



Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 11:34 pm BST

PDB ID : 6YAL
EMDB ID : EMD-10760
Title : Mammalian 48S late-stage initiation complex with beta-globin mRNA
Authors : Bochler, A.; Simonetti, A.; Guca, E.; Hashem, Y.
Deposited on : 2020-03-12
Resolution : 3.00 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:

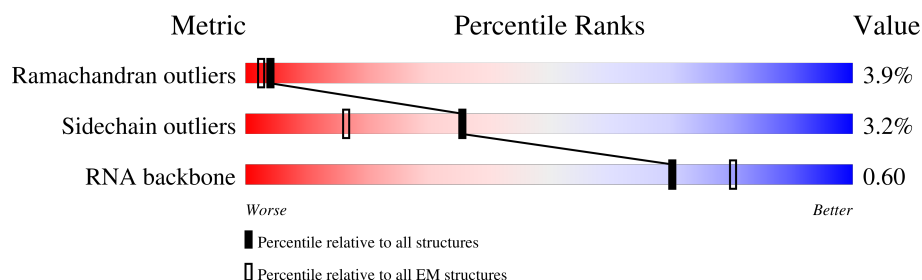
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 3.00 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	 79% 77% 16%
2	l	25	 28% 96%
3	C	209	 12% 94% 5%
4	D	264	 11% 78% 19%
5	E	226	 9% 97%
6	F	243	 23% 88% 5% 7%
7	G	263	 9% 98%
8	H	191	 15% 97%

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Mol	Chain	Length	Quality of chain
9	I	237	
10	J	192	
11	K	206	
12	L	182	
13	M	98	
14	N	158	
15	O	132	
16	P	150	
17	Q	151	
18	S	141	
19	T	135	
20	V	141	
21	W	119	
22	X	82	
23	Y	130	
24	Z	143	
25	a	133	
26	b	115	
27	c	84	
28	d	69	
29	e	56	
30	f	71	
31	g	313	
32	n	124	
33	i	133	

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Mol	Chain	Length	Quality of chain
34	2	1863	
35	A	284	
36	B	422	
37	j	111	
38	k	595	
39	U	152	
40	R	145	
41	3	42	

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 44 unique types of molecules in this entry. The entry contains 90085 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 ul41.

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
			1764	1124	317	315	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 40S 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 40S 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
			1113	701	213	196	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
			1106	698	220	184	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 40S 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 40S 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 40S ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	75	Total	C	N	O	S	0	0
			598	382	111	104	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	1744	Total	C	N	O	P	0	0
			37204	16614	6663	12187	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
			2146	1354	376	405	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
			883	549	168	162	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		

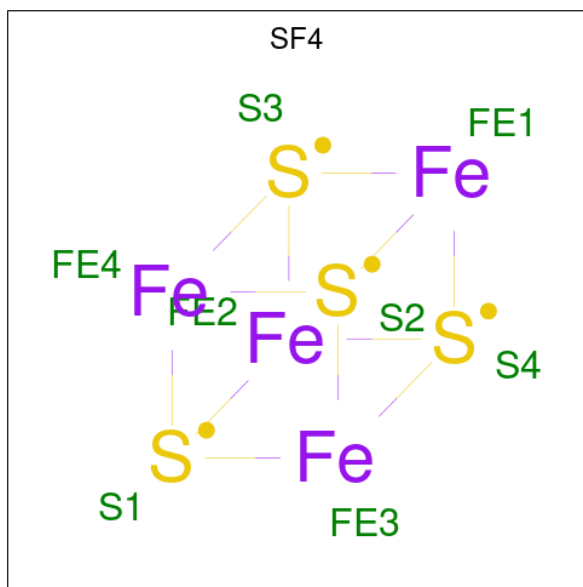
- Molecule 40 is a protein called 40S ribosomal protein uS19.

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	42	Total	C	N	O	P	0	0
			892	401	166	284	41		

- Molecule 42 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 44 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

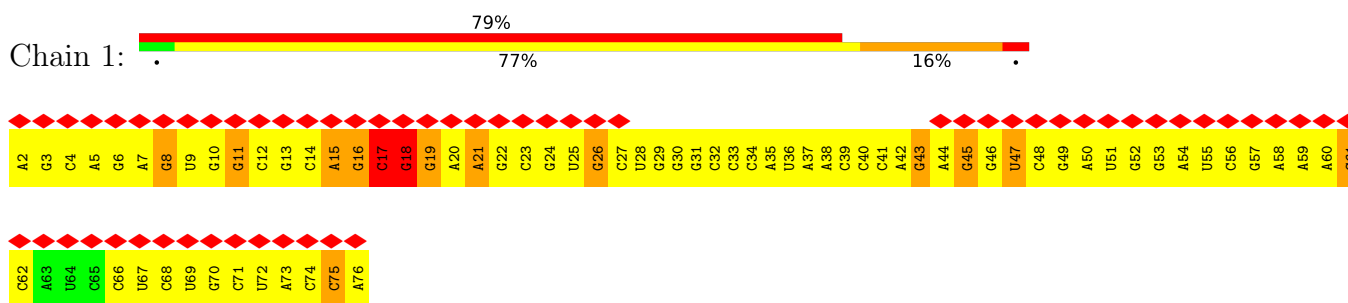


Mol	Chain	Residues	Atoms					AltConf
44	k	1	Total	C	N	O	P	0
			32	10	6	13	3	
44	k	1	Total	C	N	O	P	0
			32	10	6	13	3	

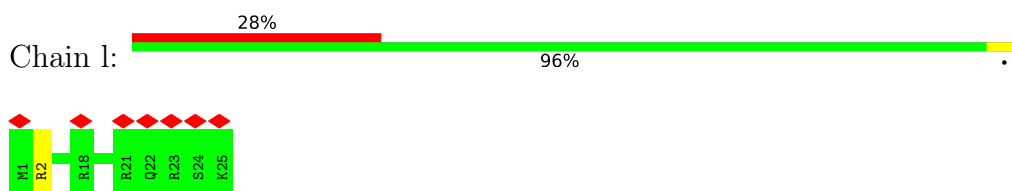
3 Residue-property plots [i](#)

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.

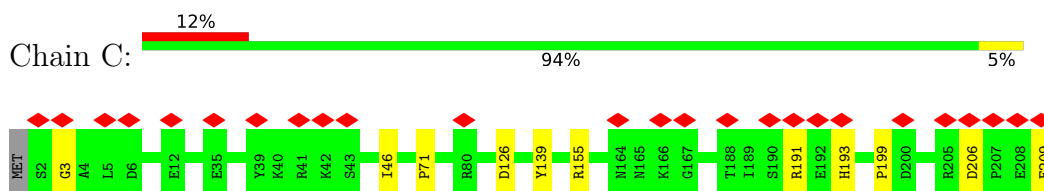
- Molecule 1: initiator methionylated tRNA



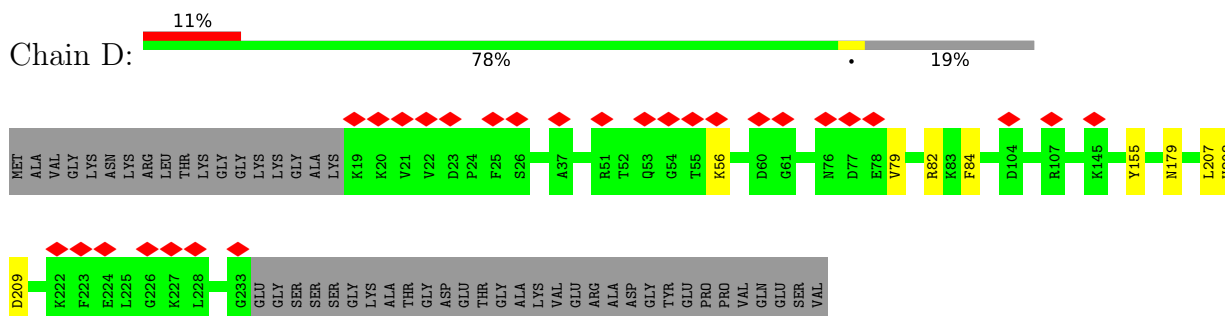
- Molecule 2: 60s ribosomal protein ul41



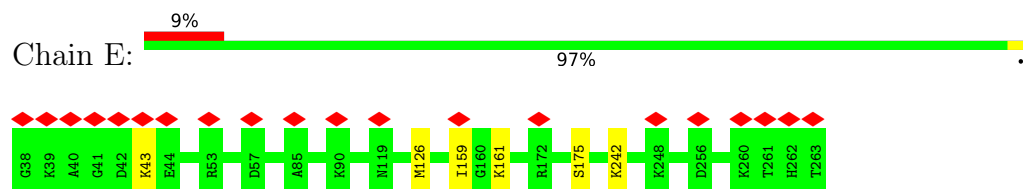
- Molecule 3: 40S ribosomal protein uS2



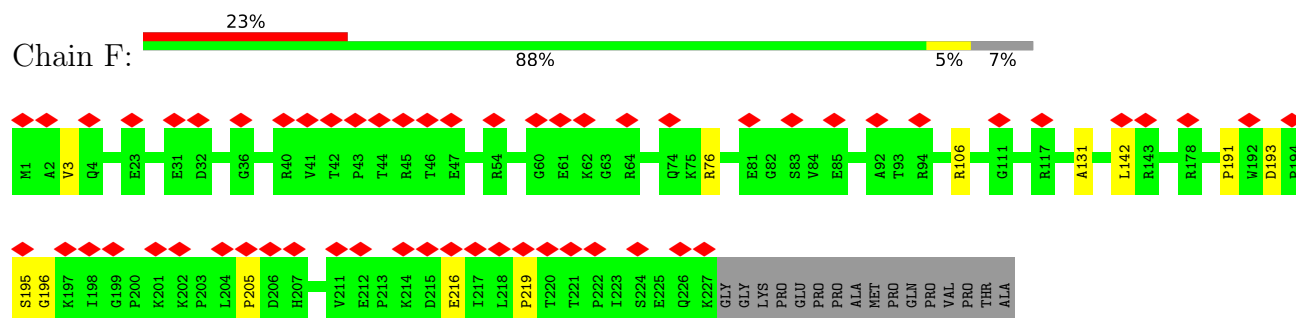
- Molecule 4: 40S ribosomal protein eS1



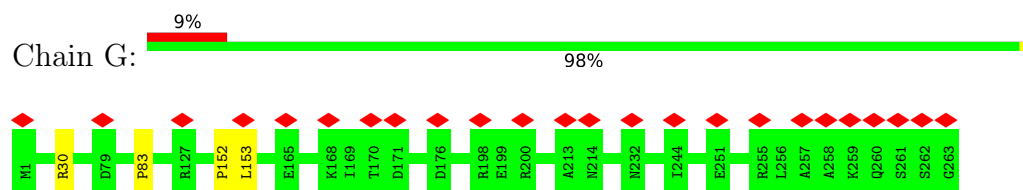
- Molecule 5: 40S ribosomal protein uS5



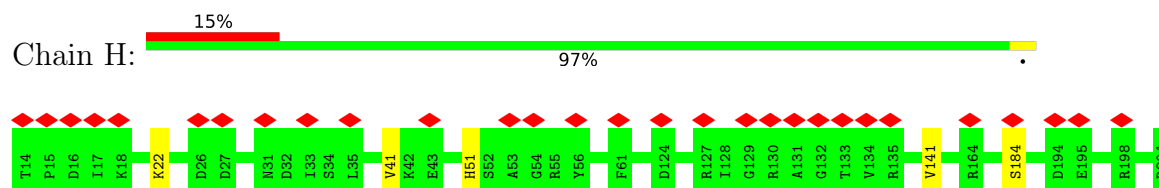
- Molecule 6: 40S Ribosomal protein uS3



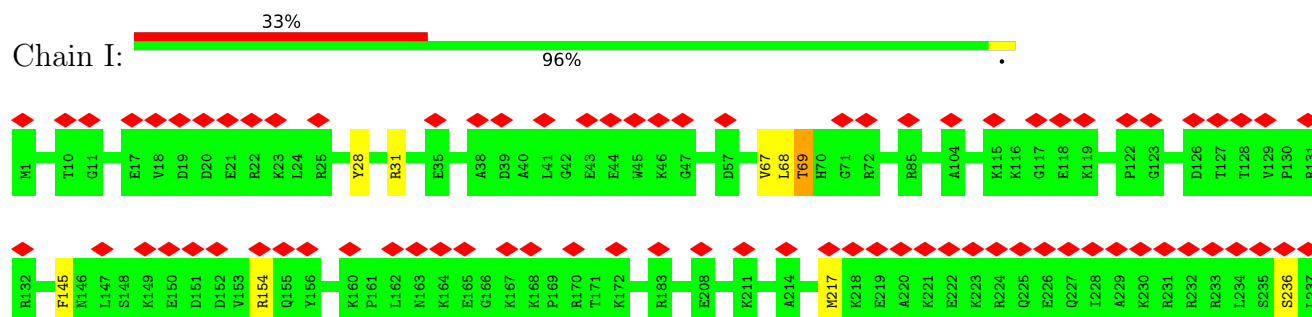
- Molecule 7: 40S ribosomal protein eS4



- Molecule 8: 40S Ribosomal protein uS7

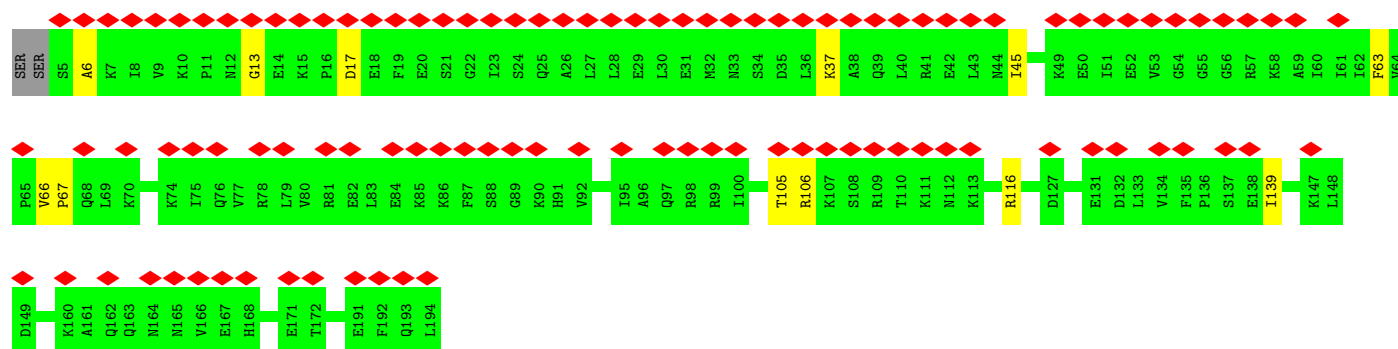


- Molecule 9: 40S ribosomal protein eS6



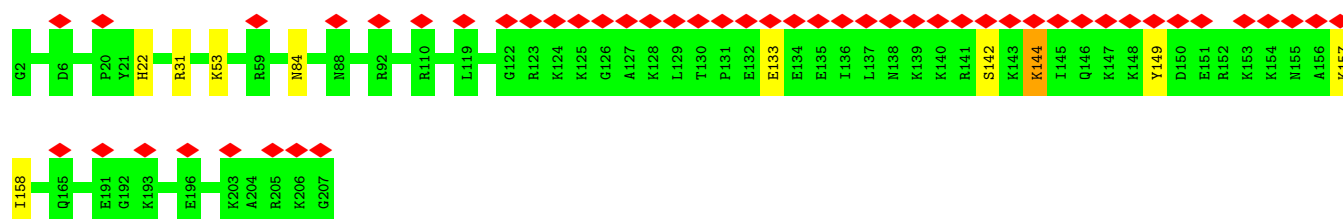
- Molecule 10: 40S ribosomal protein eS7





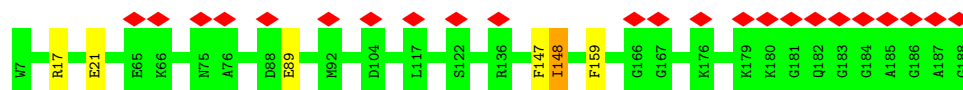
- Molecule 11: 40S ribosomal protein eS8

Chain K: 24% 95% .



- Molecule 12: 40S ribosomal protein uS4

Chain L: 13% 97% ..



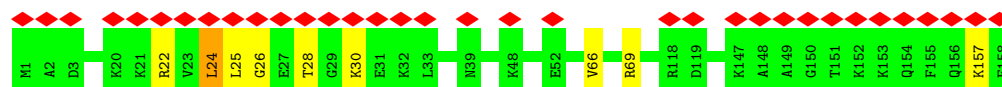
- Molecule 13: 40S ribosomal protein eS10

Chain M: 33% 89% 9% .



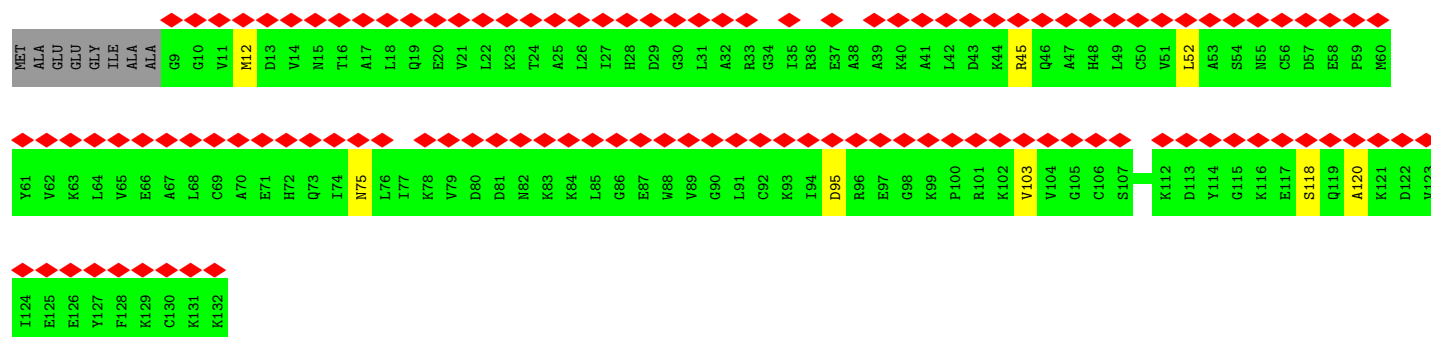
- Molecule 14: 40S ribosomal protein uS17

Chain N: 22% 94% 5% .

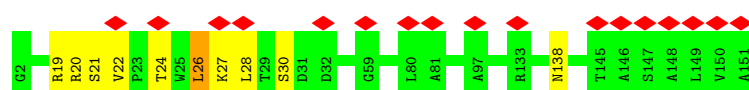


- Molecule 15: 40S ribosomal protein eS12

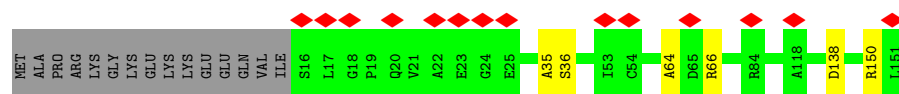
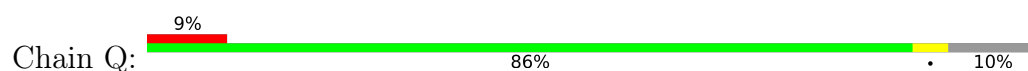
Chain O: 88% 88% 6% 6%



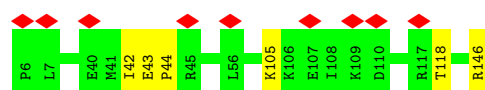
• Molecule 16: 40S ribosomal protein uS15



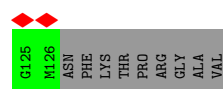
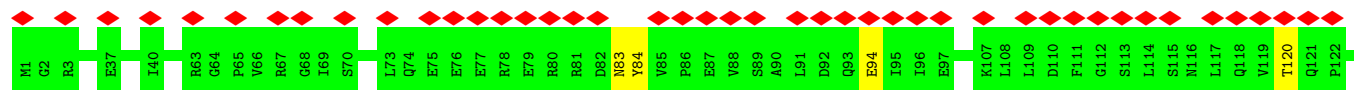
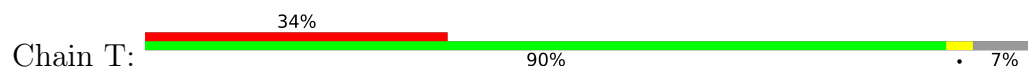
• Molecule 17: 40S ribosomal protein uS11



• Molecule 18: 40S ribosomal protein uS9

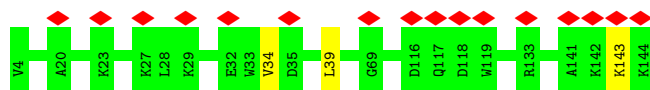


• Molecule 19: 40S ribosomal protein eS17

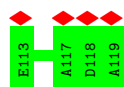
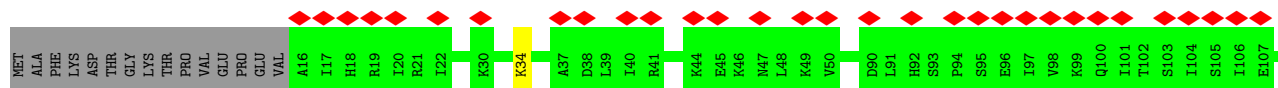
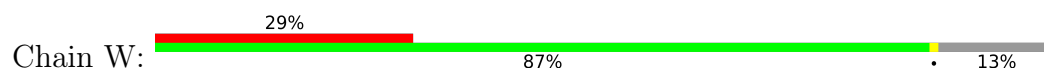


• Molecule 20: 40S ribosomal protein eS19

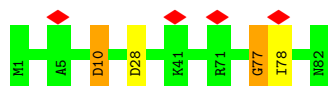




- Molecule 21: 40S ribosomal protein uS10



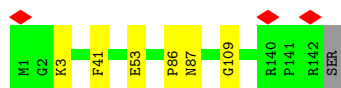
- Molecule 22: 40S ribosomal protein eS21



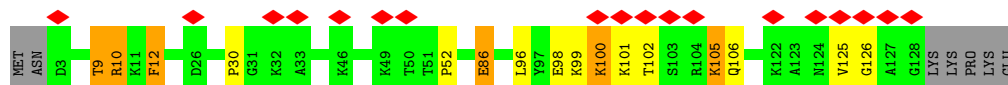
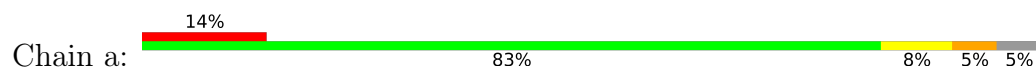
- Molecule 23: 40S ribosomal protein uS8



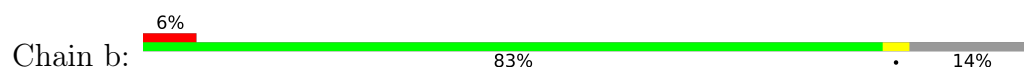
- Molecule 24: 40S ribosomal protein uS12

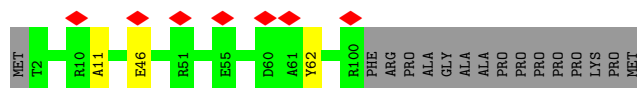


- Molecule 25: 40S ribosomal protein eS24

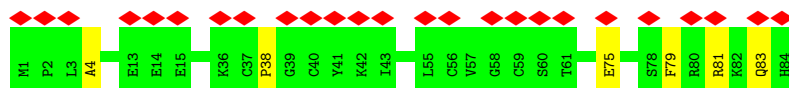


- Molecule 26: 40S ribosomal protein eS26

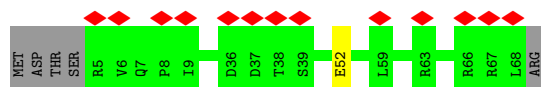




- Molecule 27: 40S ribosomal protein eS27



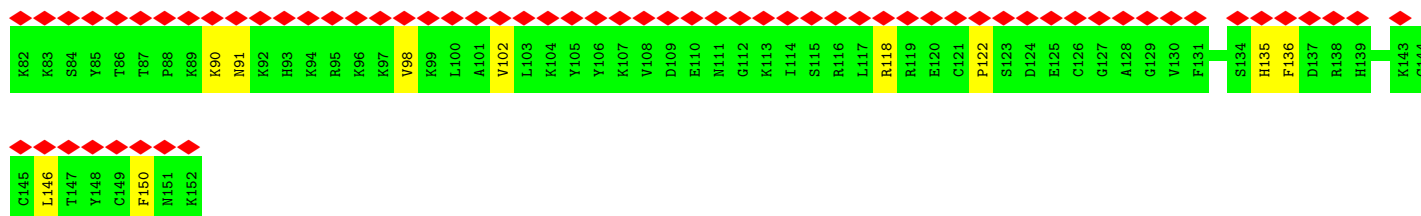
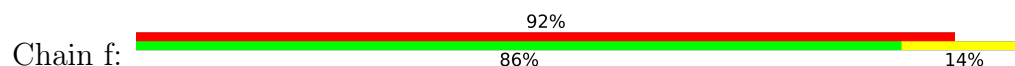
- Molecule 28: 40S ribosomal protein eS28



