	117.70
34	2	1051	A	C4-C5-C6	5.87	119.94	117.00
34	2	1414	C	N3-C4-N4	5.87	122.11	118.00
34	2	545	A	C5-C6-N1	-5.87	114.76	117.70
34	2	808	A	O4'-C1'-N9	5.87	112.90	108.20
34	2	1410	A	C5-C6-N1	-5.87	114.77	117.70
34	2	201	G	O4'-C1'-N9	5.87	112.90	108.20
34	2	1082	G	O4'-C1'-N9	5.87	112.89	108.20
34	2	1574	A	C4-C5-C6	5.87	119.93	117.00
34	2	142	C	N3-C4-N4	5.87	122.11	118.00
1	1	56	C	N3-C4-C5	-5.87	119.55	121.90
34	2	333	A	C5-C6-N1	-5.87	114.77	117.70
34	2	871	A	C4-C5-C6	5.87	119.93	117.00
34	2	1096	A	C4-C5-C6	5.87	119.93	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	796	U	O4'-C1'-N1	5.86	112.89	108.20
34	2	1031	A	C5-C6-N6	-5.86	119.01	123.70
34	2	1074	C	N3-C4-N4	5.86	122.10	118.00
34	2	1640	C	N3-C4-N4	5.86	122.11	118.00
34	2	37	C	N3-C4-N4	5.86	122.10	118.00
34	2	1692	A	C5-C6-N6	-5.86	119.01	123.70
34	2	1543	G	O4'-C1'-N9	5.86	112.89	108.20
34	2	1795	A	C4-C5-C6	5.86	119.93	117.00
34	2	1839	A	C5-C6-N6	-5.86	119.01	123.70
34	2	146	G	O4'-C1'-N9	5.86	112.89	108.20
34	2	159	A	C4-C5-C6	5.86	119.93	117.00
34	2	408	A	O4'-C1'-N9	5.86	112.89	108.20
34	2	593	C	O4'-C1'-N1	5.86	112.89	108.20
34	2	1146	A	C5-C6-N1	-5.86	114.77	117.70
34	2	237	G	OP2-P-O3'	5.86	118.08	105.20
34	2	896	C	N3-C4-C5	-5.86	119.56	121.90
34	2	969	C	N3-C4-C5	-5.86	119.56	121.90
34	2	1430	C	N3-C4-N4	5.86	122.10	118.00
34	2	1448	A	C4-C5-C6	5.86	119.93	117.00
34	2	111	A	C4-C5-C6	5.85	119.93	117.00
34	2	356	U	O4'-C1'-N1	5.85	112.88	108.20
34	2	390	C	N3-C4-N4	5.85	122.10	118.00
34	2	496	G	O4'-C1'-N9	5.85	112.88	108.20
34	2	588	G	O4'-C1'-N9	5.85	112.88	108.20
34	2	628	C	N3-C4-N4	5.85	122.10	118.00
34	2	855	G	O4'-C1'-N9	5.85	112.88	108.20
34	2	958	A	C5-C6-N6	-5.85	119.02	123.70
34	2	1035	C	N3-C4-N4	5.85	122.10	118.00
34	2	1476	A	C5-C6-N6	-5.85	119.02	123.70
34	2	307	G	O4'-C1'-N9	5.85	112.88	108.20
34	2	309	A	C4-C5-C6	5.85	119.92	117.00
34	2	382	A	C4-C5-C6	5.85	119.92	117.00
34	2	407	C	N3-C4-N4	5.85	122.09	118.00
34	2	1526	A	C4-C5-C6	5.85	119.92	117.00
34	2	50	A	C5-C6-N6	-5.85	119.02	123.70
34	2	70	G	O4'-C1'-N9	5.85	112.88	108.20
34	2	896	C	N3-C4-N4	5.85	122.09	118.00
34	2	1022	C	O4'-C1'-N1	5.85	112.88	108.20
34	2	64	A	C4-C5-C6	5.84	119.92	117.00
34	2	379	A	C4-C5-C6	5.84	119.92	117.00
34	2	923	C	N3-C4-N4	5.84	122.09	118.00
34	2	454	A	C4-C5-C6	5.84	119.92	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	584	A	C5-C6-N1	-5.84	114.78	117.70
34	2	176	U	O4'-C1'-N1	5.84	112.87	108.20
34	2	633	A	C4-C5-C6	5.84	119.92	117.00
34	2	934	A	C5-C6-N1	-5.84	114.78	117.70
34	2	481	C	N3-C4-N4	5.84	122.09	118.00
34	2	661	A	C4-C5-C6	5.84	119.92	117.00
1	1	2	A	C4-C5-C6	5.84	119.92	117.00
34	2	868	A	C5-C6-N6	-5.84	119.03	123.70
34	2	1703	C	N3-C4-N4	5.84	122.09	118.00
38	k	481	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	1	15	A	C4-C5-C6	5.84	119.92	117.00
34	2	229	A	C5-C6-N1	-5.84	114.78	117.70
34	2	314	U	O4'-C1'-N1	5.84	112.87	108.20
34	2	535	A	C4-C5-C6	5.84	119.92	117.00
34	2	1141	A	C5-C6-N1	-5.84	114.78	117.70
34	2	1227	C	N3-C4-C5	-5.84	119.57	121.90
34	2	1807	A	C5-C6-N1	-5.84	114.78	117.70
34	2	1170	U	N3-C4-O4	5.83	123.48	119.40
34	2	179	C	N3-C4-N4	5.83	122.08	118.00
34	2	651	U	O4'-C1'-N1	5.83	112.87	108.20
34	2	805	A	C5-C6-N6	-5.83	119.03	123.70
34	2	1026	A	C5-C6-N6	-5.83	119.03	123.70
34	2	1468	C	N3-C4-N4	5.83	122.08	118.00
34	2	27	A	C4-C5-C6	5.83	119.91	117.00
1	1	38	A	C4-C5-C6	5.83	119.91	117.00
34	2	1507	U	O4'-C1'-N1	5.83	112.86	108.20
34	2	275	C	O4'-C1'-N1	5.83	112.86	108.20
34	2	1185	A	C5-C6-N1	-5.83	114.79	117.70
34	2	221	A	C4-C5-C6	5.82	119.91	117.00
34	2	475	A	C5-C6-N6	-5.82	119.04	123.70
34	2	1771	G	O4'-C1'-N9	5.82	112.86	108.20
34	2	1808	G	N3-C2-N2	5.82	123.98	119.90
35	A	33	TYR	CB-CG-CD2	-5.82	117.51	121.00
34	2	660	A	C5-C6-N6	-5.82	119.04	123.70
34	2	869	G	P-O3'-C3'	5.82	126.68	119.70
34	2	966	G	O4'-C1'-N9	5.82	112.86	108.20
34	2	1674	A	C5-C6-N6	-5.82	119.04	123.70
34	2	234	C	N3-C4-N4	5.82	122.07	118.00
4	D	84	PHE	CB-CG-CD1	5.82	124.87	120.80
10	J	63	PHE	CB-CG-CD1	5.82	124.87	120.80
34	2	877	G	O4'-C1'-N9	5.82	112.85	108.20
34	2	1651	G	O4'-C1'-N9	5.82	112.85	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1655	C	N3-C4-C5	-5.82	119.57	121.90
34	2	1782	A	C5-C6-N6	-5.82	119.05	123.70
34	2	22	A	C4-C5-C6	5.81	119.91	117.00
34	2	512	A	C5-C6-N1	-5.81	114.79	117.70
34	2	947	C	N3-C4-N4	5.81	122.07	118.00
34	2	166	A	C5-C6-N1	-5.81	114.79	117.70
34	2	462	C	N3-C4-C5	-5.81	119.58	121.90
34	2	554	A	C5-C6-N6	-5.81	119.05	123.70
34	2	1019	A	C5-C6-N6	-5.81	119.05	123.70
34	2	1027	A	C5-C6-N1	-5.81	114.79	117.70
34	2	1710	A	C5-C6-N1	-5.81	114.79	117.70
34	2	595	A	C5-C6-N1	-5.81	114.79	117.70
34	2	458	A	C5-C6-N6	-5.81	119.05	123.70
34	2	819	U	O4'-C1'-N1	5.81	112.85	108.20
34	2	978	G	O4'-C1'-N9	5.81	112.85	108.20
34	2	1154	G	O4'-C1'-N9	5.81	112.85	108.20
34	2	1654	U	O4'-C1'-N1	5.81	112.85	108.20
34	2	25	A	C5-C6-N6	-5.81	119.06	123.70
34	2	1789	G	O4'-C1'-N9	5.81	112.85	108.20
34	2	510	A	O4'-C1'-N9	5.81	112.84	108.20
34	2	228	A	C5-C6-N1	-5.80	114.80	117.70
34	2	483	A	C4-C5-C6	5.80	119.90	117.00
34	2	1356	U	O4'-C1'-N1	5.80	112.84	108.20
41	3	40	C	O3'-P-O5'	5.80	115.03	104.00
34	2	459	A	O4'-C1'-N9	5.80	112.84	108.20
34	2	1344	G	O4'-C1'-N9	5.80	112.84	108.20
34	2	1673	A	C5-C6-N6	-5.80	119.06	123.70
34	2	65	C	N3-C4-N4	5.80	122.06	118.00
34	2	510	A	C4-C5-C6	5.80	119.90	117.00
34	2	835	C	O4'-C1'-N1	5.80	112.84	108.20
34	2	899	A	C5-C6-N1	-5.80	114.80	117.70
34	2	1159	C	N3-C4-C5	-5.80	119.58	121.90
34	2	1387	C	N3-C4-N4	5.80	122.06	118.00
34	2	1727	G	O4'-C1'-N9	5.80	112.84	108.20
34	2	1857	A	C4-C5-C6	5.80	119.90	117.00
34	2	295	C	O4'-C1'-N1	5.80	112.84	108.20
34	2	448	A	C4-C5-C6	5.80	119.90	117.00
34	2	68	A	C4-C5-C6	5.79	119.90	117.00
34	2	551	A	O4'-C1'-N9	5.79	112.83	108.20
34	2	1179	A	C4-C5-C6	5.79	119.90	117.00
34	2	1710	A	C5-C6-N6	-5.79	119.07	123.70
34	2	1482	A	O4'-C1'-N9	5.79	112.83	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	548	G	O4'-C1'-N9	5.79	112.83	108.20
34	2	667	G	N3-C2-N2	5.79	123.95	119.90
34	2	677	C	N3-C4-N4	5.79	122.05	118.00
34	2	857	A	C5-C6-N6	-5.79	119.07	123.70
34	2	1690	A	C5-C6-N6	-5.79	119.07	123.70
38	k	267	ARG	NE-CZ-NH2	5.79	123.19	120.30
34	2	290	A	C4-C5-C6	5.78	119.89	117.00
34	2	609	A	C4-C5-C6	5.78	119.89	117.00
34	2	1235	U	O4'-C1'-N1	5.78	112.83	108.20
34	2	293	A	C4-C5-C6	5.78	119.89	117.00
34	2	1211	C	N3-C4-C5	-5.78	119.59	121.90
44	v	748	ASP	C-N-CA	5.78	136.15	121.70
34	2	142	C	C2-N1-C1'	5.78	125.16	118.80
34	2	185	C	N3-C4-C5	-5.78	119.59	121.90
34	2	609	A	C5-C6-N1	-5.78	114.81	117.70
34	2	1433	C	N3-C4-N4	5.78	122.04	118.00
34	2	1439	C	N3-C4-N4	5.78	122.04	118.00
34	2	1658	A	C4-C5-C6	5.78	119.89	117.00
34	2	633	A	C5-C6-N1	-5.77	114.81	117.70
34	2	399	C	N3-C4-N4	5.77	122.04	118.00
31	g	101	PHE	CB-CG-CD1	5.77	124.84	120.80
34	2	13	C	N3-C4-C5	-5.77	119.59	121.90
34	2	1424	G	O4'-C1'-N9	5.77	112.82	108.20
34	2	900	A	O4'-C1'-N9	5.77	112.81	108.20
34	2	1674	A	C4-C5-C6	5.77	119.88	117.00
34	2	1248	C	N3-C4-N4	5.77	122.04	118.00
34	2	302	C	N3-C4-N4	5.76	122.03	118.00
34	2	533	C	N3-C4-C5	-5.76	119.59	121.90
34	2	1564	A	C5-C6-N6	-5.76	119.09	123.70
34	2	159	A	C5-C6-N1	-5.76	114.82	117.70
34	2	223	A	C5-C6-N6	-5.76	119.09	123.70
34	2	812	A	C5-C6-N6	-5.76	119.09	123.70
1	1	48	C	N3-C4-C5	-5.76	119.59	121.90
34	2	85	A	C4-C5-C6	5.76	119.88	117.00
34	2	218	A	C5-C6-N1	-5.76	114.82	117.70
34	2	495	G	O4'-C1'-N9	5.76	112.81	108.20
34	2	1691	C	N3-C4-C5	-5.76	119.59	121.90
34	2	1016	A	C5-C6-N1	-5.76	114.82	117.70
34	2	1086	C	N3-C4-N4	5.76	122.03	118.00
34	2	1485	A	C5-C6-N6	-5.76	119.09	123.70
34	2	658	A	C4-C5-C6	5.76	119.88	117.00
34	2	851	G	O4'-C1'-N9	5.76	112.81	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	383	U	O4'-C1'-N1	5.76	112.81	108.20
34	2	502	A	C5-C6-N1	-5.76	114.82	117.70
34	2	815	G	O4'-C1'-N9	5.76	112.81	108.20
34	2	1096	A	C5-C6-N1	-5.76	114.82	117.70
34	2	1216	A	C4-C5-C6	5.76	119.88	117.00
34	2	1499	C	N3-C4-N4	5.76	122.03	118.00
34	2	272	C	C5-C4-N4	-5.75	116.17	120.20
34	2	1051	A	C5-C6-N1	-5.75	114.82	117.70
34	2	11	A	C5-C6-N6	-5.75	119.10	123.70
34	2	54	A	C5-C6-N6	-5.75	119.10	123.70
34	2	1300	U	O4'-C1'-N1	5.75	112.80	108.20
34	2	1522	C	N3-C4-N4	5.75	122.03	118.00
34	2	1183	G	N3-C2-N2	5.75	123.93	119.90
34	2	1569	C	N3-C4-C5	-5.75	119.60	121.90
34	2	60	A	C4-C5-C6	5.75	119.88	117.00
34	2	566	A	C5-C6-N1	-5.75	114.83	117.70
34	2	1088	G	O4'-C1'-N9	5.75	112.80	108.20
34	2	1839	A	O4'-C1'-N9	5.75	112.80	108.20
34	2	401	G	O4'-C1'-N9	5.75	112.80	108.20
34	2	422	G	O4'-C1'-N9	5.75	112.80	108.20
34	2	865	A	C5-C6-N6	-5.75	119.10	123.70
34	2	909	A	C5-C6-N6	-5.75	119.10	123.70
34	2	1564	A	C5-C6-N1	-5.75	114.83	117.70
34	2	1696	C	N3-C4-C5	-5.75	119.60	121.90
1	1	44	A	C5-C6-N1	-5.75	114.83	117.70
34	2	1204	A	C5-C6-N6	-5.75	119.10	123.70
34	2	19	A	C5-C6-N1	-5.74	114.83	117.70
34	2	22	A	C5-C6-N1	-5.74	114.83	117.70
34	2	492	C	N3-C4-N4	5.74	122.02	118.00
34	2	1246	A	C5-C6-N6	-5.74	119.11	123.70
34	2	1503	G	O4'-C1'-N9	5.74	112.79	108.20
1	1	73	A	C5-C6-N6	-5.74	119.11	123.70
34	2	364	G	C5-C6-O6	-5.74	125.16	128.60
34	2	1472	A	O4'-C1'-N9	5.74	112.79	108.20
34	2	1569	C	N3-C4-N4	5.74	122.02	118.00
34	2	1699	C	N3-C4-N4	5.74	122.02	118.00
34	2	1410	A	O4'-C1'-N9	5.74	112.79	108.20
34	2	1860	A	C5-C6-N6	-5.74	119.11	123.70
34	2	1811	G	O4'-C1'-N9	5.74	112.79	108.20
49	t	197	PHE	CB-CG-CD1	5.74	124.81	120.80
34	2	1722	G	O4'-C1'-N9	5.73	112.79	108.20
34	2	1456	C	N3-C4-C5	-5.73	119.61	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1515	G	C8-N9-C1'	-5.73	119.55	127.00
1	1	10	G	C4-N9-C1'	5.73	133.95	126.50
1	1	29	G	O4'-C1'-N9	5.73	112.78	108.20
34	2	1719	A	C5-C6-N1	-5.73	114.84	117.70
34	2	1144	A	O4'-C1'-N9	5.73	112.78	108.20
34	2	1201	C	N3-C4-C5	-5.73	119.61	121.90
34	2	509	A	C5-C6-N6	-5.72	119.12	123.70
34	2	986	A	C4-C5-C6	5.72	119.86	117.00
34	2	1184	A	C5-C6-N1	-5.72	114.84	117.70
34	2	353	A	C5-C6-N1	-5.72	114.84	117.70
34	2	1449	C	C6-N1-C1'	-5.72	113.93	120.80
48	s	54	TYR	CB-CG-CD1	5.72	124.43	121.00
34	2	1016	A	C4-C5-C6	5.72	119.86	117.00
34	2	24	C	N3-C4-N4	5.72	122.00	118.00
34	2	369	C	N3-C4-N4	5.72	122.00	118.00
34	2	664	C	N3-C4-N4	5.72	122.00	118.00
34	2	1076	A	C5-C6-N6	-5.72	119.12	123.70
34	2	1205	A	C4-C5-C6	5.72	119.86	117.00
34	2	1297	A	C5-C6-N1	-5.72	114.84	117.70
34	2	1723	U	O4'-C1'-N1	5.72	112.78	108.20
34	2	1821	U	O4'-C1'-N1	5.72	112.78	108.20
34	2	319	G	O4'-C1'-N9	5.72	112.77	108.20
34	2	871	A	C5-C6-N6	-5.72	119.13	123.70
34	2	905	G	O4'-C1'-N9	5.72	112.77	108.20
1	1	20	A	C4-C5-C6	5.71	119.86	117.00
34	2	572	U	O4'-C1'-N1	5.71	112.77	108.20
34	2	1175	G	N3-C2-N2	5.71	123.90	119.90
34	2	484	C	N3-C4-N4	5.71	122.00	118.00
34	2	1247	A	C5-C6-N6	-5.71	119.13	123.70
34	2	1192	A	C5-C6-N1	-5.71	114.84	117.70
34	2	1245	C	N3-C4-C5	-5.71	119.62	121.90
34	2	1415	C	N3-C4-N4	5.71	122.00	118.00
34	2	1437	U	O4'-C1'-N1	5.71	112.77	108.20
34	2	1456	C	N3-C4-N4	5.71	122.00	118.00
34	2	1841	G	O4'-C1'-N9	5.71	112.77	108.20
34	2	59	U	O4'-C1'-N1	5.71	112.77	108.20
34	2	1670	A	C4-C5-C6	5.71	119.86	117.00
1	1	2	A	C5-C6-N1	-5.71	114.85	117.70
34	2	455	A	C5-C6-N6	-5.71	119.13	123.70
34	2	868	A	O4'-C1'-N9	5.71	112.77	108.20
34	2	1691	C	N3-C4-N4	5.70	121.99	118.00
34	2	11	A	C5-C6-N1	-5.70	114.85	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	181	A	C5-C6-N1	-5.70	114.85	117.70
34	2	1738	G	N3-C2-N2	5.70	123.89	119.90
34	2	158	A	C4-C5-C6	5.70	119.85	117.00
34	2	284	C	O4'-C1'-N1	5.70	112.76	108.20
34	2	289	G	O4'-C1'-N9	5.70	112.76	108.20
34	2	640	A	C5-C6-N1	-5.70	114.85	117.70
34	2	1810	G	O4'-C1'-N9	5.70	112.76	108.20
34	2	1289	A	C5-C6-N1	-5.70	114.85	117.70
34	2	1444	A	C5-C6-N6	-5.70	119.14	123.70
34	2	354	A	C4-C5-C6	5.69	119.85	117.00
34	2	450	A	C5-C6-N6	-5.69	119.14	123.70
34	2	1206	G	O4'-C1'-N9	5.69	112.75	108.20
34	2	1075	C	N3-C4-N4	5.69	121.98	118.00
34	2	429	A	C4-C5-C6	5.69	119.85	117.00
34	2	801	U	O4'-C1'-N1	5.69	112.75	108.20
34	2	1027	A	C4-C5-C6	5.69	119.85	117.00
34	2	1276	G	O4'-C1'-N9	5.69	112.75	108.20
34	2	1606	G	O4'-C1'-N9	5.69	112.75	108.20
1	1	5	A	O4'-C1'-N9	5.69	112.75	108.20
34	2	1382	A	C5-C6-N6	-5.69	119.15	123.70
45	w	223	PHE	CB-CG-CD1	5.69	124.78	120.80
34	2	971	G	O4'-C1'-N9	5.69	112.75	108.20
34	2	1083	A	C5-C6-N6	-5.69	119.15	123.70
34	2	1130	G	O4'-C1'-N9	5.69	112.75	108.20
34	2	1366	A	C4-C5-C6	5.69	119.84	117.00
34	2	1502	A	C5-C6-N1	-5.69	114.86	117.70
34	2	459	A	C5-C6-N1	-5.69	114.86	117.70
34	2	1195	A	C5-C6-N1	-5.69	114.86	117.70
34	2	316	C	N3-C4-N4	5.68	121.98	118.00
34	2	1086	C	N3-C4-C5	-5.68	119.63	121.90
34	2	1485	A	C4-C5-C6	5.68	119.84	117.00
34	2	99	A	O4'-C1'-N9	5.68	112.75	108.20
34	2	619	A	C5-C6-N6	-5.68	119.15	123.70
34	2	1317	G	O4'-C1'-N9	5.68	112.75	108.20
34	2	1429	C	N3-C4-N4	5.68	121.98	118.00
34	2	951	A	O4'-C1'-N9	5.68	112.75	108.20
34	2	1692	A	C5-C6-N1	-5.68	114.86	117.70
34	2	226	A	C5-C6-N1	-5.68	114.86	117.70
34	2	1592	C	N3-C4-N4	5.68	121.97	118.00
34	2	1421	G	C5-C6-O6	-5.68	125.19	128.60
34	2	297	C	N3-C4-N4	5.68	121.97	118.00
34	2	1050	G	O4'-C1'-N9	5.68	112.74	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1530	U	O4'-C1'-N1	5.68	112.74	108.20
34	2	1604	C	N3-C4-N4	5.68	121.97	118.00
34	2	603	C	N3-C4-N4	5.67	121.97	118.00
34	2	650	C	N3-C4-C5	-5.67	119.63	121.90
34	2	974	G	O4'-C1'-N9	5.67	112.74	108.20
34	2	1193	G	O4'-C1'-N9	5.67	112.74	108.20
34	2	302	C	O4'-C1'-N1	5.67	112.74	108.20
34	2	1379	A	C5-C6-N6	-5.67	119.16	123.70
34	2	117	C	N3-C4-N4	5.67	121.97	118.00
34	2	284	C	N3-C4-N4	5.67	121.97	118.00
34	2	1205	A	C5-C6-N6	-5.67	119.17	123.70
34	2	1698	C	N3-C4-C5	-5.67	119.63	121.90
34	2	1483	A	C4-C5-C6	5.67	119.83	117.00
34	2	1698	C	N3-C4-N4	5.67	121.97	118.00
34	2	1859	C	N3-C4-N4	5.67	121.97	118.00
34	2	437	A	C5-C6-N1	-5.67	114.87	117.70
34	2	1216	A	O4'-C1'-N9	5.67	112.73	108.20
34	2	382	A	O4'-C1'-N9	5.66	112.73	108.20
34	2	1179	A	C5-C6-N1	-5.66	114.87	117.70
34	2	1364	U	O4'-C1'-N1	5.66	112.73	108.20
34	2	1536	G	O4'-C1'-N9	5.66	112.73	108.20
34	2	1351	C	N3-C4-C5	-5.66	119.64	121.90
4	D	155	TYR	CB-CG-CD2	-5.66	117.60	121.00
34	2	1528	A	C4-C5-C6	5.66	119.83	117.00
1	1	32	C	N3-C4-N4	5.66	121.96	118.00
34	2	502	A	C5-C6-N6	-5.66	119.17	123.70
34	2	536	G	O4'-C1'-N9	5.66	112.73	108.20
34	2	584	A	C5-C6-N6	-5.66	119.17	123.70
34	2	891	G	O4'-C1'-N9	5.66	112.73	108.20
34	2	890	G	O4'-C1'-N9	5.66	112.72	108.20
34	2	953	A	C5-C6-N6	-5.66	119.17	123.70
34	2	1165	G	N3-C2-N2	5.66	123.86	119.90
34	2	78	C	N3-C4-C5	-5.66	119.64	121.90
34	2	628	C	N3-C4-C5	-5.66	119.64	121.90
34	2	1140	A	C5-C6-N1	-5.66	114.87	117.70
34	2	587	G	O4'-C1'-N9	5.65	112.72	108.20
34	2	1126	G	O4'-C1'-N9	5.65	112.72	108.20
34	2	1196	A	C5-C6-N6	-5.65	119.18	123.70
1	1	75	C	N3-C4-N4	5.65	121.96	118.00
34	2	1548	C	N3-C4-N4	5.65	121.96	118.00
34	2	108	G	O4'-C1'-N9	5.65	112.72	108.20
34	2	170	A	C5-C6-N1	-5.65	114.88	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	280	G	O4'-C1'-N9	5.65	112.72	108.20
34	2	416	A	C5-C6-N6	-5.65	119.18	123.70
34	2	630	A	C5-C6-N1	-5.65	114.88	117.70
34	2	1575	A	C5-C6-N1	-5.65	114.88	117.70
1	1	56	C	N3-C4-N4	5.64	121.95	118.00
34	2	76	U	O4'-C1'-N1	5.64	112.72	108.20
34	2	240	C	N3-C4-N4	5.64	121.95	118.00
34	2	618	A	C5-C6-N1	-5.64	114.88	117.70
34	2	1279	C	N3-C4-N4	5.64	121.95	118.00
34	2	329	A	C5-C6-N6	-5.64	119.19	123.70
34	2	577	A	C5-C6-N1	-5.64	114.88	117.70
34	2	1331	G	O4'-C1'-N9	5.64	112.71	108.20
34	2	1384	A	C5-C6-N6	-5.64	119.19	123.70
38	k	205	ASP	CB-CG-OD1	5.64	123.38	118.30
34	2	729	C	N3-C4-C5	-5.64	119.64	121.90
34	2	1488	U	O4'-C1'-N1	5.64	112.71	108.20
34	2	275	C	N3-C4-C5	-5.64	119.64	121.90
34	2	77	A	C5-C6-N1	-5.64	114.88	117.70
34	2	350	A	OP1-P-O3'	5.64	117.60	105.20
34	2	381	C	N3-C4-C5	-5.64	119.64	121.90
34	2	455	A	C5-C6-N1	-5.64	114.88	117.70
34	2	644	A	C5-C6-N6	-5.64	119.19	123.70
34	2	38	A	C4-C5-C6	5.63	119.82	117.00
34	2	275	C	N3-C4-N4	5.63	121.94	118.00
34	2	476	A	C5-C6-N6	-5.63	119.19	123.70
34	2	544	A	C5-C6-N1	-5.63	114.88	117.70
34	2	980	C	N3-C4-C5	-5.63	119.65	121.90
34	2	1129	A	C4-C5-C6	5.63	119.82	117.00
34	2	61	A	C5-C6-N1	-5.63	114.88	117.70
34	2	90	G	O4'-C1'-N9	5.63	112.70	108.20
34	2	283	A	C5-C6-N6	-5.63	119.19	123.70
34	2	654	A	C5-C6-N1	-5.63	114.88	117.70
34	2	993	A	C5-C6-N6	-5.63	119.19	123.70
34	2	1056	A	C4-C5-C6	5.63	119.82	117.00
34	2	1655	C	N3-C4-N4	5.63	121.94	118.00
34	2	29	G	O4'-C1'-N9	5.63	112.70	108.20
34	2	969	C	N3-C4-N4	5.63	121.94	118.00
1	1	20	A	C5-C6-N6	-5.63	119.20	123.70
13	M	70	TYR	CB-CG-CD2	-5.63	117.62	121.00
34	2	425	A	C5-C6-N1	-5.63	114.89	117.70
34	2	807	A	C4-C5-C6	5.63	119.81	117.00
34	2	1135	C	N3-C4-C5	-5.63	119.65	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1372	A	C5-C6-N6	-5.63	119.20	123.70
34	2	983	A	C5-C6-N6	-5.63	119.20	123.70
34	2	1433	C	N3-C4-C5	-5.63	119.65	121.90
34	2	1567	C	N3-C4-N4	5.63	121.94	118.00
34	2	662	A	C5-C6-N6	-5.62	119.20	123.70
34	2	1246	A	C4-C5-C6	5.62	119.81	117.00
34	2	1309	A	C4-C5-C6	5.62	119.81	117.00
34	2	1511	G	O4'-C1'-N9	5.62	112.70	108.20
34	2	1696	C	N3-C4-N4	5.62	121.94	118.00
34	2	1799	G	O4'-C1'-N9	5.62	112.70	108.20
1	1	48	C	N3-C4-N4	5.62	121.94	118.00
34	2	438	A	C4-C5-C6	5.62	119.81	117.00
34	2	1656	A	C5-C6-N6	-5.62	119.20	123.70
44	v	697	TYR	CB-CG-CD2	-5.62	117.63	121.00
34	2	174	C	N3-C4-N4	5.62	121.93	118.00
34	2	624	A	C5-C6-N6	-5.62	119.20	123.70
34	2	1075	C	N3-C4-C5	-5.62	119.65	121.90
34	2	426	G	O4'-C1'-N9	5.62	112.69	108.20
34	2	470	G	O4'-C1'-N9	5.62	112.69	108.20
34	2	491	C	N3-C4-C5	-5.62	119.65	121.90
34	2	612	C	N3-C4-N4	5.62	121.93	118.00
34	2	1652	G	O4'-C1'-N9	5.62	112.69	108.20
1	1	75	C	N3-C4-C5	-5.62	119.65	121.90
34	2	1191	A	O4'-C1'-N9	5.62	112.69	108.20
12	L	159	PHE	CB-CG-CD2	-5.62	116.87	120.80
34	2	624	A	C5-C6-N1	-5.62	114.89	117.70
34	2	658	A	C5-C6-N6	-5.62	119.21	123.70
34	2	904	A	C4-C5-C6	5.62	119.81	117.00
32	n	65	TYR	CB-CG-CD2	-5.61	117.63	121.00
34	2	67	C	C6-N1-C2	-5.61	118.05	120.30
34	2	182	C	N3-C4-C5	-5.61	119.66	121.90
45	w	323	PHE	CB-CG-CD2	-5.61	116.87	120.80
34	2	72	C	N3-C4-C5	-5.61	119.66	121.90
34	2	175	A	C5-C6-N6	-5.61	119.21	123.70
34	2	576	G	O4'-C1'-N9	5.61	112.69	108.20
34	2	1575	A	C4-C5-C6	5.61	119.81	117.00
34	2	1714	A	C5-C6-N6	-5.61	119.21	123.70
34	2	1735	C	N3-C4-N4	5.61	121.93	118.00
34	2	1221	U	O4'-C1'-N1	5.61	112.69	108.20
34	2	67	C	N3-C4-N4	5.61	121.93	118.00
34	2	98	C	O4'-C1'-N1	5.61	112.69	108.20
34	2	191	C	O4'-C1'-N1	5.61	112.69	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1159	C	N3-C4-N4	5.61	121.92	118.00
34	2	1382	A	C5-C6-N1	-5.61	114.90	117.70
34	2	458	A	C5-C6-N1	-5.61	114.90	117.70
34	2	1475	G	O4'-C1'-N9	5.61	112.68	108.20
34	2	158	A	C5-C6-N6	-5.60	119.22	123.70
34	2	675	A	C5-C6-N6	-5.60	119.22	123.70
34	2	1254	A	C4-C5-C6	5.60	119.80	117.00
34	2	218	A	O4'-C1'-N9	5.60	112.68	108.20
34	2	510	A	C5-C6-N1	-5.60	114.90	117.70
34	2	866	A	C4-C5-C6	5.60	119.80	117.00
34	2	275	C	C6-N1-C1'	-5.60	114.08	120.80
34	2	38	A	C5-C6-N6	-5.60	119.22	123.70
34	2	359	C	N3-C4-N4	5.60	121.92	118.00
34	2	1542	C	N3-C4-C5	-5.60	119.66	121.90
1	1	35	A	C5-C6-N1	-5.59	114.90	117.70
34	2	277	U	O4'-C1'-N1	5.59	112.67	108.20
34	2	573	A	O4'-C1'-N9	5.59	112.68	108.20
34	2	861	A	C5-C6-N6	-5.59	119.22	123.70
34	2	1100	G	O4'-C1'-N9	5.59	112.68	108.20
34	2	1442	A	C4-C5-C6	5.59	119.80	117.00
34	2	1533	C	N3-C4-N4	5.59	121.92	118.00
34	2	3	C	N3-C4-N4	5.59	121.92	118.00
34	2	290	A	C5-C6-N1	-5.59	114.90	117.70
34	2	46	A	C5-C6-N1	-5.59	114.90	117.70
34	2	675	A	C4-C5-C6	5.59	119.80	117.00
34	2	807	A	C5-C6-N6	-5.59	119.23	123.70
34	2	1795	A	O4'-C1'-N9	5.59	112.67	108.20
34	2	1812	A	C5-C6-N1	-5.59	114.91	117.70
1	1	35	A	C5-C6-N6	-5.59	119.23	123.70
34	2	114	G	O4'-C1'-N9	5.59	112.67	108.20
34	2	429	A	C5-C6-N6	-5.59	119.23	123.70
35	A	82	TYR	CB-CG-CD2	-5.59	117.65	121.00
40	R	15	PHE	CB-CG-CD1	5.59	124.71	120.80
34	2	1434	A	C4-C5-C6	5.59	119.79	117.00
34	2	1618	A	C5-C6-N6	-5.59	119.23	123.70
34	2	13	C	N3-C4-N4	5.59	121.91	118.00
34	2	453	C	N3-C4-N4	5.59	121.91	118.00
34	2	638	A	C5-C6-N1	-5.59	114.91	117.70
34	2	669	A	C4-C5-C6	5.59	119.79	117.00
34	2	866	A	C5-C6-N6	-5.59	119.23	123.70
34	2	1072	G	O4'-C1'-N9	5.59	112.67	108.20
34	2	1155	G	O4'-C1'-N9	5.59	112.67	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1095	G	O4'-C1'-N9	5.58	112.67	108.20
34	2	1693	C	N3-C4-C5	-5.58	119.67	121.90
34	2	1026	A	C5-C6-N1	-5.58	114.91	117.70
34	2	1212	C	N3-C4-N4	5.58	121.91	118.00
1	1	61	C	N3-C4-N4	5.58	121.91	118.00
34	2	389	C	N3-C4-N4	5.58	121.91	118.00
34	2	397	G	C4-N9-C1'	5.58	133.76	126.50
34	2	1787	A	O4'-C1'-N9	5.58	112.67	108.20
1	1	14	C	N3-C4-C5	-5.58	119.67	121.90
34	2	2	A	C5-C6-N6	-5.58	119.24	123.70
34	2	68	A	C5-C6-N1	-5.58	114.91	117.70
34	2	526	A	C4-C5-C6	5.58	119.79	117.00
34	2	580	A	O4'-C1'-N9	5.58	112.66	108.20
34	2	1340	A	C5-C6-N6	-5.58	119.24	123.70
34	2	1719	A	O4'-C1'-N9	5.58	112.66	108.20
34	2	179	C	N3-C4-C5	-5.58	119.67	121.90
34	2	831	C	N3-C4-N4	5.58	121.90	118.00
34	2	1678	C	N3-C4-N4	5.58	121.90	118.00
49	t	197	PHE	CB-CG-CD2	-5.58	116.90	120.80
34	2	1121	C	N3-C4-N4	5.58	121.90	118.00
34	2	1134	C	N3-C4-N4	5.58	121.90	118.00
34	2	1310	U	C2-N1-C1'	5.58	124.39	117.70
41	3	40	C	N3-C4-C5	-5.58	119.67	121.90
34	2	16	G	N3-C2-N2	5.57	123.80	119.90
34	2	583	C	N3-C4-N4	5.57	121.90	118.00
34	2	1397	A	C4-C5-C6	5.57	119.79	117.00
34	2	1190	A	C4-C5-C6	5.57	119.79	117.00
34	2	1278	A	C5-C6-N6	-5.57	119.24	123.70
34	2	512	A	C5-C6-N6	-5.57	119.24	123.70
34	2	315	C	N3-C4-N4	5.57	121.90	118.00
34	2	1158	C	N3-C4-N4	5.57	121.90	118.00
34	2	491	C	N3-C4-N4	5.57	121.90	118.00
34	2	594	A	C5-C6-N1	-5.57	114.92	117.70
34	2	826	A	C5-C6-N6	-5.57	119.25	123.70
34	2	166	A	O4'-C1'-N9	5.57	112.65	108.20
34	2	1845	A	C5-C6-N6	-5.57	119.25	123.70
43	y	540	ALA	N-CA-CB	5.57	117.89	110.10
34	2	613	G	O4'-C1'-N9	5.56	112.65	108.20
34	2	1812	A	O4'-C1'-N9	5.56	112.65	108.20
34	2	1054	A	C5-C6-N6	-5.56	119.25	123.70
34	2	1449	C	N3-C4-N4	5.56	121.89	118.00
34	2	1699	C	N3-C4-C5	-5.56	119.68	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1714	A	O4'-C1'-N9	5.56	112.65	108.20
1	1	20	A	C5-C6-N1	-5.56	114.92	117.70
34	2	91	A	C5-C6-N6	-5.56	119.25	123.70
34	2	448	A	C5-C6-N1	-5.56	114.92	117.70
34	2	1284	U	O4'-C1'-N1	5.56	112.65	108.20
34	2	1186	A	C5-C6-N1	-5.56	114.92	117.70
34	2	1619	U	C2-N1-C1'	5.56	124.37	117.70
34	2	80	G	O4'-C1'-N9	5.56	112.64	108.20
34	2	1399	C	N3-C4-N4	5.56	121.89	118.00
34	2	1483	A	C5-C6-N6	-5.56	119.25	123.70
34	2	922	A	O4'-C1'-N9	5.55	112.64	108.20
34	2	1205	A	C5-C6-N1	-5.55	114.92	117.70
34	2	1502	A	C5-C6-N6	-5.55	119.26	123.70
34	2	221	A	C5-C6-N1	-5.55	114.92	117.70
34	2	580	A	C5-C6-N6	-5.55	119.26	123.70
34	2	418	U	C2-N1-C1'	5.55	124.36	117.70
34	2	960	A	C5-C6-N1	-5.55	114.92	117.70
34	2	1400	U	O4'-C1'-N1	5.55	112.64	108.20
34	2	1478	C	N3-C4-N4	5.55	121.89	118.00
34	2	574	A	C4-C5-C6	5.55	119.77	117.00
34	2	1080	A	C5-C6-N1	-5.55	114.93	117.70
34	2	1080	A	C5-C6-N6	-5.55	119.26	123.70
34	2	603	C	N3-C4-C5	-5.55	119.68	121.90
34	2	645	A	C5-C6-N6	-5.55	119.26	123.70
34	2	820	C	N3-C4-N4	5.55	121.88	118.00
34	2	1287	A	C5-C6-N6	-5.55	119.26	123.70
34	2	1410	A	C4-C5-C6	5.55	119.77	117.00
34	2	1596	A	C5-C6-N1	-5.55	114.93	117.70
34	2	833	A	C5-C6-N6	-5.54	119.26	123.70
34	2	993	A	C5-C6-N1	-5.54	114.93	117.70
34	2	178	C	N3-C4-C5	-5.54	119.68	121.90
34	2	831	C	N3-C4-C5	-5.54	119.68	121.90
34	2	1396	U	O4'-C1'-N1	5.54	112.63	108.20
34	2	292	A	C5-C6-N6	-5.54	119.27	123.70
34	2	1083	A	C5-C6-N1	-5.54	114.93	117.70
34	2	1286	G	O4'-C1'-N9	5.54	112.63	108.20
34	2	1290	G	O4'-C1'-N9	5.54	112.63	108.20
34	2	1578	C	N3-C4-C5	-5.54	119.69	121.90
1	1	68	C	O4'-C1'-N1	5.54	112.63	108.20
34	2	1541	G	O4'-C1'-N9	5.54	112.63	108.20
34	2	1815	U	P-O3'-C3'	5.54	126.34	119.70
34	2	807	A	O4'-C1'-N9	5.53	112.63	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1320	G	O4'-C1'-N9	5.53	112.63	108.20
34	2	1334	G	O4'-C1'-N9	5.53	112.63	108.20
34	2	1365	A	C5-C6-N1	-5.53	114.93	117.70
34	2	535	A	O4'-C1'-N9	5.53	112.63	108.20
34	2	1237	A	C5-C6-N1	-5.53	114.93	117.70
34	2	1586	C	N3-C4-N4	5.53	121.87	118.00
1	1	28	U	O4'-C1'-N1	5.53	112.62	108.20
34	2	330	C	N3-C4-C5	-5.53	119.69	121.90
34	2	860	A	C5-C6-N6	-5.53	119.28	123.70
34	2	1185	A	O4'-C1'-N9	5.53	112.62	108.20
34	2	1280	A	C4-C5-C6	5.53	119.76	117.00
34	2	1092	G	O4'-C1'-N9	5.52	112.62	108.20
34	2	1129	A	C5-C6-N6	-5.52	119.28	123.70
34	2	1807	A	O4'-C1'-N9	5.52	112.62	108.20
34	2	297	C	N3-C4-C5	-5.52	119.69	121.90
34	2	830	C	N3-C4-N4	5.52	121.87	118.00
34	2	956	U	O4'-C1'-N1	5.52	112.62	108.20
34	2	1444	A	C5-C6-N1	-5.52	114.94	117.70
34	2	1697	G	O4'-C1'-N9	5.52	112.62	108.20
34	2	912	A	C5-C6-N6	-5.52	119.28	123.70
34	2	321	C	N3-C4-C5	-5.52	119.69	121.90
34	2	901	C	N3-C4-N4	5.52	121.86	118.00
34	2	1548	C	P-O3'-C3'	5.52	126.32	119.70
34	2	605	C	N3-C4-C5	-5.52	119.69	121.90
34	2	980	C	N3-C4-N4	5.52	121.86	118.00
34	2	1784	A	O4'-C1'-N9	5.52	112.61	108.20
46	q	239	TYR	CB-CG-CD2	-5.52	117.69	121.00
34	2	445	A	C5-C6-N6	-5.52	119.29	123.70
34	2	1844	A	O4'-C1'-N9	5.52	112.61	108.20
34	2	482	C	N3-C4-N4	5.51	121.86	118.00
34	2	835	C	N3-C4-C5	-5.51	119.69	121.90
41	3	40	C	N3-C4-N4	5.51	121.86	118.00
34	2	283	A	C5-C6-N1	-5.51	114.94	117.70
24	Z	41	PHE	CB-CG-CD2	-5.51	116.94	120.80
34	2	1472	A	C5-C6-N1	-5.51	114.94	117.70
34	2	440	C	N3-C4-N4	5.51	121.86	118.00
34	2	1540	A	C5-C6-N6	-5.51	119.29	123.70
34	2	544	A	C5-C6-N6	-5.51	119.29	123.70
34	2	940	A	C4-C5-C6	5.51	119.75	117.00
1	1	18	G	C4'-C3'-O3'	5.51	124.01	113.00
34	2	828	G	O4'-C1'-N9	5.51	112.61	108.20
34	2	873	C	N3-C4-N4	5.51	121.86	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1399	C	O4'-C1'-N1	5.51	112.61	108.20
34	2	593	C	N3-C4-N4	5.50	121.85	118.00
34	2	809	A	O4'-C1'-N9	5.50	112.60	108.20
34	2	1297	A	C5-C6-N6	-5.50	119.30	123.70
34	2	23	G	O4'-C1'-N9	5.50	112.60	108.20
34	2	1549	C	N3-C4-N4	5.50	121.85	118.00
34	2	25	A	C4-C5-C6	5.50	119.75	117.00
34	2	453	C	N3-C4-C5	-5.50	119.70	121.90
34	2	1137	G	O4'-C1'-N9	5.50	112.60	108.20
34	2	1729	G	N3-C2-N2	5.50	123.75	119.90
34	2	450	A	C5-C6-N1	-5.50	114.95	117.70
34	2	1614	A	C5-C6-N6	-5.50	119.30	123.70
34	2	1659	A	C5-C6-N1	-5.50	114.95	117.70
34	2	117	C	N3-C4-C5	-5.50	119.70	121.90
34	2	196	U	O4'-C1'-N1	5.50	112.60	108.20
34	2	560	C	N3-C4-C5	-5.50	119.70	121.90
34	2	560	C	N3-C4-N4	5.50	121.85	118.00
34	2	958	A	C5-C6-N1	-5.50	114.95	117.70
34	2	993	A	C4-C5-C6	5.50	119.75	117.00
1	1	55	U	O4'-C1'-N1	5.50	112.60	108.20
34	2	1060	C	N3-C4-C5	-5.50	119.70	121.90
34	2	1840	G	O4'-C1'-N9	5.50	112.60	108.20
34	2	551	A	C5-C6-N6	-5.50	119.30	123.70
34	2	1411	C	N3-C4-N4	5.50	121.85	118.00
43	y	384	VAL	C-N-CD	5.50	139.94	128.40
34	2	550	A	C5-C6-N1	-5.49	114.95	117.70
34	2	983	A	C5-C6-N1	-5.49	114.95	117.70
34	2	1066	A	O4'-C1'-N9	5.49	112.59	108.20
34	2	1258	C	N3-C4-C5	-5.49	119.70	121.90
34	2	798	A	C5-C6-N6	-5.49	119.31	123.70
45	w	223	PHE	CB-CG-CD2	-5.49	116.95	120.80
32	n	65	TYR	CB-CG-CD1	5.49	124.29	121.00
34	2	96	C	N3-C4-N4	5.49	121.84	118.00
34	2	643	A	C5-C6-N1	-5.49	114.95	117.70
34	2	924	G	O4'-C1'-N9	5.49	112.59	108.20
34	2	1149	C	N3-C4-N4	5.49	121.84	118.00
34	2	1551	A	C5-C6-N6	-5.49	119.31	123.70
34	2	1770	G	O4'-C1'-N9	5.49	112.59	108.20
34	2	340	C	N3-C4-C5	-5.49	119.70	121.90
34	2	526	A	O4'-C1'-N9	5.49	112.59	108.20
34	2	650	C	N3-C4-N4	5.49	121.84	118.00
34	2	823	A	C5-C6-N6	-5.49	119.31	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1360	U	C6-N1-C1'	-5.49	113.52	121.20
1	1	58	A	C5-C6-N1	-5.49	114.96	117.70
34	2	102	A	C5-C6-N1	-5.49	114.96	117.70
34	2	1260	C	N3-C4-N4	5.49	121.84	118.00
34	2	1576	C	N3-C4-N4	5.49	121.84	118.00
34	2	429	A	C5-C6-N1	-5.49	114.96	117.70
34	2	600	G	O4'-C1'-N9	5.49	112.59	108.20
34	2	846	C	N3-C4-N4	5.49	121.84	118.00
34	2	994	A	C5-C6-N6	-5.49	119.31	123.70
34	2	1551	A	C5-C6-N1	-5.49	114.96	117.70
34	2	67	C	O4'-C1'-N1	5.48	112.59	108.20
34	2	860	A	C5-C6-N1	-5.48	114.96	117.70
34	2	926	C	N3-C4-N4	5.48	121.84	118.00
34	2	1419	C	N3-C4-N4	5.48	121.84	118.00
34	2	573	A	C4-C5-C6	5.48	119.74	117.00
34	2	1257	C	N3-C4-C5	-5.48	119.71	121.90
34	2	1641	C	N3-C4-C5	-5.48	119.71	121.90
34	2	1692	A	C4-C5-C6	5.48	119.74	117.00
34	2	1694	A	C5-C6-N1	-5.48	114.96	117.70
34	2	50	A	C5-C6-N1	-5.48	114.96	117.70
34	2	1483	A	O4'-C1'-N9	5.48	112.58	108.20
1	1	38	A	O4'-C1'-N9	5.48	112.58	108.20
34	2	343	C	N3-C4-C5	-5.48	119.71	121.90
34	2	922	A	C5-C6-N6	-5.48	119.32	123.70
34	2	1242	A	C5-C6-N1	-5.48	114.96	117.70
34	2	1640	C	N3-C4-C5	-5.48	119.71	121.90
34	2	1659	A	O4'-C1'-N9	5.48	112.58	108.20
34	2	1056	A	C5-C6-N6	-5.48	119.32	123.70
34	2	1340	A	C5-C6-N1	-5.48	114.96	117.70
34	2	454	A	C5-C6-N6	-5.47	119.32	123.70
34	2	1215	C	N3-C4-N4	5.47	121.83	118.00
34	2	1510	G	O4'-C1'-N9	5.47	112.58	108.20
34	2	367	G	O4'-C1'-N9	5.47	112.58	108.20
34	2	1412	C	N3-C4-N4	5.47	121.83	118.00
34	2	435	A	C5-C6-N6	-5.47	119.32	123.70
34	2	945	G	O4'-C1'-N9	5.47	112.58	108.20
34	2	976	A	O4'-C1'-N9	5.47	112.58	108.20
41	3	51	C	N3-C4-N4	5.47	121.83	118.00
34	2	45	A	C5-C6-N6	-5.47	119.32	123.70
34	2	814	A	C5-C6-N6	-5.47	119.32	123.70
34	2	111	A	C5-C6-N1	-5.47	114.97	117.70
34	2	492	C	N3-C4-C5	-5.47	119.71	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	958	A	O4'-C1'-N9	5.47	112.57	108.20
34	2	1273	C	N3-C4-C5	-5.47	119.71	121.90
34	2	845	A	C5-C6-N6	-5.46	119.33	123.70
34	2	1435	A	O4'-C1'-N9	5.46	112.57	108.20
34	2	1450	A	C5-C6-N6	-5.46	119.33	123.70
34	2	1529	C	O4'-C1'-N1	5.46	112.57	108.20
34	2	1566	G	O4'-C1'-N9	5.46	112.57	108.20
34	2	1786	G	O4'-C1'-N9	5.46	112.57	108.20
44	v	463	ASP	C-N-CD	5.46	139.88	128.40
34	2	915	A	C5-C6-N6	-5.46	119.33	123.70
34	2	1258	C	N3-C4-N4	5.46	121.82	118.00
1	1	59	A	C5-C6-N6	-5.46	119.33	123.70
34	2	977	A	O4'-C1'-N9	5.46	112.57	108.20
34	2	1015	C	N3-C4-C5	-5.46	119.72	121.90
34	2	1031	A	O4'-C1'-N9	5.46	112.57	108.20
34	2	1163	G	O4'-C1'-N9	5.46	112.57	108.20
34	2	1307	C	N3-C4-C5	-5.46	119.72	121.90
34	2	85	A	C5-C6-N6	-5.46	119.33	123.70
34	2	1260	C	N3-C4-C5	-5.46	119.72	121.90
34	2	166	A	C5-C6-N6	-5.46	119.33	123.70
34	2	513	A	C5-C6-N6	-5.46	119.33	123.70
34	2	940	A	O4'-C1'-N9	5.46	112.57	108.20
34	2	949	C	N3-C4-N4	5.46	121.82	118.00
34	2	1628	A	C5-C6-N1	-5.46	114.97	117.70
41	3	50	C	N3-C4-N4	5.46	121.82	118.00
34	2	82	G	N3-C2-N2	5.46	123.72	119.90
34	2	659	A	C5-C6-N1	-5.46	114.97	117.70
34	2	920	G	O4'-C1'-N9	5.46	112.56	108.20
34	2	1093	G	O4'-C1'-N9	5.46	112.57	108.20
34	2	566	A	C5-C6-N6	-5.46	119.34	123.70
34	2	1347	G	O4'-C1'-N9	5.46	112.56	108.20
34	2	660	A	C4-C5-C6	5.45	119.73	117.00
34	2	1583	A	C5-C6-N6	-5.45	119.34	123.70
34	2	1679	C	N3-C4-N4	5.45	121.82	118.00
34	2	288	A	C5-C6-N1	-5.45	114.97	117.70
34	2	1010	G	O4'-C1'-N9	5.45	112.56	108.20
34	2	1430	C	N3-C4-C5	-5.45	119.72	121.90
34	2	1476	A	C5-C6-N1	-5.45	114.97	117.70
34	2	1793	G	N3-C2-N2	5.45	123.72	119.90
34	2	1795	A	C5-C6-N6	-5.45	119.34	123.70
38	k	136	ASP	C-N-CD	5.45	139.85	128.40
34	2	228	A	C5-C6-N6	-5.45	119.34	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	391	A	C4-C5-C6	5.45	119.72	117.00
34	2	826	A	C5-C6-N1	-5.45	114.98	117.70
34	2	1829	A	C5-C6-N6	-5.45	119.34	123.70
38	k	128	LYS	C-N-CD	5.45	139.84	128.40
38	k	137	PRO	C-N-CD	5.45	139.84	128.40
34	2	25	A	C5-C6-N1	-5.45	114.98	117.70
34	2	533	C	N3-C4-N4	5.45	121.81	118.00
34	2	631	A	O4'-C1'-N9	5.45	112.56	108.20
34	2	1053	C	N3-C4-C5	-5.45	119.72	121.90
34	2	1563	C	N3-C4-C5	-5.45	119.72	121.90
34	2	1766	C	P-O3'-C3'	-5.45	113.17	119.70
34	2	302	C	N3-C4-C5	-5.44	119.72	121.90
34	2	466	A	O4'-C1'-N9	5.44	112.56	108.20
34	2	1504	A	C4-C5-C6	5.44	119.72	117.00
34	2	149	A	C4-C5-C6	5.44	119.72	117.00
34	2	519	A	C4-C5-C6	5.44	119.72	117.00
34	2	590	G	O4'-C1'-N9	5.44	112.55	108.20
34	2	19	A	C5-C6-N6	-5.44	119.35	123.70
34	2	45	A	C5-C6-N1	-5.44	114.98	117.70
34	2	606	A	C5-C6-N1	-5.44	114.98	117.70
34	2	1007	A	O4'-C1'-N9	5.44	112.55	108.20
34	2	1129	A	C5-C6-N1	-5.44	114.98	117.70
42	m	201	TYR	CB-CG-CD2	-5.44	117.73	121.00
34	2	185	C	N3-C4-N4	5.44	121.81	118.00
34	2	73	C	N3-C4-N4	5.44	121.81	118.00
34	2	270	G	O4'-C1'-N9	5.44	112.55	108.20
34	2	901	C	N3-C4-C5	-5.44	119.72	121.90
38	k	176	ILE	C-N-CD	5.44	139.82	128.40
10	J	63	PHE	CB-CG-CD2	-5.44	117.00	120.80
34	2	959	A	C5-C6-N1	-5.44	114.98	117.70
34	2	1078	A	C5-C6-N6	-5.44	119.35	123.70
34	2	354	A	O4'-C1'-N9	5.43	112.55	108.20
34	2	508	G	O4'-C1'-N9	5.43	112.55	108.20
34	2	580	A	C5-C6-N1	-5.43	114.98	117.70
34	2	677	C	N3-C4-C5	-5.43	119.73	121.90
34	2	1399	C	N3-C4-C5	-5.43	119.73	121.90
34	2	118	C	N3-C4-N4	5.43	121.80	118.00
34	2	183	G	O4'-C1'-N9	5.43	112.55	108.20
34	2	304	A	C5-C6-N1	-5.43	114.98	117.70
34	2	1195	A	C5-C6-N6	-5.43	119.36	123.70
34	2	1548	C	N3-C4-C5	-5.43	119.73	121.90
34	2	845	A	O4'-C1'-N9	5.43	112.55	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	27	A	O4'-C1'-N9	5.43	112.54	108.20
34	2	550	A	C4-C5-C6	5.43	119.72	117.00
34	2	955	G	N3-C2-N2	5.43	123.70	119.90
34	2	284	C	N3-C4-C5	-5.43	119.73	121.90
34	2	1243	C	N3-C4-N4	5.43	121.80	118.00
34	2	1563	C	N3-C4-N4	5.43	121.80	118.00
34	2	111	A	C5-C6-N6	-5.43	119.36	123.70
34	2	1435	A	C5-C6-N6	-5.43	119.36	123.70
34	2	1461	A	C5-C6-N6	-5.43	119.36	123.70
34	2	845	A	C5-C6-N1	-5.42	114.99	117.70
34	2	1753	G	O4'-C1'-N9	5.42	112.54	108.20
34	2	1186	A	O4'-C1'-N9	5.42	112.54	108.20
34	2	1279	C	N3-C4-C5	-5.42	119.73	121.90
47	r	123	THR	N-CA-C	-5.42	96.36	111.00
34	2	338	A	C5-C6-N1	-5.42	114.99	117.70
34	2	408	A	C5-C6-N1	-5.42	114.99	117.70
34	2	1008	A	O4'-C1'-N9	5.42	112.54	108.20
34	2	1120	C	N3-C4-C5	-5.42	119.73	121.90
1	1	44	A	C5-C6-N6	-5.42	119.36	123.70
34	2	1039	G	O4'-C1'-N9	5.42	112.54	108.20
34	2	145	G	O4'-C1'-N9	5.42	112.53	108.20
34	2	221	A	C5-C6-N6	-5.42	119.36	123.70
34	2	1176	C	N3-C4-C5	-5.42	119.73	121.90
34	2	1618	A	C5-C6-N1	-5.42	114.99	117.70
34	2	1632	A	C5-C6-N1	-5.42	114.99	117.70
34	2	125	C	N3-C4-N4	5.42	121.79	118.00
34	2	494	G	O4'-C1'-N9	5.42	112.53	108.20
34	2	806	A	C5-C6-N1	-5.42	114.99	117.70
34	2	1019	A	C5-C6-N1	-5.42	114.99	117.70
34	2	1257	C	N3-C4-N4	5.42	121.79	118.00
34	2	73	C	N3-C4-C5	-5.42	119.73	121.90
34	2	1248	C	N3-C4-C5	-5.42	119.73	121.90
34	2	56	G	O4'-C1'-N9	5.41	112.53	108.20
34	2	110	U	O4'-C1'-N1	5.41	112.53	108.20
34	2	490	A	C5-C6-N1	-5.41	114.99	117.70
34	2	989	G	O4'-C1'-N9	5.41	112.53	108.20
34	2	1377	G	O4'-C1'-N9	5.41	112.53	108.20
34	2	1639	C	N3-C4-C5	-5.41	119.73	121.90
34	2	1752	G	O4'-C1'-N9	5.41	112.53	108.20
34	2	1863	A	C5-C6-N1	-5.41	114.99	117.70
34	2	61	A	C5-C6-N6	-5.41	119.37	123.70
1	1	32	C	N3-C4-C5	-5.41	119.74	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	912	A	C5-C6-N1	-5.41	114.99	117.70
34	2	84	A	C5-C6-N6	-5.41	119.37	123.70
34	2	605	C	N3-C4-N4	5.41	121.79	118.00
34	2	645	A	C5-C6-N1	-5.41	115.00	117.70
34	2	4	C	N3-C4-C5	-5.41	119.74	121.90
34	2	218	A	C5-C6-N6	-5.41	119.38	123.70
34	2	377	C	N3-C4-C5	-5.41	119.74	121.90
9	I	28	TYR	CB-CG-CD1	5.41	124.24	121.00
34	2	236	C	N3-C4-C5	-5.41	119.74	121.90
34	2	473	C	N3-C4-N4	5.41	121.78	118.00
34	2	1477	G	O4'-C1'-N9	5.41	112.52	108.20
34	2	1614	A	C5-C6-N1	-5.41	115.00	117.70
34	2	408	A	C5-C6-N6	-5.40	119.38	123.70
34	2	654	A	C4-C5-C6	5.40	119.70	117.00
35	A	89	ARG	NE-CZ-NH1	5.40	123.00	120.30
34	2	1200	A	O4'-C1'-N9	5.40	112.52	108.20
34	2	1204	A	C5-C6-N1	-5.40	115.00	117.70
34	2	1552	C	N3-C4-C5	-5.40	119.74	121.90
34	2	189	G	N3-C2-N2	5.40	123.68	119.90
34	2	351	U	OP2-P-O3'	5.40	117.08	105.20
34	2	661	A	C5-C6-N1	-5.40	115.00	117.70
34	2	669	A	O4'-C1'-N9	5.40	112.52	108.20
34	2	988	A	C5-C6-N1	-5.40	115.00	117.70
34	2	1359	C	N3-C4-C5	-5.40	119.74	121.90
34	2	178	C	N3-C4-N4	5.40	121.78	118.00
34	2	290	A	C5-C6-N6	-5.40	119.38	123.70
34	2	511	A	O4'-C1'-N9	5.40	112.52	108.20
34	2	882	A	C5-C6-N1	-5.40	115.00	117.70
1	1	76	A	C5-C6-N1	-5.39	115.00	117.70
34	2	2	A	C5-C6-N1	-5.39	115.00	117.70
34	2	515	A	C5-C6-N1	-5.39	115.00	117.70
34	2	633	A	C5-C6-N6	-5.39	119.38	123.70
1	1	74	C	N3-C4-C5	-5.39	119.74	121.90
34	2	127	C	N3-C4-N4	5.39	121.78	118.00
34	2	507	C	N3-C4-C5	-5.39	119.74	121.90
34	2	1859	C	N3-C4-C5	-5.39	119.74	121.90
34	2	104	A	C5-C6-N1	-5.39	115.00	117.70
34	2	323	G	O4'-C1'-N9	5.39	112.51	108.20
34	2	1241	G	O4'-C1'-N9	5.39	112.51	108.20
34	2	1480	A	C5-C6-N6	-5.39	119.39	123.70
34	2	440	C	N3-C4-C5	-5.39	119.74	121.90
34	2	836	C	N3-C4-N4	5.39	121.77	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	921	G	O4'-C1'-N9	5.39	112.51	108.20
34	2	1450	A	C5-C6-N1	-5.39	115.01	117.70
34	2	316	C	N3-C4-C5	-5.39	119.75	121.90
34	2	993	A	O4'-C1'-N9	5.39	112.51	108.20
34	2	303	G	P-O3'-C3'	5.39	126.16	119.70
34	2	400	G	O4'-C1'-N9	5.39	112.51	108.20
34	2	1362	G	O4'-C1'-N9	5.39	112.51	108.20
34	2	1812	A	C5-C6-N6	-5.39	119.39	123.70
34	2	1860	A	C5-C6-N1	-5.39	115.01	117.70
5	E	175	SER	N-CA-CB	5.38	118.58	110.50
34	2	77	A	C5-C6-N6	-5.38	119.39	123.70
34	2	476	A	C5-C6-N1	-5.38	115.01	117.70
34	2	841	G	O4'-C1'-N9	5.38	112.51	108.20
34	2	1857	A	O4'-C1'-N9	5.38	112.51	108.20
34	2	809	A	C5-C6-N1	-5.38	115.01	117.70
34	2	1144	A	C5-C6-N6	-5.38	119.39	123.70
44	v	386	ASN	C-N-CD	5.38	139.70	128.40
34	2	94	G	O4'-C1'-N9	5.38	112.51	108.20
34	2	835	C	N3-C4-N4	5.38	121.77	118.00
34	2	1435	A	C5-C6-N1	-5.38	115.01	117.70
34	2	1783	G	N3-C2-N2	5.38	123.67	119.90
30	f	135	HIS	CA-CB-CG	5.38	122.75	113.60
34	2	421	G	O4'-C1'-N9	5.38	112.50	108.20
34	2	484	C	N3-C4-C5	-5.38	119.75	121.90
34	2	294	C	N3-C4-N4	5.38	121.76	118.00
34	2	521	A	O4'-C1'-N9	5.38	112.50	108.20
34	2	1374	A	C5-C6-N1	-5.38	115.01	117.70
34	2	1782	A	C5-C6-N1	-5.38	115.01	117.70
34	2	14	C	N3-C4-N4	5.37	121.76	118.00
34	2	821	A	C5-C6-N6	-5.37	119.40	123.70
34	2	1226	C	N3-C4-C5	-5.37	119.75	121.90
34	2	1418	G	N3-C2-N2	5.37	123.66	119.90
34	2	1740	A	C5-C6-N6	-5.37	119.40	123.70
34	2	354	A	C5-C6-N6	-5.37	119.40	123.70
34	2	1144	A	C5-C6-N1	-5.37	115.02	117.70
34	2	1420	G	O4'-C1'-N9	5.37	112.50	108.20
42	m	201	TYR	CB-CG-CD1	5.37	124.22	121.00
34	2	865	A	O4'-C1'-N9	5.37	112.50	108.20
34	2	1328	A	C4-C5-C6	5.37	119.68	117.00
34	2	1745	C	C5-C4-N4	-5.37	116.44	120.20
34	2	1078	A	C5-C6-N1	-5.37	115.02	117.70
34	2	1602	A	O4'-C1'-N9	5.37	112.49	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	997	A	C4-C5-C6	5.36	119.68	117.00
34	2	1552	C	N3-C4-N4	5.36	121.75	118.00
34	2	670	G	O4'-C1'-N9	5.36	112.49	108.20
34	2	158	A	C5-C6-N1	-5.36	115.02	117.70
34	2	338	A	O4'-C1'-N9	5.36	112.49	108.20
34	2	463	A	O4'-C1'-N9	5.36	112.49	108.20
34	2	827	G	O4'-C1'-N9	5.36	112.49	108.20
34	2	1468	C	N3-C4-C5	-5.36	119.76	121.90
34	2	1705	C	N3-C4-N4	5.36	121.75	118.00
34	2	407	C	N3-C4-C5	-5.36	119.76	121.90
34	2	83	A	C5-C6-N1	-5.36	115.02	117.70
34	2	557	C	N3-C4-N4	5.36	121.75	118.00
34	2	654	A	O4'-C1'-N9	5.36	112.49	108.20
34	2	928	G	O4'-C1'-N9	5.36	112.49	108.20
34	2	654	A	C5-C6-N6	-5.36	119.42	123.70
34	2	1261	A	C5-C6-N1	-5.36	115.02	117.70
34	2	1442	A	C5-C6-N1	-5.36	115.02	117.70
34	2	450	A	O4'-C1'-N9	5.35	112.48	108.20
34	2	1047	G	O4'-C1'-N9	5.35	112.48	108.20
34	2	564	A	C5-C6-N1	-5.35	115.02	117.70
34	2	997	A	C5-C6-N1	-5.35	115.02	117.70
34	2	1773	G	O4'-C1'-N9	5.35	112.48	108.20
34	2	1844	A	C5-C6-N6	-5.35	119.42	123.70
34	2	221	A	O4'-C1'-N9	5.35	112.48	108.20
34	2	985	C	N3-C4-C5	-5.35	119.76	121.90
34	2	1102	C	N3-C4-C5	-5.35	119.76	121.90
34	2	398	A	C5-C6-N1	-5.35	115.03	117.70
34	2	515	A	C4-C5-C6	5.35	119.67	117.00
34	2	979	A	C5-C6-N1	-5.35	115.03	117.70
34	2	1048	A	C5-C6-N1	-5.35	115.03	117.70
34	2	52	G	O4'-C1'-N9	5.35	112.48	108.20
34	2	62	G	O4'-C1'-N9	5.35	112.48	108.20
1	1	15	A	C5-C6-N1	-5.34	115.03	117.70
34	2	516	A	C5-C6-N6	-5.34	119.42	123.70
34	2	806	A	C5-C6-N6	-5.34	119.42	123.70
34	2	850	A	O4'-C1'-N9	5.34	112.47	108.20
34	2	1256	A	C5-C6-N1	-5.34	115.03	117.70
34	2	1379	A	C5-C6-N1	-5.34	115.03	117.70
34	2	861	A	C5-C6-N1	-5.34	115.03	117.70
34	2	926	C	N3-C4-C5	-5.34	119.76	121.90
34	2	1215	C	N3-C4-C5	-5.34	119.76	121.90
34	2	1695	C	O4'-C1'-N1	5.34	112.47	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	159	A	C5-C6-N6	-5.34	119.43	123.70
34	2	299	G	O4'-C1'-N9	5.34	112.47	108.20
34	2	1054	A	C5-C6-N1	-5.34	115.03	117.70
34	2	1467	C	N3-C4-C5	-5.34	119.76	121.90
34	2	1019	A	O4'-C1'-N9	5.34	112.47	108.20
34	2	91	A	C5-C6-N1	-5.34	115.03	117.70
34	2	1051	A	C5-C6-N6	-5.34	119.43	123.70
34	2	1726	A	C5-C6-N1	-5.34	115.03	117.70
34	2	3	C	N3-C4-C5	-5.33	119.77	121.90
34	2	1348	G	O4'-C1'-N9	5.33	112.47	108.20
34	2	976	A	C5-C6-N1	-5.33	115.03	117.70
34	2	1081	C	O4'-C1'-N1	5.33	112.47	108.20
34	2	1214	C	N3-C4-C5	-5.33	119.77	121.90
34	2	1448	A	C5-C6-N1	-5.33	115.03	117.70
34	2	197	U	C6-N1-C1'	-5.33	113.74	121.20
34	2	551	A	C5-C6-N1	-5.33	115.03	117.70
34	2	1287	A	C5-C6-N1	-5.33	115.03	117.70
34	2	868	A	C5-C6-N1	-5.33	115.03	117.70
34	2	493	C	N3-C4-C5	-5.33	119.77	121.90
34	2	366	A	O4'-C1'-N9	5.32	112.46	108.20
34	2	660	A	C5-C6-N1	-5.32	115.04	117.70
34	2	511	A	C5-C6-N6	-5.32	119.44	123.70
34	2	562	U	O4'-C1'-N1	5.32	112.46	108.20
34	2	618	A	C5-C6-N6	-5.32	119.44	123.70
34	2	805	A	C5-C6-N1	-5.32	115.04	117.70
34	2	1140	A	O4'-C1'-N9	5.32	112.46	108.20
34	2	1413	C	N3-C4-C5	-5.32	119.77	121.90
34	2	1479	A	C5-C6-N6	-5.32	119.44	123.70
34	2	1746	C	C5-C4-N4	-5.32	116.48	120.20
34	2	42	A	C5-C6-N6	-5.32	119.44	123.70
34	2	78	C	N3-C4-N4	5.32	121.72	118.00
34	2	1478	C	N3-C4-C5	-5.32	119.77	121.90
34	2	122	G	O4'-C1'-N9	5.32	112.45	108.20
34	2	214	A	C5-C6-N1	-5.32	115.04	117.70
34	2	295	C	N3-C4-N4	5.32	121.72	118.00
34	2	661	A	C5-C6-N6	-5.32	119.45	123.70
34	2	104	A	O4'-C1'-N9	5.32	112.45	108.20
34	2	435	A	O4'-C1'-N9	5.32	112.45	108.20
34	2	985	C	N3-C4-N4	5.32	121.72	118.00
34	2	1397	A	C5-C6-N6	-5.32	119.45	123.70
34	2	1484	C	O4'-C1'-N1	5.32	112.45	108.20
34	2	1589	A	C5-C6-N1	-5.32	115.04	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1635	A	C5-C6-N1	-5.32	115.04	117.70
34	2	1184	A	O4'-C1'-N9	5.31	112.45	108.20
34	2	1146	A	C5-C6-N6	-5.31	119.45	123.70
34	2	35	C	N3-C4-C5	-5.31	119.78	121.90
34	2	60	A	C5-C6-N1	-5.31	115.05	117.70
34	2	150	A	C4-C5-C6	5.31	119.66	117.00
34	2	329	A	C5-C6-N1	-5.31	115.05	117.70
34	2	609	A	C5-C6-N6	-5.31	119.45	123.70
34	2	804	A	O4'-C1'-N9	5.31	112.45	108.20
34	2	1288	C	N3-C4-N4	5.31	121.72	118.00
34	2	1212	C	N3-C4-C5	-5.31	119.78	121.90
34	2	1330	G	C5-C6-O6	-5.31	125.42	128.60
34	2	1482	A	C5-C6-N1	-5.31	115.05	117.70
34	2	1522	C	N3-C4-C5	-5.31	119.78	121.90
34	2	1795	A	C5-C6-N1	-5.31	115.05	117.70
34	2	174	C	N3-C4-C5	-5.30	119.78	121.90
34	2	295	C	N3-C4-C5	-5.30	119.78	121.90
34	2	625	G	O4'-C1'-N9	5.30	112.44	108.20
34	2	830	C	N3-C4-C5	-5.30	119.78	121.90
34	2	320	G	O4'-C1'-N9	5.30	112.44	108.20
1	1	54	A	C5-C6-N1	-5.30	115.05	117.70
34	2	226	A	C5-C6-N6	-5.30	119.46	123.70
34	2	513	A	C5-C6-N1	-5.30	115.05	117.70
34	2	535	A	C5-C6-N1	-5.30	115.05	117.70
34	2	1537	C	N3-C4-N4	5.30	121.71	118.00
30	f	150	PHE	CB-CG-CD1	5.30	124.51	120.80
34	2	127	C	N3-C4-C5	-5.30	119.78	121.90
34	2	373	G	O4'-C1'-N9	5.30	112.44	108.20
34	2	644	A	C5-C6-N1	-5.30	115.05	117.70
34	2	1089	A	C5-C6-N6	-5.30	119.46	123.70
34	2	798	A	C5-C6-N1	-5.30	115.05	117.70
34	2	1158	C	N3-C4-C5	-5.30	119.78	121.90
34	2	1216	A	C5-C6-N1	-5.30	115.05	117.70
34	2	1446	G	O4'-C1'-N9	5.30	112.44	108.20
34	2	1283	A	C5-C6-N1	-5.29	115.05	117.70
34	2	1658	A	C5-C6-N6	-5.29	119.46	123.70
1	1	60	A	C5-C6-N1	-5.29	115.05	117.70
34	2	808	A	C4-C5-C6	5.29	119.65	117.00
34	2	992	A	C5-C6-N6	-5.29	119.47	123.70
34	2	1196	A	C5-C6-N1	-5.29	115.05	117.70
34	2	1565	G	O4'-C1'-N9	5.29	112.43	108.20
34	2	1776	G	O4'-C1'-N9	5.29	112.44	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	199	G	O4'-C1'-N9	5.29	112.43	108.20
34	2	223	A	C5-C6-N1	-5.29	115.06	117.70
34	2	328	G	O4'-C1'-N9	5.29	112.43	108.20
34	2	910	U	O4'-C1'-N1	5.29	112.43	108.20
34	2	1018	U	C2-N1-C1'	5.29	124.05	117.70
34	2	1031	A	C5-C6-N1	-5.29	115.05	117.70
34	2	1324	G	O4'-C1'-N9	5.29	112.43	108.20
34	2	1414	C	N3-C4-C5	-5.29	119.78	121.90
34	2	19	A	O4'-C1'-N9	5.29	112.43	108.20
34	2	390	C	N3-C4-C5	-5.29	119.78	121.90
34	2	1196	A	O4'-C1'-N9	5.29	112.43	108.20
34	2	1527	C	N3-C4-C5	-5.29	119.78	121.90
35	A	82	TYR	CB-CG-CD1	5.29	124.17	121.00
34	2	473	C	N3-C4-C5	-5.29	119.78	121.90
34	2	970	C	N3-C4-C5	-5.29	119.78	121.90
34	2	1066	A	C5-C6-N1	-5.29	115.06	117.70
34	2	1237	A	C5-C6-N6	-5.29	119.47	123.70
34	2	1625	A	C5-C6-N6	-5.29	119.47	123.70
34	2	1731	G	O4'-C1'-N9	5.29	112.43	108.20
34	2	42	A	C5-C6-N1	-5.29	115.06	117.70
34	2	655	G	O4'-C1'-N9	5.29	112.43	108.20
34	2	1718	G	O4'-C1'-N9	5.29	112.43	108.20
34	2	84	A	C5-C6-N1	-5.28	115.06	117.70
34	2	459	A	C5-C6-N6	-5.28	119.47	123.70
34	2	1043	C	N3-C4-C5	-5.28	119.79	121.90
34	2	1540	A	C5-C6-N1	-5.28	115.06	117.70
41	3	64	A	C5-C6-N1	-5.28	115.06	117.70
34	2	227	A	O4'-C1'-N9	5.28	112.43	108.20
34	2	1378	A	C5-C6-N1	-5.28	115.06	117.70
34	2	206	A	O4'-C1'-N9	5.28	112.42	108.20
34	2	472	G	N3-C2-N2	5.28	123.60	119.90
34	2	1513	C	C6-N1-C1'	-5.28	114.46	120.80
34	2	506	A	C5-C6-N6	-5.28	119.48	123.70
34	2	165	G	C4-N9-C1'	5.28	133.36	126.50
34	2	351	U	O4'-C1'-N1	5.28	112.42	108.20
34	2	826	A	O4'-C1'-N9	5.28	112.42	108.20
34	2	1338	U	O4'-C1'-N1	5.28	112.42	108.20
34	2	1411	C	N3-C4-C5	-5.28	119.79	121.90
34	2	1740	A	C5-C6-N1	-5.28	115.06	117.70
34	2	591	G	O4'-C1'-N9	5.28	112.42	108.20
34	2	833	A	C5-C6-N1	-5.28	115.06	117.70
34	2	951	A	C5-C6-N1	-5.28	115.06	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	863	G	O4'-C1'-N9	5.27	112.42	108.20
34	2	987	G	C8-N9-C1'	-5.27	120.14	127.00
34	2	142	C	C6-N1-C1'	-5.27	114.47	120.80
34	2	1375	A	C5-C6-N1	-5.27	115.06	117.70
1	1	12	C	N3-C4-C5	-5.27	119.79	121.90
22	X	10	ASP	N-CA-CB	5.27	120.09	110.60
34	2	404	A	C5-C6-N1	-5.27	115.06	117.70
34	2	1714	A	C5-C6-N1	-5.27	115.06	117.70
1	1	57	G	O4'-C1'-N9	5.27	112.42	108.20
34	2	49	C	N3-C4-C5	-5.27	119.79	121.90
34	2	1264	C	N3-C4-C5	-5.27	119.79	121.90
34	2	1807	A	C5-C6-N6	-5.27	119.48	123.70
34	2	564	A	C5-C6-N6	-5.27	119.49	123.70
38	k	388	PHE	CB-CG-CD1	5.27	124.49	120.80
41	3	50	C	N3-C4-C5	-5.27	119.79	121.90
34	2	1195	A	O4'-C1'-N9	5.27	112.41	108.20
34	2	1613	C	N3-C4-C5	-5.27	119.79	121.90
1	1	52	G	O4'-C1'-N9	5.26	112.41	108.20
3	C	139	TYR	CB-CG-CD2	-5.26	117.84	121.00
34	2	873	C	N3-C4-C5	-5.26	119.79	121.90
34	2	1524	C	N3-C4-C5	-5.26	119.80	121.90
34	2	908	C	N3-C4-N4	5.26	121.68	118.00
34	2	1015	C	N3-C4-N4	5.26	121.68	118.00
1	1	17	C	O4'-C1'-N1	5.26	112.41	108.20
34	2	67	C	N3-C4-C5	-5.26	119.80	121.90
34	2	1576	C	N3-C4-C5	-5.26	119.80	121.90
34	2	1632	A	C5-C6-N6	-5.26	119.49	123.70
34	2	1829	A	C5-C6-N1	-5.26	115.07	117.70
34	2	232	A	C5-C6-N1	-5.26	115.07	117.70
34	2	466	A	C4-C5-C6	5.26	119.63	117.00
34	2	503	G	O4'-C1'-N9	5.26	112.41	108.20
34	2	850	A	C5-C6-N6	-5.26	119.49	123.70
34	2	1096	A	C5-C6-N6	-5.26	119.49	123.70
34	2	1129	A	O4'-C1'-N9	5.26	112.41	108.20
34	2	1186	A	C5-C6-N6	-5.26	119.49	123.70
34	2	16	G	O4'-C1'-N9	5.26	112.41	108.20
34	2	60	A	C5-C6-N6	-5.26	119.50	123.70
34	2	454	A	C5-C6-N1	-5.26	115.07	117.70
34	2	659	A	C5-C6-N6	-5.26	119.50	123.70
34	2	812	A	C5-C6-N1	-5.26	115.07	117.70
34	2	899	A	C5-C6-N6	-5.26	119.50	123.70
34	2	804	A	C5-C6-N1	-5.25	115.07	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1166	A	C4-C5-C6	5.25	119.63	117.00
34	2	1571	G	O4'-C1'-N9	5.25	112.40	108.20
1	1	2	A	C5-C6-N6	-5.25	119.50	123.70
1	1	11	G	O4'-C1'-N9	5.25	112.40	108.20
34	2	338	A	C5-C6-N6	-5.25	119.50	123.70
34	2	540	C	N3-C4-C5	-5.25	119.80	121.90
34	2	547	U	O4'-C1'-N1	5.25	112.40	108.20
34	2	814	A	O4'-C1'-N9	5.25	112.40	108.20
34	2	1528	A	C5-C6-N1	-5.25	115.07	117.70
34	2	1646	A	C5-C6-N1	-5.25	115.07	117.70
34	2	1705	C	N3-C4-C5	-5.25	119.80	121.90
34	2	363	G	O4'-C1'-N9	5.25	112.40	108.20
34	2	1058	A	C5-C6-N1	-5.25	115.08	117.70
34	2	1087	C	N3-C4-C5	-5.25	119.80	121.90
34	2	1465	A	C5-C6-N1	-5.25	115.08	117.70
34	2	1470	A	C5-C6-N1	-5.25	115.08	117.70
1	1	73	A	C5-C6-N1	-5.25	115.08	117.70
34	2	846	C	N3-C4-C5	-5.25	119.80	121.90
34	2	1064	G	N3-C2-N2	5.25	123.57	119.90
34	2	1134	C	N3-C4-C5	-5.25	119.80	121.90
34	2	1384	A	C5-C6-N1	-5.25	115.08	117.70
34	2	1578	C	N3-C4-N4	5.25	121.67	118.00
34	2	290	A	O4'-C1'-N9	5.25	112.40	108.20
34	2	1857	A	C5-C6-N6	-5.25	119.50	123.70
34	2	601	G	O4'-C1'-N9	5.24	112.39	108.20
34	2	1372	A	O4'-C1'-N9	5.24	112.39	108.20
34	2	1480	A	C5-C6-N1	-5.24	115.08	117.70
38	k	516	PHE	CB-CG-CD1	5.24	124.47	120.80
34	2	662	A	C5-C6-N1	-5.24	115.08	117.70
34	2	619	A	C5-C6-N1	-5.24	115.08	117.70
34	2	1008	A	C5-C6-N1	-5.24	115.08	117.70
34	2	1845	A	C5-C6-N1	-5.24	115.08	117.70
34	2	538	C	N3-C4-C5	-5.24	119.81	121.90
34	2	804	A	C5-C6-N6	-5.24	119.51	123.70
34	2	1673	A	C5-C6-N1	-5.24	115.08	117.70
34	2	371	C	N3-C4-N4	5.24	121.67	118.00
34	2	576	G	N3-C2-N2	5.24	123.57	119.90
34	2	1374	A	C5-C6-N6	-5.24	119.51	123.70
34	2	1612	G	N3-C2-N2	5.24	123.57	119.90
34	2	38	A	C5-C6-N1	-5.24	115.08	117.70
34	2	1267	C	N3-C4-N4	5.24	121.67	118.00
34	2	1694	A	C5-C6-N6	-5.24	119.51	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	39	C	O4'-C1'-N1	5.23	112.39	108.20
34	2	64	A	C5-C6-N1	-5.23	115.08	117.70
34	2	847	C	N3-C4-N4	5.23	121.66	118.00
34	2	866	A	C5-C6-N1	-5.23	115.08	117.70
34	2	438	A	C5-C6-N6	-5.23	119.52	123.70
34	2	1032	A	C5-C6-N1	-5.23	115.08	117.70
34	2	1782	A	O4'-C1'-N9	5.23	112.39	108.20
34	2	652	G	N1-C6-O6	5.23	123.04	119.90
34	2	107	A	C5-C6-N1	-5.23	115.08	117.70
34	2	415	G	O4'-C1'-N9	5.23	112.38	108.20
35	A	100	ASP	CB-CG-OD2	-5.23	113.59	118.30
34	2	1316	G	O4'-C1'-N9	5.23	112.38	108.20
43	y	329	ILE	C-N-CD	5.23	139.38	128.40
34	2	857	A	C5-C6-N1	-5.23	115.09	117.70
34	2	1147	G	O4'-C1'-N9	5.23	112.38	108.20
34	2	27	A	C5-C6-N1	-5.22	115.09	117.70
34	2	1076	A	C5-C6-N1	-5.22	115.09	117.70
34	2	1140	A	C5-C6-N6	-5.22	119.52	123.70
34	2	1184	A	C5-C6-N6	-5.22	119.52	123.70
34	2	1314	G	O4'-C1'-N9	5.22	112.38	108.20
34	2	1405	A	O4'-C1'-N9	5.22	112.38	108.20
34	2	1419	C	N3-C4-C5	-5.22	119.81	121.90
34	2	80	G	O3'-P-O5'	5.22	113.92	104.00
34	2	142	C	N3-C4-C5	-5.22	119.81	121.90
34	2	326	A	C5-C6-N6	-5.22	119.52	123.70
34	2	658	A	C5-C6-N1	-5.22	115.09	117.70
34	2	1059	C	N3-C4-N4	5.22	121.66	118.00
34	2	1182	U	C1'-O4'-C4'	5.22	114.08	109.90
34	2	1192	A	O4'-C1'-N9	5.22	112.38	108.20
34	2	78	C	C2-N1-C1'	5.22	124.54	118.80
34	2	382	A	C5-C6-N1	-5.22	115.09	117.70
34	2	1038	A	O4'-C1'-N9	5.22	112.38	108.20
34	2	546	U	O4'-C1'-N1	5.22	112.38	108.20
34	2	1690	A	C5-C6-N1	-5.22	115.09	117.70
34	2	1542	C	N3-C4-N4	5.22	121.65	118.00
34	2	1730	A	C5-C6-N1	-5.22	115.09	117.70
34	2	1162	G	O4'-C1'-N9	5.22	112.37	108.20
50	u	115	LYS	N-CA-CB	5.22	119.99	110.60
34	2	636	G	O4'-C1'-N9	5.21	112.37	108.20
34	2	814	A	C5-C6-N1	-5.21	115.09	117.70
34	2	949	C	N3-C4-C5	-5.21	119.81	121.90
34	2	1532	A	O4'-C1'-N9	5.21	112.37	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	w	53	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	1	23	C	N3-C4-C5	-5.21	119.81	121.90
34	2	948	G	O4'-C1'-N9	5.21	112.37	108.20
34	2	1539	C	C5-C4-N4	-5.21	116.55	120.20
34	2	1180	G	O4'-C1'-N9	5.21	112.37	108.20
34	2	1231	G	O4'-C1'-N9	5.21	112.37	108.20
34	2	1717	G	O4'-C1'-N9	5.21	112.37	108.20
13	M	70	TYR	CB-CG-CD1	5.21	124.12	121.00
34	2	6	G	O4'-C1'-N9	5.21	112.37	108.20
34	2	1497	C	N3-C4-C5	-5.21	119.82	121.90
34	2	389	C	N3-C4-C5	-5.21	119.82	121.90
34	2	656	U	O4'-C1'-N1	5.21	112.36	108.20
34	2	40	A	C5-C6-N1	-5.20	115.10	117.70
34	2	1038	A	C5-C6-N1	-5.20	115.10	117.70
34	2	1123	C	N3-C4-C5	-5.20	119.82	121.90
34	2	915	A	C5-C6-N1	-5.20	115.10	117.70
34	2	1586	C	N3-C4-C5	-5.20	119.82	121.90
34	2	167	G	O4'-C1'-N9	5.20	112.36	108.20
34	2	675	A	C5-C6-N1	-5.20	115.10	117.70
34	2	918	A	O4'-C1'-N9	5.20	112.36	108.20
47	r	123	THR	N-CA-CB	5.20	120.18	110.30
34	2	1030	A	O4'-C1'-N9	5.20	112.36	108.20
34	2	1508	C	N3-C4-C5	-5.20	119.82	121.90
1	1	8	G	O4'-C1'-N9	5.20	112.36	108.20
34	2	53	C	N3-C4-C5	-5.20	119.82	121.90
34	2	677	C	O4'-C1'-N1	5.20	112.36	108.20
34	2	1530	U	C2-N1-C1'	5.20	123.94	117.70
34	2	1800	A	O4'-C1'-N9	5.20	112.36	108.20
34	2	205	G	N3-C2-N2	5.19	123.53	119.90
34	2	369	C	N3-C4-C5	-5.19	119.82	121.90
34	2	429	A	O4'-C1'-N9	5.19	112.35	108.20
34	2	545	A	P-O3'-C3'	5.19	125.93	119.70
34	2	836	C	N3-C4-C5	-5.19	119.82	121.90
34	2	1247	A	C5-C6-N1	-5.19	115.10	117.70
34	2	1254	A	C5-C6-N1	-5.19	115.10	117.70
34	2	1675	G	O4'-C1'-N9	5.19	112.35	108.20
34	2	151	C	N3-C4-C5	-5.19	119.82	121.90
34	2	80	G	OP2-P-O3'	-5.19	93.78	105.20
34	2	157	U	O4'-C1'-N1	5.19	112.35	108.20
34	2	181	A	C5-C6-N6	-5.19	119.55	123.70
34	2	463	A	C5-C6-N1	-5.19	115.11	117.70
43	y	123	THR	C-N-CD	5.19	139.29	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	160	U	O4'-C1'-N1	5.18	112.35	108.20
34	2	405	A	C5-C6-N1	-5.18	115.11	117.70
34	2	1025	G	O4'-C1'-N9	5.18	112.35	108.20
49	t	522	TYR	CB-CG-CD2	-5.18	117.89	121.00
34	2	595	A	C5-C6-N6	-5.18	119.55	123.70
34	2	1327	C	N3-C4-N4	5.18	121.63	118.00
34	2	1372	A	C5-C6-N1	-5.18	115.11	117.70
34	2	1537	C	N3-C4-C5	-5.18	119.83	121.90
34	2	235	C	C5-C4-N4	-5.18	116.57	120.20
34	2	416	A	C5-C6-N1	-5.18	115.11	117.70
34	2	1312	C	N3-C4-C5	-5.18	119.83	121.90
34	2	1805	C	N3-C4-C5	-5.18	119.83	121.90
34	2	371	C	N3-C4-C5	-5.18	119.83	121.90
34	2	557	C	N3-C4-C5	-5.18	119.83	121.90
34	2	593	C	N3-C4-C5	-5.18	119.83	121.90
34	2	824	G	O4'-C1'-N9	5.18	112.34	108.20
34	2	1630	C	N3-C4-C5	-5.18	119.83	121.90
34	2	1793	G	O4'-C1'-N9	5.18	112.34	108.20
34	2	99	A	C5-C6-N1	-5.17	115.11	117.70
34	2	609	A	O4'-C1'-N9	5.17	112.34	108.20
34	2	1337	C	N3-C4-C5	-5.17	119.83	121.90
34	2	1549	C	N3-C4-C5	-5.17	119.83	121.90
34	2	446	C	N3-C4-C5	-5.17	119.83	121.90
34	2	798	A	O4'-C1'-N9	5.17	112.34	108.20
34	2	1295	A	C5-C6-N1	-5.17	115.11	117.70
34	2	1321	G	O4'-C1'-N9	5.17	112.34	108.20
34	2	1636	A	C5-C6-N1	-5.17	115.11	117.70
48	s	204	LYS	N-CA-CB	5.17	119.91	110.60
34	2	1243	C	N3-C4-C5	-5.17	119.83	121.90
34	2	293	A	C5-C6-N6	-5.17	119.57	123.70
34	2	164	A	O4'-C1'-N9	5.17	112.33	108.20
34	2	445	A	O4'-C1'-N9	5.17	112.33	108.20
34	2	458	A	O4'-C1'-N9	5.17	112.33	108.20
34	2	899	A	O4'-C1'-N9	5.17	112.33	108.20
34	2	1337	C	O4'-C1'-N1	5.17	112.33	108.20
34	2	509	A	O4'-C1'-N9	5.17	112.33	108.20
34	2	1785	A	O4'-C1'-N9	5.17	112.33	108.20
41	3	51	C	N3-C4-C5	-5.17	119.83	121.90
34	2	77	A	O4'-C1'-N9	5.16	112.33	108.20
34	2	502	A	O4'-C1'-N9	5.16	112.33	108.20
34	2	1674	A	C5-C6-N1	-5.16	115.12	117.70
38	k	551	LEU	CB-CG-CD2	5.16	119.78	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	22	G	O4'-C1'-N9	5.16	112.33	108.20
34	2	292	A	C5-C6-N1	-5.16	115.12	117.70
34	2	915	A	O4'-C1'-N9	5.16	112.33	108.20
34	2	1431	C	N3-C4-C5	-5.16	119.84	121.90
34	2	1491	G	O4'-C1'-N9	5.16	112.33	108.20
34	2	1557	C	N3-C4-C5	-5.16	119.84	121.90
34	2	1730	A	C5-C6-N6	-5.16	119.57	123.70
34	2	240	C	N3-C4-C5	-5.16	119.84	121.90
34	2	526	A	C5-C6-N6	-5.16	119.58	123.70
34	2	967	G	N3-C2-N2	5.16	123.51	119.90
34	2	1432	C	O4'-C1'-N1	5.16	112.33	108.20
34	2	1751	G	O4'-C1'-N9	5.16	112.32	108.20
34	2	1825	A	C5-C6-N1	-5.16	115.12	117.70
34	2	1837	G	O4'-C1'-N9	5.16	112.32	108.20
34	2	202	U	O4'-C1'-N1	5.15	112.32	108.20
34	2	1131	C	N3-C4-C5	-5.15	119.84	121.90
34	2	427	G	O4'-C1'-N9	5.15	112.32	108.20
34	2	359	C	N3-C4-C5	-5.15	119.84	121.90
34	2	953	A	O4'-C1'-N9	5.15	112.32	108.20
34	2	992	A	C5-C6-N1	-5.15	115.12	117.70
34	2	1401	A	O4'-C1'-N9	5.15	112.32	108.20
34	2	1803	A	C5-C6-N1	-5.15	115.12	117.70
34	2	1361	G	O4'-C1'-N9	5.15	112.32	108.20
34	2	1592	C	N3-C4-C5	-5.15	119.84	121.90
34	2	985	C	O4'-C1'-N1	5.15	112.32	108.20
34	2	1509	G	O4'-C1'-N9	5.15	112.32	108.20
34	2	1803	A	O4'-C1'-N9	5.15	112.32	108.20
1	1	73	A	O4'-C1'-N9	5.15	112.32	108.20
34	2	835	C	C6-N1-C1'	-5.15	114.62	120.80
34	2	1544	U	O4'-C1'-N1	5.15	112.32	108.20
34	2	813	G	N3-C2-N2	5.14	123.50	119.90
34	2	1479	A	C5-C6-N1	-5.14	115.13	117.70
34	2	1832	U	O4'-C1'-N1	5.14	112.32	108.20
34	2	1845	A	O4'-C1'-N9	5.14	112.32	108.20
34	2	48	C	N3-C4-C5	-5.14	119.84	121.90
34	2	431	C	N3-C4-C5	-5.14	119.84	121.90
34	2	644	A	O4'-C1'-N9	5.14	112.31	108.20
34	2	938	G	N3-C2-N2	5.14	123.50	119.90
34	2	1442	A	C5-C6-N6	-5.14	119.59	123.70
1	1	38	A	C5-C6-N1	-5.14	115.13	117.70
34	2	333	A	C5-C6-N6	-5.14	119.59	123.70
34	2	519	A	C5-C6-N1	-5.14	115.13	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1701	G	O4'-C1'-N9	5.14	112.31	108.20
34	2	435	A	C5-C6-N1	-5.14	115.13	117.70
34	2	1058	A	C5-C6-N6	-5.14	119.59	123.70
34	2	565	A	C5-C6-N1	-5.14	115.13	117.70
34	2	922	A	C5-C6-N1	-5.14	115.13	117.70
34	2	92	A	C5-C6-N1	-5.14	115.13	117.70
34	2	118	C	N3-C4-C5	-5.14	119.85	121.90
34	2	518	A	C5-C6-N1	-5.14	115.13	117.70
34	2	91	A	O4'-C1'-N9	5.13	112.31	108.20
34	2	318	U	O4'-C1'-N1	5.13	112.31	108.20
34	2	372	C	N3-C4-C5	-5.13	119.85	121.90
34	2	649	G	O4'-C1'-N9	5.13	112.31	108.20
34	2	854	A	C5-C6-N6	-5.13	119.59	123.70
34	2	1291	A	C5-C6-N6	-5.13	119.59	123.70
34	2	1330	G	O4'-C1'-N9	5.13	112.31	108.20
34	2	1024	A	C5-C6-N1	-5.13	115.13	117.70
31	g	101	PHE	CB-CG-CD2	-5.13	117.21	120.80
34	2	1219	A	O4'-C1'-N9	5.13	112.30	108.20
27	c	65	GLN	C-N-CD	5.13	139.17	128.40
34	2	175	A	C5-C6-N1	-5.13	115.14	117.70
34	2	483	A	O4'-C1'-N9	5.13	112.30	108.20
34	2	566	A	O4'-C1'-N9	5.13	112.30	108.20
34	2	1322	U	C2-N1-C1'	5.13	123.86	117.70
34	2	968	A	C5-C6-N6	-5.12	119.60	123.70
34	2	1434	A	O4'-C1'-N9	5.12	112.30	108.20
34	2	820	C	N3-C4-C5	-5.12	119.85	121.90
34	2	932	G	O4'-C1'-N9	5.12	112.30	108.20
34	2	371	C	O4'-C1'-N1	5.12	112.30	108.20
34	2	402	G	O4'-C1'-N9	5.12	112.30	108.20
34	2	623	C	N3-C4-C5	-5.12	119.85	121.90
34	2	673	G	O4'-C1'-N9	5.12	112.30	108.20
34	2	909	A	C5-C6-N1	-5.12	115.14	117.70
34	2	965	U	O4'-C1'-N1	5.12	112.30	108.20
34	2	1020	A	C5-C6-N1	-5.12	115.14	117.70
34	2	1087	C	N3-C4-N4	5.12	121.58	118.00
34	2	1568	G	O4'-C1'-N9	5.12	112.30	108.20
34	2	1744	G	O4'-C1'-N9	5.12	112.30	108.20
36	B	194	LYS	N-CA-CB	5.12	119.82	110.60
34	2	1066	A	C5-C6-N6	-5.12	119.60	123.70
34	2	10	G	N3-C2-N2	5.12	123.48	119.90
34	2	448	A	O4'-C1'-N9	5.12	112.30	108.20
34	2	545	A	O4'-C1'-N9	5.12	112.29	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1583	A	C5-C6-N1	-5.12	115.14	117.70
34	2	1145	A	C5-C6-N1	-5.12	115.14	117.70
34	2	1149	C	N3-C4-C5	-5.12	119.85	121.90
34	2	1499	C	N3-C4-C5	-5.12	119.85	121.90
34	2	1809	A	C5-C6-N6	-5.12	119.61	123.70
34	2	1371	G	O4'-C1'-N9	5.11	112.29	108.20
34	2	1274	A	C5-C6-N1	-5.11	115.14	117.70
34	2	1647	G	O4'-C1'-N9	5.11	112.29	108.20
37	j	95	TYR	C-N-CA	5.11	134.48	121.70
45	w	143	ASN	C-N-CA	5.11	134.48	121.70
34	2	388	A	C5-C6-N1	-5.11	115.14	117.70
34	2	482	C	N3-C4-C5	-5.11	119.86	121.90
34	2	1164	G	O4'-C1'-N9	5.11	112.29	108.20
34	2	1670	A	C5-C6-N1	-5.11	115.15	117.70
45	w	179	MET	CG-SD-CE	-5.11	92.03	100.20
34	2	84	A	O4'-C1'-N9	5.11	112.28	108.20
34	2	1229	G	O4'-C1'-N9	5.11	112.28	108.20
34	2	1609	A	C5-C6-N1	-5.11	115.15	117.70
34	2	1664	G	O4'-C1'-N9	5.11	112.28	108.20
34	2	7	G	O4'-C1'-N9	5.10	112.28	108.20
34	2	1275	C	N3-C4-C5	-5.10	119.86	121.90
34	2	1629	A	O4'-C1'-N9	5.10	112.28	108.20
34	2	589	A	O4'-C1'-N9	5.10	112.28	108.20
34	2	1078	A	O4'-C1'-N9	5.10	112.28	108.20
34	2	1170	U	C6-N1-C1'	-5.10	114.06	121.20
34	2	1327	C	N3-C4-C5	-5.10	119.86	121.90
34	2	141	A	P-O3'-C3'	5.10	125.82	119.70
34	2	900	A	C5-C6-N6	-5.10	119.62	123.70
34	2	1835	C	N3-C4-C5	-5.10	119.86	121.90
34	2	908	C	N3-C4-C5	-5.09	119.86	121.90
34	2	1353	A	C5-C6-N6	-5.09	119.62	123.70
34	2	1847	C	N3-C4-N4	5.09	121.57	118.00
34	2	353	A	C4-C5-C6	5.09	119.55	117.00
34	2	366	A	C5-C6-N1	-5.09	115.15	117.70
34	2	907	C	N3-C4-C5	-5.09	119.86	121.90
41	3	64	A	C5-C6-N6	-5.09	119.62	123.70
34	2	379	A	O4'-C1'-N9	5.09	112.27	108.20
34	2	1394	G	O4'-C1'-N9	5.09	112.27	108.20
34	2	1521	G	O4'-C1'-N9	5.09	112.27	108.20
48	s	88	MET	CG-SD-CE	-5.09	92.06	100.20
34	2	437	A	C5-N7-C8	5.09	106.44	103.90
34	2	583	C	N3-C4-C5	-5.09	119.86	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1516	C	O4'-C1'-N1	5.09	112.27	108.20
34	2	333	A	O4'-C1'-N9	5.09	112.27	108.20
34	2	438	A	C5-C6-N1	-5.09	115.16	117.70
27	c	37	CYS	C-N-CD	5.09	139.08	128.40
34	2	934	A	O4'-C1'-N9	5.09	112.27	108.20
34	2	1004	A	C5-C6-N1	-5.09	115.16	117.70
34	2	229	A	C5-C6-N6	-5.08	119.63	123.70
34	2	288	A	O4'-C1'-N9	5.08	112.27	108.20
34	2	1410	A	C5-C6-N6	-5.08	119.63	123.70
44	v	799	TYR	CB-CG-CD2	-5.08	117.95	121.00
34	2	337	G	O4'-C1'-N9	5.08	112.27	108.20
34	2	858	A	O4'-C1'-N9	5.08	112.27	108.20
34	2	871	A	C5-C6-N1	-5.08	115.16	117.70
34	2	1483	A	C5-C6-N1	-5.08	115.16	117.70
34	2	1216	A	P-O3'-C3'	5.08	125.80	119.70
34	2	1380	C	N3-C4-C5	-5.08	119.87	121.90
34	2	58	C	N3-C4-C5	-5.08	119.87	121.90
34	2	1246	A	C5-C6-N1	-5.08	115.16	117.70
34	2	919	G	O4'-C1'-N9	5.07	112.26	108.20
34	2	1032	A	O4'-C1'-N9	5.07	112.26	108.20
34	2	1178	A	O4'-C1'-N9	5.07	112.26	108.20
34	2	1601	G	N3-C2-N2	5.07	123.45	119.90
34	2	1777	C	N3-C4-N4	5.07	121.55	118.00
34	2	1839	A	C5-C6-N1	-5.07	115.16	117.70
34	2	1849	G	O4'-C1'-N9	5.07	112.26	108.20
34	2	306	C	N3-C4-C5	-5.07	119.87	121.90
34	2	1407	G	O4'-C1'-N9	5.07	112.26	108.20
34	2	102	A	C5-C6-N6	-5.07	119.64	123.70
34	2	1384	A	O4'-C1'-N9	5.07	112.26	108.20
34	2	1457	G	N3-C2-N2	5.07	123.45	119.90
43	y	265	LYS	C-N-CD	5.07	139.04	128.40
34	2	339	A	C5-C6-N1	-5.07	115.17	117.70
34	2	968	A	O4'-C1'-N9	5.07	112.25	108.20
34	2	1048	A	O4'-C1'-N9	5.07	112.25	108.20
34	2	1608	G	O4'-C1'-N9	5.07	112.25	108.20
34	2	1585	C	N3-C4-C5	-5.07	119.87	121.90
43	y	268	LYS	C-N-CD	5.07	139.04	128.40
34	2	1383	G	O4'-C1'-N9	5.06	112.25	108.20
34	2	1777	C	O4'-C1'-N1	5.06	112.25	108.20
34	2	823	A	O4'-C1'-N9	5.06	112.25	108.20
44	v	394	LYS	C-N-CD	5.06	139.03	128.40
34	2	44	U	O4'-C1'-N1	5.06	112.25	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	372	C	N3-C4-N4	5.06	121.54	118.00
34	2	431	C	N3-C4-N4	5.06	121.54	118.00
34	2	856	G	O4'-C1'-N9	5.06	112.25	108.20
34	2	1266	G	O4'-C1'-N9	5.06	112.25	108.20
34	2	1850	C	N3-C4-C5	-5.06	119.88	121.90
36	B	279	LYS	C-N-CD	5.06	139.02	128.40
34	2	960	A	C5-C6-N6	-5.06	119.65	123.70
34	2	1487	G	O4'-C1'-N9	5.06	112.25	108.20
34	2	168	C	N3-C4-C5	-5.05	119.88	121.90
34	2	1261	A	C5-C6-N6	-5.05	119.66	123.70
34	2	1851	G	O4'-C1'-N9	5.05	112.24	108.20
34	2	574	A	C5-C6-N1	-5.05	115.17	117.70
34	2	805	A	O4'-C1'-N9	5.05	112.24	108.20
34	2	1305	C	N3-C4-C5	-5.05	119.88	121.90
34	2	393	G	O4'-C1'-N9	5.05	112.24	108.20
34	2	858	A	C5-C6-N1	-5.05	115.17	117.70
34	2	957	G	O4'-C1'-N9	5.05	112.24	108.20
34	2	1826	A	C5-C6-N6	-5.05	119.66	123.70
43	y	363	ALA	C-N-CD	5.05	139.01	128.40
34	2	332	C	N3-C4-C5	-5.05	119.88	121.90
34	2	847	C	N3-C4-C5	-5.05	119.88	121.90
34	2	1166	A	O4'-C1'-N9	5.05	112.24	108.20
34	2	1809	A	C5-C6-N1	-5.05	115.17	117.70
49	t	415	TYR	CB-CG-CD2	-5.05	117.97	121.00
34	2	897	G	O4'-C1'-N9	5.05	112.24	108.20
34	2	994	A	O4'-C1'-N9	5.05	112.24	108.20
34	2	622	C	N3-C4-C5	-5.05	119.88	121.90
34	2	843	A	O4'-C1'-N9	5.05	112.24	108.20
34	2	1777	C	N3-C4-C5	-5.05	119.88	121.90
43	y	25	GLN	C-N-CD	5.04	138.99	128.40
43	y	332	THR	C-N-CD	5.04	138.99	128.40
34	2	283	A	O4'-C1'-N9	5.04	112.23	108.20
34	2	849	C	N3-C4-N4	5.04	121.53	118.00
34	2	1004	A	O4'-C1'-N9	5.04	112.23	108.20
34	2	1036	G	O4'-C1'-N9	5.04	112.23	108.20
34	2	1098	G	O4'-C1'-N9	5.04	112.23	108.20
34	2	1213	A	C5-C6-N1	-5.04	115.18	117.70
34	2	1397	A	C5-C6-N1	-5.04	115.18	117.70
34	2	1451	A	C5-C6-N6	-5.04	119.67	123.70
34	2	1589	A	O4'-C1'-N9	5.04	112.23	108.20
34	2	39	A	O4'-C1'-N9	5.04	112.23	108.20
34	2	1549	C	O4'-C1'-N1	5.04	112.23	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1583	A	O4'-C1'-N9	5.04	112.23	108.20
34	2	1824	U	O4'-C1'-N1	5.04	112.23	108.20
34	2	1333	C	N3-C4-C5	-5.04	119.88	121.90
34	2	934	A	C5-C6-N6	-5.04	119.67	123.70
34	2	483	A	C5-C6-N1	-5.04	115.18	117.70
34	2	1341	G	O4'-C1'-N9	5.04	112.23	108.20
1	1	74	C	O4'-C1'-N1	5.04	112.23	108.20
34	2	620	U	O4'-C1'-N1	5.04	112.23	108.20
34	2	1494	A	C5-C6-N6	-5.04	119.67	123.70
34	2	171	A	C5-C6-N1	-5.03	115.18	117.70
34	2	311	C	O4'-C1'-N1	5.03	112.23	108.20
34	2	823	A	C5-C6-N1	-5.03	115.18	117.70
34	2	887	G	C6-C5-N7	-5.03	127.38	130.40
34	2	1426	C	N3-C4-C5	-5.03	119.89	121.90
34	2	1449	C	N3-C4-C5	-5.03	119.89	121.90
34	2	951	A	C5-C6-N6	-5.03	119.68	123.70
34	2	47	G	O4'-C1'-N9	5.03	112.22	108.20
34	2	410	G	O4'-C1'-N9	5.03	112.22	108.20
34	2	1224	A	C5-C6-N1	-5.03	115.19	117.70
34	2	1418	G	O4'-C1'-N9	5.03	112.22	108.20
34	2	916	A	C5-N7-C8	5.03	106.41	103.90
34	2	1412	C	N3-C4-C5	-5.03	119.89	121.90
34	2	1024	A	O4'-C1'-N9	5.02	112.22	108.20
34	2	1181	C	N3-C4-C5	-5.02	119.89	121.90
34	2	1303	U	C5-C4-O4	-5.02	122.89	125.90
1	1	60	A	O4'-C1'-N9	5.02	112.22	108.20
34	2	58	C	O4'-C1'-N1	5.02	112.22	108.20
34	2	615	G	N3-C2-N2	5.02	123.42	119.90
34	2	916	A	O4'-C1'-N9	5.02	112.22	108.20
34	2	1027	A	O4'-C1'-N9	5.02	112.22	108.20
44	v	415	ASN	C-N-CD	5.02	138.95	128.40
45	w	245	ALA	N-CA-CB	5.02	117.13	110.10
34	2	938	G	O4'-C1'-N9	5.02	112.22	108.20
34	2	1135	C	N3-C4-N4	5.02	121.51	118.00
34	2	1299	C	N3-C4-C5	-5.02	119.89	121.90
34	2	1432	C	N3-C4-C5	-5.02	119.89	121.90
34	2	181	A	O4'-C1'-N9	5.02	112.21	108.20
34	2	279	G	O4'-C1'-N9	5.02	112.21	108.20
34	2	569	C	N3-C4-C5	-5.02	119.89	121.90
34	2	1532	A	C5-C6-N1	-5.02	115.19	117.70
34	2	1857	A	C5-C6-N1	-5.02	115.19	117.70
34	2	1423	C	C5-C4-N4	-5.01	116.69	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1142	C	C5-C4-N4	-5.01	116.69	120.20
34	2	1529	C	N3-C4-C5	-5.01	119.89	121.90
34	2	83	A	O4'-C1'-N9	5.01	112.21	108.20
34	2	86	C	N3-C4-C5	-5.01	119.89	121.90
34	2	364	G	O4'-C1'-N9	5.01	112.21	108.20
34	2	1024	A	C5-C6-N6	-5.01	119.69	123.70
34	2	1469	G	O4'-C1'-N9	5.01	112.21	108.20
34	2	1635	A	C5-C6-N6	-5.01	119.69	123.70
34	2	42	A	O4'-C1'-N9	5.01	112.20	108.20
34	2	464	G	O4'-C1'-N9	5.01	112.20	108.20
34	2	79	A	C4'-C3'-C2'	-5.00	97.59	102.60
34	2	615	G	O4'-C1'-N9	5.00	112.20	108.20
34	2	83	A	C5-C6-N6	-5.00	119.70	123.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	17	C	C3',C2'
1	1	18	G	C3'
34	2	1244	C4J	C4'