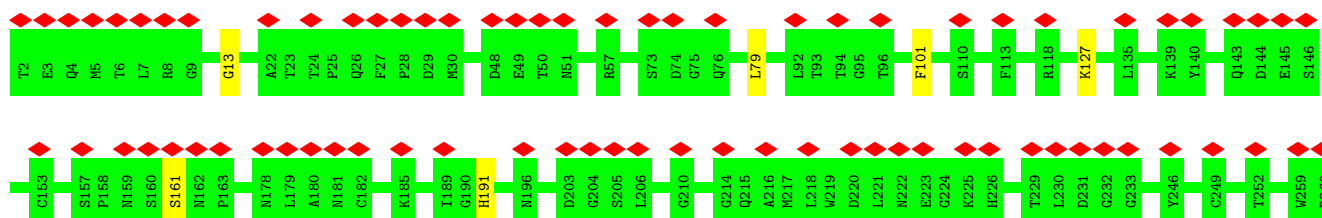
- Molecule 29: 40S ribosomal protein uS14



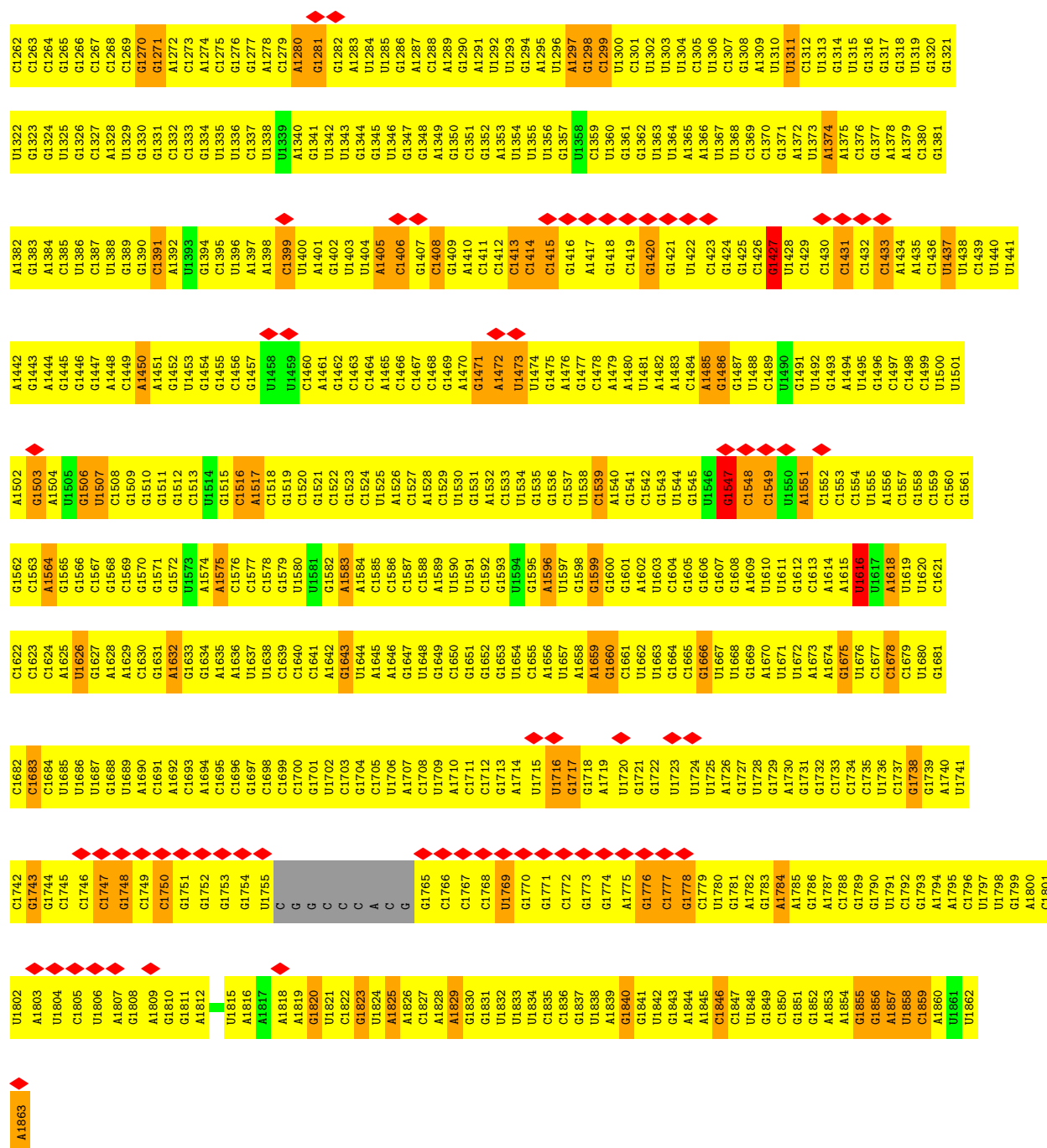
- Molecule 30: 40S ribosomal protein eS31

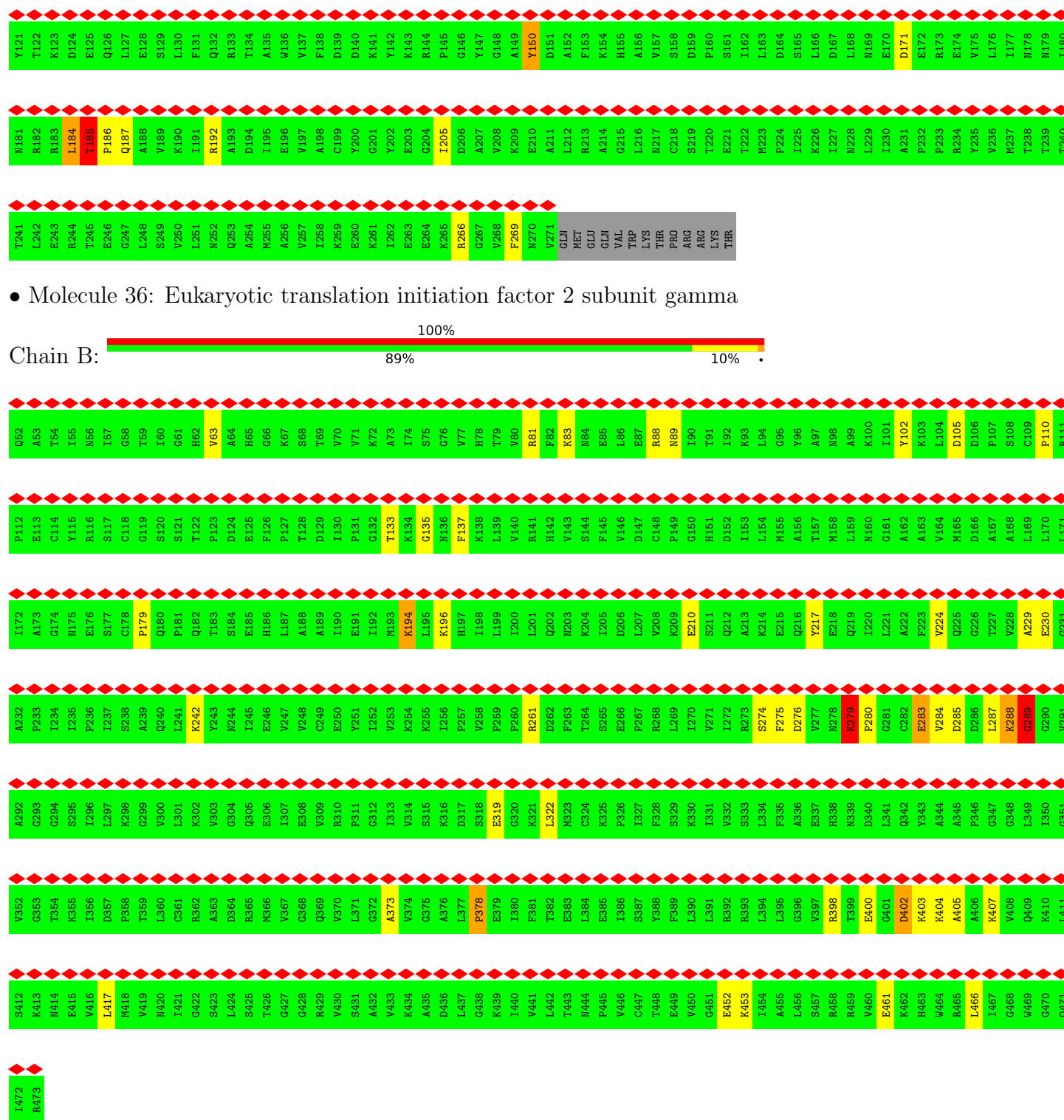


- Molecule 31: ribosomal protein RACK1

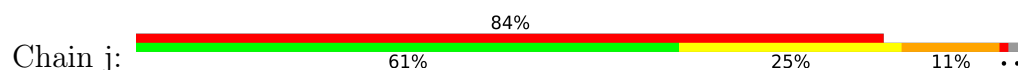


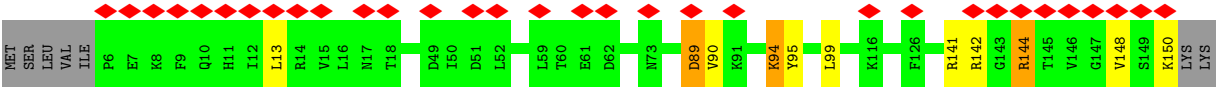
G1202	A1141	C1081	U1021	U961	C901	G841	C	C	A661	G601	U541	C481	G421	A361
G1203	C1142	G1082	C1022	U962	U902	G842	G	C	A662	U602	G542	C482	G422	G362
A1204	C1143	A1083	A1023	C963	G	A843	G	C	G663	C603	G543	A483	A423	G363
A1205	A1144	G1084	A1024	U964	G784	U844	C	C	G664	G604	U544	C484	G424	G364
G1206	A1145	U965	G1025	U965	G785	U845	C	C	U665	C605	A544	U485	A425	U365
G1207	A1146	C1086	A1026	G966	G786	C846	C	C	G666	A606	A545	C486	G426	A366
G1208	U1147	C1087	A1027	G967	C787	C847	C	C	G667	G607	U546	C487	G427	G367
C1209	U1148	G1088	C1028	U968	C788	G848	U728	U728	G668	C608	U547	C488	G428	U368
A1210	C1149	A1089	G1029	C969	C788	C849	C729	C729	A669	G609	U547	C489	A429	G369
C1211	U1150	C1090	C1030	U970	G789	A850	G	C	G670	A490	G548	C490	G430	G370
A1212	G1151	U1091	A1031	G971	G789	C851	C730	C730	U671	C611	G549	C491	C431	C371
C1213	G1152	G1092	A1032	G972	A790	C852	C731	C731	U672	C612	A550	C492	C432	C372
A1214	G1154	C1093	G1033	C973	A791	U853	C732	C732	G673	G613	A551	C493	U433	G373
C1215	U1155	U1094	U1034	G974	A854	A854	G733	G733	G674	C614	U552	C494	U434	G374
A1216	U1156	C1095	C1035	C975	G855	G855	C733	C733	A675	G615	G553	C495	A435	G375
G1217	U1157	A1096	G1036	U976	C793	C856	C734	C734	U676	G616	A554	G497	G436	C376
C1218	C1158	U1097	G1037	A977	G794	A857	C735	C735	C677	U617	G555	G497	G437	C377
A1219	C1159	G1098	A978	G978	G794	C857	C736	C736	U678	A618	U556	A498	U378	U378
G1220	U1160	C1099	U1039	A979	U795	U859	C737	C737	U679	A619	C557	A439	A379	C380
U1221	G1161	G1100	G1040	C980	U796	A860	U737	U737	C680	U620	C558	C500	C440	C381
G1222	U1162	G1101	U1041	C981	U796	A861	U738	U738	U681	U621	A559	U501	G441	C382
C1223	G1163	C1102	U1042	G982	A798	U862	U739	U739	G682	C622	C560	A502	G442	U383
A1224	G1164	G1103	C1043	A983	C799	C863	U740	U740	U683	C623	U561	G503	C443	G384
G1225	U1165	U1104	G1044	C984	U800	G864	G740	G740	G684	A624	U562	U504	U444	U385
C1226	A1166	C1105	A1045	C985	U801	A865	C741	C741	U685	G625	U563	G505	A445	G386
G1227	U1167	G1106	A1046	A986	U802	A866	U742	U742	G686	C626	A564	A506	C446	U387
U1228	U1168	U1107	G1047	G987	U803	U867	C743	C743	U687	U627	U565	C507	C447	G387
C1229	A1169	U1108	A1048	A988	A804	G868	U744	U744	G688	C628	A566	G508	A448	U388
U1230	U1170	G1109	C1049	G989	A805	C869	C744	C744	U689	C629	U567	A509	C449	C389
G1231	C1171	C990	G1050	C990	A806	G870	U745	U745	U688	A630	C569	A510	A450	C390
C1232	G1172	U1110	A1051	G991	A807	C871	C746	C746	G	U632	U570	A511	U451	C391
C1233	U1173	C1112	C1052	A992	A808	C872	G747	G747	G	A633	U571	A512	C452	C392
U1234	U1174	G1113	G1053	A993	U930	C873	U748	U748	G	C634	U572	A513	C453	C393
C1235	G1175	C1114	G1055	G995	U931	U810	G749	C749	U	C635	A573	A515	A454	G394
A1236	A1176	U1115	A1056	C996	C933	A812	C749	C749	A	C636	A574	A516	A455	G395
U1238	A1177	C1116	U1057	U997	U935	C813	G750	G750	C	U637	C575	C517	G457	U396
U1239	A1178	U1117	A1058	U998	U936	A814	C751	C751	G	A638	G576	C518	A458	A398
C1240	G1180	G1117	C1059	U999	U937	G815	C752	C752	G	U639	A577	A519	A459	C399
G1241	C1181	U1118	U1060	U1000	U938	G816	C	C	G	A640	G578	U520	G460	G400
A1242	U1182	C1119	G1061	G1001	U938	U817	C	C	G	U641	G579	A521	G461	G401
C1243	G1183	C1120	U1062	C1002	A940	U879	U	U	C	U642	A580	C522	C462	G402
A1244	A1184	G1121	C1063	C1003	U941	C880	C	C	G	A643	U581	A523	A463	G403
C1245	A1185	U1122	G1064	A1004	U942	U881	C	C	U	A644	C582	G524	G464	A404
A1246	A1186	C1123	U1065	A1005	U942	A821	C	C	U	A645	C583	G525	C465	A405
U1247	C1187	G1124	A1066	G1006	U944	A822	C	C	C	U646	A584	A526	A466	U406
C1248	U1188	G1125	G1067	A1007	C944	C824	U	U	G	U647	U585	C527	G467	C407
A1249	U1189	U1126	U1068	A1008	U945	U883	C	C	C	U648	U586	C527	A468	A408
C1250	U1190	C1127	U1069	C947	C825	C825	C	C	C	C650	G587	U528	C469	G409
G1251	A1191	G1128	G1070	G948	A826	U885	U	U	C	U651	G588	C529	G470	G410
A1252	A1192	U1129	C1071	U949	G827	C827	C	C	C	A589	C589	C471	C471	G411
G1253	G1193	G1130	G1072	U1011	C948	U886	U	U	C	G582	G590	U530	C472	U412
A1254	U1194	C1131	A1073	U1012	U950	G887	U	U	C	C653	G591	U531	C473	U413
A1255	A1195	U1132	C1074	G952	C830	U888	A	A	G	C654	G592	U532	A474	C414
C1256	U1196	C1015	A953	U953	C831	U889	C	C	A	A655	G592	U532	A475	G415
U1257	U1197	C1134	G1075	G954	G832	G890	C	C	C	C656	C593	C533	A476	A416
C1258	U1198	U1135	U1076	G954	G832	G891	U	U	C	U657	A594	G534	U477	U417
U1259	G1199	G1136	U1077	G955	A833	G891	C	C	C	U658	A595	A478	U478	U418
C1260	U1200	G1137	A1078	U956	G834	U892	G	G	A	A659	U597	G536	C419	C420
A1261	C1201	U1138	A1079	A1020	C835	U893	A	A	G	A660	C598	G537	C490	
		A1139	A958		C836	U894	U	U	C		U599	C538		
		U895	C837		C837	U895	C	C	C		G600	C539		
		C896	C838		C838	U896	C	C	C			C540		
		G897	C839		C839	U897	C	C	C					
		G898	U840		U840	U898	C	C	C					
		A899				A900	C	C	C					



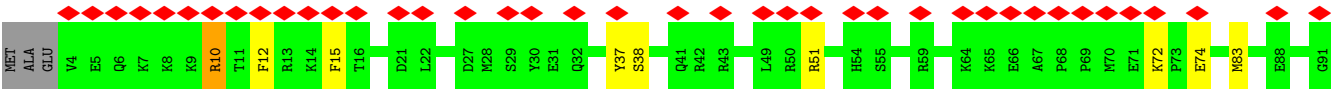
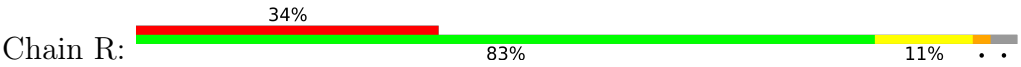


• Molecule 37: eukaryotic translation initiation factor 1A

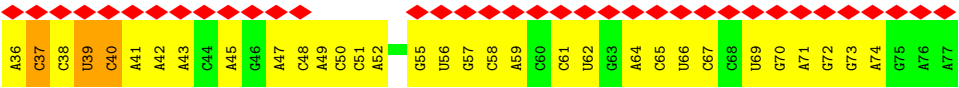
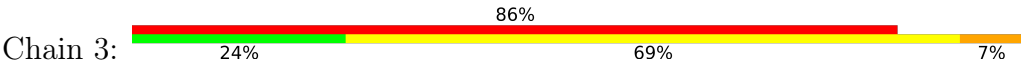




• Molecule 40: 40S ribosomal protein uS19



• Molecule 41: beta-globin mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252000	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	0.147	Depositor
Minimum map value	-0.078	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: C4J, SF4, T6A, GNP, 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	1.37	0/241	0.93	0/305
3	C	0.97	0/1680	0.97	1/2283 (0.0%)
4	D	0.90	0/1769	0.98	2/2367 (0.1%)
5	E	0.91	0/1779	0.94	1/2399 (0.0%)
6	F	0.97	0/1792	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	0/1133	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	0.98	0/1124	0.95	2/1500 (0.1%)
25	a	1.04	1/1038 (0.1%)	1.06	3/1380 (0.2%)
26	b	1.06	0/802	0.96	0/1076
27	c	0.93	0/673	0.97	1/902 (0.1%)
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	0/604	1.01	2/810 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	1.09	0/478	0.99	0/628
34	2	1.59	70/41567 (0.2%)	2.40	4350/64783 (6.7%)
35	A	0.79	1/2177 (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	1/893 (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	0.91	1/998 (0.1%)	1.29	29/1553 (1.9%)
All	All	1.32	104/95467 (0.1%)	1.85	4672/137696 (3.4%)

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
33	i	0	3
34	2	1	47
35	A	0	7
36	B	0	8
37	j	0	12
38	k	0	33
39	U	0	3
All	All	4	144

All (104) 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	-35.48	0.52	1.34
38	k	378	LEU	C-N	34.32	1.94	1.33
1	1	17	C	O3'-P	32.13	1.99	1.61
38	k	408	ASN	C-N	-28.69	0.68	1.34
1	1	17	C	C2'-O2'	-25.99	1.07	1.41
38	k	109	VAL	C-N	25.78	1.79	1.33
38	k	104	GLU	C-N	-25.64	0.75	1.34
38	k	481	ASP	C-N	-23.70	0.79	1.34
38	k	531	ARG	C-N	-22.54	0.82	1.34
38	k	440	GLN	C-N	22.43	1.85	1.34
34	2	80	G	O3'-P	-21.96	1.34	1.61
1	1	18	G	O3'-P	21.68	1.87	1.61
38	k	241	ASP	C-N	-21.55	0.84	1.34
34	2	239	U	O3'-P	-20.59	1.36	1.61
34	2	350	A	O3'-P	18.98	1.83	1.61
41	3	39	U	O3'-P	-17.77	1.39	1.61
1	1	18	G	C3'-O3'	-16.68	1.18	1.42
36	B	289	GLY	N-CA	-14.38	1.24	1.46
38	k	150	SER	C-N	-13.59	1.02	1.34
38	k	268	TYR	C-N	-13.56	1.02	1.34
34	2	351	U	O3'-P	-13.55	1.44	1.61
38	k	513	LYS	C-N	13.32	1.64	1.34
1	1	16	G	O3'-P	-12.63	1.46	1.61
38	k	160	LEU	C-N	-12.40	1.05	1.34
1	1	37	T6A	O3'-P	11.69	1.75	1.61
25	a	9	THR	C-N	11.64	1.60	1.34
38	k	493	ASP	C-N	-10.72	1.09	1.34
34	2	1170	U	O3'-P	-10.31	1.48	1.61
35	A	184	LEU	C-N	10.10	1.57	1.34
34	2	1171	G	O3'-P	-9.17	1.50	1.61
22	X	77	GLY	C-N	8.96	1.54	1.34
1	1	18	G	C1'-N9	-7.92	1.35	1.46
34	2	67	C	O3'-P	7.77	1.70	1.61
37	j	95	TYR	C-N	-7.73	1.16	1.34
34	2	1182	U	N3-C4	7.50	1.45	1.38
34	2	1170	U	C2-N3	6.94	1.42	1.37
34	2	1809	A	N7-C5	-6.53	1.35	1.39
38	k	179	ALA	C-N	6.43	1.48	1.34
34	2	916	A	N7-C5	-6.36	1.35	1.39
34	2	1023	A	N7-C5	-6.34	1.35	1.39
34	2	822	A	N7-C5	-6.20	1.35	1.39
34	2	1141	A	N7-C5	-6.19	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	2	1185	A	N7-C5	-6.12	1.35	1.39
34	2	1170	U	C1'-N1	6.07	1.57	1.48
34	2	960	A	N7-C5	-6.06	1.35	1.39
34	2	1584	A	N7-C5	-6.02	1.35	1.39
34	2	206	A	N7-C5	-5.93	1.35	1.39
34	2	437	A	N7-C5	-5.93	1.35	1.39
34	2	1815	U	O3'-P	-5.89	1.54	1.61
34	2	237	G	C2-N3	5.86	1.37	1.32
34	2	1628	A	N7-C5	-5.85	1.35	1.39
34	2	1192	A	N7-C5	-5.67	1.35	1.39
1	1	17	C	C3'-O3'	-5.64	1.34	1.42
34	2	1283	A	N7-C5	-5.62	1.35	1.39
34	2	577	A	N7-C5	-5.61	1.35	1.39
34	2	994	A	N7-C5	-5.61	1.35	1.39
34	2	190	A	N7-C5	-5.60	1.35	1.39
34	2	1178	A	N7-C5	-5.60	1.35	1.39
34	2	102	A	N7-C5	-5.59	1.35	1.39
34	2	1066	A	N7-C5	-5.59	1.35	1.39
34	2	1182	U	N1-C6	5.58	1.43	1.38
34	2	1045	A	N7-C5	-5.57	1.35	1.39
34	2	1629	A	N7-C5	-5.54	1.35	1.39
34	2	1353	A	N7-C5	-5.48	1.35	1.39
34	2	1714	A	N7-C5	-5.47	1.35	1.39
34	2	1635	A	N7-C5	-5.46	1.35	1.39
34	2	1784	A	N7-C5	-5.42	1.35	1.39
34	2	1186	A	N7-C5	-5.41	1.36	1.39
34	2	1730	A	N7-C5	-5.35	1.36	1.39
34	2	235	C	N3-C4	5.34	1.37	1.33
34	2	1440	U	C2-N3	5.34	1.41	1.37
34	2	1740	A	N7-C5	-5.34	1.36	1.39
34	2	554	A	N7-C5	-5.33	1.36	1.39
34	2	1046	A	N7-C5	-5.33	1.36	1.39
34	2	537	G	C2-N3	5.32	1.37	1.32
34	2	318	U	C2-N3	5.30	1.41	1.37
34	2	1615	A	N7-C5	-5.30	1.36	1.39
34	2	171	A	N7-C5	-5.29	1.36	1.39
34	2	80	G	N1-C2	5.24	1.42	1.37
34	2	1182	U	C2-N3	5.23	1.41	1.37
34	2	1539	C	N3-C4	5.23	1.37	1.33
34	2	474	A	N7-C5	-5.23	1.36	1.39
34	2	1645	A	N7-C5	-5.20	1.36	1.39
34	2	1170	U	C5-C6	5.19	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	2	92	A	N7-C5	-5.18	1.36	1.39
34	2	229	A	N7-C5	-5.17	1.36	1.39
34	2	1745	C	N3-C4	5.14	1.37	1.33
34	2	304	A	N7-C5	-5.11	1.36	1.39
34	2	439	A	N7-C5	-5.09	1.36	1.39
34	2	272	C	N3-C4	5.08	1.37	1.33
34	2	1767	C	N3-C4	5.08	1.37	1.33
1	1	71	C	N3-C4	5.08	1.37	1.33
1	1	60	A	N7-C5	-5.07	1.36	1.39
34	2	402	G	C2-N3	5.06	1.36	1.32
34	2	1747	C	N3-C4	5.06	1.37	1.33
34	2	1303	U	C2-N3	5.05	1.41	1.37
34	2	1774	G	N1-C2	5.05	1.41	1.37
34	2	1170	U	N1-C2	-5.04	1.34	1.38
34	2	1772	C	N3-C4	5.04	1.37	1.33
36	B	288	LYS	C-N	-5.03	1.24	1.33
1	1	70	G	N1-C2	5.02	1.41	1.37
34	2	827	G	N1-C2	5.02	1.41	1.37
34	2	1183	G	C2-N3	5.01	1.36	1.32

All (4672) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	160	LEU	O-C-N	35.02	178.73	122.70
38	k	531	ARG	C-N-CA	-34.37	35.77	121.70
38	k	531	ARG	CA-C-N	-33.52	43.46	117.20
38	k	378	LEU	CA-C-N	-27.38	61.45	116.20
38	k	408	ASN	O-C-N	-25.78	81.45	122.70
38	k	160	LEU	CA-C-N	-25.44	61.22	117.20
38	k	160	LEU	C-N-CA	-25.00	59.19	121.70
38	k	348	TYR	O-C-N	-21.55	88.21	122.70
38	k	378	LEU	C-N-CA	-21.51	77.13	122.30
38	k	481	ASP	O-C-N	-21.39	88.48	122.70
34	2	271	G	P-O3'-C3'	21.36	145.33	119.70
38	k	531	ARG	O-C-N	20.05	154.79	122.70
38	k	317	VAL	C-N-CD	-18.91	79.00	120.60
34	2	351	U	P-O3'-C3'	18.69	142.12	119.70
38	k	513	LYS	O-C-N	-17.29	95.03	122.70
1	1	17	C	C4'-C3'-O3'	16.33	145.65	113.00
38	k	493	ASP	O-C-N	16.31	148.80	122.70
34	2	1854	A	P-O3'-C3'	15.81	138.68	119.70
38	k	455	ILE	O-C-N	-15.60	97.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	104	GLU	O-C-N	-15.52	97.87	122.70
38	k	109	VAL	O-C-N	-14.76	98.12	123.20
25	a	12	PHE	CB-CA-C	14.67	139.75	110.40
34	2	1027	A	N1-C6-N6	14.61	127.36	118.60
34	2	997	A	N1-C6-N6	14.49	127.30	118.60
34	2	1556	A	N1-C6-N6	14.37	127.22	118.60
34	2	1405	A	N1-C6-N6	14.30	127.18	118.60
38	k	481	ASP	C-N-CA	14.22	157.26	121.70
34	2	1417	A	N1-C6-N6	14.18	127.11	118.60
34	2	1032	A	N1-C6-N6	14.07	127.04	118.60
1	1	17	C	O3'-P-O5'	13.88	130.38	104.00
34	2	519	A	N1-C6-N6	13.81	126.88	118.60
34	2	68	A	N1-C6-N6	13.79	126.87	118.60
1	1	54	A	N1-C6-N6	13.78	126.87	118.60
34	2	1007	A	N1-C6-N6	13.72	126.83	118.60
34	2	173	A	N1-C6-N6	13.70	126.82	118.60
1	1	60	A	N1-C6-N6	13.69	126.81	118.60
34	2	640	A	N1-C6-N6	13.66	126.80	118.60
34	2	1575	A	N1-C6-N6	13.65	126.79	118.60
34	2	1190	A	N1-C6-N6	13.59	126.75	118.60
34	2	1289	A	N1-C6-N6	13.59	126.75	118.60
34	2	834	G	O4'-C1'-N9	13.54	119.03	108.20
34	2	550	A	N1-C6-N6	13.51	126.71	118.60
41	3	39	U	P-O3'-C3'	13.49	135.89	119.70
34	2	425	A	N1-C6-N6	13.47	126.69	118.60
34	2	1825	A	N1-C6-N6	13.44	126.66	118.60
1	1	18	G	O3'-P-O5'	13.40	129.46	104.00
34	2	1803	A	N1-C6-N6	13.40	126.64	118.60
34	2	1526	A	N1-C6-N6	13.35	126.61	118.60
34	2	309	A	N1-C6-N6	13.33	126.60	118.60
34	2	959	A	N1-C6-N6	13.32	126.59	118.60
34	2	1200	A	N1-C6-N6	13.25	126.55	118.60
34	2	1109	A	N1-C6-N6	13.25	126.55	118.60
34	2	1048	A	N1-C6-N6	13.22	126.53	118.60
34	2	986	A	N1-C6-N6	13.22	126.53	118.60
1	1	16	G	O3'-P-O5'	13.20	129.08	104.00
34	2	1216	A	N1-C6-N6	13.20	126.52	118.60
34	2	1646	A	N1-C6-N6	13.18	126.51	118.60
34	2	545	A	N1-C6-N6	13.18	126.51	118.60
34	2	1448	A	N1-C6-N6	13.12	126.47	118.60
34	2	423	A	N1-C6-N6	13.11	126.47	118.60
34	2	940	A	N1-C6-N6	13.10	126.46	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	79	A	N1-C6-N6	13.09	126.45	118.60
34	2	1609	A	N1-C6-N6	13.08	126.45	118.60
34	2	1141	A	N1-C6-N6	13.05	126.43	118.60
34	2	1853	A	N1-C6-N6	13.04	126.43	118.60
34	2	904	A	N1-C6-N6	13.03	126.42	118.60
34	2	977	A	N1-C6-N6	13.03	126.42	118.60
34	2	1274	A	N1-C6-N6	13.03	126.42	118.60
1	1	21	A	N1-C6-N6	13.02	126.41	118.60
34	2	1272	A	N1-C6-N6	12.99	126.40	118.60
34	2	233	A	N1-C6-N6	12.99	126.39	118.60
34	2	1800	A	N1-C6-N6	12.96	126.38	118.60
34	2	350	A	N1-C6-N6	12.95	126.37	118.60
34	2	22	A	N1-C6-N6	12.95	126.37	118.60
34	2	1719	A	N1-C6-N6	12.94	126.36	118.60
34	2	1596	A	N1-C6-N6	12.93	126.36	118.60
34	2	988	A	N1-C6-N6	12.92	126.35	118.60
34	2	64	A	N1-C6-N6	12.91	126.34	118.60
34	2	509	A	N1-C6-N6	12.90	126.34	118.60
34	2	405	A	N1-C6-N6	12.86	126.31	118.60
34	2	164	A	N1-C6-N6	12.84	126.31	118.60
34	2	1854	A	N1-C6-N6	12.82	126.29	118.60
1	1	38	A	N1-C6-N6	12.81	126.28	118.60
34	2	631	A	N1-C6-N6	12.81	126.28	118.60
34	2	1016	A	N1-C6-N6	12.79	126.27	118.60
34	2	1465	A	N1-C6-N6	12.78	126.27	118.60
34	2	589	A	N1-C6-N6	12.77	126.26	118.60
34	2	339	A	N1-C6-N6	12.76	126.26	118.60
34	2	1726	A	N1-C6-N6	12.76	126.26	118.60
38	k	493	ASP	CA-C-N	-12.75	89.15	117.20
34	2	490	A	N1-C6-N6	12.73	126.24	118.60
34	2	882	A	N1-C6-N6	12.72	126.23	118.60
1	1	76	A	N1-C6-N6	12.72	126.23	118.60
34	2	1375	A	N1-C6-N6	12.72	126.23	118.60
34	2	1179	A	N1-C6-N6	12.71	126.23	118.60
34	2	1636	A	N1-C6-N6	12.67	126.20	118.60
34	2	630	A	N1-C6-N6	12.67	126.20	118.60
34	2	1020	A	N1-C6-N6	12.67	126.20	118.60
34	2	638	A	N1-C6-N6	12.65	126.19	118.60
34	2	404	A	N1-C6-N6	12.64	126.19	118.60
34	2	1177	A	N1-C6-N6	12.64	126.18	118.60
34	2	103	A	N1-C6-N6	12.63	126.18	118.60
34	2	1365	A	N1-C6-N6	12.63	126.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1242	A	N1-C6-N6	12.63	126.18	118.60
34	2	807	A	N1-C6-N6	12.62	126.17	118.60
34	2	388	A	N1-C6-N6	12.62	126.17	118.60
34	2	535	A	N1-C6-N6	12.62	126.17	118.60
34	2	1349	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	227	A	N1-C6-N6	12.61	126.17	118.60
34	2	382	A	N1-C6-N6	12.60	126.16	118.60
34	2	448	A	N1-C6-N6	12.60	126.16	118.60
34	2	479	A	N1-C6-N6	12.60	126.16	118.60
34	2	214	A	N1-C6-N6	12.60	126.16	118.60
34	2	398	A	N1-C6-N6	12.60	126.16	118.60
34	2	1589	A	N1-C6-N6	12.60	126.16	118.60
34	2	1863	A	N1-C6-N6	12.60	126.16	118.60
34	2	1378	A	N1-C6-N6	12.59	126.16	118.60
34	2	1710	A	N1-C6-N6	12.59	126.15	118.60
34	2	99	A	N1-C6-N6	12.59	126.15	118.60
34	2	643	A	N1-C6-N6	12.59	126.15	118.60
34	2	1692	A	N1-C6-N6	12.58	126.15	118.60
34	2	1213	A	N1-C6-N6	12.57	126.14	118.60
34	2	1532	A	N1-C6-N6	12.56	126.14	118.60
41	3	52	A	N1-C6-N6	12.56	126.14	118.60
34	2	366	A	N1-C6-N6	12.56	126.14	118.60
34	2	1470	A	N1-C6-N6	12.55	126.13	118.60
34	2	565	A	N1-C6-N6	12.54	126.12	118.60
34	2	510	A	N1-C6-N6	12.53	126.12	118.60
34	2	288	A	N1-C6-N6	12.53	126.12	118.60
34	2	1145	A	N1-C6-N6	12.52	126.11	118.60
34	2	1659	A	N1-C6-N6	12.51	126.11	118.60
34	2	518	A	N1-C6-N6	12.51	126.11	118.60
34	2	1472	A	N1-C6-N6	12.51	126.11	118.60
34	2	1038	A	N1-C6-N6	12.51	126.10	118.60
34	2	1224	A	N1-C6-N6	12.50	126.10	118.60
34	2	584	A	N1-C6-N6	12.49	126.09	118.60
34	2	458	A	N1-C6-N6	12.48	126.09	118.60
34	2	953	A	N1-C6-N6	12.47	126.08	118.60
34	2	483	A	N1-C6-N6	12.47	126.08	118.60
34	2	976	A	N1-C6-N6	12.46	126.08	118.60
34	2	232	A	N1-C6-N6	12.45	126.07	118.60
34	2	1026	A	N1-C6-N6	12.45	126.07	118.60
34	2	50	A	N1-C6-N6	12.42	126.05	118.60
34	2	85	A	N1-C6-N6	12.40	126.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1564	A	N1-C6-N6	12.40	126.04	118.60
34	2	979	A	N1-C6-N6	12.38	126.03	118.60
34	2	858	A	N1-C6-N6	12.38	126.03	118.60
34	2	11	A	N1-C6-N6	12.37	126.02	118.60
34	2	502	A	N1-C6-N6	12.37	126.02	118.60
34	2	854	A	N1-C6-N6	12.37	126.02	118.60
34	2	1476	A	N1-C6-N6	12.37	126.02	118.60
34	2	1005	A	N1-C6-N6	12.36	126.02	118.60
34	2	994	A	N1-C6-N6	12.36	126.02	118.60
34	2	1236	A	N1-C6-N6	12.36	126.02	118.60
34	2	107	A	N1-C6-N6	12.35	126.01	118.60
34	2	1295	A	N1-C6-N6	12.35	126.01	118.60
34	2	1401	A	N1-C6-N6	12.35	126.01	118.60
34	2	958	A	N1-C6-N6	12.35	126.01	118.60
34	2	1118	A	N1-C6-N6	12.34	126.00	118.60
34	2	809	A	N1-C6-N6	12.33	126.00	118.60
34	2	512	A	N1-C6-N6	12.31	125.99	118.60
34	2	523	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	445	A	N1-C6-N6	12.30	125.98	118.60
34	2	1280	A	N1-C6-N6	12.29	125.98	118.60
34	2	354	A	N1-C6-N6	12.29	125.97	118.60
34	2	1482	A	N1-C6-N6	12.27	125.96	118.60
34	2	455	A	N1-C6-N6	12.27	125.96	118.60
34	2	1775	A	N1-C6-N6	12.26	125.96	118.60
34	2	1204	A	N1-C6-N6	12.25	125.95	118.60
34	2	1670	A	N1-C6-N6	12.25	125.95	118.60
34	2	574	A	N1-C6-N6	12.24	125.95	118.60
34	2	1008	A	N1-C6-N6	12.24	125.94	118.60
34	2	868	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	1328	A	N1-C6-N6	12.23	125.94	118.60
34	2	1382	A	N1-C6-N6	12.23	125.94	118.60
34	2	1782	A	N1-C6-N6	12.23	125.94	118.60
34	2	27	A	N1-C6-N6	12.22	125.93	118.60
34	2	450	A	N1-C6-N6	12.22	125.93	118.60
34	2	1019	A	N1-C6-N6	12.22	125.93	118.60
34	2	1444	A	N1-C6-N6	12.22	125.93	118.60
34	2	1844	A	N1-C6-N6	12.22	125.93	118.60
1	1	20	A	N1-C6-N6	12.21	125.93	118.60
34	2	25	A	N1-C6-N6	12.21	125.93	118.60
34	2	141	A	N1-C6-N6	12.21	125.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1083	A	N1-C6-N6	12.21	125.92	118.60
34	2	1366	A	N1-C6-N6	12.20	125.92	118.60
34	2	1625	A	N1-C6-N6	12.19	125.91	118.60
34	2	559	A	N1-C6-N6	12.18	125.91	118.60
34	2	463	A	N1-C6-N6	12.18	125.91	118.60
34	2	805	A	N1-C6-N6	12.18	125.91	118.60
34	2	1073	A	N1-C6-N6	12.17	125.90	118.60
34	2	660	A	N1-C6-N6	12.16	125.90	118.60
34	2	573	A	N1-C6-N6	12.16	125.89	118.60
34	2	1205	A	N1-C6-N6	12.15	125.89	118.60
34	2	1860	A	N1-C6-N6	12.15	125.89	118.60
34	2	1502	A	N1-C6-N6	12.15	125.89	118.60
34	2	1031	A	N1-C6-N6	12.14	125.89	118.60
34	2	166	A	N1-C6-N6	12.14	125.89	118.60
34	2	812	A	N1-C6-N6	12.14	125.88	118.60
34	2	983	A	N1-C6-N6	12.13	125.88	118.60
1	1	59	A	N1-C6-N6	12.13	125.88	118.60
34	2	624	A	N1-C6-N6	12.13	125.88	118.60
34	2	1297	A	N1-C6-N6	12.12	125.87	118.60
34	2	40	A	N1-C6-N6	12.12	125.87	118.60
34	2	857	A	N1-C6-N6	12.11	125.87	118.60
34	2	993	A	N1-C6-N6	12.11	125.86	118.60
34	2	1451	A	N1-C6-N6	12.11	125.86	118.60
34	2	361	A	N1-C6-N6	12.10	125.86	118.60
34	2	1080	A	N1-C6-N6	12.10	125.86	118.60
1	1	35	A	N1-C6-N6	12.09	125.86	118.60
34	2	1004	A	N1-C6-N6	12.08	125.84	118.60
34	2	1496	G	N1-C6-O6	12.07	127.14	119.90
34	2	1690	A	N1-C6-N6	12.06	125.84	118.60
34	2	223	A	N1-C6-N6	12.06	125.84	118.60
34	2	1674	A	N1-C6-N6	12.06	125.83	118.60
34	2	566	A	N1-C6-N6	12.05	125.83	118.60
34	2	1340	A	N1-C6-N6	12.05	125.83	118.60
34	2	1146	A	N1-C6-N6	12.05	125.83	118.60
34	2	544	A	N1-C6-N6	12.04	125.83	118.60
34	2	1379	A	N1-C6-N6	12.04	125.83	118.60
34	2	511	A	N1-C6-N6	12.04	125.82	118.60
34	2	850	A	N1-C6-N6	12.04	125.82	118.60
1	1	44	A	N1-C6-N6	12.03	125.82	118.60
34	2	228	A	N1-C6-N6	12.02	125.81	118.60
34	2	633	A	N1-C6-N6	12.01	125.81	118.60
34	2	1673	A	N1-C6-N6	12.01	125.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	516	A	N1-C6-N6	12.01	125.81	118.60
34	2	283	A	N1-C6-N6	12.01	125.81	118.60
34	2	1839	A	N1-C6-N6	12.01	125.81	118.60
34	2	429	A	N1-C6-N6	12.00	125.80	118.60
34	2	1574	A	N1-C6-N6	12.00	125.80	118.60
34	2	860	A	N1-C6-N6	11.98	125.79	118.60
34	2	808	A	N1-C6-N6	11.98	125.79	118.60
34	2	476	A	N1-C6-N6	11.98	125.79	118.60
34	2	861	A	N1-C6-N6	11.98	125.79	118.60
34	2	147	A	N1-C6-N6	11.97	125.78	118.60
34	2	525	G	N1-C6-O6	11.97	127.08	119.90
34	2	1219	A	N1-C6-N6	11.97	125.78	118.60
34	2	159	A	N1-C6-N6	11.97	125.78	118.60
34	2	1076	A	N1-C6-N6	11.97	125.78	118.60
34	2	329	A	N1-C6-N6	11.96	125.78	118.60
34	2	826	A	N1-C6-N6	11.97	125.78	118.60
34	2	1398	A	N1-C6-N6	11.97	125.78	118.60
34	2	19	A	N1-C6-N6	11.96	125.78	118.60
34	2	1247	A	N1-C6-N6	11.96	125.78	118.60
1	1	73	A	N1-C6-N6	11.96	125.77	118.60
34	2	644	A	N1-C6-N6	11.95	125.77	118.60
34	2	645	A	N1-C6-N6	11.95	125.77	118.60
34	2	1196	A	N1-C6-N6	11.95	125.77	118.60
34	2	1353	A	N1-C6-N6	11.95	125.77	118.60
34	2	1551	A	N1-C6-N6	11.95	125.77	118.60
34	2	580	A	N1-C6-N6	11.94	125.77	118.60
34	2	1129	A	N1-C6-N6	11.94	125.76	118.60
41	3	36	A	N1-C6-N6	11.94	125.76	118.60
34	2	619	A	N1-C6-N6	11.93	125.76	118.60
34	2	158	A	N1-C6-N6	11.93	125.76	118.60
34	2	1195	A	N1-C6-N6	11.93	125.76	118.60
34	2	609	A	N1-C6-N6	11.92	125.75	118.60
34	2	918	A	N1-C6-N6	11.92	125.75	118.60
34	2	1372	A	N1-C6-N6	11.92	125.75	118.60
34	2	2	A	N1-C6-N6	11.91	125.75	118.60
34	2	912	A	N1-C6-N6	11.91	125.75	118.60
34	2	1051	A	N1-C6-N6	11.91	125.75	118.60
34	2	968	A	N1-C6-N6	11.91	125.75	118.60
34	2	1618	A	N1-C6-N6	11.91	125.74	118.60
34	2	218	A	N1-C6-N6	11.90	125.74	118.60
34	2	61	A	N1-C6-N6	11.90	125.74	118.60
34	2	1434	A	N1-C6-N6	11.90	125.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	326	A	N1-C6-N6	11.90	125.74	118.60
34	2	1614	A	N1-C6-N6	11.90	125.74	118.60
34	2	77	A	N1-C6-N6	11.89	125.74	118.60
34	2	1249	A	N1-C6-N6	11.89	125.73	118.60
34	2	521	A	N1-C6-N6	11.89	125.73	118.60
34	2	899	A	N1-C6-N6	11.88	125.73	118.60
34	2	91	A	N1-C6-N6	11.88	125.73	118.60
34	2	909	A	N1-C6-N6	11.88	125.73	118.60
34	2	416	A	N1-C6-N6	11.88	125.73	118.60
34	2	871	A	N1-C6-N6	11.88	125.72	118.60
34	2	658	A	N1-C6-N6	11.87	125.72	118.60
34	2	475	A	N1-C6-N6	11.87	125.72	118.60
38	k	455	ILE	C-N-CA	-11.87	92.02	121.70
34	2	1812	A	N1-C6-N6	11.87	125.72	118.60
34	2	662	A	N1-C6-N6	11.86	125.72	118.60
34	2	1845	A	N1-C6-N6	11.85	125.71	118.60
34	2	1054	A	N1-C6-N6	11.85	125.71	118.60
34	2	654	A	N1-C6-N6	11.84	125.71	118.60
34	2	290	A	N1-C6-N6	11.84	125.70	118.60
34	2	1384	A	N1-C6-N6	11.84	125.70	118.60
34	2	887	G	N1-C6-O6	11.84	127.00	119.90
34	2	379	A	N1-C6-N6	11.83	125.70	118.60
34	2	1246	A	N1-C6-N6	11.83	125.70	118.60
34	2	1139	A	N1-C6-N6	11.83	125.69	118.60
34	2	1517	A	N1-C6-N6	11.82	125.69	118.60
34	2	45	A	N1-C6-N6	11.82	125.69	118.60
34	2	38	A	N1-C6-N6	11.82	125.69	118.60
34	2	54	A	N1-C6-N6	11.82	125.69	118.60
34	2	1291	A	N1-C6-N6	11.81	125.69	118.60
34	2	675	A	N1-C6-N6	11.81	125.69	118.60
1	1	2	A	N1-C6-N6	11.81	125.69	118.60
34	2	798	A	N1-C6-N6	11.81	125.68	118.60
34	2	1287	A	N1-C6-N6	11.80	125.68	118.60
34	2	293	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	1078	A	N1-C6-N6	11.80	125.68	118.60
34	2	833	A	N1-C6-N6	11.80	125.68	118.60
34	2	1807	A	N1-C6-N6	11.79	125.68	118.60
34	2	221	A	N1-C6-N6	11.79	125.67	118.60
34	2	900	A	N1-C6-N6	11.79	125.67	118.60
34	2	1787	A	N1-C6-N6	11.78	125.67	118.60
34	2	459	A	N1-C6-N6	11.78	125.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1450	A	N1-C6-N6	11.78	125.67	118.60
34	2	1096	A	N1-C6-N6	11.78	125.67	118.60
34	2	1714	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	595	A	N1-C6-N6	11.77	125.66	118.60
34	2	865	A	N1-C6-N6	11.76	125.66	118.60
34	2	618	A	N1-C6-N6	11.75	125.65	118.60
34	2	111	A	N1-C6-N6	11.75	125.65	118.60
34	2	175	A	N1-C6-N6	11.74	125.65	118.60
34	2	337	G	N1-C6-O6	11.74	126.94	119.90
34	2	1045	A	N1-C6-N6	11.74	125.64	118.60
34	2	866	A	N1-C6-N6	11.74	125.64	118.60
34	2	454	A	N1-C6-N6	11.72	125.64	118.60
34	2	1494	A	N1-C6-N6	11.72	125.64	118.60
34	2	1540	A	N1-C6-N6	11.72	125.63	118.60
34	2	1795	A	N1-C6-N6	11.72	125.63	118.60
34	2	226	A	N1-C6-N6	11.72	125.63	118.60
34	2	1184	A	N1-C6-N6	11.71	125.63	118.60
34	2	1483	A	N1-C6-N6	11.71	125.63	118.60
34	2	333	A	N1-C6-N6	11.70	125.62	118.60
34	2	806	A	N1-C6-N6	11.70	125.62	118.60
34	2	1826	A	N1-C6-N6	11.70	125.62	118.60
34	2	551	A	N1-C6-N6	11.69	125.61	118.60
34	2	513	A	N1-C6-N6	11.69	125.61	118.60
34	2	814	A	N1-C6-N6	11.68	125.61	118.60
34	2	1435	A	N1-C6-N6	11.68	125.61	118.60
34	2	922	A	N1-C6-N6	11.67	125.60	118.60
34	2	1144	A	N1-C6-N6	11.67	125.60	118.60
34	2	1140	A	N1-C6-N6	11.65	125.59	118.60
34	2	1237	A	N1-C6-N6	11.65	125.59	118.60