All (245) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	18	G	Sidechain
1	1	26	G	Sidechain
34	2	1044	G	Sidechain
34	2	1161	G	Sidechain
34	2	1170	U	Sidechain
34	2	1171	G	Sidechain
34	2	1182	U	Sidechain
34	2	1183	G	Sidechain
34	2	1191	A	Sidechain
34	2	1192	A	Sidechain
34	2	1236	A	Sidechain
34	2	1252	G	Sidechain
34	2	1255	A	Sidechain
34	2	126	G	Sidechain
34	2	1304	U	Sidechain
34	2	1405	A	Sidechain
34	2	1427	G	Sidechain
34	2	1437	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
34	2	1438	U	Sidechain
34	2	146	G	Sidechain
34	2	148	U	Sidechain
34	2	1547	G	Sidechain
34	2	1564	A	Sidechain
34	2	1599	G	Sidechain
34	2	1616	U	Sidechain
34	2	1738	G	Sidechain
34	2	1750	C	Sidechain
34	2	1769	U	Sidechain
34	2	1776	G	Sidechain
34	2	1784	A	Sidechain
34	2	1840	G	Sidechain
34	2	195	C	Sidechain
34	2	211	U	Sidechain
34	2	240	C	Sidechain
34	2	318	U	Sidechain
34	2	39	A	Sidechain
34	2	435	A	Sidechain
34	2	526	A	Sidechain
34	2	554	A	Sidechain
34	2	574	A	Sidechain
34	2	576	G	Sidechain
34	2	660	A	Sidechain
34	2	71	G	Sidechain
34	2	76	U	Sidechain
34	2	82	G	Sidechain
34	2	869	G	Sidechain
34	2	951	A	Sidechain
34	2	997	A	Sidechain
35	A	150	TYR	Sidechain
35	A	184	LEU	Peptide
35	A	185	THR	Peptide
35	A	186	PRO	Peptide
35	A	187	GLN	Peptide
35	A	192	ARG	Sidechain
35	A	39	TYR	Sidechain
36	B	110	PRO	Peptide
36	B	133	THR	Peptide
36	B	287	LEU	Peptide
36	B	288	LYS	Peptide,Mainchain
36	B	289	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
36	B	322	LEU	Peptide
36	B	373	ALA	Peptide
3	C	193	HIS	Peptide
4	D	208	HIS	Peptide
9	I	217	MET	Mainchain
9	I	68	LEU	Peptide
9	I	69	THR	Peptide
10	J	105	THR	Peptide
10	J	66	VAL	Peptide
11	K	144	LYS	Peptide
11	K	157	LYS	Peptide
12	L	147	PHE	Peptide
12	L	148	ILE	Peptide
13	M	1	MET	Peptide
13	M	34	GLU	Peptide
13	M	35	LEU	Peptide
13	M	43	LEU	Peptide
13	M	96	ARG	Sidechain
17	Q	35	ALA	Peptide
17	Q	36	SER	Peptide
18	S	42	ILE	Peptide
18	S	43	GLU	Peptide
39	U	89	ASP	Peptide
39	U	94	LYS	Peptide
39	U	99	LEU	Peptide
22	X	77	GLY	Mainchain
25	a	126	GLY	Peptide
26	b	46	GLU	Peptide
27	c	81	ARG	Peptide
29	e	28	HIS	Peptide
29	e	32	ARG	Peptide
29	e	49	ASP	Peptide
29	e	52	PHE	Peptide
30	f	90	LYS	Peptide
33	i	126	LYS	Peptide
33	i	78	GLY	Peptide
33	i	82	ARG	Sidechain
37	j	15	GLY	Peptide
37	j	16	LYS	Peptide
37	j	18	GLU	Peptide
37	j	19	ASN	Peptide
37	j	22	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
37	j	23	LYS	Peptide
37	j	24	ARG	Peptide
37	j	25	GLU	Peptide
37	j	28	PHE	Peptide
37	j	29	LYS	Peptide,Mainchain
37	j	92	ILE	Peptide
38	k	129	PRO	Peptide
38	k	130	ASN	Peptide
38	k	131	LEU	Peptide
38	k	132	GLY	Peptide
38	k	133	LYS	Peptide
38	k	134	TYR	Peptide
38	k	137	PRO	Peptide
38	k	138	PRO	Peptide
38	k	150	SER	Mainchain
38	k	173	VAL	Peptide
38	k	175	GLN	Peptide
38	k	176	ILE	Peptide
38	k	192	ASP	Peptide
38	k	193	GLU	Peptide
38	k	208	HIS	Sidechain
38	k	237	ILE	Mainchain
38	k	241	ASP	Mainchain
38	k	268	TYR	Mainchain
38	k	272	VAL	Mainchain
38	k	290	TYR	Sidechain
38	k	348	TYR	Peptide,Mainchain
38	k	408	ASN	Mainchain
38	k	438	HIS	Peptide
38	k	455	ILE	Peptide,Mainchain
38	k	481	ASP	Mainchain
38	k	513	LYS	Mainchain
38	k	531	ARG	Mainchain
38	k	535	PHE	Sidechain
38	k	569	ASP	Peptide
38	k	574	ARG	Sidechain
38	k	96	ARG	Sidechain
46	q	108	ARG	Peptide
46	q	173	TYR	Sidechain
46	q	190	TYR	Sidechain
46	q	194	ALA	Peptide
46	q	223	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
46	q	298	VAL	Peptide
47	r	122	SER	Peptide
47	r	126	GLY	Peptide
47	r	152	TYR	Sidechain
47	r	177	CYS	Peptide
47	r	243	LEU	Peptide
47	r	304	LEU	Peptide
47	r	306	LYS	Peptide
47	r	307	PRO	Peptide
47	r	350	TYR	Sidechain
47	r	99	TYR	Sidechain
48	s	200	ASN	Peptide
49	t	317	TYR	Sidechain
49	t	350	PHE	Peptide
49	t	375	LEU	Peptide
49	t	376	THR	Peptide
49	t	434	ASN	Peptide
50	u	117	THR	Peptide
50	u	120	ARG	Sidechain
50	u	169	TYR	Sidechain
50	u	217	ALA	Peptide
50	u	249	LEU	Peptide
50	u	259	ASN	Peptide
50	u	335	SER	Peptide
50	u	42	LEU	Peptide
50	u	56	ASP	Peptide
44	v	325	THR	Peptide
44	v	346	ASP	Peptide
44	v	356	LEU	Peptide
44	v	363	GLU	Peptide
44	v	365	ASN	Peptide
44	v	366	LEU	Peptide
44	v	367	GLY	Peptide
44	v	368	GLU	Peptide
44	v	369	GLY	Peptide
44	v	383	TYR	Peptide
44	v	385	TYR	Peptide
44	v	386	ASN	Peptide
44	v	390	ALA	Peptide
44	v	392	TYR	Peptide
44	v	408	LEU	Peptide
44	v	412	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
44	v	413	PHE	Peptide
44	v	414	ALA	Peptide
44	v	415	ASN	Peptide
44	v	416	PRO	Peptide
44	v	418	ILE	Peptide
44	v	419	PHE	Peptide
44	v	425	LEU	Peptide
44	v	426	GLU	Peptide
44	v	427	GLU	Peptide
44	v	429	GLU	Peptide
44	v	431	LEU	Peptide
44	v	434	VAL	Peptide
44	v	437	PRO	Peptide
44	v	462	THR	Peptide
44	v	463	ASP	Peptide
44	v	466	SER	Peptide
44	v	467	GLN	Peptide
44	v	468	GLU	Peptide
44	v	469	TYR	Peptide
44	v	489	TYR	Peptide
44	v	490	LEU	Peptide
44	v	492	GLU	Peptide
44	v	495	THR	Peptide
44	v	496	THR	Peptide
44	v	499	ILE	Peptide
44	v	501	ARG	Peptide
44	v	513	LYS	Peptide
44	v	523	LEU	Peptide
44	v	556	TYR	Peptide
44	v	557	ALA	Peptide
44	v	558	LYS	Peptide
44	v	559	ASP	Peptide
44	v	583	TYR	Sidechain
44	v	655	LEU	Peptide
44	v	656	GLN	Peptide
44	v	697	TYR	Sidechain
44	v	725	PRO	Peptide
45	w	17	HIS	Peptide
45	w	219	LEU	Peptide
45	w	220	PHE	Peptide
45	w	236	PHE	Peptide
45	w	268	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
45	w	27	SER	Peptide
45	w	270	ARG	Sidechain
45	w	32	TYR	Peptide
45	w	50	MET	Peptide
45	w	52	ASP	Peptide
43	y	245	LEU	Mainchain
43	y	368	ILE	Peptide
43	y	385	PRO	Peptide
43	y	398	PHE	Peptide
43	y	417	GLN	Peptide
43	y	43	TRP	Peptide
43	y	495	SER	Peptide
43	y	505	ALA	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	
2	l	23/25 (92%)	23 (100%)	0	0	100	100
3	C	206/208 (99%)	177 (86%)	21 (10%)	8 (4%)	2	21
4	D	213/264 (81%)	186 (87%)	21 (10%)	6 (3%)	4	27
5	E	224/226 (99%)	208 (93%)	14 (6%)	2 (1%)	14	48
6	F	225/227 (99%)	202 (90%)	14 (6%)	9 (4%)	2	21
7	G	261/263 (99%)	233 (89%)	24 (9%)	4 (2%)	8	39
8	H	189/191 (99%)	169 (89%)	17 (9%)	3 (2%)	8	38
9	I	235/237 (99%)	209 (89%)	22 (9%)	4 (2%)	7	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	188/190 (99%)	161 (86%)	18 (10%)	9 (5%)	2	17
11	K	204/206 (99%)	178 (87%)	20 (10%)	6 (3%)	3	27
12	L	180/182 (99%)	167 (93%)	11 (6%)	2 (1%)	12	45
13	M	96/98 (98%)	74 (77%)	16 (17%)	6 (6%)	1	13
14	N	156/158 (99%)	130 (83%)	22 (14%)	4 (3%)	4	28
15	O	122/132 (92%)	105 (86%)	13 (11%)	4 (3%)	3	25
16	P	148/150 (99%)	130 (88%)	11 (7%)	7 (5%)	2	18
17	Q	134/151 (89%)	119 (89%)	12 (9%)	3 (2%)	5	32
18	S	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	40
19	T	124/135 (92%)	112 (90%)	8 (6%)	4 (3%)	3	25
20	V	139/145 (96%)	128 (92%)	8 (6%)	3 (2%)	5	32
21	W	102/119 (86%)	93 (91%)	9 (9%)	0	100	100
22	X	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	29
23	Y	127/130 (98%)	117 (92%)	6 (5%)	4 (3%)	3	26
24	Z	140/142 (99%)	129 (92%)	7 (5%)	4 (3%)	3	27
25	a	124/133 (93%)	104 (84%)	10 (8%)	10 (8%)	1	8
26	b	97/115 (84%)	86 (89%)	10 (10%)	1 (1%)	13	46
27	c	82/84 (98%)	56 (68%)	16 (20%)	10 (12%)	0	4
28	d	62/69 (90%)	57 (92%)	4 (6%)	1 (2%)	8	38
29	e	51/53 (96%)	40 (78%)	7 (14%)	4 (8%)	1	9
30	f	69/71 (97%)	51 (74%)	12 (17%)	6 (9%)	0	7
31	g	311/313 (99%)	273 (88%)	33 (11%)	5 (2%)	8	38
32	n	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	9	40
33	i	57/59 (97%)	49 (86%)	7 (12%)	1 (2%)	7	35
35	A	264/266 (99%)	233 (88%)	25 (10%)	6 (2%)	5	31
36	B	420/422 (100%)	352 (84%)	48 (11%)	20 (5%)	2	17
37	j	107/144 (74%)	64 (60%)	27 (25%)	16 (15%)	0	2
38	k	577/595 (97%)	431 (75%)	95 (16%)	51 (9%)	0	7
39	U	141/152 (93%)	123 (87%)	12 (8%)	6 (4%)	2	19
40	R	138/145 (95%)	107 (78%)	18 (13%)	13 (9%)	0	6
42	m	363/548 (66%)	336 (93%)	25 (7%)	2 (1%)	22	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	y	601/1350 (44%)	457 (76%)	85 (14%)	59 (10%)	0	6
44	v	548/913 (60%)	446 (81%)	72 (13%)	30 (6%)	1	15
45	w	417/445 (94%)	349 (84%)	57 (14%)	11 (3%)	4	28
46	q	270/272 (99%)	226 (84%)	32 (12%)	12 (4%)	2	19
47	r	322/352 (92%)	267 (83%)	42 (13%)	13 (4%)	2	21
48	s	213/218 (98%)	201 (94%)	10 (5%)	2 (1%)	14	48
49	t	370/564 (66%)	328 (89%)	38 (10%)	4 (1%)	12	45
50	u	363/374 (97%)	308 (85%)	47 (13%)	8 (2%)	5	32
All	All	9695/11534 (84%)	8260 (85%)	1047 (11%)	388 (4%)	4	21

All (388) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	191	ARG
4	D	78	GLU
4	D	209	ASP
6	F	3	VAL
6	F	193	ASP
6	F	219	PRO
8	H	41	VAL
9	I	69	THR
10	J	106	ARG
11	K	158	ILE
12	L	148	ILE
13	M	35	LEU
14	N	66	VAL
14	N	157	LYS
15	O	95	ASP
16	P	19	ARG
16	P	20	ARG
20	V	34	VAL
23	Y	30	CYS
25	a	10	ARG
25	a	100	LYS
25	a	102	THR
25	a	105	LYS
27	c	36	LYS
27	c	37	CYS
27	c	73	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	c	77	CYS
29	e	25	SER
30	f	102	VAL
35	A	171	ASP
35	A	185	THR
35	A	266	ARG
36	B	194	LYS
36	B	279	LYS
36	B	280	PRO
36	B	283	GLU
36	B	289	GLY
36	B	402	ASP
36	B	405	ALA
37	j	16	LYS
37	j	20	GLU
37	j	21	SER
37	j	24	ARG
37	j	44	ASN
37	j	66	ARG
37	j	72	ASN
37	j	75	ASP
37	j	94	LYS
38	k	20	LYS
38	k	58	CYS
38	k	134	TYR
38	k	140	TRP
38	k	176	ILE
38	k	316	TYR
38	k	318	PRO
38	k	331	PHE
38	k	333	VAL
38	k	348	TYR
38	k	435	ALA
38	k	439	PRO
38	k	456	ASP
38	k	526	THR
38	k	528	LEU
39	U	90	VAL
39	U	144	ARG
40	R	126	VAL
40	R	142	ILE
43	y	4	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	y	7	ARG
43	y	8	PRO
43	y	79	GLN
43	y	80	GLN
43	y	123	THR
43	y	160	CYS
43	y	164	LEU
43	y	173	LEU
43	y	219	ASN
43	y	284	TRP
43	y	329	ILE
43	y	345	ASP
44	v	342	LYS
44	v	376	PHE
44	v	391	THR
44	v	392	TYR
44	v	464	PRO
44	v	490	LEU
44	v	499	ILE
44	v	558	LYS
44	v	749	TRP
45	w	50	MET
45	w	51	VAL
45	w	200	SER
45	w	221	VAL
46	q	224	PRO
46	q	299	SER
46	q	318	ILE
47	r	305	PHE
48	s	204	LYS
50	u	334	VAL
50	u	335	SER
50	u	336	HIS
3	C	46	ILE
4	D	81	PHE
5	E	159	ILE
6	F	131	ALA
10	J	17	ASP
10	J	67	PRO
10	J	139	ILE
13	M	34	GLU
13	M	36	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	24	LEU
15	O	118	SER
16	P	24	THR
17	Q	66	ARG
17	Q	138	ASP
18	S	44	PRO
20	V	143	LYS
22	X	10	ASP
23	Y	58	ALA
24	Z	87	ASN
25	a	86	GLU
27	c	70	LYS
30	f	98	VAL
36	B	63	VAL
36	B	224	VAL
36	B	229	ALA
36	B	398	ARG
36	B	403	LYS
36	B	452	GLU
37	j	29	LYS
37	j	46	ARG
38	k	132	GLY
38	k	185	GLY
38	k	187	ILE
38	k	322	LEU
38	k	329	LEU
38	k	338	ASN
38	k	342	VAL
38	k	345	MET
38	k	358	GLY
38	k	408	ASN
38	k	514	THR
38	k	527	TYR
40	R	12	PHE
40	R	133	ILE
40	R	134	GLY
40	R	135	ALA
43	y	62	ARG
43	y	116	GLU
43	y	120	ASN
43	y	167	ASN
43	y	168	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	y	188	TYR
43	y	241	ILE
43	y	270	GLN
43	y	286	SER
43	y	331	ILE
44	v	377	ASN
44	v	422	GLU
44	v	458	ILE
44	v	459	MET
44	v	487	GLN
44	v	498	GLU
45	w	28	VAL
46	q	179	ILE
46	q	240	ALA
47	r	159	GLN
47	r	205	ILE
49	t	378	TYR
50	u	57	ASP
4	D	207	LEU
6	F	205	PRO
8	H	22	LYS
9	I	236	SER
10	J	13	GLY
12	L	21	GLU
15	O	75	ASN
16	P	30	SER
18	S	118	THR
19	T	83	ASN
19	T	94	GLU
23	Y	71	LYS
24	Z	86	PRO
24	Z	109	GLY
25	a	30	PRO
25	a	52	PRO
25	a	106	GLN
27	c	38	PRO
27	c	78	SER
27	c	83	GLN
28	d	52	GLU
29	e	24	CYS
31	g	13	GLY
31	g	161	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	n	112	ASN
33	i	79	SER
35	A	55	ARG
36	B	89	ASN
36	B	135	GLY
36	B	179	PRO
36	B	378	PRO
37	j	42	LEU
37	j	74	SER
38	k	88	CYS
38	k	98	PRO
38	k	175	GLN
38	k	327	ALA
38	k	380	GLU
38	k	395	ARG
38	k	448	PRO
38	k	477	GLY
38	k	585	ASP
40	R	10	ARG
40	R	83	MET
43	y	42	THR
43	y	187	GLN
43	y	211	HIS
43	y	212	HIS
43	y	214	GLN
43	y	215	SER
43	y	223	PRO
43	y	267	PRO
43	y	328	SER
43	y	348	ILE
43	y	373	ASP
43	y	399	ASN
43	y	540	ALA
44	v	339	ALA
44	v	370	VAL
44	v	383	TYR
44	v	390	ALA
44	v	428	SER
44	v	493	LYS
44	v	655	LEU
46	q	228	MET
47	r	35	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	r	167	TYR
47	r	312	ALA
49	t	273	SER
49	t	500	LEU
50	u	108	ASN
3	C	71	PRO
3	C	155	ARG
4	D	56	LYS
5	E	161	LYS
7	G	30	ARG
7	G	153	LEU
10	J	6	ALA
10	J	37	LYS
10	J	116	ARG
11	K	22	HIS
11	K	31	ARG
11	K	144	LYS
13	M	94	LEU
15	O	120	ALA
16	P	22	VAL
16	P	26	LEU
16	P	138	ASN
17	Q	64	ALA
19	T	84	TYR
22	X	28	ASP
24	Z	53	GLU
25	a	9	THR
26	b	11	ALA
27	c	41	TYR
29	e	8	TRP
30	f	91	ASN
30	f	122	PRO
31	g	127	LYS
35	A	40	ASN
38	k	133	LYS
38	k	265	PRO
38	k	321	ASN
38	k	337	ALA
38	k	446	MET
38	k	450	GLN
39	U	89	ASP
39	U	95	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	R	140	ARG
42	m	244	ASN
42	m	295	ALA
43	y	41	ARG
43	y	119	ASP
43	y	162	ASP
43	y	165	ARG
43	y	231	GLU
43	y	363	ALA
43	y	486	HIS
43	y	497	LEU
43	y	505	ALA
44	v	431	LEU
44	v	707	ARG
45	w	26	LEU
45	w	76	THR
46	q	109	ARG
46	q	114	ALA
46	q	178	ASP
47	r	54	GLN
47	r	90	ASP
50	u	192	TYR
3	C	199	PRO
4	D	179	ASN
6	F	142	LEU
6	F	216	GLU
7	G	83	PRO
8	H	184	SER
11	K	53	LYS
11	K	133	GLU
19	T	120	THR
20	V	39	LEU
25	a	96	LEU
27	c	4	ALA
30	f	136	PHE
30	f	146	LEU
35	A	59	ILE
36	B	196	LYS
36	B	461	GLU
37	j	25	GLU
38	k	191	LYS
38	k	330	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	k	379	GLY
39	U	141	ARG
39	U	148	VAL
40	R	38	SER
40	R	74	GLU
40	R	130	ARG
43	y	81	VAL
43	y	225	SER
43	y	227	SER
43	y	229	HIS
43	y	233	ARG
43	y	237	LEU
43	y	268	LYS
43	y	421	GLU
44	v	416	PRO
44	v	423	ASN
45	w	326	VAL
46	q	94	LEU
47	r	125	TYR
47	r	154	PRO
47	r	178	LYS
47	r	183	SER
49	t	294	LEU
50	u	118	PRO
3	C	126	ASP
3	C	206	ASP
6	F	191	PRO
9	I	154	ARG
13	M	2	LEU
29	e	36	LEU
31	g	191	HIS
36	B	105	ASP
37	j	23	LYS
37	j	27	VAL
38	k	319	THR
43	y	26	PRO
43	y	327	LEU
44	v	358	VAL
45	w	22	LEU
45	w	48	THR
50	u	193	THR
3	C	3	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	152	PRO
13	M	3	MET
14	N	26	GLY
38	k	99	ILE
38	k	100	PRO
38	k	137	PRO
43	y	347	ILE
44	v	374	ILE
47	r	112	ILE
43	y	121	ILE
45	w	91	ILE
46	q	138	PRO
6	F	196	GLY
10	J	45	ILE
23	Y	29	PRO
31	g	275	ILE
38	k	177	PRO
38	k	237	ILE
43	y	170	VAL
43	y	269	PRO
44	v	324	ILE
44	v	424	ILE
46	q	87	PRO
9	I	67	VAL
40	R	129	GLY
48	s	78	PRO