34	2	1485	A	N1-C6-N6	11.65	125.59	118.60
34	2	661	A	N1-C6-N6	11.64	125.59	118.60
34	2	1278	A	N1-C6-N6	11.64	125.59	118.60
34	2	659	A	N1-C6-N6	11.64	125.58	118.60
34	2	915	A	N1-C6-N6	11.64	125.58	118.60
34	2	229	A	N1-C6-N6	11.63	125.58	118.60
34	2	292	A	N1-C6-N6	11.63	125.58	118.60
34	2	181	A	N1-C6-N6	11.62	125.57	118.60
34	2	1829	A	N1-C6-N6	11.61	125.57	118.60
34	2	408	A	N1-C6-N6	11.61	125.57	118.60
34	2	466	A	N1-C6-N6	11.61	125.57	118.60
34	2	553	G	N1-C6-O6	11.61	126.86	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	934	A	N1-C6-N6	11.59	125.56	118.60
34	2	1480	A	N1-C6-N6	11.59	125.55	118.60
34	2	84	A	N1-C6-N6	11.58	125.55	118.60
34	2	1186	A	N1-C6-N6	11.57	125.55	118.60
34	2	1410	A	N1-C6-N6	11.57	125.55	118.60
34	2	42	A	N1-C6-N6	11.57	125.54	118.60
34	2	435	A	N1-C6-N6	11.57	125.54	118.60
34	2	1694	A	N1-C6-N6	11.55	125.53	118.60
34	2	1740	A	N1-C6-N6	11.54	125.53	118.60
34	2	823	A	N1-C6-N6	11.54	125.52	118.60
34	2	1056	A	N1-C6-N6	11.52	125.51	118.60
34	2	1115	A	N1-C6-N6	11.51	125.51	118.60
38	k	481	ASP	CA-C-N	11.49	142.49	117.20
34	2	1583	A	N1-C6-N6	11.49	125.49	118.60
34	2	338	A	N1-C6-N6	11.48	125.49	118.60
34	2	1255	A	N1-C6-N6	11.46	125.48	118.60
34	2	1374	A	N1-C6-N6	11.46	125.48	118.60
34	2	1632	A	N1-C6-N6	11.46	125.48	118.60
37	j	29	LYS	O-C-N	-11.45	104.37	122.70
34	2	1479	A	N1-C6-N6	11.43	125.46	118.60
34	2	564	A	N1-C6-N6	11.40	125.44	118.60
34	2	60	A	N1-C6-N6	11.39	125.43	118.60
34	2	102	A	N1-C6-N6	11.38	125.43	118.60
34	2	1717	G	N1-C6-O6	11.38	126.73	119.90
34	2	1442	A	N1-C6-N6	11.38	125.43	118.60
34	2	1397	A	N1-C6-N6	11.37	125.42	118.60
34	2	821	A	N1-C6-N6	11.32	125.39	118.60
34	2	1656	A	N1-C6-N6	11.32	125.39	118.60
34	2	1461	A	N1-C6-N6	11.30	125.38	118.60
34	2	804	A	N1-C6-N6	11.30	125.38	118.60
34	2	960	A	N1-C6-N6	11.30	125.38	118.60
34	2	992	A	N1-C6-N6	11.30	125.38	118.60
1	1	53	G	N1-C6-O6	11.28	126.67	119.90
34	2	1066	A	N1-C6-N6	11.28	125.37	118.60
34	2	204	G	N1-C6-O6	11.27	126.66	119.90
34	2	201	G	N1-C6-O6	11.27	126.66	119.90
41	3	64	A	N1-C6-N6	11.27	125.36	118.60
34	2	88	G	N1-C6-O6	11.24	126.65	119.90
34	2	1651	G	N1-C6-O6	11.24	126.65	119.90
34	2	594	A	N1-C6-N6	11.23	125.34	118.60
34	2	46	A	N1-C6-N6	11.22	125.33	118.60
34	2	438	A	N1-C6-N6	11.21	125.32	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1058	A	N1-C6-N6	11.21	125.33	118.60
34	2	1857	A	N1-C6-N6	11.19	125.31	118.60
34	2	1730	A	N1-C6-N6	11.18	125.31	118.60
34	2	300	G	N1-C6-O6	11.17	126.60	119.90
34	2	1178	A	N1-C6-N6	11.17	125.30	118.60
34	2	1628	A	N1-C6-N6	11.15	125.29	118.60
34	2	83	A	N1-C6-N6	11.15	125.29	118.60
34	2	1605	G	N1-C6-O6	11.15	126.59	119.90
34	2	1261	A	N1-C6-N6	11.13	125.28	118.60
34	2	1371	G	N1-C6-O6	11.11	126.57	119.90
34	2	1137	G	N1-C6-O6	11.10	126.56	119.90
34	2	1658	A	N1-C6-N6	11.08	125.25	118.60
1	1	8	G	P-O3'-C3'	11.07	132.99	119.70
34	2	421	G	N1-C6-O6	11.07	126.54	119.90
34	2	1635	A	N1-C6-N6	11.07	125.24	118.60
34	2	1743	G	N1-C6-O6	11.04	126.52	119.90
1	1	70	G	N1-C6-O6	11.02	126.51	119.90
34	2	146	G	N1-C6-O6	11.00	126.50	119.90
34	2	304	A	N1-C6-N6	10.99	125.19	118.60
34	2	526	A	N1-C6-N6	10.99	125.19	118.60
34	2	542	G	N1-C6-O6	10.97	126.48	119.90
34	2	1024	A	N1-C6-N6	10.95	125.17	118.60
34	2	1809	A	N1-C6-N6	10.95	125.17	118.60
34	2	579	G	N1-C6-O6	10.94	126.47	119.90
38	k	104	GLU	C-N-CA	10.93	149.03	121.70
34	2	1770	G	N1-C6-O6	10.93	126.46	119.90
34	2	663	G	N1-C6-O6	10.92	126.45	119.90
34	2	1820	G	N1-C6-O6	10.92	126.45	119.90
34	2	951	A	N1-C6-N6	10.91	125.15	118.60
34	2	208	G	N1-C6-O6	10.90	126.44	119.90
34	2	437	A	N1-C6-N6	10.89	125.14	118.60
34	2	1424	G	N1-C6-O6	10.89	126.44	119.90
1	1	3	G	N1-C6-O6	10.89	126.43	119.90
37	j	29	LYS	C-N-CA	-10.88	94.49	121.70
34	2	156	G	N1-C6-O6	10.87	126.42	119.90
34	2	1117	G	N1-C6-O6	10.87	126.42	119.90
34	2	206	A	N1-C6-N6	10.86	125.12	118.60
1	1	43	G	N1-C6-O6	10.85	126.41	119.90
34	2	577	A	N1-C6-N6	10.84	125.11	118.60
34	2	506	A	N1-C6-N6	10.84	125.10	118.60
34	2	62	G	N1-C6-O6	10.79	126.38	119.90
34	2	525	G	C5-C6-O6	-10.79	122.12	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	7	G	N1-C6-O6	10.79	126.37	119.90
34	2	1256	A	N1-C6-N6	10.78	125.07	118.60
34	2	869	G	N1-C6-O6	10.77	126.36	119.90
34	2	1732	G	N1-C6-O6	10.75	126.35	119.90
34	2	1799	G	N1-C6-O6	10.75	126.35	119.90
34	2	843	A	N1-C6-N6	10.74	125.05	118.60
38	k	104	GLU	CA-C-N	10.74	140.82	117.20
34	2	1753	G	N1-C6-O6	10.73	126.34	119.90
34	2	1528	A	N1-C6-N6	10.73	125.04	118.60
34	2	1752	G	N1-C6-O6	10.72	126.33	119.90
34	2	401	G	N1-C6-O6	10.71	126.33	119.90
34	2	474	A	N1-C6-N6	10.70	125.02	118.60
34	2	1283	A	N1-C6-N6	10.69	125.01	118.60
34	2	104	A	N1-C6-N6	10.68	125.01	118.60
34	2	1079	A	N1-C6-N6	10.67	125.00	118.60
34	2	1202	G	N1-C6-O6	10.67	126.30	119.90
34	2	80	G	N1-C6-O6	10.66	126.30	119.90
34	2	186	G	N1-C6-O6	10.66	126.29	119.90
34	2	279	G	N1-C6-O6	10.66	126.29	119.90
34	2	1776	G	N1-C6-O6	10.65	126.29	119.90
34	2	39	A	N1-C6-N6	10.64	124.99	118.60
34	2	1688	G	N1-C6-O6	10.64	126.28	119.90
34	2	170	A	N1-C6-N6	10.63	124.98	118.60
34	2	203	G	N1-C6-O6	10.63	126.28	119.90
34	2	1266	G	N1-C6-O6	10.63	126.28	119.90
34	2	1774	G	N1-C6-O6	10.62	126.27	119.90
34	2	995	G	N1-C6-O6	10.61	126.27	119.90
34	2	1784	A	N1-C6-N6	10.61	124.97	118.60
34	2	607	G	N1-C6-O6	10.60	126.26	119.90
34	2	1496	G	C5-C6-O6	-10.59	122.25	128.60
34	2	606	A	N1-C6-N6	10.59	124.95	118.60
34	2	1778	G	N1-C6-O6	10.58	126.25	119.90
34	2	1642	A	N1-C6-N6	10.57	124.94	118.60
34	2	1392	A	N1-C6-N6	10.57	124.94	118.60
34	2	515	A	N1-C6-N6	10.56	124.94	118.60
34	2	1455	G	N1-C6-O6	10.56	126.23	119.90
34	2	167	G	N1-C6-O6	10.55	126.23	119.90
38	k	408	ASN	CA-C-N	10.56	140.42	117.20
34	2	310	G	N1-C6-O6	10.55	126.23	119.90
34	2	320	G	N1-C6-O6	10.55	126.23	119.90
34	2	1515	G	N1-C6-O6	10.55	126.23	119.90
34	2	1061	G	N1-C6-O6	10.53	126.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1828	A	N1-C6-N6	10.53	124.92	118.60
34	2	1748	G	N1-C6-O6	10.53	126.22	119.90
34	2	1185	A	N1-C6-N6	10.52	124.91	118.60
34	2	52	G	N1-C6-O6	10.52	126.21	119.90
34	2	1160	G	N1-C6-O6	10.51	126.21	119.90
34	2	353	A	N1-C6-N6	10.51	124.91	118.60
34	2	1701	G	N1-C6-O6	10.51	126.21	119.90
34	2	1254	A	N1-C6-N6	10.51	124.90	118.60
34	2	1169	A	N1-C6-N6	10.47	124.88	118.60
34	2	1023	A	N1-C6-N6	10.46	124.88	118.60
34	2	384	G	N1-C6-O6	10.45	126.17	119.90
34	2	1170	U	P-O3'-C3'	10.45	132.24	119.70
34	2	29	G	N1-C6-O6	10.44	126.16	119.90
34	2	1849	G	N1-C6-O6	10.43	126.16	119.90
34	2	1565	G	N1-C6-O6	10.41	126.15	119.90
34	2	932	G	N1-C6-O6	10.40	126.14	119.90
34	2	1731	G	N1-C6-O6	10.40	126.14	119.90
34	2	500	G	N1-C6-O6	10.40	126.14	119.90
34	2	669	A	N1-C6-N6	10.40	124.84	118.60
34	2	1162	G	N1-C6-O6	10.40	126.14	119.90
34	2	1171	G	O3'-P-O5'	10.40	123.75	104.00
34	2	596	G	N1-C6-O6	10.39	126.14	119.90
34	2	210	G	N1-C6-O6	10.39	126.13	119.90
34	2	670	G	N1-C6-O6	10.39	126.13	119.90
34	2	1331	G	N1-C6-O6	10.39	126.13	119.90
34	2	945	G	N1-C6-O6	10.38	126.13	119.90
34	2	534	G	N1-C6-O6	10.38	126.13	119.90
34	2	1348	G	N1-C6-O6	10.37	126.12	119.90
34	2	92	A	N1-C6-N6	10.36	124.82	118.60
34	2	323	G	N1-C6-O6	10.35	126.11	119.90
34	2	1545	G	N1-C6-O6	10.34	126.11	119.90
34	2	1223	G	N1-C6-O6	10.34	126.11	119.90
34	2	400	G	N1-C6-O6	10.34	126.10	119.90
34	2	1744	G	N1-C6-O6	10.33	126.10	119.90
34	2	1046	A	N1-C6-N6	10.33	124.80	118.60
34	2	1823	G	N1-C6-O6	10.32	126.09	119.90
34	2	1334	G	N1-C6-O6	10.31	126.09	119.90
34	2	1208	G	N1-C6-O6	10.31	126.09	119.90
34	2	1361	G	N1-C6-O6	10.31	126.08	119.90
34	2	1324	G	N1-C6-O6	10.31	126.08	119.90
34	2	1781	G	N1-C6-O6	10.29	126.08	119.90
34	2	1794	A	N1-C6-N6	10.29	124.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1841	G	N1-C6-O6	10.29	126.07	119.90
34	2	1454	G	N1-C6-O6	10.29	126.07	119.90
34	2	1487	G	N1-C6-O6	10.28	126.07	119.90
34	2	1605	G	C5-C6-O6	-10.28	122.43	128.60
34	2	1754	G	N1-C6-O6	10.28	126.07	119.90
34	2	1347	G	N1-C6-O6	10.27	126.06	119.90
34	2	41	G	N1-C6-O6	10.27	126.06	119.90
34	2	95	G	N1-C6-O6	10.27	126.06	119.90
34	2	1511	G	N1-C6-O6	10.26	126.06	119.90
34	2	1510	G	N1-C6-O6	10.26	126.06	119.90
34	2	461	G	N1-C6-O6	10.26	126.05	119.90
34	2	123	G	N1-C6-O6	10.24	126.04	119.90
34	2	634	G	N1-C6-O6	10.23	126.04	119.90
34	2	1100	G	N1-C6-O6	10.23	126.04	119.90
34	2	1286	G	N1-C6-O6	10.23	126.04	119.90
34	2	1602	A	N1-C6-N6	10.23	124.74	118.60
34	2	916	A	N1-C6-N6	10.23	124.74	118.60
34	2	1810	G	N1-C6-O6	10.22	126.03	119.90
34	2	553	G	C5-C6-O6	-10.22	122.47	128.60
34	2	204	G	C5-C6-O6	-10.22	122.47	128.60
34	2	536	G	N1-C6-O6	10.20	126.02	119.90
34	2	1790	G	N1-C6-O6	10.20	126.02	119.90
34	2	920	G	N1-C6-O6	10.19	126.02	119.90
34	2	931	G	N1-C6-O6	10.18	126.01	119.90
34	2	1477	G	N1-C6-O6	10.18	126.01	119.90
38	k	493	ASP	C-N-CA	-10.18	96.25	121.70
34	2	1037	G	N1-C6-O6	10.17	126.00	119.90
34	2	828	G	N1-C6-O6	10.16	126.00	119.90
34	2	403	G	N1-C6-O6	10.16	126.00	119.90
34	2	1136	G	N1-C6-O6	10.16	126.00	119.90
34	2	1519	G	N1-C6-O6	10.16	125.99	119.90
34	2	1606	G	N1-C6-O6	10.16	125.99	119.90
34	2	300	G	C5-C6-O6	-10.15	122.51	128.60
34	2	822	A	N1-C6-N6	10.15	124.69	118.60
34	2	1629	A	N1-C6-N6	10.15	124.69	118.60
34	2	1666	G	N1-C6-O6	10.15	125.99	119.90
34	2	1837	G	N1-C6-O6	10.15	125.99	119.90
34	2	385	G	N1-C6-O6	10.14	125.99	119.90
34	2	978	G	N1-C6-O6	10.14	125.98	119.90
34	2	1607	G	N1-C6-O6	10.13	125.98	119.90
34	2	1180	G	N1-C6-O6	10.13	125.98	119.90
34	2	524	G	N1-C6-O6	10.13	125.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1164	G	N1-C6-O6	10.12	125.97	119.90
34	2	1786	G	N1-C6-O6	10.12	125.97	119.90
34	2	23	G	N1-C6-O6	10.11	125.97	119.90
34	2	1851	G	N1-C6-O6	10.11	125.97	119.90
34	2	457	G	N1-C6-O6	10.11	125.97	119.90
34	2	190	A	N1-C6-N6	10.11	124.67	118.60
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	815	G	N1-C6-O6	10.08	125.95	119.90
34	2	1840	G	N1-C6-O6	10.08	125.95	119.90
34	2	319	G	N1-C6-O6	10.08	125.95	119.90
34	2	212	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	1722	G	N1-C6-O6	10.07	125.94	119.90
34	2	1558	G	N1-C6-O6	10.06	125.93	119.90
34	2	1785	A	N1-C6-N6	10.05	124.63	118.60
34	2	948	G	N1-C6-O6	10.05	125.93	119.90
34	2	1265	G	N1-C6-O6	10.04	125.92	119.90
34	2	325	G	N1-C6-O6	10.03	125.92	119.90
34	2	1067	G	N1-C6-O6	10.03	125.92	119.90
34	2	1314	G	N1-C6-O6	10.03	125.92	119.90
34	2	1771	G	N1-C6-O6	10.03	125.92	119.90
34	2	555	G	N1-C6-O6	10.03	125.92	119.90
34	2	649	G	N1-C6-O6	10.02	125.91	119.90
34	2	208	G	C5-C6-O6	-10.02	122.59	128.60
34	2	274	G	N1-C6-O6	10.02	125.91	119.90
34	2	870	G	N1-C6-O6	10.01	125.91	119.90
34	2	542	G	C5-C6-O6	-10.00	122.60	128.60
34	2	6	G	N1-C6-O6	10.00	125.90	119.90
34	2	1092	G	N1-C6-O6	9.99	125.90	119.90
1	1	29	G	N1-C6-O6	9.97	125.88	119.90
34	2	1506	G	N1-C6-O6	9.97	125.88	119.90
34	2	1855	G	N1-C6-O6	9.97	125.88	119.90
34	2	1036	G	N1-C6-O6	9.97	125.88	119.90
34	2	66	G	N1-C6-O6	9.97	125.88	119.90
34	2	1664	G	N1-C6-O6	9.97	125.88	119.90
34	2	1718	G	N1-C6-O6	9.96	125.88	119.90
34	2	600	G	N1-C6-O6	9.96	125.88	119.90
34	2	1566	G	N1-C6-O6	9.96	125.88	119.90
34	2	827	G	N1-C6-O6	9.96	125.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	468	G	N1-C6-O6	9.96	125.87	119.90
34	2	1001	G	N1-C6-O6	9.95	125.87	119.90
34	2	393	G	N1-C6-O6	9.95	125.87	119.90
34	2	1452	G	N1-C6-O6	9.95	125.87	119.90
34	2	1509	G	N1-C6-O6	9.94	125.86	119.90
34	2	1220	G	N1-C6-O6	9.92	125.85	119.90
34	2	1093	G	N1-C6-O6	9.91	125.85	119.90
34	2	1752	G	C5-C6-O6	-9.90	122.66	128.60
34	2	289	G	N1-C6-O6	9.90	125.84	119.90
34	2	1050	G	N1-C6-O6	9.90	125.84	119.90
1	1	53	G	C5-C6-O6	-9.89	122.66	128.60
34	2	1229	G	N1-C6-O6	9.88	125.83	119.90
34	2	625	G	N1-C6-O6	9.88	125.83	119.90
34	2	972	G	N1-C6-O6	9.87	125.82	119.90
34	2	601	G	N1-C6-O6	9.87	125.82	119.90
34	2	1207	G	N1-C6-O6	9.87	125.82	119.90
34	2	1571	G	N1-C6-O6	9.87	125.82	119.90
34	2	201	G	C5-C6-O6	-9.86	122.69	128.60
34	2	903	G	N1-C6-O6	9.85	125.81	119.90
34	2	1341	G	N1-C6-O6	9.85	125.81	119.90
34	2	1584	A	N1-C6-N6	9.85	124.51	118.60
34	2	803	G	N1-C6-O6	9.84	125.81	119.90
34	2	122	G	N1-C6-O6	9.84	125.81	119.90
34	2	146	G	C5-C6-O6	-9.84	122.69	128.60
34	2	1443	G	N1-C6-O6	9.83	125.80	119.90
34	2	1778	G	C5-C6-O6	-9.83	122.70	128.60
1	1	22	G	N1-C6-O6	9.83	125.80	119.90
34	2	1653	G	N1-C6-O6	9.83	125.80	119.90
34	2	345	G	N1-C6-O6	9.82	125.79	119.90
34	2	1122	G	N1-C6-O6	9.82	125.79	119.90
34	2	1316	G	N1-C6-O6	9.81	125.79	119.90
34	2	1649	G	N1-C6-O6	9.81	125.79	119.90
34	2	307	G	N1-C6-O6	9.81	125.79	119.90
34	2	409	G	N1-C6-O6	9.81	125.78	119.90
34	2	1101	G	N1-C6-O6	9.81	125.78	119.90
34	2	274	G	C5-C6-O6	-9.80	122.72	128.60
34	2	1323	G	N1-C6-O6	9.79	125.78	119.90
1	1	3	G	C5-C6-O6	-9.79	122.72	128.60
34	2	919	G	N1-C6-O6	9.79	125.78	119.90
34	2	1025	G	N1-C6-O6	9.78	125.77	119.90
34	2	1416	G	N1-C6-O6	9.78	125.77	119.90
34	2	303	G	N1-C6-O6	9.78	125.77	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	47	G	N1-C6-O6	9.78	125.77	119.90
34	2	1669	G	N1-C6-O6	9.78	125.77	119.90
34	2	1320	G	N1-C6-O6	9.77	125.76	119.90
34	2	943	G	N1-C6-O6	9.76	125.76	119.90
34	2	1568	G	N1-C6-O6	9.76	125.76	119.90
34	2	411	G	N1-C6-O6	9.76	125.76	119.90
34	2	1675	G	N1-C6-O6	9.76	125.76	119.90
34	2	1615	A	N1-C6-N6	9.76	124.45	118.60
34	2	1572	G	N1-C6-O6	9.75	125.75	119.90
34	2	1130	G	N1-C6-O6	9.74	125.74	119.90
34	2	1006	G	N1-C6-O6	9.73	125.74	119.90
34	2	974	G	N1-C6-O6	9.72	125.73	119.90
34	2	1561	G	N1-C6-O6	9.72	125.73	119.90
34	2	434	G	N1-C6-O6	9.72	125.73	119.90
34	2	636	G	N1-C6-O6	9.71	125.73	119.90
34	2	897	G	N1-C6-O6	9.71	125.73	119.90
34	2	1125	G	N1-C6-O6	9.71	125.72	119.90
34	2	1232	G	N1-C6-O6	9.71	125.72	119.90
34	2	898	G	N1-C6-O6	9.71	125.72	119.90
34	2	56	G	N1-C6-O6	9.70	125.72	119.90
34	2	856	G	N1-C6-O6	9.70	125.72	119.90
34	2	981	G	N1-C6-O6	9.70	125.72	119.90
34	2	1137	G	C5-C6-O6	-9.70	122.78	128.60
34	2	156	G	C5-C6-O6	-9.69	122.78	128.60
34	2	1774	G	C5-C6-O6	-9.69	122.78	128.60
34	2	855	G	N1-C6-O6	9.69	125.71	119.90
1	1	52	G	N1-C6-O6	9.69	125.71	119.90
34	2	1033	G	N1-C6-O6	9.69	125.71	119.90
34	2	464	G	N1-C6-O6	9.69	125.71	119.90
1	1	57	G	N1-C6-O6	9.68	125.71	119.90
34	2	1748	G	C5-C6-O6	-9.68	122.79	128.60
1	1	11	G	N1-C6-O6	9.67	125.70	119.90
34	2	271	G	N1-C6-O6	9.67	125.70	119.90
34	2	952	G	N1-C6-O6	9.67	125.70	119.90
34	2	1697	G	N1-C6-O6	9.66	125.70	119.90
34	2	149	A	N1-C6-N6	9.66	124.39	118.60
34	2	427	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	1072	G	N1-C6-O6	9.65	125.69	119.90
34	2	1776	G	C5-C6-O6	-9.65	122.81	128.60