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	
2	I	24/24 (100%)	23 (96%)	1 (4%)	25	54
3	C	174/174 (100%)	173 (99%)	1 (1%)	84	92
4	D	196/231 (85%)	192 (98%)	4 (2%)	50	72
5	E	187/187 (100%)	184 (98%)	3 (2%)	58	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	190/190 (100%)	187 (98%)	3 (2%)	58	76
7	G	225/225 (100%)	225 (100%)	0	100	100
8	H	161/161 (100%)	159 (99%)	2 (1%)	67	82
9	I	207/207 (100%)	206 (100%)	1 (0%)	86	93
10	J	170/170 (100%)	170 (100%)	0	100	100
11	K	177/177 (100%)	176 (99%)	1 (1%)	84	92
12	L	157/157 (100%)	155 (99%)	2 (1%)	65	81
13	M	89/89 (100%)	89 (100%)	0	100	100
14	N	142/142 (100%)	136 (96%)	6 (4%)	25	54
15	O	104/108 (96%)	100 (96%)	4 (4%)	28	57
16	P	130/130 (100%)	126 (97%)	4 (3%)	35	62
17	Q	106/119 (89%)	105 (99%)	1 (1%)	75	87
18	S	117/117 (100%)	115 (98%)	2 (2%)	56	75
19	T	114/121 (94%)	114 (100%)	0	100	100
20	V	113/116 (97%)	113 (100%)	0	100	100
21	W	94/107 (88%)	93 (99%)	1 (1%)	70	83
22	X	67/67 (100%)	67 (100%)	0	100	100
23	Y	112/113 (99%)	112 (100%)	0	100	100
24	Z	114/114 (100%)	113 (99%)	1 (1%)	75	87
25	a	108/115 (94%)	101 (94%)	7 (6%)	14	42
26	b	87/99 (88%)	86 (99%)	1 (1%)	70	83
27	c	76/76 (100%)	73 (96%)	3 (4%)	27	57
28	d	57/62 (92%)	57 (100%)	0	100	100
29	e	47/47 (100%)	45 (96%)	2 (4%)	25	54
30	f	64/64 (100%)	63 (98%)	1 (2%)	58	76
31	g	272/272 (100%)	271 (100%)	1 (0%)	89	95
32	n	66/66 (100%)	65 (98%)	1 (2%)	60	78
33	i	49/49 (100%)	47 (96%)	2 (4%)	26	55
35	A	238/238 (100%)	231 (97%)	7 (3%)	37	63
36	B	354/354 (100%)	328 (93%)	26 (7%)	11	38
37	j	92/123 (75%)	69 (75%)	23 (25%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	k	523/523 (100%)	466 (89%)	57 (11%)	5	25
39	U	125/132 (95%)	120 (96%)	5 (4%)	27	56
40	R	126/130 (97%)	119 (94%)	7 (6%)	17	47
42	m	329/494 (67%)	327 (99%)	2 (1%)	84	92
43	y	554/1233 (45%)	467 (84%)	87 (16%)	2	14
44	v	501/812 (62%)	489 (98%)	12 (2%)	44	67
45	w	384/406 (95%)	380 (99%)	4 (1%)	73	85
46	q	239/239 (100%)	237 (99%)	2 (1%)	79	88
47	r	293/310 (94%)	290 (99%)	3 (1%)	73	85
48	s	190/193 (98%)	190 (100%)	0	100	100
49	t	342/515 (66%)	341 (100%)	1 (0%)	91	96
50	u	327/335 (98%)	327 (100%)	0	100	100
All	All	8613/10133 (85%)	8322 (97%)	291 (3%)	34	60