34	2	113	G	N1-C6-O6	9.64	125.68	119.90
34	2	1047	G	N1-C6-O6	9.63	125.68	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	70	G	C5-C6-O6	-9.63	122.82	128.60
34	2	1599	G	N1-C6-O6	9.62	125.67	119.90
1	1	43	G	C5-C6-O6	-9.62	122.83	128.60
34	2	1462	G	N1-C6-O6	9.62	125.67	119.90
34	2	906	G	N1-C6-O6	9.60	125.66	119.90
34	2	1103	G	N1-C6-O6	9.60	125.66	119.90
34	2	1183	G	N1-C6-O6	9.60	125.66	119.90
34	2	1608	G	N1-C6-O6	9.60	125.66	119.90
34	2	1645	A	N1-C6-N6	9.60	124.36	118.60
34	2	1104	G	N1-C6-O6	9.59	125.66	119.90
34	2	1362	G	N1-C6-O6	9.59	125.66	119.90
34	2	360	G	N1-C6-O6	9.59	125.65	119.90
34	2	499	G	N1-C6-O6	9.59	125.65	119.90
34	2	460	G	N1-C6-O6	9.58	125.65	119.90
34	2	1446	G	N1-C6-O6	9.58	125.65	119.90
34	2	337	G	C5-C6-O6	-9.58	122.85	128.60
34	2	1727	G	N1-C6-O6	9.58	125.65	119.90
34	2	1085	G	N1-C6-O6	9.57	125.64	119.90
34	2	1218	G	N1-C6-O6	9.57	125.64	119.90
34	2	891	G	N1-C6-O6	9.57	125.64	119.90
34	2	1598	G	N1-C6-O6	9.57	125.64	119.90
34	2	1225	G	N1-C6-O6	9.56	125.64	119.90
34	2	1231	G	N1-C6-O6	9.56	125.64	119.90
1	1	30	G	N1-C6-O6	9.56	125.64	119.90
34	2	20	G	N1-C6-O6	9.56	125.64	119.90
34	2	1523	G	N1-C6-O6	9.56	125.64	119.90
34	2	1753	G	C5-C6-O6	-9.55	122.87	128.60
34	2	1721	G	N1-C6-O6	9.55	125.63	119.90
1	1	18	G	O4'-C1'-N9	9.52	115.82	108.20
34	2	395	G	N1-C6-O6	9.52	125.61	119.90
34	2	971	G	N1-C6-O6	9.51	125.61	119.90
34	2	29	G	C5-C6-O6	-9.51	122.90	128.60
34	2	1475	G	N1-C6-O6	9.51	125.61	119.90
34	2	1163	G	N1-C6-O6	9.50	125.60	119.90
34	2	1633	G	N1-C6-O6	9.50	125.60	119.90
34	2	1789	G	N1-C6-O6	9.50	125.60	119.90
34	2	587	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	1535	G	N1-C6-O6	9.49	125.60	119.90
34	2	1394	G	N1-C6-O6	9.49	125.59	119.90
34	2	1471	G	N1-C6-O6	9.49	125.59	119.90
34	2	495	G	N1-C6-O6	9.48	125.59	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1321	G	N1-C6-O6	9.47	125.58	119.90
34	2	1486	G	N1-C6-O6	9.47	125.58	119.90
34	2	456	G	N1-C6-O6	9.46	125.58	119.90
34	2	1309	A	N1-C6-N6	9.46	124.28	118.60
34	2	887	G	C5-C6-O6	-9.46	122.93	128.60
34	2	145	G	N1-C6-O6	9.46	125.57	119.90
1	1	8	G	N1-C6-O6	9.45	125.57	119.90
34	2	1241	G	N1-C6-O6	9.45	125.57	119.90
34	2	1098	G	N1-C6-O6	9.44	125.57	119.90
34	2	930	G	N1-C6-O6	9.44	125.56	119.90
34	2	186	G	C5-C6-O6	-9.43	122.94	128.60
38	k	268	TYR	O-C-N	-9.43	107.61	122.70
38	k	150	SER	CA-C-N	-9.43	96.46	117.20
34	2	320	G	C5-C6-O6	-9.42	122.95	128.60
34	2	1830	G	N1-C6-O6	9.41	125.55	119.90
38	k	272	VAL	CA-C-N	-9.41	96.51	117.20
34	2	421	G	C5-C6-O6	-9.40	122.96	128.60
34	2	1770	G	C5-C6-O6	-9.40	122.96	128.60
34	2	508	G	N1-C6-O6	9.40	125.54	119.90
34	2	590	G	N1-C6-O6	9.40	125.54	119.90
34	2	1565	G	C5-C6-O6	-9.40	122.96	128.60
34	2	1521	G	N1-C6-O6	9.40	125.54	119.90
34	2	1570	G	N1-C6-O6	9.40	125.54	119.90
34	2	430	G	N1-C6-O6	9.39	125.53	119.90
34	2	938	G	N1-C6-O6	9.39	125.53	119.90
34	2	1290	G	N1-C6-O6	9.39	125.53	119.90
34	2	367	G	N1-C6-O6	9.38	125.53	119.90
34	2	1811	G	N1-C6-O6	9.37	125.52	119.90
34	2	1418	G	N1-C6-O6	9.36	125.52	119.90
34	2	494	G	N1-C6-O6	9.36	125.52	119.90
34	2	1852	G	N1-C6-O6	9.36	125.52	119.90
34	2	375	G	N1-C6-O6	9.36	125.51	119.90
34	2	1427	G	N1-C6-O6	9.35	125.51	119.90
34	2	1206	G	N1-C6-O6	9.35	125.51	119.90
1	1	16	G	N1-C6-O6	9.34	125.50	119.90
34	2	1277	G	N1-C6-O6	9.34	125.50	119.90
34	2	351	U	OP1-P-O3'	-9.33	84.66	105.20
1	1	13	G	N1-C6-O6	9.32	125.50	119.90
34	2	995	G	C5-C6-O6	-9.31	123.01	128.60
34	2	1455	G	C5-C6-O6	-9.31	123.01	128.60
34	2	80	G	C5-C6-O6	-9.30	123.02	128.60
34	2	1744	G	C5-C6-O6	-9.30	123.02	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1579	G	N1-C6-O6	9.30	125.48	119.90
34	2	1371	G	C5-C6-O6	-9.29	123.03	128.60
34	2	1531	G	N1-C6-O6	9.29	125.48	119.90
34	2	1536	G	N1-C6-O6	9.29	125.48	119.90
34	2	62	G	C5-C6-O6	-9.29	123.03	128.60
34	2	183	G	N1-C6-O6	9.29	125.47	119.90
34	2	498	A	N1-C6-N6	9.29	124.17	118.60
34	2	1172	G	N1-C6-O6	9.27	125.46	119.90
34	2	279	G	C5-C6-O6	-9.26	123.04	128.60
34	2	813	G	N1-C6-O6	9.26	125.46	119.90
34	2	1308	G	N1-C6-O6	9.26	125.46	119.90
34	2	1416	G	C5-C6-O6	-9.26	123.04	128.60
34	2	1147	G	N1-C6-O6	9.25	125.45	119.90
34	2	422	G	N1-C6-O6	9.25	125.45	119.90
34	2	1841	G	C5-C6-O6	-9.24	123.05	128.60
34	2	534	G	C5-C6-O6	-9.24	123.06	128.60
34	2	108	G	N1-C6-O6	9.23	125.44	119.90
34	2	579	G	C5-C6-O6	-9.23	123.06	128.60
34	2	7	G	C5-C6-O6	-9.22	123.07	128.60
34	2	1044	G	N1-C6-O6	9.21	125.42	119.90
34	2	1010	G	N1-C6-O6	9.21	125.42	119.90
34	2	426	G	N1-C6-O6	9.20	125.42	119.90
34	2	503	G	N1-C6-O6	9.20	125.42	119.90
34	2	1593	G	N1-C6-O6	9.20	125.42	119.90
34	2	1061	G	C5-C6-O6	-9.19	123.09	128.60
34	2	1671	U	P-O3'-C3'	9.19	130.72	119.70
34	2	401	G	C5-C6-O6	-9.18	123.09	128.60
34	2	385	G	C5-C6-O6	-9.18	123.09	128.60
34	2	1126	G	N1-C6-O6	9.18	125.41	119.90
34	2	155	G	N1-C6-O6	9.18	125.41	119.90
34	2	199	G	N1-C6-O6	9.17	125.40	119.90
34	2	237	G	C5-C6-O6	-9.17	123.10	128.60
34	2	496	G	N1-C6-O6	9.17	125.40	119.90
34	2	1294	G	N1-C6-O6	9.17	125.40	119.90
34	2	1251	G	N1-C6-O6	9.16	125.40	119.90
34	2	1781	G	C5-C6-O6	-9.16	123.11	128.60
34	2	578	G	N1-C6-O6	9.15	125.39	119.90
34	2	588	G	N1-C6-O6	9.15	125.39	119.90
34	2	604	G	N1-C6-O6	9.13	125.38	119.90
34	2	167	G	C5-C6-O6	-9.13	123.12	128.60
34	2	1106	G	N1-C6-O6	9.12	125.37	119.90
34	2	500	G	C5-C6-O6	-9.12	123.13	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1160	G	C5-C6-O6	-9.11	123.13	128.60
34	2	212	G	C5-C6-O6	-9.11	123.13	128.60
34	2	592	G	N1-C6-O6	9.11	125.37	119.90
34	2	1631	G	N1-C6-O6	9.11	125.37	119.90
34	2	1030	A	N1-C6-N6	9.11	124.06	118.60
34	2	1171	G	N1-C6-O6	9.10	125.36	119.90
34	2	1447	G	N1-C6-O6	9.10	125.36	119.90
34	2	663	G	C5-C6-O6	-9.10	123.14	128.60
37	j	82	ARG	NE-CZ-NH1	9.10	124.85	120.30
34	2	400	G	C5-C6-O6	-9.09	123.14	128.60
34	2	955	G	N1-C6-O6	9.09	125.36	119.90
34	2	1425	G	N1-C6-O6	9.08	125.35	119.90
34	2	238	G	N1-C6-O6	9.08	125.35	119.90
34	2	1344	G	N1-C6-O6	9.08	125.35	119.90
34	2	655	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	1731	G	C5-C6-O6	-9.07	123.16	128.60
34	2	350	A	O3'-P-O5'	-9.07	86.77	104.00
34	2	1647	G	N1-C6-O6	9.06	125.33	119.90
34	2	555	G	C5-C6-O6	-9.05	123.17	128.60
34	2	824	G	N1-C6-O6	9.05	125.33	119.90
34	2	114	G	N1-C6-O6	9.05	125.33	119.90
34	2	989	G	N1-C6-O6	9.04	125.33	119.90
34	2	1515	G	C5-C6-O6	-9.04	123.17	128.60
34	2	1681	G	N1-C6-O6	9.04	125.33	119.90
34	2	1040	G	N1-C6-O6	9.04	125.32	119.90
34	2	1271	G	N1-C6-O6	9.04	125.32	119.90
34	2	123	G	C5-C6-O6	-9.03	123.18	128.60
34	2	1402	G	N1-C6-O6	9.02	125.31	119.90
34	2	945	G	C5-C6-O6	-9.02	123.19	128.60
34	2	1383	G	N1-C6-O6	9.02	125.31	119.90
34	2	1192	A	N1-C6-N6	9.01	124.01	118.60
34	2	1717	G	C5-C6-O6	-9.00	123.20	128.60
34	2	1754	G	C5-C6-O6	-9.00	123.20	128.60
34	2	441	G	N1-C6-O6	9.00	125.30	119.90
34	2	1634	G	N1-C6-O6	8.99	125.30	119.90
34	2	1454	G	C5-C6-O6	-8.99	123.21	128.60
34	2	1607	G	C5-C6-O6	-8.98	123.21	128.60
34	2	1193	G	N1-C6-O6	8.98	125.29	119.90
34	2	967	G	N1-C6-O6	8.97	125.28	119.90
34	2	1751	G	N1-C6-O6	8.97	125.28	119.90
34	2	828	G	C5-C6-O6	-8.97	123.22	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	932	G	C5-C6-O6	-8.97	123.22	128.60
34	2	1100	G	C5-C6-O6	-8.97	123.22	128.60
34	2	457	G	C5-C6-O6	-8.96	123.22	128.60
34	2	842	G	N1-C6-O6	8.96	125.28	119.90
34	2	1136	G	C5-C6-O6	-8.97	123.22	128.60
34	2	1469	G	N1-C6-O6	8.96	125.28	119.90
34	2	1512	G	N1-C6-O6	8.96	125.28	119.90
34	2	88	G	C5-C6-O6	-8.96	123.22	128.60
34	2	1222	G	N1-C6-O6	8.96	125.28	119.90
34	2	1786	G	C5-C6-O6	-8.95	123.23	128.60
34	2	1519	G	C5-C6-O6	-8.95	123.23	128.60
34	2	1651	G	C5-C6-O6	-8.95	123.23	128.60
35	A	184	LEU	C-N-CA	8.94	144.05	121.70
34	2	153	G	N1-C6-O6	8.94	125.26	119.90
34	2	634	G	C5-C6-O6	-8.94	123.24	128.60
34	2	403	G	C5-C6-O6	-8.94	123.24	128.60
34	2	874	G	N1-C6-O6	8.94	125.26	119.90
34	2	925	G	N1-C6-O6	8.94	125.26	119.90
34	2	1055	G	N1-C6-O6	8.94	125.26	119.90
34	2	1773	G	N1-C6-O6	8.93	125.26	119.90
34	2	827	G	C5-C6-O6	-8.93	123.24	128.60
34	2	1612	G	N1-C6-O6	8.93	125.25	119.90
34	2	1739	G	N1-C6-O6	8.93	125.25	119.90
34	2	1199	G	N1-C6-O6	8.92	125.25	119.90
34	2	1361	G	C5-C6-O6	-8.92	123.25	128.60
34	2	273	G	N1-C6-O6	8.92	125.25	119.90
34	2	1281	G	N1-C6-O6	8.92	125.25	119.90
34	2	928	G	N1-C6-O6	8.91	125.25	119.90
34	2	966	G	N1-C6-O6	8.91	125.25	119.90
34	2	1334	G	C5-C6-O6	-8.90	123.26	128.60
34	2	576	G	N1-C6-O6	8.90	125.24	119.90
34	2	319	G	C5-C6-O6	-8.89	123.27	128.60
34	2	1424	G	C5-C6-O6	-8.89	123.27	128.60
34	2	1208	G	C5-C6-O6	-8.88	123.27	128.60
34	2	982	G	N1-C6-O6	8.88	125.22	119.90
34	2	126	G	N1-C6-O6	8.87	125.22	119.90
34	2	322	G	N1-C6-O6	8.87	125.22	119.90
34	2	607	G	C5-C6-O6	-8.87	123.28	128.60
34	2	817	G	N1-C6-O6	8.86	125.22	119.90
34	2	16	G	N1-C6-O6	8.86	125.22	119.90
34	2	222	G	N1-C6-O6	8.86	125.22	119.90
34	2	646	G	N1-C6-O6	8.85	125.21	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1729	G	N1-C6-O6	8.85	125.21	119.90
34	2	310	G	C5-C6-O6	-8.85	123.29	128.60
34	2	472	G	N1-C6-O6	8.84	125.20	119.90
34	2	1286	G	C5-C6-O6	-8.84	123.30	128.60
34	2	1566	G	C5-C6-O6	-8.84	123.30	128.60
34	2	1155	G	N1-C6-O6	8.84	125.20	119.90
34	2	1627	G	N1-C6-O6	8.84	125.20	119.90
34	2	1649	G	C5-C6-O6	-8.84	123.30	128.60
34	2	424	G	N1-C6-O6	8.83	125.20	119.90
34	2	954	G	N1-C6-O6	8.83	125.20	119.90
34	2	1324	G	C5-C6-O6	-8.83	123.30	128.60
1	1	16	G	OP2-P-O3'	-8.83	85.77	105.20
34	2	1487	G	C5-C6-O6	-8.83	123.30	128.60
34	2	1037	G	C5-C6-O6	-8.82	123.31	128.60
34	2	41	G	C5-C6-O6	-8.82	123.31	128.60
38	k	241	ASP	CA-C-N	-8.82	97.80	117.20
34	2	270	G	N1-C6-O6	8.81	125.19	119.90
34	2	1606	G	C5-C6-O6	-8.81	123.31	128.60
36	B	288	LYS	C-N-CA	8.81	140.80	122.30
34	2	75	G	N1-C6-O6	8.81	125.18	119.90
34	2	177	G	N1-C6-O6	8.81	125.18	119.90
34	2	1345	G	N1-C6-O6	8.81	125.18	119.90
34	2	1390	G	N1-C6-O6	8.80	125.18	119.90
34	2	1831	G	N1-C6-O6	8.79	125.18	119.90
34	2	903	G	C5-C6-O6	-8.79	123.33	128.60
34	2	1194	G	N1-C6-O6	8.79	125.17	119.90
34	2	341	G	N1-C6-O6	8.79	125.17	119.90
34	2	987	G	N1-C6-O6	8.79	125.17	119.90
34	2	1317	G	N1-C6-O6	8.79	125.17	119.90
34	2	837	G	N1-C6-O6	8.78	125.17	119.90
34	2	1510	G	C5-C6-O6	-8.78	123.33	128.60
34	2	1701	G	C5-C6-O6	-8.78	123.33	128.60
34	2	467	G	N1-C6-O6	8.78	125.17	119.90
34	2	1082	G	N1-C6-O6	8.78	125.17	119.90
34	2	1229	G	C5-C6-O6	-8.78	123.33	128.60
34	2	1820	G	C5-C6-O6	-8.78	123.33	128.60
34	2	1562	G	N1-C6-O6	8.77	125.16	119.90
34	2	1493	G	N1-C6-O6	8.77	125.16	119.90
34	2	323	G	C5-C6-O6	-8.77	123.34	128.60
34	2	1125	G	C5-C6-O6	-8.77	123.34	128.60
34	2	613	G	C5-C6-O6	-8.76	123.34	128.60
34	2	1326	G	N1-C6-O6	8.76	125.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	187	C	O4'-C1'-N1	8.76	115.21	108.20
34	2	864	G	N1-C6-O6	8.76	125.16	119.90
34	2	184	G	N1-C6-O6	8.76	125.15	119.90
1	1	24	G	N1-C6-O6	8.75	125.15	119.90
34	2	205	G	N1-C6-O6	8.75	125.15	119.90
34	2	1154	G	N1-C6-O6	8.75	125.15	119.90
34	2	1547	G	N1-C6-O6	8.75	125.15	119.90
34	2	1127	G	N1-C6-O6	8.75	125.15	119.90
34	2	1732	G	C5-C6-O6	-8.75	123.35	128.60
34	2	1318	G	N1-C6-O6	8.74	125.15	119.90
34	2	1381	G	N1-C6-O6	8.74	125.14	119.90
34	2	1771	G	C5-C6-O6	-8.74	123.36	128.60
34	2	1029	G	N1-C6-O6	8.73	125.14	119.90
34	2	1743	G	C5-C6-O6	-8.73	123.36	128.60
1	1	46	G	N1-C6-O6	8.72	125.13	119.90
34	2	1095	G	N1-C6-O6	8.72	125.13	119.90
34	2	1276	G	N1-C6-O6	8.72	125.13	119.90
34	2	1175	G	N1-C6-O6	8.71	125.13	119.90
34	2	591	G	C5-C6-O6	-8.71	123.37	128.60
34	2	863	G	N1-C6-O6	8.71	125.12	119.90
34	2	298	G	N1-C6-O6	8.71	125.12	119.90
34	2	1601	G	N1-C6-O6	8.71	125.12	119.90
34	2	47	G	C5-C6-O6	-8.70	123.38	128.60
34	2	877	G	N1-C6-O6	8.71	125.12	119.90
34	2	1217	G	N1-C6-O6	8.70	125.12	119.90
34	2	1409	G	N1-C6-O6	8.71	125.12	119.90
34	2	815	G	C5-C6-O6	-8.70	123.38	128.60
34	2	397	G	N1-C6-O6	8.70	125.12	119.90
34	2	536	G	C5-C6-O6	-8.69	123.38	128.60
34	2	1808	G	N1-C6-O6	8.70	125.12	119.90
34	2	497	G	N1-C6-O6	8.69	125.11	119.90
34	2	1153	G	N1-C6-O6	8.69	125.11	119.90
34	2	74	G	N1-C6-O6	8.69	125.11	119.90
34	2	991	G	N1-C6-O6	8.69	125.11	119.90
34	2	1117	G	C5-C6-O6	-8.68	123.39	128.60
34	2	373	G	N1-C6-O6	8.68	125.11	119.90
34	2	921	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	1793	G	N1-C6-O6	8.67	125.10	119.90
34	2	1001	G	C5-C6-O6	-8.67	123.40	128.60
34	2	1377	G	N1-C6-O6	8.67	125.10	119.90
34	2	6	G	C5-C6-O6	-8.67	123.40	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	26	G	N1-C6-O6	8.66	125.10	119.90
34	2	394	G	C5-C6-O6	-8.66	123.40	128.60
34	2	667	G	N1-C6-O6	8.66	125.09	119.90
34	2	543	U	O4'-C1'-N1	8.66	115.12	108.20
34	2	1783	G	N1-C6-O6	8.66	125.09	119.90
34	2	1619	U	O4'-C1'-N1	8.65	115.12	108.20
34	2	1036	G	C5-C6-O6	-8.65	123.41	128.60
34	2	1704	G	N1-C6-O6	8.65	125.09	119.90
34	2	625	G	C5-C6-O6	-8.65	123.41	128.60
34	2	1477	G	C5-C6-O6	-8.65	123.41	128.60
34	2	870	G	C5-C6-O6	-8.64	123.42	128.60
34	2	470	G	N1-C6-O6	8.64	125.08	119.90
34	2	924	G	N1-C6-O6	8.63	125.08	119.90
34	2	71	G	N1-C6-O6	8.62	125.08	119.90
34	2	370	G	N1-C6-O6	8.62	125.08	119.90
34	2	1851	G	C5-C6-O6	-8.62	123.42	128.60
34	2	1389	G	N1-C6-O6	8.62	125.07	119.90
34	2	1509	G	C5-C6-O6	-8.62	123.43	128.60
34	2	1503	G	N1-C6-O6	8.62	125.07	119.90
34	2	596	G	C5-C6-O6	-8.61	123.43	128.60
34	2	616	G	N1-C6-O6	8.62	125.07	119.90
34	2	1506	G	C5-C6-O6	-8.61	123.43	128.60
34	2	410	G	N1-C6-O6	8.61	125.07	119.90
34	2	1511	G	C5-C6-O6	-8.61	123.44	128.60
34	2	1202	G	C5-C6-O6	-8.60	123.44	128.60
34	2	841	G	N1-C6-O6	8.60	125.06	119.90
34	2	906	G	C5-C6-O6	-8.60	123.44	128.60
34	2	442	G	N1-C6-O6	8.59	125.06	119.90
34	2	832	G	N1-C6-O6	8.59	125.06	119.90
34	2	929	G	N1-C6-O6	8.59	125.06	119.90
34	2	1164	G	C5-C6-O6	-8.59	123.44	128.60
34	2	1420	G	N1-C6-O6	8.59	125.05	119.90
34	2	1722	G	C5-C6-O6	-8.59	123.45	128.60
34	2	415	G	N1-C6-O6	8.59	125.05	119.90
34	2	848	G	N1-C6-O6	8.59	125.05	119.90
34	2	931	G	C5-C6-O6	-8.59	123.45	128.60
34	2	150	A	N1-C6-N6	8.58	123.75	118.60
34	2	1572	G	C5-C6-O6	-8.58	123.45	128.60
34	2	1191	A	N1-C6-N6	8.58	123.75	118.60
34	2	1253	G	N1-C6-O6	8.58	125.05	119.90
1	1	29	G	C5-C6-O6	-8.57	123.46	128.60
34	2	94	G	N1-C6-O6	8.57	125.04	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1655	C	C2-N1-C1'	8.57	128.22	118.80
34	2	1039	G	N1-C6-O6	8.57	125.04	119.90
34	2	436	G	N1-C6-O6	8.56	125.04	119.90
34	2	957	G	N1-C6-O6	8.56	125.04	119.90
34	2	1138	G	N1-C6-O6	8.56	125.04	119.90
34	2	1600	G	N1-C6-O6	8.56	125.04	119.90
34	2	673	G	N1-C6-O6	8.55	125.03	119.90
34	2	1738	G	N1-C6-O6	8.55	125.03	119.90