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	l	2	ARG
3	C	209	GLU
4	D	71	LEU
4	D	76	ASN
4	D	82	ARG
4	D	191	ASP
5	E	43	LYS
5	E	126	MET
5	E	242	LYS
6	F	76	ARG
6	F	106	ARG
6	F	195	SER
8	H	51	HIS
8	H	141	VAL
9	I	31	ARG
11	K	84	ASN
12	L	17	ARG
12	L	89	GLU
14	N	22	ARG
14	N	24	LEU
14	N	25	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	28	THR
14	N	30	LYS
14	N	69	ARG
15	O	12	MET
15	O	45	ARG
15	O	52	LEU
15	O	103	VAL
16	P	21	SER
16	P	26	LEU
16	P	27	LYS
16	P	28	LEU
17	Q	150	ARG
18	S	105	LYS
18	S	146	ARG
21	W	34	LYS
24	Z	3	LYS
25	a	10	ARG
25	a	12	PHE
25	a	98	GLU
25	a	99	LYS
25	a	100	LYS
25	a	101	LYS
25	a	105	LYS
26	b	59	PHE
27	c	64	CYS
27	c	73	LEU
27	c	79	PHE
29	e	23	VAL
29	e	39	CYS
30	f	118	ARG
31	g	79	LEU
32	n	106	GLN
33	i	80	LEU
33	i	82	ARG
35	A	38	GLU
35	A	45	MET
35	A	54	ARG
35	A	55	ARG
35	A	150	TYR
35	A	185	THR
35	A	205	ILE
36	B	81	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	B	83	LYS
36	B	88	ARG
36	B	102	TYR
36	B	137	PHE
36	B	210	GLU
36	B	217	TYR
36	B	230	GLU
36	B	242	LYS
36	B	261	ARG
36	B	274	SER
36	B	275	PHE
36	B	276	ASP
36	B	279	LYS
36	B	283	GLU
36	B	284	VAL
36	B	285	ASP
36	B	319	GLU
36	B	378	PRO
36	B	400	GLU
36	B	402	ASP
36	B	404	LYS
36	B	407	LYS
36	B	417	LEU
36	B	453	LYS
36	B	466	LEU
37	j	7	LYS
37	j	13	ARG
37	j	29	LYS
37	j	34	GLU
37	j	40	LYS
37	j	41	MET
37	j	42	LEU
37	j	44	ASN
37	j	46	ARG
37	j	52	PHE
37	j	57	ARG
37	j	62	ARG
37	j	64	LYS
37	j	65	LEU
37	j	66	ARG
37	j	68	LYS
37	j	70	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	j	72	ASN
37	j	82	ARG
37	j	91	VAL
37	j	101	ARG
37	j	103	LEU
37	j	111	GLU
38	k	20	LYS
38	k	33	ARG
38	k	40	GLU
38	k	45	SER
38	k	64	LYS
38	k	74	ASN
38	k	79	LEU
38	k	96	ARG
38	k	97	LEU
38	k	112	ASN
38	k	114	ILE
38	k	117	SER
38	k	131	LEU
38	k	133	LYS
38	k	135	ASP
38	k	150	SER
38	k	153	GLN
38	k	154	ASN
38	k	162	ASP
38	k	187	ILE
38	k	190	ARG
38	k	191	LYS
38	k	194	THR
38	k	205	ASP
38	k	224	ARG
38	k	245	SER
38	k	268	TYR
38	k	294	SER
38	k	311	ILE
38	k	312	PHE
38	k	313	LEU
38	k	316	TYR
38	k	319	THR
38	k	320	GLU
38	k	322	LEU
38	k	325	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	k	326	ASP
38	k	328	SER
38	k	329	LEU
38	k	332	LYS
38	k	336	THR
38	k	339	GLU
38	k	343	LYS
38	k	344	LYS
38	k	347	MET
38	k	419	LYS
38	k	433	ARG
38	k	439	PRO
38	k	443	THR
38	k	481	ASP
38	k	485	ILE
38	k	526	THR
38	k	528	LEU
38	k	569	ASP
38	k	576	ARG
38	k	579	LYS
38	k	598	ASP
39	U	13	LEU
39	U	94	LYS
39	U	142	ARG
39	U	144	ARG
39	U	150	LYS
40	R	10	ARG
40	R	51	ARG
40	R	72	LYS
40	R	100	LYS
40	R	130	ARG
40	R	140	ARG
40	R	141	PHE
42	m	339	ASN
42	m	500	LYS
43	y	4	TYR
43	y	6	GLN
43	y	9	GLU
43	y	12	LEU
43	y	13	LYS
43	y	14	ARG
43	y	25	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	y	28	LEU
43	y	29	ASP
43	y	39	LYS
43	y	60	ASP
43	y	68	LYS
43	y	79	GLN
43	y	83	ILE
43	y	113	LEU
43	y	120	ASN
43	y	123	THR
43	y	126	SER
43	y	133	SER
43	y	135	GLU
43	y	145	LEU
43	y	149	TRP
43	y	150	VAL
43	y	151	LYS
43	y	154	TRP
43	y	160	CYS
43	y	162	ASP
43	y	173	LEU
43	y	176	ASP
43	y	179	GLN
43	y	180	GLN
43	y	183	LYS
43	y	186	LEU
43	y	193	GLU
43	y	195	ARG
43	y	198	CYS
43	y	200	ASN
43	y	206	SER
43	y	207	GLN
43	y	208	ILE
43	y	209	GLN
43	y	210	ARG
43	y	212	HIS
43	y	220	LEU
43	y	225	SER
43	y	228	MET
43	y	232	THR
43	y	234	LEU
43	y	236	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	y	237	LEU
43	y	242	SER
43	y	246	TRP
43	y	250	PHE
43	y	254	GLU
43	y	257	HIS
43	y	259	LEU
43	y	265	LYS
43	y	268	LYS
43	y	271	LEU
43	y	276	TYR
43	y	278	LYS
43	y	283	PHE
43	y	285	LYS
43	y	290	LEU
43	y	291	PHE
43	y	299	LEU
43	y	303	SER
43	y	304	ARG
43	y	305	GLU
43	y	306	MET
43	y	307	ARG
43	y	323	LEU
43	y	324	LEU
43	y	340	ARG
43	y	341	LEU
43	y	342	LEU
43	y	343	ASP
43	y	344	MET
43	y	347	ILE
43	y	350	GLU
43	y	351	LYS
43	y	354	ARG
43	y	355	LEU
43	y	358	LEU
43	y	359	LEU
43	y	381	GLN
43	y	546	LYS
44	v	342	LYS
44	v	366	LEU
44	v	389	LEU
44	v	396	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	v	397	MET
44	v	425	LEU
44	v	430	ASN
44	v	521	ARG
44	v	542	GLU
44	v	556	TYR
44	v	615	GLN
44	v	707	ARG
45	w	7	THR
45	w	94	MET
45	w	193	LYS
45	w	269	LYS
46	q	187	HIS
46	q	249	VAL
47	r	70	LEU
47	r	104	MET
47	r	168	ARG
49	t	544	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	40	ASN
4	D	76	ASN
8	H	29	GLN
8	H	65	GLN
11	K	84	ASN
16	P	90	HIS
24	Z	16	HIS
26	b	80	HIS
30	f	111	ASN
30	f	135	HIS
31	g	191	HIS
35	A	114	HIS
37	j	17	ASN
37	j	37	GLN
37	j	60	HIS
37	j	72	ASN
38	k	153	GLN
38	k	208	HIS
38	k	450	GLN
38	k	520	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	k	549	GLN
38	k	578	ASN
38	k	593	ASN
42	m	296	ASN
42	m	377	HIS
42	m	479	GLN
42	m	486	ASN
43	y	10	ASN
43	y	73	GLN
43	y	80	GLN
43	y	82	ASN
43	y	120	ASN
43	y	122	GLN
43	y	179	GLN
43	y	204	HIS
43	y	207	GLN
43	y	209	GLN
43	y	211	HIS
43	y	229	HIS
43	y	236	GLN
43	y	292	HIS
43	y	301	HIS
43	y	309	ASN
43	y	352	GLN
43	y	381	GLN
43	y	434	ASN
43	y	512	GLN
44	v	326	HIS
44	v	355	GLN
44	v	377	ASN
44	v	399	GLN
44	v	430	ASN
44	v	465	HIS
44	v	522	GLN
44	v	576	HIS
44	v	662	GLN
44	v	674	HIS
44	v	701	HIS
44	v	736	HIS
45	w	348	HIS
45	w	349	GLN
46	q	139	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	r	54	GLN
47	r	141	GLN
49	t	387	HIS
49	t	495	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	13 (17%)	3 (4%)
34	2	1735/1863 (93%)	248 (14%)	8 (0%)
41	3	44/45 (97%)	29 (65%)	2 (4%)
All	All	1853/1983 (93%)	290 (15%)	13 (0%)