34	2	70	G	N1-C6-O6	8.55	125.03	119.90
34	2	911	G	N1-C6-O6	8.54	125.03	119.90
38	k	513	LYS	C-N-CA	8.54	143.06	121.70
1	1	17	C	P-O3'-C3'	8.54	129.95	119.70
34	2	289	G	C5-C6-O6	-8.54	123.47	128.60
34	2	189	G	N1-C6-O6	8.54	125.02	119.90
34	2	1360	U	O4'-C1'-N1	8.53	115.03	108.20
34	2	280	G	N1-C6-O6	8.53	125.02	119.90
34	2	674	G	N1-C6-O6	8.53	125.02	119.90
34	2	972	G	C5-C6-O6	-8.53	123.48	128.60
34	2	1810	G	C5-C6-O6	-8.53	123.48	128.60
34	2	402	G	N1-C6-O6	8.53	125.02	119.90
34	2	1545	G	C5-C6-O6	-8.52	123.49	128.60
34	2	1765	G	N1-C6-O6	8.52	125.01	119.90
34	2	1282	G	N1-C6-O6	8.52	125.01	119.90
34	2	1266	G	C5-C6-O6	-8.51	123.49	128.60
34	2	375	G	C5-C6-O6	-8.51	123.50	128.60
34	2	10	G	N1-C6-O6	8.50	125.00	119.90
34	2	1165	G	N1-C6-O6	8.50	125.00	119.90
34	2	1314	G	C5-C6-O6	-8.50	123.50	128.60
34	2	1207	G	C5-C6-O6	-8.49	123.50	128.60
34	2	1457	G	N1-C6-O6	8.49	124.99	119.90
34	2	615	G	N1-C6-O6	8.48	124.99	119.90
34	2	1790	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	1504	A	N1-C6-N6	8.47	123.69	118.60
34	2	387	G	N1-C6-O6	8.47	124.98	119.90
34	2	307	G	C5-C6-O6	-8.46	123.52	128.60
34	2	1167	G	N1-C6-O6	8.46	124.97	119.90
34	2	1571	G	C5-C6-O6	-8.46	123.53	128.60
34	2	1823	G	C5-C6-O6	-8.45	123.53	128.60
34	2	943	G	C5-C6-O6	-8.45	123.53	128.60
34	2	601	G	C5-C6-O6	-8.45	123.53	128.60
34	2	1643	G	N1-C6-O6	8.45	124.97	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1298	G	N1-C6-O6	8.44	124.97	119.90
34	2	325	G	C5-C6-O6	-8.44	123.53	128.60
34	2	1047	G	C5-C6-O6	-8.44	123.54	128.60
34	2	1718	G	C5-C6-O6	-8.44	123.54	128.60
34	2	1837	G	C5-C6-O6	-8.44	123.54	128.60
34	2	52	G	C5-C6-O6	-8.44	123.54	128.60
34	2	1232	G	C5-C6-O6	-8.44	123.54	128.60
34	2	1541	G	N1-C6-O6	8.43	124.96	119.90
38	k	241	ASP	O-C-N	8.43	136.19	122.70
34	2	282	G	N1-C6-O6	8.43	124.95	119.90
34	2	328	G	N1-C6-O6	8.42	124.95	119.90
34	2	1270	G	N1-C6-O6	8.42	124.95	119.90
34	2	1265	G	C5-C6-O6	-8.42	123.55	128.60
34	2	317	G	N1-C6-O6	8.41	124.95	119.90
34	2	345	G	C5-C6-O6	-8.41	123.56	128.60
34	2	952	G	C5-C6-O6	-8.41	123.56	128.60
34	2	1352	G	N1-C6-O6	8.41	124.94	119.90
34	2	180	G	N1-C6-O6	8.40	124.94	119.90
34	2	1350	G	N1-C6-O6	8.40	124.94	119.90
34	2	537	G	N1-C6-O6	8.39	124.93	119.90
34	2	1025	G	C5-C6-O6	-8.39	123.57	128.60
34	2	917	G	N1-C6-O6	8.38	124.93	119.90
34	2	505	G	N1-C6-O6	8.38	124.93	119.90
34	2	1452	G	C5-C6-O6	-8.38	123.57	128.60
34	2	1357	G	N1-C6-O6	8.37	124.92	119.90
34	2	427	G	C5-C6-O6	-8.37	123.58	128.60
34	2	237	G	N1-C6-O6	8.37	124.92	119.90
34	2	1088	G	N1-C6-O6	8.36	124.92	119.90
34	2	1443	G	C5-C6-O6	-8.37	123.58	128.60
34	2	1231	G	C5-C6-O6	-8.36	123.58	128.60
34	2	1652	G	N1-C6-O6	8.36	124.92	119.90
1	1	10	G	N1-C6-O6	8.35	124.91	119.90
34	2	82	G	N1-C6-O6	8.35	124.91	119.90
34	2	1341	G	C5-C6-O6	-8.35	123.59	128.60
34	2	1446	G	C5-C6-O6	-8.35	123.59	128.60
34	2	1130	G	C5-C6-O6	-8.34	123.59	128.60
34	2	90	G	N1-C6-O6	8.34	124.91	119.90
34	2	1543	G	N1-C6-O6	8.33	124.90	119.90
34	2	549	G	N1-C6-O6	8.33	124.90	119.90
34	2	1830	G	C5-C6-O6	-8.33	123.61	128.60
34	2	1445	G	C5-C6-O6	-8.32	123.61	128.60
34	2	1093	G	C5-C6-O6	-8.32	123.61	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1414	C	C2-N1-C1'	8.32	127.95	118.80
34	2	1688	G	C5-C6-O6	-8.32	123.61	128.60
35	A	184	LEU	O-C-N	8.32	136.01	122.70
34	2	548	G	N1-C6-O6	8.31	124.89	119.90
1	1	19	G	N1-C6-O6	8.31	124.89	119.90
34	2	1166	A	N1-C6-N6	8.31	123.59	118.60
34	2	56	G	C5-C6-O6	-8.31	123.61	128.60
34	2	1362	G	C5-C6-O6	-8.31	123.61	128.60
34	2	1568	G	C5-C6-O6	-8.31	123.62	128.60
34	2	1835	C	O4'-C1'-N1	8.30	114.84	108.20
34	2	851	G	N1-C6-O6	8.29	124.88	119.90
34	2	33	G	N1-C6-O6	8.29	124.87	119.90
34	2	1252	G	N1-C6-O6	8.29	124.87	119.90
34	2	1407	G	N1-C6-O6	8.29	124.87	119.90
34	2	1006	G	C5-C6-O6	-8.27	123.64	128.60
34	2	803	G	C5-C6-O6	-8.27	123.64	128.60
34	2	649	G	C5-C6-O6	-8.27	123.64	128.60
1	1	52	G	C5-C6-O6	-8.26	123.64	128.60
34	2	1119	C	O4'-C1'-N1	8.26	114.81	108.20
34	2	1101	G	C5-C6-O6	-8.26	123.65	128.60
34	2	1135	C	C2-N1-C1'	8.26	127.88	118.80
34	2	1323	G	C5-C6-O6	-8.26	123.65	128.60
34	2	1713	G	N1-C6-O6	8.26	124.85	119.90
34	2	1475	G	C5-C6-O6	-8.26	123.65	128.60
34	2	384	G	C5-C6-O6	-8.25	123.65	128.60
34	2	1535	G	C5-C6-O6	-8.25	123.65	128.60
34	2	670	G	C5-C6-O6	-8.24	123.66	128.60
34	2	468	G	C5-C6-O6	-8.24	123.66	128.60
34	2	898	G	C5-C6-O6	-8.24	123.66	128.60
34	2	981	G	C5-C6-O6	-8.23	123.66	128.60
34	2	1697	G	C5-C6-O6	-8.23	123.66	128.60
34	2	360	G	C5-C6-O6	-8.22	123.67	128.60
34	2	948	G	C5-C6-O6	-8.22	123.67	128.60
34	2	905	G	N1-C6-O6	8.22	124.83	119.90
1	1	7	A	O4'-C1'-N9	8.21	114.77	108.20
34	2	834	G	N1-C6-O6	8.21	124.82	119.90
34	2	1582	G	N1-C6-O6	8.20	124.82	119.90
1	1	30	G	C5-C6-O6	-8.20	123.68	128.60
34	2	1666	G	C5-C6-O6	-8.20	123.68	128.60
34	2	1347	G	C5-C6-O6	-8.19	123.68	128.60
34	2	66	G	C5-C6-O6	-8.18	123.69	128.60
34	2	428	G	N1-C6-O6	8.17	124.80	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	876	G	N1-C6-O6	8.17	124.80	119.90
34	2	381	C	O4'-C1'-N1	8.17	114.73	108.20
34	2	1050	G	C5-C6-O6	-8.16	123.70	128.60
34	2	122	G	C5-C6-O6	-8.15	123.71	128.60
34	2	165	G	N1-C6-O6	8.15	124.79	119.90
34	2	74	G	O4'-C1'-N9	8.14	114.72	108.20
34	2	1103	G	C5-C6-O6	-8.14	123.71	128.60
34	2	1849	G	C5-C6-O6	-8.14	123.72	128.60
34	2	600	G	C5-C6-O6	-8.13	123.72	128.60
34	2	1348	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	974	G	C5-C6-O6	-8.11	123.73	128.60
34	2	303	G	C5-C6-O6	-8.11	123.73	128.60
34	2	1856	G	N1-C6-O6	8.11	124.76	119.90
22	X	78	ILE	N-CA-C	8.10	132.88	111.00
34	2	1664	G	C5-C6-O6	-8.10	123.74	128.60
34	2	1843	G	N1-C6-O6	8.10	124.76	119.90
34	2	937	C	O4'-C1'-N1	8.10	114.68	108.20
1	1	66	C	O4'-C1'-N1	8.09	114.67	108.20
34	2	140	U	O4'-C1'-N1	8.09	114.67	108.20
34	2	461	G	C5-C6-O6	-8.09	123.75	128.60
34	2	849	C	C2-N1-C1'	8.09	127.69	118.80
34	2	879	U	O4'-C1'-N1	8.09	114.67	108.20
34	2	1660	G	N1-C6-O6	8.08	124.75	119.90
1	1	11	G	C5-C6-O6	-8.07	123.76	128.60
34	2	95	G	C5-C6-O6	-8.07	123.76	128.60
34	2	1595	G	N1-C6-O6	8.07	124.74	119.90
34	2	1072	G	C5-C6-O6	-8.05	123.77	128.60
34	2	422	G	C5-C6-O6	-8.05	123.77	128.60
34	2	1267	C	O4'-C1'-N1	8.05	114.64	108.20
34	2	1241	G	C5-C6-O6	-8.04	123.77	128.60
34	2	1427	G	C5-C6-O6	-8.04	123.77	128.60
34	2	1675	G	C5-C6-O6	-8.04	123.78	128.60
34	2	880	C	O4'-C1'-N1	8.04	114.63	108.20
34	2	1218	G	C5-C6-O6	-8.04	123.78	128.60
34	2	729	C	O4'-C1'-N1	8.03	114.62	108.20
38	k	272	VAL	O-C-N	8.03	135.55	122.70
34	2	352	C	O4'-C1'-N1	8.03	114.62	108.20
34	2	1147	G	C5-C6-O6	-8.03	123.78	128.60
34	2	494	G	C5-C6-O6	-8.02	123.79	128.60
34	2	409	G	C5-C6-O6	-8.02	123.79	128.60
34	2	848	G	P-O3'-C3'	8.01	129.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1727	G	C5-C6-O6	-8.01	123.79	128.60
34	2	322	G	O4'-C1'-N9	8.01	114.61	108.20
34	2	1608	G	C5-C6-O6	-8.00	123.80	128.60
1	1	25	U	O4'-C1'-N1	7.99	114.59	108.20
34	2	856	G	C5-C6-O6	-7.99	123.81	128.60
34	2	395	G	C5-C6-O6	-7.99	123.81	128.60
34	2	1099	C	O4'-C1'-N1	7.97	114.58	108.20
34	2	495	G	C5-C6-O6	-7.97	123.82	128.60
34	2	1290	G	C5-C6-O6	-7.97	123.82	128.60
34	2	1206	G	C5-C6-O6	-7.97	123.82	128.60
34	2	1806	U	O4'-C1'-N1	7.97	114.57	108.20
34	2	587	G	C5-C6-O6	-7.96	123.82	128.60
34	2	568	C	O4'-C1'-N1	7.96	114.57	108.20
34	2	989	G	C5-C6-O6	-7.96	123.82	128.60
34	2	37	C	O4'-C1'-N1	7.96	114.57	108.20
34	2	508	G	C5-C6-O6	-7.96	123.82	128.60
34	2	1053	C	O4'-C1'-N1	7.96	114.57	108.20
34	2	1094	C	O4'-C1'-N1	7.96	114.57	108.20
34	2	1789	G	C5-C6-O6	-7.96	123.82	128.60
34	2	891	G	C5-C6-O6	-7.96	123.83	128.60
34	2	499	G	C5-C6-O6	-7.95	123.83	128.60
34	2	1225	G	C5-C6-O6	-7.95	123.83	128.60
34	2	430	G	C5-C6-O6	-7.94	123.83	128.60
34	2	1847	C	O4'-C1'-N1	7.94	114.55	108.20
34	2	1669	G	C5-C6-O6	-7.93	123.84	128.60
34	2	1331	G	C5-C6-O6	-7.93	123.84	128.60
34	2	1779	C	O4'-C1'-N1	7.93	114.55	108.20
34	2	1210	A	N1-C6-N6	7.93	123.36	118.60
34	2	1106	G	C5-C6-O6	-7.93	123.84	128.60
34	2	1486	G	C5-C6-O6	-7.93	123.84	128.60
34	2	1471	G	C5-C6-O6	-7.92	123.85	128.60
34	2	439	A	N1-C6-N6	7.92	123.35	118.60
34	2	1598	G	C5-C6-O6	-7.92	123.85	128.60
34	2	939	U	O4'-C1'-N1	7.92	114.53	108.20
34	2	1162	G	C5-C6-O6	-7.92	123.85	128.60
34	2	1201	C	O4'-C1'-N1	7.92	114.53	108.20
34	2	481	C	O4'-C1'-N1	7.92	114.53	108.20
34	2	460	G	C5-C6-O6	-7.91	123.86	128.60
1	1	8	G	C5-C6-O6	-7.90	123.86	128.60
34	2	1067	G	C5-C6-O6	-7.90	123.86	128.60
34	2	113	G	C5-C6-O6	-7.89	123.87	128.60
34	2	869	G	C5-C6-O6	-7.89	123.87	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1421	G	N1-C6-O6	7.88	124.63	119.90
34	2	376	C	O4'-C1'-N1	7.88	114.50	108.20
1	1	62	C	O4'-C1'-N1	7.88	114.50	108.20
34	2	235	C	O4'-C1'-N1	7.88	114.50	108.20
34	2	1223	G	C5-C6-O6	-7.87	123.88	128.60
34	2	431	C	O4'-C1'-N1	7.87	114.50	108.20
34	2	1855	G	C5-C6-O6	-7.87	123.88	128.60
34	2	489	G	N1-C6-O6	7.87	124.62	119.90
1	1	6	G	O4'-C1'-N9	7.86	114.49	108.20
34	2	923	C	O4'-C1'-N1	7.86	114.49	108.20
34	2	1135	C	O4'-C1'-N1	7.84	114.47	108.20
34	2	464	G	C5-C6-O6	-7.84	123.90	128.60
38	k	272	VAL	C-N-CA	-7.83	102.11	121.70
34	2	590	G	C5-C6-O6	-7.83	123.90	128.60
34	2	1220	G	C5-C6-O6	-7.83	123.90	128.60
34	2	1599	G	C5-C6-O6	-7.83	123.91	128.60
34	2	1840	G	C5-C6-O6	-7.83	123.91	128.60
34	2	1122	G	C5-C6-O6	-7.82	123.91	128.60
34	2	975	C	O4'-C1'-N1	7.81	114.45	108.20
34	2	1561	G	C5-C6-O6	-7.81	123.91	128.60
34	2	653	C	O4'-C1'-N1	7.81	114.45	108.20
34	2	469	C	O4'-C1'-N1	7.81	114.45	108.20
34	2	1120	C	O4'-C1'-N1	7.80	114.44	108.20
34	2	299	G	N1-C6-O6	7.79	124.58	119.90
34	2	380	C	O4'-C1'-N1	7.79	114.44	108.20
34	2	837	G	C5-C6-O6	-7.79	123.92	128.60
34	2	1852	G	C5-C6-O6	-7.79	123.93	128.60
34	2	446	C	O4'-C1'-N1	7.77	114.42	108.20
34	2	118	C	O4'-C1'-N1	7.77	114.42	108.20
34	2	1316	G	C5-C6-O6	-7.77	123.94	128.60
34	2	550	A	O4'-C1'-N9	7.76	114.41	108.20
34	2	1033	G	C5-C6-O6	-7.76	123.94	128.60
34	2	1187	C	O4'-C1'-N1	7.76	114.41	108.20
34	2	890	G	C5-C6-O6	-7.76	123.94	128.60
34	2	830	C	O4'-C1'-N1	7.75	114.40	108.20
34	2	919	G	C5-C6-O6	-7.75	123.95	128.60
34	2	69	C	O4'-C1'-N1	7.74	114.39	108.20
34	2	1411	C	O4'-C1'-N1	7.74	114.39	108.20
34	2	197	U	O4'-C1'-N1	7.74	114.39	108.20
34	2	1102	C	O4'-C1'-N1	7.74	114.39	108.20
34	2	210	G	C5-C6-O6	-7.73	123.96	128.60
34	2	1028	C	O4'-C1'-N1	7.73	114.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	13	G	C5-C6-O6	-7.73	123.96	128.60
34	2	496	G	C5-C6-O6	-7.73	123.96	128.60
34	2	1653	G	C5-C6-O6	-7.73	123.96	128.60
34	2	635	C	O4'-C1'-N1	7.72	114.38	108.20
34	2	1811	G	C5-C6-O6	-7.72	123.97	128.60
34	2	179	C	O4'-C1'-N1	7.72	114.38	108.20
34	2	876	G	O4'-C1'-N9	7.72	114.38	108.20
34	2	1407	G	P-O3'-C3'	7.72	128.96	119.70
34	2	312	C	O4'-C1'-N1	7.72	114.37	108.20
34	2	1405	A	C5-C6-N6	-7.71	117.53	123.70
34	2	1639	C	O4'-C1'-N1	7.71	114.37	108.20
34	2	106	C	O4'-C1'-N1	7.71	114.37	108.20
34	2	560	C	O4'-C1'-N1	7.71	114.36	108.20
34	2	1112	C	O4'-C1'-N1	7.71	114.36	108.20
34	2	1558	G	C5-C6-O6	-7.71	123.98	128.60
34	2	820	C	O4'-C1'-N1	7.70	114.36	108.20
34	2	1633	G	C5-C6-O6	-7.70	123.98	128.60
34	2	1105	C	O4'-C1'-N1	7.70	114.36	108.20
34	2	1556	A	C5-C6-N6	-7.70	117.54	123.70
34	2	1182	U	O4'-C1'-N1	7.69	114.36	108.20
34	2	1121	C	O4'-C1'-N1	7.69	114.35	108.20
1	1	51	U	O4'-C1'-N1	7.69	114.35	108.20
34	2	203	G	C5-C6-O6	-7.69	123.99	128.60
34	2	306	C	O4'-C1'-N1	7.68	114.34	108.20
34	2	920	G	C5-C6-O6	-7.68	123.99	128.60
34	2	1417	A	C5-C6-N6	-7.68	117.56	123.70
34	2	183	G	C5-C6-O6	-7.67	124.00	128.60
34	2	456	G	C5-C6-O6	-7.67	124.00	128.60
34	2	933	C	O4'-C1'-N1	7.67	114.34	108.20
34	2	875	C	O4'-C1'-N1	7.67	114.34	108.20
1	1	57	G	C5-C6-O6	-7.67	124.00	128.60
34	2	367	G	C5-C6-O6	-7.67	124.00	128.60
34	2	1745	C	N3-C4-N4	7.66	123.36	118.00
34	2	352	C	N3-C4-C5	-7.66	118.84	121.90
25	a	125	VAL	C-N-CA	-7.66	106.22	122.30
34	2	1043	C	O4'-C1'-N1	7.66	114.32	108.20
34	2	946	C	O4'-C1'-N1	7.65	114.32	108.20
34	2	901	C	O4'-C1'-N1	7.64	114.32	108.20
34	2	30	C	O4'-C1'-N1	7.64	114.31	108.20
34	2	434	G	C5-C6-O6	-7.64	124.02	128.60
34	2	1681	G	C5-C6-O6	-7.64	124.02	128.60
34	2	1123	C	O4'-C1'-N1	7.64	114.31	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1517	A	O4'-C1'-N9	7.64	114.31	108.20
34	2	35	C	O4'-C1'-N1	7.63	114.31	108.20
34	2	522	C	O4'-C1'-N1	7.63	114.30	108.20
34	2	1799	G	C5-C6-O6	-7.63	124.02	128.60
34	2	20	G	C5-C6-O6	-7.63	124.03	128.60
34	2	926	C	O4'-C1'-N1	7.63	114.30	108.20
1	1	22	G	C5-C6-O6	-7.62	124.03	128.60
34	2	930	G	C5-C6-O6	-7.62	124.03	128.60
34	2	1497	C	O4'-C1'-N1	7.61	114.29	108.20
34	2	332	C	O4'-C1'-N1	7.61	114.29	108.20
34	2	971	G	C5-C6-O6	-7.61	124.04	128.60
34	2	1741	U	O4'-C1'-N1	7.61	114.29	108.20
34	2	48	C	O4'-C1'-N1	7.60	114.28	108.20
34	2	1862	U	O4'-C1'-N1	7.60	114.28	108.20
34	2	1092	G	C5-C6-O6	-7.60	124.04	128.60
34	2	1268	C	O4'-C1'-N1	7.60	114.28	108.20
34	2	1709	U	O4'-C1'-N1	7.59	114.27	108.20
34	2	1053	C	C2-N1-C1'	7.59	127.14	118.80
34	2	1805	C	O4'-C1'-N1	7.59	114.27	108.20
34	2	369	C	O4'-C1'-N1	7.58	114.27	108.20
34	2	1002	C	O4'-C1'-N1	7.58	114.27	108.20
34	2	1090	C	O4'-C1'-N1	7.58	114.26	108.20
34	2	414	C	O4'-C1'-N1	7.58	114.26	108.20
34	2	731	C	O4'-C1'-N1	7.58	114.26	108.20
34	2	1733	C	O4'-C1'-N1	7.58	114.26	108.20
34	2	411	G	C5-C6-O6	-7.57	124.06	128.60
34	2	23	G	C5-C6-O6	-7.57	124.06	128.60
34	2	558	C	O4'-C1'-N1	7.56	114.25	108.20
34	2	348	C	O4'-C1'-N1	7.56	114.25	108.20
34	2	1275	C	O4'-C1'-N1	7.56	114.25	108.20
34	2	1227	C	O4'-C1'-N1	7.56	114.25	108.20
34	2	96	C	O4'-C1'-N1	7.55	114.24	108.20
34	2	628	C	O4'-C1'-N1	7.55	114.24	108.20
34	2	626	C	O4'-C1'-N1	7.55	114.24	108.20
34	2	878	U	O4'-C1'-N1	7.54	114.23	108.20
34	2	873	C	O4'-C1'-N1	7.54	114.23	108.20
34	2	1333	C	O4'-C1'-N1	7.54	114.23	108.20
34	2	79	A	C5-C6-N6	-7.54	117.67	123.70
38	k	241	ASP	C-N-CA	-7.54	102.86	121.70
34	2	997	A	C5-C6-N6	-7.53	117.67	123.70
1	1	61	C	O4'-C1'-N1	7.53	114.22	108.20
34	2	231	C	O4'-C1'-N1	7.53	114.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1180	G	C5-C6-O6	-7.53	124.08	128.60
34	2	896	C	O4'-C1'-N1	7.53	114.22	108.20
34	2	1010	G	C5-C6-O6	-7.52	124.09	128.60
34	2	1468	C	O4'-C1'-N1	7.52	114.22	108.20
34	2	272	C	N3-C4-N4	7.52	123.26	118.00
34	2	1683	C	O4'-C1'-N1	7.52	114.22	108.20
34	2	1536	G	C5-C6-O6	-7.51	124.09	128.60
34	2	839	C	O4'-C1'-N1	7.51	114.21	108.20
34	2	236	C	O4'-C1'-N1	7.51	114.21	108.20
34	2	916	A	C4-C5-C6	7.50	120.75	117.00
34	2	1801	C	O4'-C1'-N1	7.50	114.20	108.20
34	2	728	U	O4'-C1'-N1	7.49	114.19	108.20
34	2	145	G	C5-C6-O6	-7.49	124.11	128.60