All (290) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	9	U
1	1	11	G
1	1	15	A
1	1	16	G
1	1	17	C
1	1	18	G
1	1	19	G
1	1	21	A
1	1	43	G
1	1	45	G
1	1	47	U
1	1	61	C
1	1	75	C
34	2	4	C
34	2	33	G
34	2	41	G
34	2	42	A
34	2	44	U
34	2	46	A
34	2	56	G
34	2	67	C
34	2	68	A
34	2	72	C
34	2	73	C
34	2	74	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	76	U
34	2	77	A
34	2	79	A
34	2	80	G
34	2	113	G
34	2	143	U
34	2	147	A
34	2	148	U
34	2	181	A
34	2	182	C
34	2	191	C
34	2	197	U
34	2	202	U
34	2	223	A
34	2	226	A
34	2	274	G
34	2	277	U
34	2	278	U
34	2	296	U
34	2	297	C
34	2	299	G
34	2	300	G
34	2	309	A
34	2	310	G
34	2	311	C
34	2	315	C
34	2	316	C
34	2	317	G
34	2	322	G
34	2	337	G
34	2	347	C
34	2	352	C
34	2	354	A
34	2	358	U
34	2	373	G
34	2	375	G
34	2	376	C
34	2	399	C
34	2	418	U
34	2	438	A
34	2	439	A
34	2	440	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	457	G
34	2	462	C
34	2	463	A
34	2	464	G
34	2	472	G
34	2	477	U
34	2	483	A
34	2	492	C
34	2	515	A
34	2	522	C
34	2	542	G
34	2	543	U
34	2	546	U
34	2	547	U
34	2	554	A
34	2	558	C
34	2	577	A
34	2	579	G
34	2	580	A
34	2	583	C
34	2	584	A
34	2	596	G
34	2	597	U
34	2	598	C
34	2	618	A
34	2	633	A
34	2	658	A
34	2	659	A
34	2	661	A
34	2	662	A
34	2	678	U
34	2	679	U
34	2	680	G
34	2	681	U
34	2	682	G
34	2	729	C
34	2	732	C
34	2	733	G
34	2	734	C
34	2	735	C
34	2	736	C
34	2	737	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	738	U
34	2	739	U
34	2	740	G
34	2	741	C
34	2	742	C
34	2	743	U
34	2	744	C
34	2	746	C
34	2	747	G
34	2	748	G
34	2	749	C
34	2	750	G
34	2	751	C
34	2	785	G
34	2	786	C
34	2	787	C
34	2	788	C
34	2	789	G
34	2	790	A
34	2	791	A
34	2	793	C
34	2	794	G
34	2	795	U
34	2	807	A
34	2	818	U
34	2	819	U
34	2	835	C
34	2	843	A
34	2	849	C
34	2	864	G
34	2	865	A
34	2	868	A
34	2	869	G
34	2	870	G
34	2	874	G
34	2	883	U
34	2	884	U
34	2	906	G
34	2	907	C
34	2	909	A
34	2	913	U
34	2	916	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	929	G
34	2	951	A
34	2	967	G
34	2	986	A
34	2	987	G
34	2	988	A
34	2	1004	A
34	2	1013	U
34	2	1019	A
34	2	1045	A
34	2	1057	U
34	2	1058	A
34	2	1081	C
34	2	1082	G
34	2	1103	G
34	2	1107	U
34	2	1109	A
34	2	1111	U
34	2	1112	C
34	2	1113	C
34	2	1115	A
34	2	1116	U
34	2	1117	G
34	2	1144	A
34	2	1145	A
34	2	1150	U
34	2	1211	C
34	2	1217	G
34	2	1219	A
34	2	1238	U
34	2	1247	A
34	2	1252	G
34	2	1253	G
34	2	1255	A
34	2	1260	C
34	2	1270	G
34	2	1271	G
34	2	1280	A
34	2	1281	G
34	2	1296	U
34	2	1297	A
34	2	1298	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	1299	C
34	2	1311	U
34	2	1367	U
34	2	1374	A
34	2	1391	C
34	2	1399	C
34	2	1406	C
34	2	1408	C
34	2	1413	C
34	2	1414	C
34	2	1415	C
34	2	1420	G
34	2	1427	G
34	2	1431	C
34	2	1433	C
34	2	1450	A
34	2	1471	G
34	2	1472	A
34	2	1473	U
34	2	1485	A
34	2	1486	G
34	2	1503	G
34	2	1506	G
34	2	1507	U
34	2	1516	C
34	2	1517	A
34	2	1539	C
34	2	1547	G
34	2	1548	C
34	2	1549	C
34	2	1551	A
34	2	1575	A
34	2	1580	U
34	2	1583	A
34	2	1596	A
34	2	1616	U
34	2	1618	A
34	2	1632	A
34	2	1643	G
34	2	1659	A
34	2	1660	G
34	2	1666	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2	1675	G
34	2	1678	C
34	2	1683	C
34	2	1706	U
34	2	1707	A
34	2	1708	C
34	2	1716	U
34	2	1717	G
34	2	1743	G
34	2	1747	C
34	2	1748	G
34	2	1777	C
34	2	1778	G
34	2	1816	A
34	2	1818	A
34	2	1819	A
34	2	1820	G
34	2	1823	G
34	2	1825	A
34	2	1829	A
34	2	1846	C
34	2	1855	G
34	2	1856	G
34	2	1858	U
34	2	1859	C
34	2	1863	A
41	3	34	C
41	3	35	A
41	3	36	A
41	3	37	C
41	3	39	U
41	3	40	C
41	3	41	A
41	3	42	A
41	3	43	A
41	3	45	A
41	3	47	A
41	3	48	C
41	3	49	A
41	3	55	G
41	3	56	U
41	3	57	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	3	58	C
41	3	59	A
41	3	61	C
41	3	62	U
41	3	65	C
41	3	66	U
41	3	67	C
41	3	69	U
41	3	70	G
41	3	71	A
41	3	72	G
41	3	73	G
41	3	74	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	8	G
1	1	17	C
1	1	18	G
34	2	74	G
34	2	739	U
34	2	912	A
34	2	1012	U
34	2	1112	C
34	2	1270	G
34	2	1716	U
34	2	1857	A
41	3	36	A
41	3	39	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	C4J	2	1244	34	24,29,30	0.78	1 (4%)	29,42,45	1.03	1 (3%)
1	T6A	1	37	1	27,34,35	1.05	2 (7%)	29,49,52	2.65	9 (31%)