34	2	980	C	O4'-C1'-N1	7.49	114.19	108.20
34	2	848	G	O4'-C1'-N9	7.49	114.19	108.20
34	2	273	G	C5-C6-O6	-7.48	124.11	128.60
34	2	426	G	C5-C6-O6	-7.48	124.11	128.60
34	2	1063	C	O4'-C1'-N1	7.48	114.19	108.20
34	2	1735	C	O4'-C1'-N1	7.48	114.19	108.20
34	2	374	U	O4'-C1'-N1	7.48	114.19	108.20
34	2	1604	C	O4'-C1'-N1	7.48	114.18	108.20
34	2	1746	C	N3-C4-N4	7.48	123.24	118.00
34	2	629	C	O4'-C1'-N1	7.48	114.18	108.20
34	2	881	U	O4'-C1'-N1	7.47	114.18	108.20
34	2	978	G	C5-C6-O6	-7.47	124.12	128.60
34	2	1294	G	C5-C6-O6	-7.46	124.12	128.60
34	2	393	G	C5-C6-O6	-7.46	124.12	128.60
34	2	1523	G	C5-C6-O6	-7.46	124.12	128.60
34	2	1678	C	O4'-C1'-N1	7.46	114.17	108.20
34	2	1684	C	O4'-C1'-N1	7.46	114.17	108.20
34	2	220	C	O4'-C1'-N1	7.45	114.16	108.20
34	2	1013	U	O4'-C1'-N1	7.45	114.16	108.20
34	2	1321	G	C5-C6-O6	-7.45	124.13	128.60
34	2	1163	G	C5-C6-O6	-7.45	124.13	128.60
34	2	1466	C	O4'-C1'-N1	7.44	114.15	108.20
34	2	1370	C	O4'-C1'-N1	7.44	114.15	108.20
34	2	1553	C	O4'-C1'-N1	7.43	114.15	108.20
34	2	239	U	O4'-C1'-N1	7.43	114.14	108.20
34	2	969	C	O4'-C1'-N1	7.43	114.14	108.20
34	2	1425	G	C5-C6-O6	-7.42	124.14	128.60
1	1	32	C	O4'-C1'-N1	7.42	114.14	108.20
34	2	165	G	O4'-C1'-N9	7.42	114.14	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	944	C	O4'-C1'-N1	7.42	114.14	108.20
34	2	1299	C	C2-N1-C1'	7.42	126.97	118.80
34	2	1846	C	O4'-C1'-N1	7.42	114.14	108.20
34	2	1705	C	O4'-C1'-N1	7.42	114.14	108.20
34	2	1768	C	N3-C4-N4	7.41	123.19	118.00
34	2	235	C	N3-C4-N4	7.41	123.19	118.00
34	2	1539	C	N3-C4-N4	7.41	123.19	118.00
34	2	570	U	O4'-C1'-N1	7.41	114.13	108.20
1	1	71	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	271	G	C5-C6-O6	-7.40	124.16	128.60
34	2	1394	G	C5-C6-O6	-7.40	124.16	128.60
34	2	1330	G	N1-C6-O6	7.40	124.34	119.90
34	2	206	A	C4-C5-C6	7.40	120.70	117.00
34	2	359	C	O4'-C1'-N1	7.40	114.12	108.20
34	2	278	U	O4'-C1'-N1	7.40	114.12	108.20
34	2	305	U	O4'-C1'-N1	7.40	114.12	108.20
34	2	1087	C	O4'-C1'-N1	7.40	114.12	108.20
34	2	1178	A	C4-C5-C6	7.39	120.70	117.00
34	2	1788	C	O4'-C1'-N1	7.39	114.11	108.20
1	1	14	C	O4'-C1'-N1	7.39	114.11	108.20
34	2	1772	C	O4'-C1'-N1	7.39	114.11	108.20
34	2	154	U	O4'-C1'-N1	7.39	114.11	108.20
34	2	327	C	O4'-C1'-N1	7.39	114.11	108.20
34	2	517	C	O4'-C1'-N1	7.39	114.11	108.20
34	2	1402	G	C5-C6-O6	-7.39	124.17	128.60
34	2	73	C	P-O3'-C3'	7.38	128.56	119.70
34	2	324	C	O4'-C1'-N1	7.38	114.11	108.20
34	2	1749	C	O4'-C1'-N1	7.38	114.11	108.20
34	2	1142	C	N3-C4-N4	7.38	123.17	118.00
34	2	538	C	N3-C4-N4	7.38	123.17	118.00
34	2	1624	C	O4'-C1'-N1	7.38	114.10	108.20
41	3	38	C	O4'-C1'-N1	7.38	114.10	108.20
34	2	36	U	O4'-C1'-N1	7.38	114.10	108.20
34	2	1522	C	O4'-C1'-N1	7.37	114.10	108.20
34	2	86	C	O4'-C1'-N1	7.37	114.10	108.20
1	1	4	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	538	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	1085	G	C5-C6-O6	-7.36	124.18	128.60
34	2	1436	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	954	G	O4'-C1'-N9	7.36	114.09	108.20
38	k	150	SER	O-C-N	7.36	134.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1622	C	O4'-C1'-N1	7.36	114.09	108.20
34	2	443	C	O4'-C1'-N1	7.36	114.08	108.20
34	2	552	U	O4'-C1'-N1	7.36	114.08	108.20
1	1	60	A	C4-C5-C6	7.35	120.67	117.00
34	2	420	C	O4'-C1'-N1	7.35	114.08	108.20
34	2	608	C	O4'-C1'-N1	7.35	114.08	108.20
34	2	1749	C	N3-C4-N4	7.35	123.14	118.00
34	2	1183	G	C5-C6-O6	-7.34	124.19	128.60
34	2	1414	C	C6-N1-C1'	-7.34	111.99	120.80
34	2	199	G	C5-C6-O6	-7.34	124.19	128.60
34	2	927	C	O4'-C1'-N1	7.34	114.07	108.20
34	2	1131	C	O4'-C1'-N1	7.34	114.07	108.20
34	2	1655	C	C6-N1-C1'	-7.34	111.99	120.80
34	2	1734	C	O4'-C1'-N1	7.34	114.07	108.20
34	2	193	C	O4'-C1'-N1	7.34	114.07	108.20
34	2	1226	C	O4'-C1'-N1	7.34	114.07	108.20
34	2	432	C	O4'-C1'-N1	7.34	114.07	108.20
34	2	533	C	O4'-C1'-N1	7.34	114.07	108.20
34	2	1310	U	O4'-C1'-N1	7.34	114.07	108.20
34	2	484	C	O4'-C1'-N1	7.33	114.07	108.20
34	2	270	G	C5-C6-O6	-7.33	124.20	128.60
34	2	1209	C	O4'-C1'-N1	7.33	114.07	108.20
34	2	178	C	O4'-C1'-N1	7.33	114.06	108.20
34	2	507	C	O4'-C1'-N1	7.33	114.06	108.20
34	2	668	U	O4'-C1'-N1	7.33	114.06	108.20
34	2	1105	C	C2-N1-C1'	7.32	126.86	118.80
34	2	1387	C	O4'-C1'-N1	7.32	114.06	108.20
34	2	1456	C	O4'-C1'-N1	7.32	114.06	108.20
34	2	1742	C	O4'-C1'-N1	7.32	114.06	108.20
34	2	1214	C	O4'-C1'-N1	7.32	114.06	108.20
34	2	1624	C	N3-C4-N4	7.32	123.12	118.00
34	2	1156	U	O4'-C1'-N1	7.31	114.05	108.20
1	1	12	C	O4'-C1'-N1	7.31	114.05	108.20
34	2	1343	U	O4'-C1'-N1	7.31	114.05	108.20
34	2	1273	C	O4'-C1'-N1	7.31	114.05	108.20
34	2	1176	C	O4'-C1'-N1	7.30	114.04	108.20
34	2	1007	A	C5-C6-N6	-7.30	117.86	123.70
34	2	1104	G	C5-C6-O6	-7.30	124.22	128.60
34	2	1332	C	O4'-C1'-N1	7.30	114.04	108.20
34	2	1768	C	O4'-C1'-N1	7.30	114.04	108.20
34	2	949	C	O4'-C1'-N1	7.29	114.04	108.20
34	2	1200	A	C5-C6-N6	-7.29	117.86	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1531	G	C5-C6-O6	-7.29	124.22	128.60
34	2	1836	C	O4'-C1'-N1	7.29	114.03	108.20
34	2	162	C	O4'-C1'-N1	7.29	114.03	108.20
34	2	331	C	O4'-C1'-N1	7.29	114.03	108.20
34	2	1415	C	O4'-C1'-N1	7.29	114.03	108.20
34	2	1802	U	O4'-C1'-N1	7.29	114.03	108.20
34	2	1114	C	O4'-C1'-N1	7.29	114.03	108.20
34	2	1311	U	O4'-C1'-N1	7.29	114.03	108.20
34	2	1850	C	O4'-C1'-N1	7.29	114.03	108.20
34	2	928	G	C5-C6-O6	-7.28	124.23	128.60
34	2	1041	U	O4'-C1'-N1	7.28	114.02	108.20
34	2	1537	C	O4'-C1'-N1	7.28	114.02	108.20
34	2	1181	C	O4'-C1'-N1	7.28	114.02	108.20
34	2	413	U	O4'-C1'-N1	7.27	114.02	108.20
34	2	1128	C	O4'-C1'-N1	7.27	114.02	108.20
1	1	23	C	O4'-C1'-N1	7.27	114.01	108.20
34	2	1158	C	O4'-C1'-N1	7.27	114.01	108.20
34	2	1027	A	C5-C6-N6	-7.26	117.89	123.70
34	2	424	G	C5-C6-O6	-7.26	124.24	128.60
34	2	1385	C	O4'-C1'-N1	7.26	114.01	108.20
34	2	1252	G	C5-C6-O6	-7.26	124.25	128.60
34	2	162	C	N3-C4-N4	7.25	123.08	118.00
34	2	632	U	O4'-C1'-N1	7.25	114.00	108.20
34	2	1498	C	O4'-C1'-N1	7.25	114.00	108.20
34	2	1796	C	O4'-C1'-N1	7.25	114.00	108.20
34	2	1032	A	C5-C6-N6	-7.25	117.90	123.70
34	2	1320	G	C5-C6-O6	-7.25	124.25	128.60
34	2	1736	U	O4'-C1'-N1	7.25	114.00	108.20
34	2	567	U	O4'-C1'-N1	7.25	114.00	108.20
34	2	1345	G	C5-C6-O6	-7.25	124.25	128.60
34	2	1563	C	O4'-C1'-N1	7.25	114.00	108.20
34	2	219	U	O4'-C1'-N1	7.25	114.00	108.20
34	2	191	C	N3-C4-N4	7.24	123.07	118.00
34	2	987	G	C5-C6-O6	-7.24	124.26	128.60
34	2	1042	U	O4'-C1'-N1	7.24	113.99	108.20
34	2	1676	U	O4'-C1'-N1	7.24	113.99	108.20
34	2	844	U	O4'-C1'-N1	7.24	113.99	108.20
34	2	1772	C	N3-C4-N4	7.24	123.07	118.00
34	2	1277	G	C5-C6-O6	-7.24	124.26	128.60
34	2	1173	U	O4'-C1'-N1	7.24	113.99	108.20
34	2	53	C	O4'-C1'-N1	7.23	113.98	108.20
34	2	217	U	O4'-C1'-N1	7.23	113.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1185	A	C4-C5-C6	7.23	120.61	117.00
34	2	1426	C	O4'-C1'-N1	7.23	113.98	108.20
34	2	173	A	C5-C6-N6	-7.22	117.92	123.70
1	1	27	C	N3-C4-N4	7.22	123.06	118.00
34	2	641	U	O4'-C1'-N1	7.22	113.98	108.20
34	2	407	C	O4'-C1'-N1	7.21	113.97	108.20
34	2	1143	C	O4'-C1'-N1	7.21	113.97	108.20
34	2	1631	G	C5-C6-O6	-7.21	124.27	128.60
34	2	227	A	C4-C5-C6	7.21	120.61	117.00
34	2	1322	U	O4'-C1'-N1	7.21	113.97	108.20
34	2	1499	C	O4'-C1'-N1	7.21	113.97	108.20
34	2	1848	U	O4'-C1'-N1	7.21	113.97	108.20
1	1	49	G	O4'-C1'-N9	7.21	113.97	108.20
34	2	406	U	O4'-C1'-N1	7.21	113.97	108.20
34	2	847	C	O4'-C1'-N1	7.21	113.97	108.20
38	k	109	VAL	CA-C-N	7.21	130.62	116.20
34	2	1028	C	N3-C4-N4	7.21	123.04	118.00
34	2	24	C	O4'-C1'-N1	7.21	113.96	108.20
34	2	627	U	O4'-C1'-N1	7.20	113.96	108.20
34	2	1124	C	O4'-C1'-N1	7.20	113.96	108.20
34	2	1409	G	C5-C6-O6	-7.20	124.28	128.60
34	2	1543	G	C5-C6-O6	-7.20	124.28	128.60
34	2	192	U	O4'-C1'-N1	7.20	113.96	108.20
34	2	1671	U	O4'-C1'-N1	7.20	113.96	108.20
34	2	213	C	N3-C4-N4	7.20	123.04	118.00
34	2	392	C	O4'-C1'-N1	7.20	113.96	108.20
34	2	1077	U	O4'-C1'-N1	7.20	113.96	108.20
34	2	1562	G	O4'-C1'-N9	7.20	113.96	108.20
34	2	377	C	O4'-C1'-N1	7.19	113.95	108.20
34	2	671	U	O4'-C1'-N1	7.19	113.95	108.20
34	2	108	G	C5-C6-O6	-7.19	124.29	128.60
34	2	532	U	O4'-C1'-N1	7.19	113.95	108.20
34	2	1520	C	O4'-C1'-N1	7.19	113.95	108.20
34	2	588	G	C5-C6-O6	-7.19	124.29	128.60
34	2	947	C	O4'-C1'-N1	7.18	113.95	108.20
34	2	309	A	C5-C6-N6	-7.18	117.95	123.70
34	2	1512	G	C5-C6-O6	-7.18	124.29	128.60
34	2	1555	U	O4'-C1'-N1	7.18	113.94	108.20
34	2	368	U	O4'-C1'-N1	7.18	113.94	108.20
34	2	846	C	O4'-C1'-N1	7.18	113.94	108.20
34	2	1586	C	O4'-C1'-N1	7.18	113.94	108.20
34	2	1054	A	O4'-C1'-N9	7.17	113.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1447	G	C5-C6-O6	-7.17	124.30	128.60
34	2	1023	A	C4-C5-C6	7.17	120.58	117.00
34	2	1593	G	C5-C6-O6	-7.17	124.30	128.60
34	2	17	C	O4'-C1'-N1	7.16	113.93	108.20
34	2	286	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	1319	U	O4'-C1'-N1	7.16	113.93	108.20
34	2	1248	C	O4'-C1'-N1	7.16	113.93	108.20
34	2	1585	C	O4'-C1'-N1	7.16	113.93	108.20
34	2	153	G	C5-C6-O6	-7.16	124.31	128.60
34	2	994	A	C4-C5-C6	7.16	120.58	117.00
34	2	1570	G	C5-C6-O6	-7.16	124.31	128.60
34	2	1804	U	O4'-C1'-N1	7.16	113.93	108.20
34	2	1547	G	C5-C6-O6	-7.16	124.31	128.60
1	1	4	C	N3-C4-N4	7.15	123.01	118.00
34	2	855	G	C5-C6-O6	-7.15	124.31	128.60
34	2	1040	G	C5-C6-O6	-7.15	124.31	128.60
34	2	1172	G	C5-C6-O6	-7.15	124.31	128.60
1	1	46	G	C5-C6-O6	-7.15	124.31	128.60
34	2	15	U	O4'-C1'-N1	7.15	113.92	108.20
34	2	28	U	O4'-C1'-N1	7.15	113.92	108.20
34	2	1353	A	C4-C5-C6	7.15	120.58	117.00
34	2	1567	C	O4'-C1'-N1	7.15	113.92	108.20
1	1	75	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	213	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	355	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	480	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	578	G	C5-C6-O6	-7.15	124.31	128.60
34	2	813	G	C5-C6-O6	-7.15	124.31	128.60
35	A	184	LEU	CA-C-N	-7.15	101.47	117.20
34	2	527	C	O4'-C1'-N1	7.15	113.92	108.20
34	2	364	G	N1-C6-O6	7.14	124.19	119.90
34	2	1045	A	C4-C5-C6	7.14	120.57	117.00
34	2	89	C	O4'-C1'-N1	7.14	113.91	108.20
34	2	569	C	O4'-C1'-N1	7.14	113.91	108.20
34	2	605	C	O4'-C1'-N1	7.14	113.91	108.20
34	2	1467	C	O4'-C1'-N1	7.14	113.91	108.20
34	2	114	G	C5-C6-O6	-7.14	124.32	128.60
1	1	27	C	O4'-C1'-N1	7.14	113.91	108.20
34	2	1592	C	O4'-C1'-N1	7.13	113.91	108.20
34	2	1650	C	O4'-C1'-N1	7.13	113.91	108.20
1	1	16	G	C5-C6-O6	-7.13	124.32	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	730	C	O4'-C1'-N1	7.13	113.91	108.20
34	2	344	U	O4'-C1'-N1	7.13	113.90	108.20
1	1	71	C	N3-C4-N4	7.13	122.99	118.00
34	2	437	A	C4-C5-C6	7.13	120.56	117.00
34	2	519	A	C5-C6-N6	-7.12	118.00	123.70
34	2	1634	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	347	C	O4'-C1'-N1	7.12	113.89	108.20
34	2	86	C	N3-C4-N4	7.12	122.98	118.00
34	2	838	C	O4'-C1'-N1	7.12	113.89	108.20
34	2	1301	C	O4'-C1'-N1	7.11	113.89	108.20
34	2	1769	U	O4'-C1'-N1	7.11	113.89	108.20
34	2	447	C	O4'-C1'-N1	7.11	113.89	108.20
34	2	1359	C	N3-C4-N4	7.11	122.98	118.00
34	2	441	G	C5-C6-O6	-7.11	124.33	128.60
34	2	462	C	O4'-C1'-N1	7.11	113.89	108.20
22	X	78	ILE	N-CA-CB	-7.10	94.47	110.80
34	2	970	C	O4'-C1'-N1	7.10	113.88	108.20
34	2	1312	C	O4'-C1'-N1	7.10	113.88	108.20
34	2	18	C	N3-C4-N4	7.10	122.97	118.00
34	2	655	G	C5-C6-O6	-7.10	124.34	128.60
34	2	938	G	C5-C6-O6	-7.10	124.34	128.60
34	2	1430	C	O4'-C1'-N1	7.10	113.88	108.20
34	2	636	G	C5-C6-O6	-7.10	124.34	128.60
34	2	913	U	O4'-C1'-N1	7.10	113.88	108.20
34	2	1055	G	C5-C6-O6	-7.10	124.34	128.60
34	2	1423	C	N3-C4-N4	7.10	122.97	118.00
34	2	412	U	O4'-C1'-N1	7.10	113.88	108.20
34	2	598	C	O4'-C1'-N1	7.10	113.88	108.20
1	1	72	U	O4'-C1'-N1	7.09	113.88	108.20
34	2	1647	G	C5-C6-O6	-7.09	124.34	128.60
34	2	1720	U	O4'-C1'-N1	7.09	113.87	108.20
34	2	151	C	O4'-C1'-N1	7.09	113.87	108.20
34	2	799	C	O4'-C1'-N1	7.09	113.87	108.20
34	2	961	U	O4'-C1'-N1	7.09	113.87	108.20
34	2	17	C	N3-C4-N4	7.09	122.96	118.00
34	2	1750	C	O4'-C1'-N1	7.08	113.87	108.20
34	2	954	G	C5-C6-O6	-7.08	124.35	128.60
34	2	117	C	O4'-C1'-N1	7.08	113.86	108.20
34	2	336	C	N3-C4-N4	7.08	122.95	118.00
34	2	1560	C	O4'-C1'-N1	7.08	113.86	108.20
34	2	18	C	O4'-C1'-N1	7.08	113.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1000	U	O4'-C1'-N1	7.08	113.86	108.20
34	2	187	C	N3-C4-N4	7.07	122.95	118.00
34	2	503	G	C5-C6-O6	-7.07	124.36	128.60
34	2	1021	U	O4'-C1'-N1	7.07	113.86	108.20
34	2	1009	U	O4'-C1'-N1	7.07	113.86	108.20
34	2	1621	C	O4'-C1'-N1	7.07	113.85	108.20
34	2	1711	C	O4'-C1'-N1	7.07	113.85	108.20
34	2	885	U	O4'-C1'-N1	7.06	113.85	108.20
34	2	581	U	O4'-C1'-N1	7.06	113.85	108.20
34	2	1822	C	O4'-C1'-N1	7.06	113.85	108.20
1	1	54	A	C5-C6-N6	-7.06	118.05	123.70
34	2	1527	C	O4'-C1'-N1	7.06	113.85	108.20
34	2	330	C	O4'-C1'-N1	7.06	113.85	108.20
34	2	194	C	N3-C4-N4	7.06	122.94	118.00
34	2	1623	C	N3-C4-N4	7.05	122.94	118.00
34	2	1673	A	O4'-C1'-N9	7.05	113.84	108.20
34	2	1747	C	N3-C4-N4	7.05	122.94	118.00
41	3	51	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	1257	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	1524	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	1670	A	O4'-C1'-N9	7.05	113.84	108.20
34	2	1682	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	611	C	O4'-C1'-N1	7.05	113.84	108.20
34	2	1200	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	198	U	O4'-C1'-N1	7.04	113.83	108.20
34	2	1699	C	O4'-C1'-N1	7.04	113.83	108.20
34	2	1584	A	C4-C5-C6	7.04	120.52	117.00
34	2	639	U	O4'-C1'-N1	7.04	113.83	108.20
34	2	1170	U	O4'-C1'-N1	7.04	113.83	108.20
34	2	1478	C	O4'-C1'-N1	7.04	113.83	108.20
34	2	842	G	C5-C6-O6	-7.03	124.38	128.60
34	2	1184	A	C4-C5-C6	7.03	120.52	117.00
34	2	1521	G	C5-C6-O6	-7.03	124.38	128.60
41	3	50	C	O4'-C1'-N1	7.03	113.83	108.20
34	2	486	C	O4'-C1'-N1	7.03	113.83	108.20
34	2	529	C	O4'-C1'-N1	7.03	113.83	108.20
34	2	1661	C	O4'-C1'-N1	7.03	113.83	108.20
34	2	817	G	C5-C6-O6	-7.03	124.38	128.60
34	2	1418	G	C5-C6-O6	-7.03	124.38	128.60
34	2	1698	C	O4'-C1'-N1	7.03	113.82	108.20
34	2	1779	C	N3-C4-N4	7.03	122.92	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	200	U	O4'-C1'-N1	7.02	113.82	108.20
34	2	1433	C	O4'-C1'-N1	7.02	113.82	108.20
34	2	1489	C	N3-C4-N4	7.02	122.92	118.00
34	2	81	U	O4'-C1'-N1	7.02	113.81	108.20
34	2	666	C	O4'-C1'-N1	7.02	113.82	108.20
34	2	487	C	O4'-C1'-N1	7.02	113.81	108.20
34	2	990	C	O4'-C1'-N1	7.02	113.81	108.20
34	2	1153	G	C5-C6-O6	-7.01	124.39	128.60
34	2	1258	C	O4'-C1'-N1	7.01	113.81	108.20
34	2	1425	G	O4'-C1'-N9	7.01	113.81	108.20
34	2	1380	C	O4'-C1'-N1	7.00	113.80	108.20