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
34	C4J	2	1244	34	1/1/7/7	9/16/34/35	0/2/2/2
1	T6A	1	37	1	-	6/19/41/42	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	37	T6A	C5-C4	2.54	1.47	1.40
1	1	37	T6A	O4'-C1'	2.20	1.44	1.41
34	2	1244	C4J	C1'-C5	-2.10	1.45	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	T6A	C12-N11-C10	8.53	136.15	121.94
1	1	37	T6A	C2-N1-C6	7.05	122.64	116.59
1	1	37	T6A	C14-C12-C13	3.72	116.53	110.19
1	1	37	T6A	N3-C2-N1	-3.61	123.04	128.68
34	2	1244	C4J	C4-N3-C2	-3.45	121.10	125.46
1	1	37	T6A	N6-C6-N1	3.07	122.83	118.72
1	1	37	T6A	O10-C10-N6	-2.96	118.62	123.62
1	1	37	T6A	C4-C5-N7	-2.80	106.48	109.40
1	1	37	T6A	C14-C12-N11	2.69	118.61	111.72
1	1	37	T6A	N6-C10-N11	2.10	116.70	113.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	2	1244	C4J	C4'

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	37	T6A	C14-C12-N11-C10
34	2	1244	C4J	C31-C3-N3-C2
34	2	1244	C4J	C31-C3-N3-C4
34	2	1244	C4J	N3-C3-C31-C32
34	2	1244	C4J	C3-C31-C32-C34
34	2	1244	C4J	C3-C31-C32-N33
1	1	37	T6A	N11-C12-C13-ODA
1	1	37	T6A	N11-C12-C13-ODB
1	1	37	T6A	C13-C12-C14-C15
34	2	1244	C4J	N33-C32-C34-O36
34	2	1244	C4J	C31-C32-C34-O36
1	1	37	T6A	O4'-C4'-C5'-O5'
34	2	1244	C4J	N33-C32-C34-O35
1	1	37	T6A	C13-C12-N11-C10
34	2	1244	C4J	C31-C32-C34-O35

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
53	GNP	k	705	-	29,34,34	1.77	6 (20%)	33,54,54	2.16	6 (18%)
51	SF4	k	701	38	0,12,12	-	-	-		
53	GNP	k	704	52	29,34,34	1.76	6 (20%)	33,54,54	2.15	6 (18%)
51	SF4	k	702	38	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	GNP	k	705	-	-	5/14/38/38	0/3/3/3
51	SF4	k	701	38	-	-	0/6/5/5
53	GNP	k	704	52	-	6/14/38/38	0/3/3/3
51	SF4	k	702	38	-	-	0/6/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	k	705	GNP	PG-O2G	-4.55	1.44	1.56
53	k	704	GNP	PG-O2G	-4.54	1.44	1.56
53	k	704	GNP	C6-N1	4.07	1.40	1.33
53	k	705	GNP	PB-O2B	-4.01	1.45	1.56
53	k	705	GNP	C6-N1	3.84	1.39	1.33
53	k	704	GNP	PB-O2B	-3.73	1.46	1.56
53	k	705	GNP	C5-C6	3.16	1.46	1.41
53	k	704	GNP	C5-C6	3.15	1.46	1.41
53	k	705	GNP	C8-N7	-2.74	1.29	1.34
53	k	704	GNP	C8-N7	-2.70	1.29	1.34
53	k	704	GNP	C2-N1	2.63	1.40	1.35
53	k	705	GNP	C2-N1	2.43	1.39	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	k	704	GNP	C5-C6-N1	-7.91	112.62	123.43
53	k	705	GNP	C5-C6-N1	-7.87	112.67	123.43
53	k	705	GNP	C2-N1-C6	6.08	125.59	115.93
53	k	704	GNP	C2-N1-C6	6.02	125.49	115.93
53	k	705	GNP	N3-C2-N1	-3.76	122.21	127.22
53	k	704	GNP	N3-C2-N1	-3.75	122.22	127.22
53	k	704	GNP	O2G-PG-O3G	-2.55	100.83	107.64
53	k	705	GNP	O2G-PG-O3G	-2.52	100.93	107.64
53	k	705	GNP	C4-C5-C6	-2.49	118.42	120.80
53	k	704	GNP	C4-C5-C6	-2.38	118.53	120.80
53	k	704	GNP	O3G-PG-O1G	-2.15	108.06	113.45
53	k	705	GNP	O3G-PG-O1G	-2.10	108.17	113.45

There are no chirality outliers.

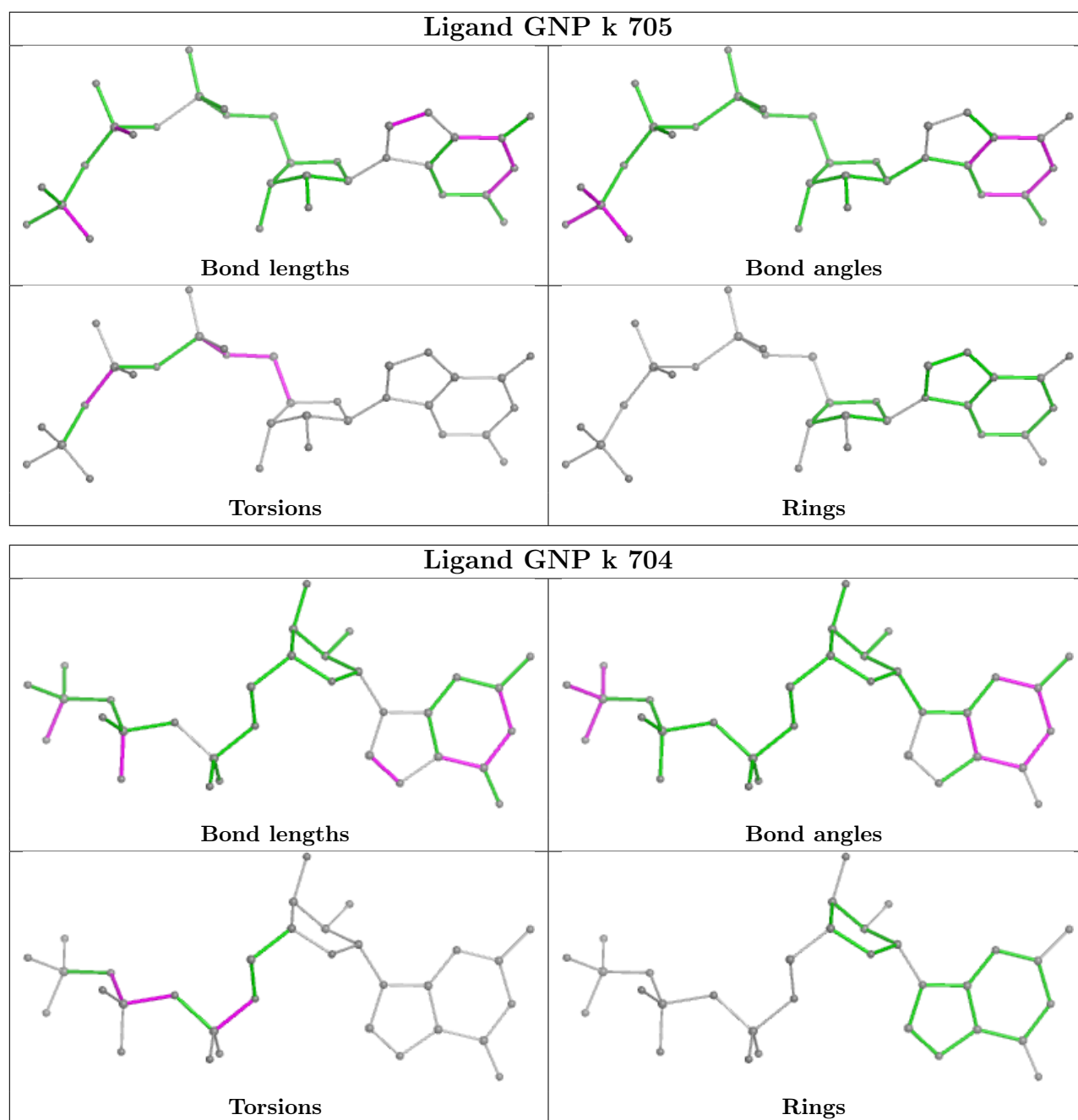
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	k	704	GNP	PG-N3B-PB-O1B
53	k	704	GNP	PG-N3B-PB-O3A
53	k	704	GNP	PA-O3A-PB-O1B
53	k	704	GNP	PA-O3A-PB-O2B
53	k	705	GNP	PG-N3B-PB-O1B
53	k	705	GNP	C5'-O5'-PA-O3A
53	k	705	GNP	C5'-O5'-PA-O2A
53	k	704	GNP	C5'-O5'-PA-O3A
53	k	705	GNP	C4'-C5'-O5'-PA
53	k	705	GNP	O4'-C4'-C5'-O5'
53	k	704	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
-----	-------	------------------

Mol	Chain	Number of breaks
38	k	23
34	2	4
44	v	4
1	1	2
39	U	1
25	a	1
37	j	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	P	8.58
1	k	521:ASP	C	522:PHE	N	2.98
1	U	142:ARG	C	143:GLY	N	2.92
1	k	451:ILE	C	452:GLU	N	2.79
1	k	373:GLU	C	374:ILE	N	2.70
1	k	550:THR	C	551:LEU	N	2.35
1	v	326:HIS	C	327:ALA	N	2.25
1	k	518:VAL	C	519:GLU	N	2.16
1	v	532:SER	C	533:GLU	N	2.16
1	k	486:ASP	C	487:GLU	N	2.09
1	k	591:SER	C	592:GLY	N	2.02
1	k	411:TYR	C	412:LYS	N	2.01
1	1	17:C	O3'	18:G	P	1.99
1	k	378:LEU	C	379:GLY	N	1.94
1	1	18:G	O3'	19:G	P	1.87
1	k	440:GLN	C	441:PHE	N	1.85
1	2	350:A	O3'	351:U	P	1.83
1	v	748:ASP	C	749:TRP	N	1.81
1	k	109:VAL	C	110:GLY	N	1.79
1	k	513:LYS	C	514:THR	N	1.64
1	a	9:THR	C	10:ARG	N	1.60
1	2	239:U	O3'	240:C	P	1.36
1	2	80:G	O3'	81:U	P	1.34
1	j	95:TYR	C	96:ASN	N	1.16
1	v	762:ASN	C	763:GLY	N	1.12
1	k	493:ASP	C	494:SER	N	1.09
1	k	160:LEU	C	161:GLU	N	1.05
1	k	150:SER	C	151:GLU	N	1.02
1	k	268:TYR	C	269:ILE	N	1.02
1	k	241:ASP	C	242:GLU	N	0.84

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	k	531:ARG	C	532:VAL	N	0.82
1	k	481:ASP	C	482:VAL	N	0.79
1	k	104:GLU	C	105:VAL	N	0.75
1	k	408:ASN	C	409:VAL	N	0.68
1	k	562:LEU	C	563:GLU	N	0.52
1	k	455:ILE	C	456:ASP	N	0.44

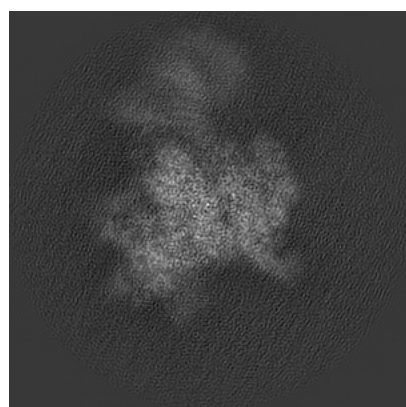
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10761. These allow visual inspection of the internal detail of the map and identification of artifacts.

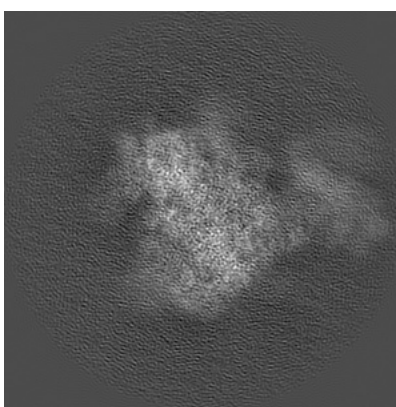
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

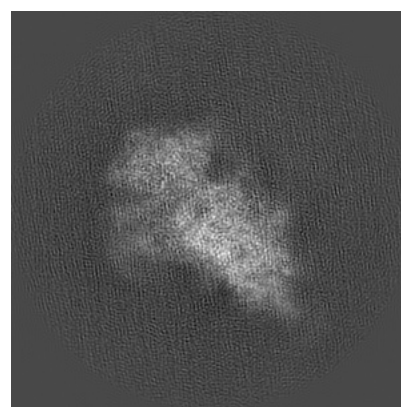
6.1.1 Primary map



X



Y

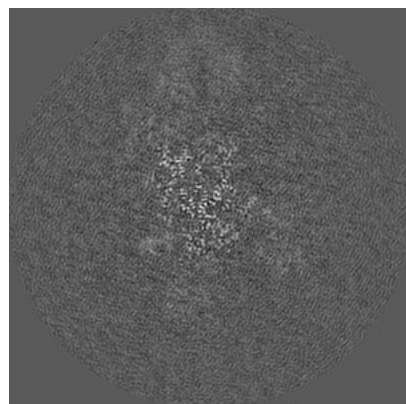


Z

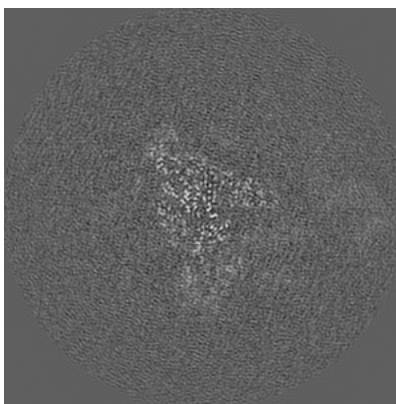
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

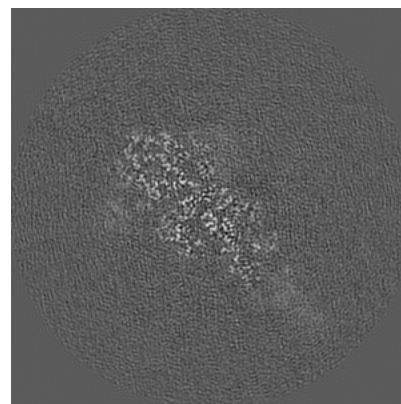
6.2.1 Primary map



X Index: 192



Y Index: 192

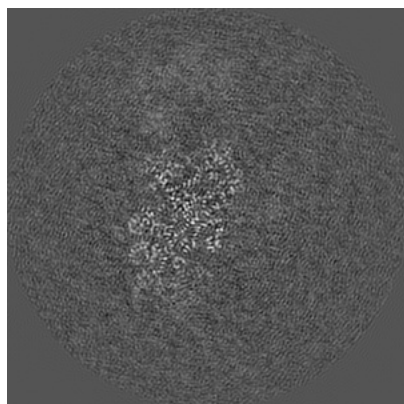


Z Index: 192

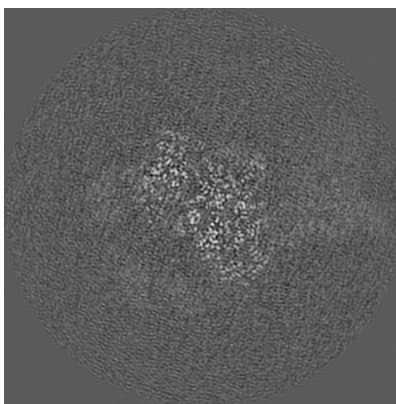
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

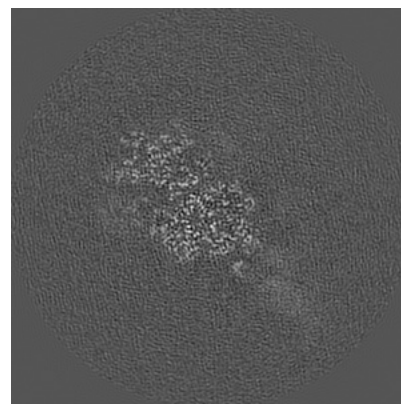
6.3.1 Primary map



X Index: 210



Y Index: 165

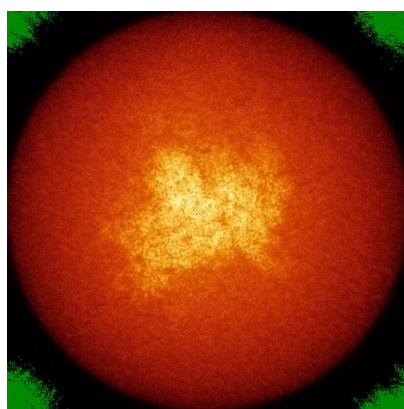


Z Index: 199

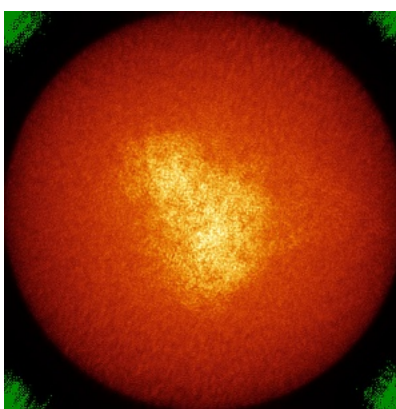
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

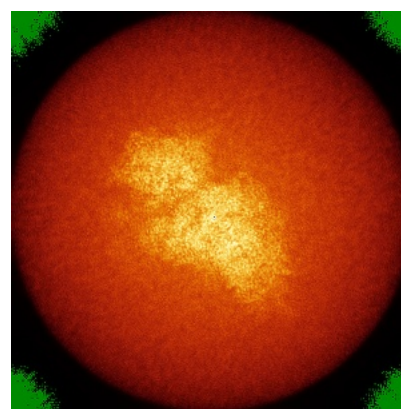
6.4.1 Primary map



X



Y

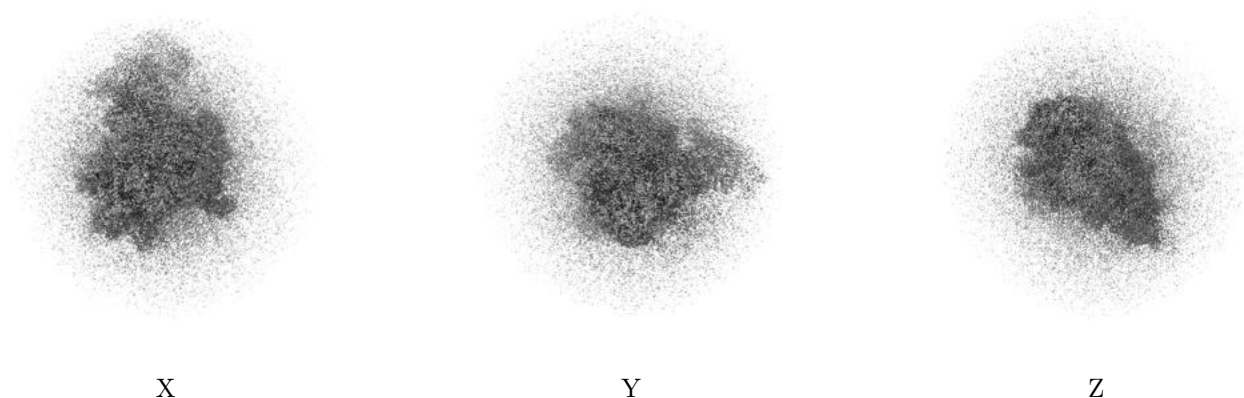


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

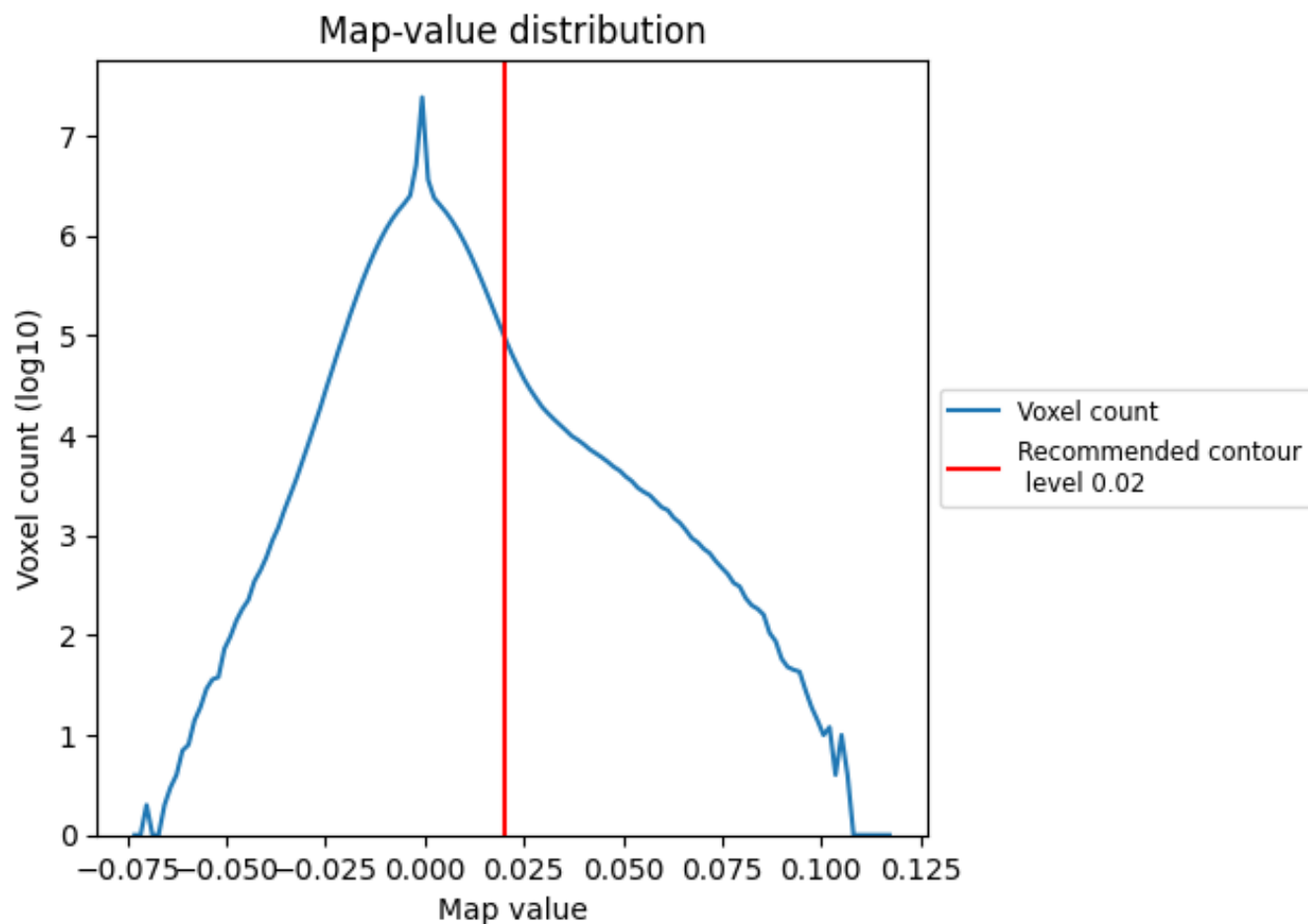
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

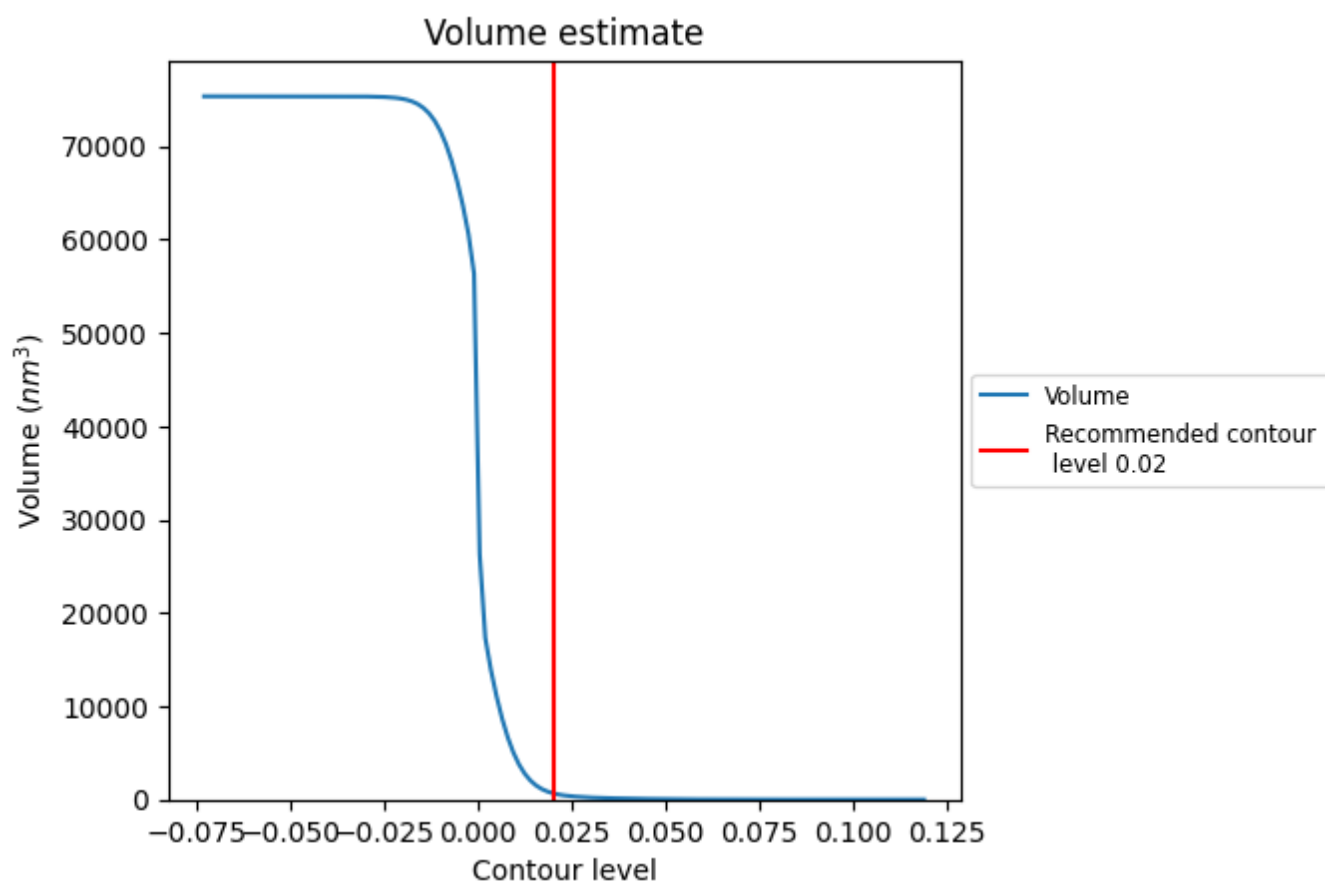
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

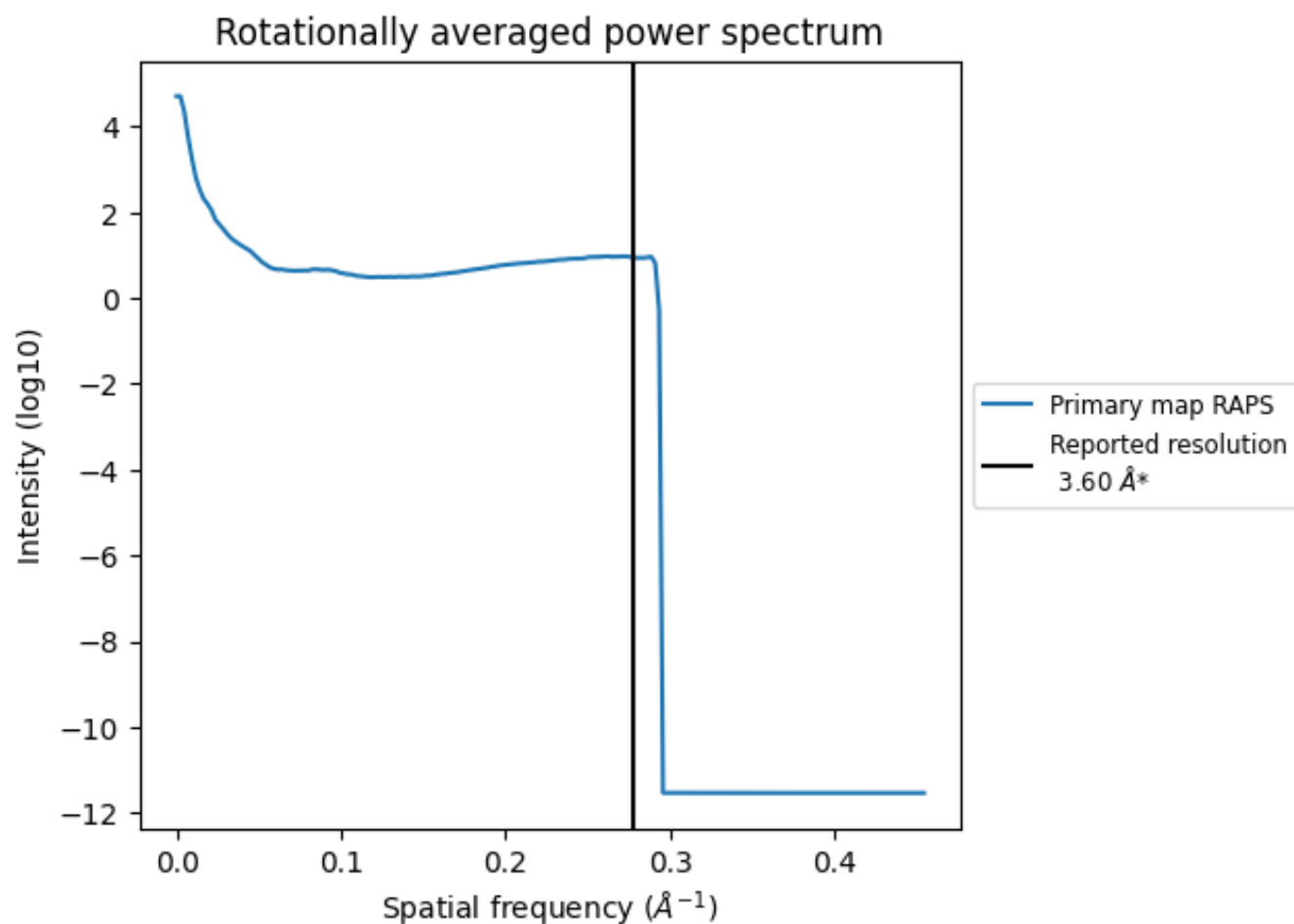
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 665 nm³; this corresponds to an approximate mass of 600 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 0.278 \AA^{-1}

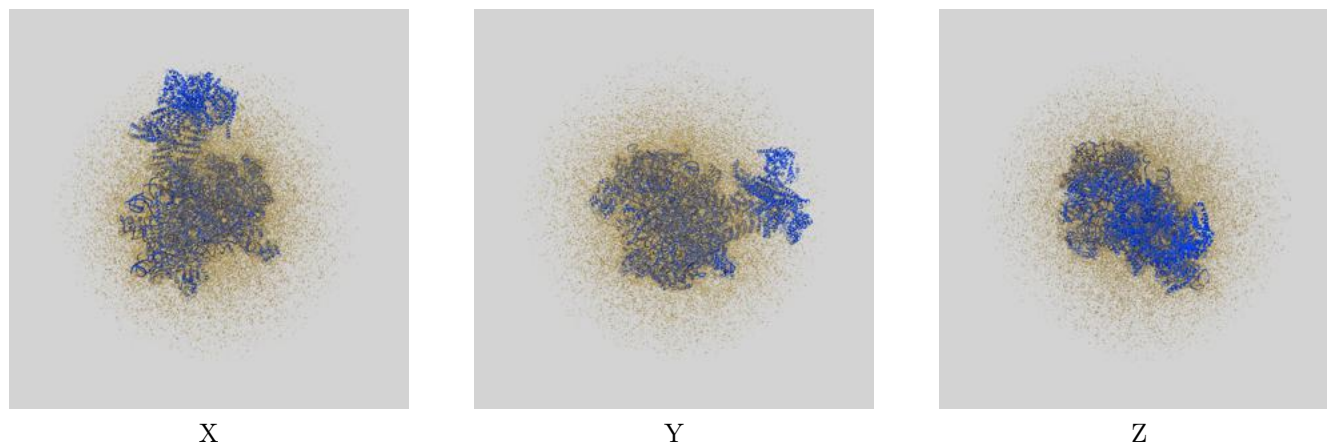
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

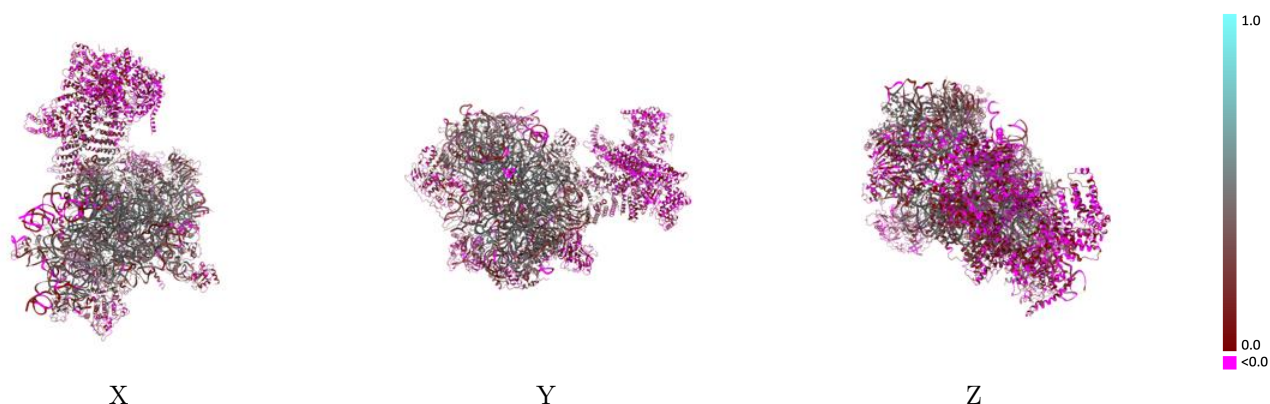
This section contains information regarding the fit between EMDB map EMD-10761 and PDB model 6YAM. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



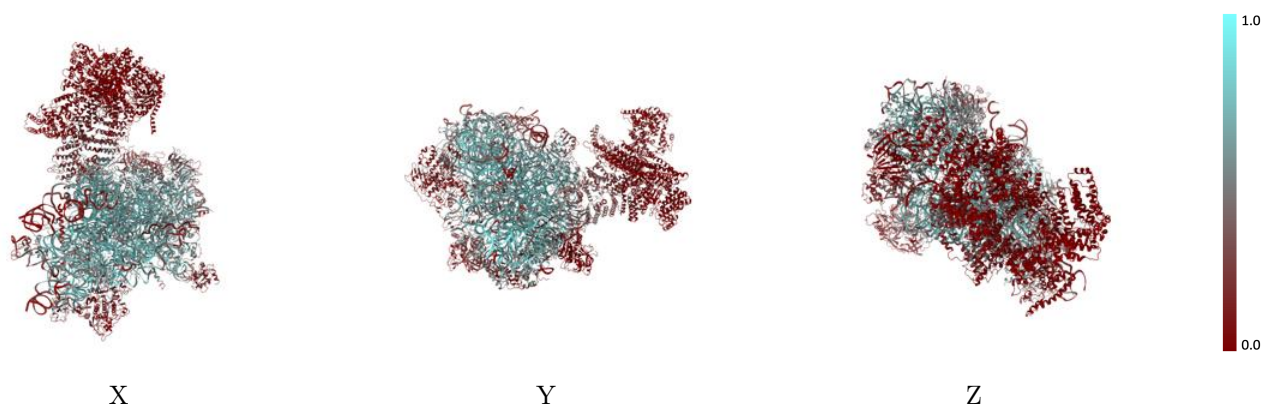
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



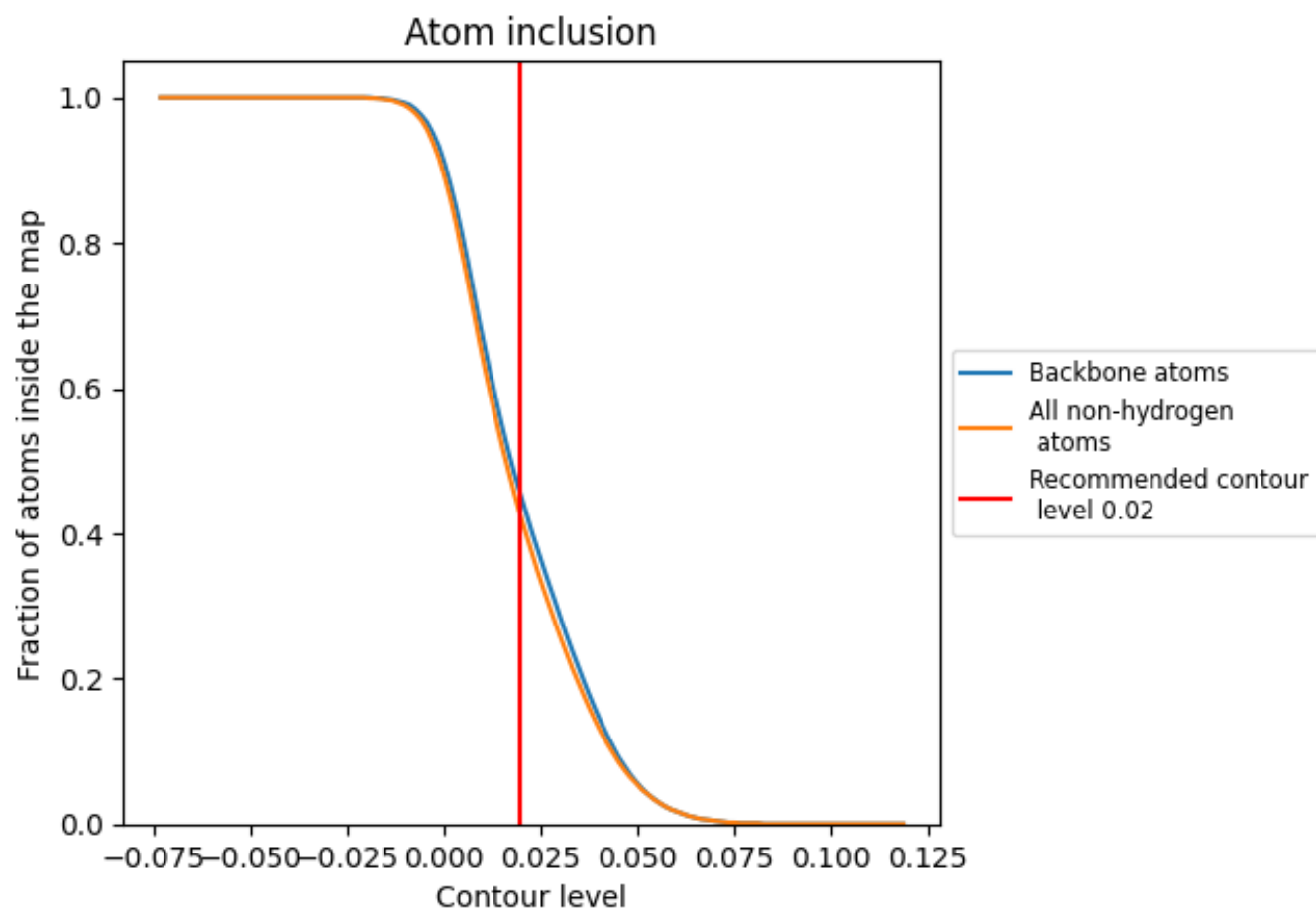
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 42% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4230	 0.2570
1	 0.3490	 0.1490
2	 0.6960	 0.3870
3	 0.1620	 0.0600
A	 0.1180	 0.1080
B	 0.0240	 0.0050
C	 0.6030	 0.3790
D	 0.5460	 0.3610
E	 0.6360	 0.4040
F	 0.5000	 0.3230
G	 0.6070	 0.3860
H	 0.5760	 0.3590
I	 0.4210	 0.2830
J	 0.3600	 0.2360
K	 0.5100	 0.3180
L	 0.6150	 0.3760
M	 0.4890	 0.2770
N	 0.5550	 0.3550
O	 0.1390	 0.0940
P	 0.5750	 0.3590
Q	 0.5710	 0.3550
R	 0.4470	 0.2960
S	 0.6060	 0.3790
T	 0.4870	 0.2970
U	 0.5170	 0.3340
V	 0.5880	 0.3760
W	 0.4870	 0.3130
X	 0.5810	 0.3810
Y	 0.6950	 0.4320
Z	 0.6580	 0.4060
a	 0.5160	 0.3190
b	 0.6540	 0.4120
c	 0.4990	 0.3270
d	 0.5230	 0.3360
e	 0.5150	 0.2410



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.1920	 0.1410
g	 0.4210	 0.2840
i	 0.4080	 0.2680
j	 0.2650	 0.2090
k	 0.1380	 0.1510
l	 0.5110	 0.3240
m	 0.0210	 0.0430
n	 0.4280	 0.2780
q	 0.0160	 0.0020
r	 0.0150	 -0.0050
s	 0.0010	 0.0140
t	 0.0030	 0.0140
u	 0.0090	 0.0180
v	 0.1510	 0.1240
w	 0.0330	 0.0340
y	 0.1500	 0.1290