34	2	1186	A	C4-C5-C6	7.00	120.50	117.00
1	1	31	G	O4'-C1'-N9	7.00	113.80	108.20
34	2	185	C	O4'-C1'-N1	7.00	113.80	108.20
34	2	1065	U	O4'-C1'-N1	7.00	113.80	108.20
34	2	1283	A	C4-C5-C6	6.99	120.50	117.00
34	2	1773	G	C5-C6-O6	-6.99	124.40	128.60
34	2	1003	C	O4'-C1'-N1	6.99	113.79	108.20
34	2	1809	A	C4-C5-C6	6.99	120.50	117.00
34	2	93	U	O4'-C1'-N1	6.99	113.79	108.20
34	2	664	C	O4'-C1'-N1	6.99	113.79	108.20
34	2	973	C	O4'-C1'-N1	6.99	113.79	108.20
35	A	269	PHE	CB-CG-CD2	-6.99	115.91	120.80
34	2	1500	U	O4'-C1'-N1	6.99	113.79	108.20
34	2	635	C	N3-C4-N4	6.99	122.89	118.00
34	2	906	G	O4'-C1'-N9	6.99	113.79	108.20
34	2	1326	G	C5-C6-O6	-6.99	124.41	128.60
34	2	209	C	N3-C4-N4	6.98	122.89	118.00
34	2	1376	C	O4'-C1'-N1	6.98	113.79	108.20
34	2	222	G	C5-C6-O6	-6.98	124.41	128.60
34	2	1737	C	O4'-C1'-N1	6.98	113.78	108.20
34	2	38	A	O4'-C1'-N9	6.98	113.78	108.20
34	2	730	C	N3-C4-N4	6.98	122.88	118.00
1	1	40	C	O4'-C1'-N1	6.98	113.78	108.20
38	k	388	PHE	CB-CG-CD2	-6.97	115.92	120.80
34	2	1376	C	N3-C4-N4	6.97	122.88	118.00
34	2	174	C	O4'-C1'-N1	6.97	113.77	108.20
34	2	1766	C	O4'-C1'-N1	6.97	113.77	108.20
34	2	233	A	C5-C6-N6	-6.97	118.13	123.70
34	2	1360	U	C2-N1-C1'	6.97	126.06	117.70
34	2	548	G	C5-C6-O6	-6.96	124.42	128.60
34	2	824	G	C5-C6-O6	-6.96	124.42	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	955	G	C5-C6-O6	-6.96	124.42	128.60
34	2	163	U	O4'-C1'-N1	6.96	113.77	108.20
34	2	612	C	O4'-C1'-N1	6.96	113.76	108.20
34	2	1082	G	C5-C6-O6	-6.96	124.43	128.60
34	2	1281	G	C5-C6-O6	-6.96	124.43	128.60
34	2	173	A	C4-C5-C6	6.95	120.48	117.00
34	2	963	C	O4'-C1'-N1	6.95	113.76	108.20
34	2	236	C	N3-C4-N4	6.95	122.86	118.00
34	2	1035	C	O4'-C1'-N1	6.95	113.76	108.20
1	1	24	G	C5-C6-O6	-6.95	124.43	128.60
34	2	990	C	N3-C4-N4	6.95	122.86	118.00
34	2	1155	G	C5-C6-O6	-6.95	124.43	128.60
34	2	1390	G	C5-C6-O6	-6.95	124.43	128.60
34	2	557	C	O4'-C1'-N1	6.94	113.75	108.20
34	2	1271	G	C5-C6-O6	-6.94	124.44	128.60
34	2	1640	C	O4'-C1'-N1	6.93	113.75	108.20
34	2	321	C	O4'-C1'-N1	6.93	113.75	108.20
34	2	452	C	N3-C4-N4	6.93	122.85	118.00
34	2	837	G	O4'-C1'-N9	6.93	113.75	108.20
34	2	471	C	O4'-C1'-N1	6.93	113.74	108.20
34	2	929	G	C5-C6-O6	-6.93	124.44	128.60
34	2	1766	C	O3'-P-O5'	6.93	117.17	104.00
34	2	1071	C	O4'-C1'-N1	6.93	113.74	108.20
34	2	30	C	N3-C4-N4	6.92	122.85	118.00
34	2	1335	U	O4'-C1'-N1	6.92	113.74	108.20
34	2	1141	A	C4-C5-C6	6.92	120.46	117.00
34	2	1395	C	O4'-C1'-N1	6.92	113.74	108.20
34	2	1383	G	C5-C6-O6	-6.92	124.45	128.60
34	2	1539	C	O4'-C1'-N1	6.92	113.73	108.20
34	2	449	C	O4'-C1'-N1	6.92	113.73	108.20
34	2	941	U	O4'-C1'-N1	6.92	113.73	108.20
34	2	1628	A	C4-C5-C6	6.92	120.46	117.00
34	2	491	C	O4'-C1'-N1	6.91	113.73	108.20
34	2	1233	C	N3-C4-N4	6.91	122.84	118.00
34	2	1429	C	O4'-C1'-N1	6.91	113.73	108.20
34	2	592	G	C5-C6-O6	-6.91	124.45	128.60
34	2	602	U	O4'-C1'-N1	6.91	113.73	108.20
34	2	1493	G	C5-C6-O6	-6.91	124.45	128.60
1	1	60	A	C5-C6-N6	-6.91	118.17	123.70
34	2	336	C	O4'-C1'-N1	6.91	113.73	108.20
34	2	982	G	C5-C6-O6	-6.91	124.45	128.60
34	2	1253	G	C5-C6-O6	-6.91	124.45	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	18	G	P-O3'-C3'	6.91	127.99	119.70
34	2	465	C	O4'-C1'-N1	6.91	113.72	108.20
34	2	544	A	O4'-C1'-N9	6.91	113.72	108.20
34	2	1111	U	C2-N1-C1'	6.91	125.99	117.70
34	2	1308	G	C5-C6-O6	-6.91	124.46	128.60
34	2	1747	C	O4'-C1'-N1	6.90	113.72	108.20
34	2	124	U	O4'-C1'-N1	6.90	113.72	108.20
34	2	1389	G	C5-C6-O6	-6.90	124.46	128.60
34	2	1745	C	O4'-C1'-N1	6.90	113.72	108.20
34	2	301	C	O4'-C1'-N1	6.90	113.72	108.20
34	2	556	U	O4'-C1'-N1	6.90	113.72	108.20
34	2	806	A	O4'-C1'-N9	6.90	113.72	108.20
34	2	1712	C	O4'-C1'-N1	6.90	113.72	108.20
34	2	1002	C	N3-C4-N4	6.90	122.83	118.00
34	2	1462	G	C5-C6-O6	-6.90	124.46	128.60
34	2	1703	C	O4'-C1'-N1	6.89	113.72	108.20
34	2	646	G	C5-C6-O6	-6.89	124.46	128.60
34	2	895	U	O4'-C1'-N1	6.89	113.71	108.20
34	2	1217	G	C5-C6-O6	-6.89	124.47	128.60
34	2	71	G	O4'-C1'-N9	6.89	113.71	108.20
34	2	1039	G	C5-C6-O6	-6.89	124.47	128.60
34	2	1730	A	C4-C5-C6	6.89	120.44	117.00
34	2	378	U	O4'-C1'-N1	6.88	113.71	108.20
34	2	586	U	O4'-C1'-N1	6.88	113.71	108.20
34	2	822	A	C4-C5-C6	6.88	120.44	117.00
1	1	18	G	OP1-P-O3'	-6.88	90.06	105.20
34	2	1297	A	C4-C5-C6	6.88	120.44	117.00
34	2	1091	U	O4'-C1'-N1	6.88	113.70	108.20
34	2	147	A	C4-C5-C6	6.88	120.44	117.00
34	2	1714	A	C4-C5-C6	6.88	120.44	117.00
34	2	68	A	C5-C6-N6	-6.88	118.20	123.70
34	2	343	C	O4'-C1'-N1	6.87	113.70	108.20
34	2	452	C	O4'-C1'-N1	6.87	113.70	108.20
34	2	470	G	C5-C6-O6	-6.87	124.47	128.60
34	2	864	G	C5-C6-O6	-6.87	124.48	128.60
34	2	1825	A	C5-C6-N6	-6.87	118.20	123.70
1	1	41	C	O4'-C1'-N1	6.87	113.69	108.20
34	2	1833	U	O4'-C1'-N1	6.87	113.69	108.20
34	2	1838	U	O4'-C1'-N1	6.87	113.69	108.20
34	2	322	G	C5-C6-O6	-6.87	124.48	128.60
34	2	396	U	O4'-C1'-N1	6.87	113.69	108.20
34	2	1679	C	O4'-C1'-N1	6.87	113.69	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1294	G	O4'-C1'-N9	6.87	113.69	108.20
34	2	197	U	C2-N1-C1'	6.86	125.94	117.70
34	2	650	C	O4'-C1'-N1	6.86	113.69	108.20
34	2	1098	G	C5-C6-O6	-6.86	124.48	128.60
34	2	123	G	O4'-C1'-N9	6.86	113.69	108.20
34	2	585	U	O4'-C1'-N1	6.86	113.68	108.20
34	2	1412	C	O4'-C1'-N1	6.86	113.68	108.20
34	2	935	U	O4'-C1'-N1	6.85	113.68	108.20
34	2	1167	G	C5-C6-O6	-6.85	124.49	128.60
34	2	1751	G	C5-C6-O6	-6.85	124.49	128.60
1	1	12	C	N3-C4-N4	6.85	122.79	118.00
34	2	875	C	N3-C4-N4	6.85	122.80	118.00
34	2	1472	A	C4-C5-C6	6.85	120.42	117.00
34	2	1230	C	O4'-C1'-N1	6.85	113.68	108.20
34	2	1562	G	C5-C6-O6	-6.85	124.49	128.60
34	2	286	C	N3-C4-N4	6.85	122.79	118.00
34	2	349	U	O4'-C1'-N1	6.84	113.67	108.20
34	2	604	G	C5-C6-O6	-6.84	124.50	128.60
25	a	86	GLU	N-CA-CB	6.84	122.91	110.60
34	2	561	U	O4'-C1'-N1	6.84	113.67	108.20
34	2	1463	C	O4'-C1'-N1	6.84	113.67	108.20
34	2	1473	U	O4'-C1'-N1	6.84	113.67	108.20
34	2	1728	U	O4'-C1'-N1	6.83	113.67	108.20
34	2	1215	C	O4'-C1'-N1	6.83	113.66	108.20
34	2	1315	U	O4'-C1'-N1	6.83	113.66	108.20
34	2	925	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	802	U	O4'-C1'-N1	6.83	113.66	108.20
34	2	1154	G	C5-C6-O6	-6.83	124.50	128.60
34	2	321	C	N3-C4-N4	6.82	122.78	118.00
34	2	1834	U	O4'-C1'-N1	6.82	113.66	108.20
34	2	334	U	O4'-C1'-N1	6.82	113.66	108.20
34	2	1318	G	C5-C6-O6	-6.82	124.51	128.60
34	2	1750	C	N3-C4-N4	6.82	122.78	118.00
34	2	209	C	O4'-C1'-N1	6.82	113.66	108.20
34	2	399	C	O4'-C1'-N1	6.82	113.66	108.20
34	2	14	C	O4'-C1'-N1	6.82	113.65	108.20
34	2	672	U	O4'-C1'-N1	6.82	113.65	108.20
34	2	451	U	O4'-C1'-N1	6.81	113.65	108.20
34	2	1239	U	O4'-C1'-N1	6.81	113.65	108.20
34	2	34	U	O4'-C1'-N1	6.81	113.64	108.20
34	2	622	C	N3-C4-N4	6.81	122.76	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	480	C	N3-C4-N4	6.80	122.76	118.00
34	2	1423	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	363	G	N1-C6-O6	6.80	123.98	119.90
34	2	863	G	C5-C6-O6	-6.80	124.52	128.60
34	2	936	U	O4'-C1'-N1	6.79	113.64	108.20
34	2	810	U	O4'-C1'-N1	6.79	113.64	108.20
34	2	911	G	O4'-C1'-N9	6.79	113.63	108.20
34	2	1203	G	C5-C6-O6	-6.79	124.52	128.60
34	2	540	C	N3-C4-N4	6.79	122.75	118.00
34	2	1381	G	C5-C6-O6	-6.79	124.53	128.60
34	2	488	C	O4'-C1'-N1	6.79	113.63	108.20
34	2	615	G	C5-C6-O6	-6.79	124.53	128.60
34	2	1325	U	O4'-C1'-N1	6.79	113.63	108.20
34	2	597	U	O4'-C1'-N1	6.78	113.63	108.20
34	2	358	U	O4'-C1'-N1	6.78	113.62	108.20
34	2	216	U	O4'-C1'-N1	6.78	113.62	108.20
34	2	1575	A	C5-C6-N6	-6.78	118.28	123.70
34	2	1843	G	O4'-C1'-N9	6.78	113.62	108.20
41	3	40	C	OP2-P-O3'	-6.78	90.30	105.20
34	2	674	G	C5-C6-O6	-6.77	124.54	128.60
34	2	849	C	O4'-C1'-N1	6.77	113.62	108.20
34	2	531	U	O4'-C1'-N1	6.77	113.62	108.20
34	2	1554	C	O4'-C1'-N1	6.77	113.62	108.20
34	2	94	G	C5-C6-O6	-6.77	124.54	128.60
34	2	1793	G	C5-C6-O6	-6.77	124.54	128.60
34	2	144	U	O4'-C1'-N1	6.77	113.61	108.20
34	2	317	G	P-O3'-C3'	6.77	127.82	119.70
34	2	1827	C	O4'-C1'-N1	6.77	113.62	108.20
34	2	966	G	C5-C6-O6	-6.77	124.54	128.60
34	2	1116	U	O4'-C1'-N1	6.77	113.61	108.20
34	2	233	A	C4-C5-C6	6.76	120.38	117.00
34	2	1263	C	O4'-C1'-N1	6.76	113.61	108.20
34	2	1803	A	C5-C6-N6	-6.76	118.29	123.70
34	2	1233	C	O4'-C1'-N1	6.76	113.61	108.20
34	2	611	C	N3-C4-N4	6.76	122.73	118.00
1	1	34	C	N3-C4-N4	6.76	122.73	118.00
34	2	832	G	C5-C6-O6	-6.76	124.54	128.60
34	2	960	A	C4-C5-C6	6.76	120.38	117.00
34	2	1159	C	O4'-C1'-N1	6.76	113.61	108.20
34	2	16	G	C5-C6-O6	-6.76	124.55	128.60
34	2	415	G	C5-C6-O6	-6.76	124.55	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1463	C	N3-C4-N4	6.76	122.73	118.00
1	1	21	A	C5-C6-N6	-6.75	118.30	123.70
13	M	57	TYR	CB-CG-CD2	-6.75	116.95	121.00
34	2	97	U	O4'-C1'-N1	6.75	113.60	108.20
34	2	311	C	N3-C4-N4	6.75	122.73	118.00
34	2	1251	G	C5-C6-O6	-6.75	124.55	128.60
34	2	1464	C	O4'-C1'-N1	6.75	113.60	108.20
34	2	1559	C	N3-C4-N4	6.75	122.72	118.00
34	2	294	C	O4'-C1'-N1	6.75	113.60	108.20
34	2	1070	C	O4'-C1'-N1	6.75	113.60	108.20
34	2	1591	U	O4'-C1'-N1	6.75	113.60	108.20
34	2	571	U	O4'-C1'-N1	6.75	113.60	108.20
1	1	36	U	O4'-C1'-N1	6.74	113.59	108.20
34	2	626	C	N3-C4-N4	6.74	122.72	118.00
34	2	852	C	O4'-C1'-N1	6.74	113.59	108.20
34	2	1066	A	C4-C5-C6	6.74	120.37	117.00
34	2	1508	C	O4'-C1'-N1	6.74	113.59	108.20
34	2	520	U	O4'-C1'-N1	6.74	113.59	108.20
34	2	550	A	C5-C6-N6	-6.74	118.31	123.70
34	2	1662	U	O4'-C1'-N1	6.74	113.59	108.20
34	2	373	G	C5-C6-O6	-6.74	124.56	128.60
34	2	1122	G	O4'-C1'-N9	6.74	113.59	108.20
34	2	1135	C	C6-N1-C1'	-6.74	112.71	120.80
34	2	100	U	O4'-C1'-N1	6.74	113.59	108.20
34	2	598	C	N3-C4-N4	6.74	122.72	118.00
34	2	1263	C	N3-C4-N4	6.74	122.72	118.00
34	2	1615	A	C4-C5-C6	6.74	120.37	117.00
34	2	471	C	N3-C4-N4	6.74	122.72	118.00
34	2	1086	C	O4'-C1'-N1	6.74	113.59	108.20
34	2	465	C	N3-C4-N4	6.73	122.71	118.00
34	2	468	G	O4'-C1'-N9	6.73	113.59	108.20
34	2	194	C	O4'-C1'-N1	6.73	113.58	108.20
34	2	397	G	C5-C6-O6	-6.73	124.56	128.60
34	2	504	U	O4'-C1'-N1	6.73	113.58	108.20
34	2	1292	U	O4'-C1'-N1	6.73	113.58	108.20
34	2	1595	G	C5-C6-O6	-6.73	124.56	128.60
34	2	1655	C	O4'-C1'-N1	6.73	113.58	108.20
9	I	145	PHE	CB-CG-CD1	6.73	125.51	120.80
34	2	1305	C	O4'-C1'-N1	6.72	113.58	108.20
34	2	1420	G	C5-C6-O6	-6.72	124.56	128.60
34	2	874	G	C5-C6-O6	-6.72	124.57	128.60
34	2	1725	U	O4'-C1'-N1	6.72	113.58	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1404	U	O4'-C1'-N1	6.72	113.58	108.20
1	1	58	A	C4-C5-C6	6.72	120.36	117.00
34	2	1858	U	O4'-C1'-N1	6.72	113.58	108.20
34	2	69	C	N3-C4-N4	6.72	122.70	118.00
34	2	872	C	N3-C4-N4	6.72	122.70	118.00
34	2	1853	A	C5-C6-N6	-6.72	118.33	123.70
34	2	523	A	C5-C6-N1	-6.71	114.34	117.70
38	k	513	LYS	CA-C-N	6.71	131.97	117.20
34	2	126	G	C5-C6-O6	-6.71	124.57	128.60
34	2	1542	C	O4'-C1'-N1	6.71	113.57	108.20
34	2	67	C	OP2-P-O3'	6.71	119.96	105.20
34	2	355	C	N3-C4-N4	6.71	122.70	118.00
34	2	594	A	C4-C5-C6	6.71	120.36	117.00
34	2	665	U	O4'-C1'-N1	6.71	113.57	108.20
34	2	1029	G	C5-C6-O6	-6.71	124.58	128.60
34	2	1497	C	N3-C4-N4	6.71	122.69	118.00
34	2	1588	C	O4'-C1'-N1	6.71	113.56	108.20
34	2	5	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	298	G	C5-C6-O6	-6.70	124.58	128.60
34	2	350	A	C5-C6-N6	-6.70	118.34	123.70
34	2	418	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	797	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	1044	G	C5-C6-O6	-6.70	124.58	128.60
34	2	1199	G	C5-C6-O6	-6.70	124.58	128.60
34	2	640	A	C5-C6-N6	-6.70	118.34	123.70
34	2	1787	A	C5-C6-N1	-6.70	114.35	117.70
34	2	115	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	229	A	C4-C5-C6	6.70	120.35	117.00
34	2	575	C	O4'-C1'-N1	6.70	113.56	108.20
34	2	1299	C	O4'-C1'-N1	6.70	113.56	108.20
34	2	1637	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	105	U	O4'-C1'-N1	6.70	113.56	108.20
34	2	402	G	N3-C2-N2	6.70	124.59	119.90
34	2	977	A	C5-C6-N6	-6.70	118.34	123.70
34	2	1682	C	N3-C4-N4	6.70	122.69	118.00
34	2	1767	C	O4'-C1'-N1	6.70	113.56	108.20
34	2	1831	G	C5-C6-O6	-6.70	124.58	128.60
34	2	529	C	N3-C4-N4	6.69	122.69	118.00
34	2	539	C	N3-C4-N4	6.69	122.69	118.00
34	2	1822	C	N3-C4-N4	6.69	122.69	118.00
34	2	420	C	N3-C4-N4	6.69	122.68	118.00
34	2	1638	U	O4'-C1'-N1	6.69	113.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	155	G	C5-C6-O6	-6.69	124.59	128.60
34	2	1503	G	C5-C6-O6	-6.69	124.59	128.60
34	2	168	C	O4'-C1'-N1	6.69	113.55	108.20
34	2	973	C	N3-C4-N4	6.69	122.68	118.00
34	2	1740	A	C4-C5-C6	6.69	120.34	117.00
34	2	33	G	C5-C6-O6	-6.68	124.59	128.60
34	2	911	G	C5-C6-O6	-6.68	124.59	128.60
34	2	917	G	C5-C6-O6	-6.68	124.59	128.60
34	2	473	C	O4'-C1'-N1	6.68	113.55	108.20
34	2	1062	U	O4'-C1'-N1	6.68	113.55	108.20
34	2	1171	G	C5-C6-O6	-6.68	124.59	128.60
34	2	391	A	N1-C6-N6	6.68	122.61	118.60
34	2	472	G	C5-C6-O6	-6.68	124.59	128.60
34	2	841	G	C5-C6-O6	-6.68	124.59	128.60
34	2	999	U	O4'-C1'-N1	6.68	113.54	108.20
34	2	177	G	C5-C6-O6	-6.68	124.59	128.60
34	2	291	U	O4'-C1'-N1	6.68	113.54	108.20
34	2	1109	A	C5-C6-N6	-6.68	118.36	123.70
34	2	1289	A	C5-C6-N6	-6.68	118.36	123.70
34	2	1354	U	O4'-C1'-N1	6.68	113.54	108.20
34	2	387	G	C5-C6-O6	-6.68	124.59	128.60
34	2	876	G	C5-C6-O6	-6.68	124.59	128.60
34	2	1070	C	N3-C4-N4	6.68	122.67	118.00
34	2	1700	C	O4'-C1'-N1	6.68	113.54	108.20
34	2	942	U	O4'-C1'-N1	6.67	113.54	108.20
34	2	1095	G	C5-C6-O6	-6.67	124.59	128.60
34	2	1484	C	N3-C4-N4	6.67	122.67	118.00
1	1	34	C	O4'-C1'-N1	6.67	113.54	108.20
34	2	1808	G	C5-C6-O6	-6.67	124.60	128.60
34	2	87	U	O4'-C1'-N1	6.67	113.53	108.20
34	2	1767	C	N3-C4-N4	6.67	122.67	118.00
34	2	1192	A	C4-C5-C6	6.67	120.33	117.00
34	2	1613	C	O4'-C1'-N1	6.66	113.53	108.20
34	2	75	G	O4'-C1'-N9	6.66	113.53	108.20
34	2	230	C	O4'-C1'-N1	6.66	113.53	108.20
34	2	642	U	O4'-C1'-N1	6.66	113.53	108.20
34	2	1355	U	O4'-C1'-N1	6.66	113.53	108.20
34	2	1143	C	N3-C4-N4	6.66	122.66	118.00
34	2	1351	C	O4'-C1'-N1	6.66	113.53	108.20
34	2	1618	A	O4'-C1'-N9	6.66	113.53	108.20
41	3	37	C	O4'-C1'-N1	6.66	113.53	108.20
34	2	193	C	N3-C4-N4	6.66	122.66	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	808	A	C5-C6-N6	-6.66	118.38	123.70
34	2	991	G	C5-C6-O6	-6.66	124.61	128.60
34	2	1108	U	O4'-C1'-N1	6.65	113.52	108.20
34	2	1685	U	O4'-C1'-N1	6.65	113.52	108.20
34	2	1612	G	C5-C6-O6	-6.65	124.61	128.60
34	2	102	A	C4-C5-C6	6.65	120.33	117.00
34	2	838	C	N3-C4-N4	6.65	122.65	118.00
34	2	957	G	C5-C6-O6	-6.65	124.61	128.60
34	2	1346	U	O4'-C1'-N1	6.64	113.52	108.20
34	2	1721	G	C5-C6-O6	-6.64	124.61	128.60
34	2	57	U	O4'-C1'-N1	6.64	113.52	108.20
34	2	619	A	C4-C5-C6	6.64	120.32	117.00
34	2	1440	U	O4'-C1'-N1	6.64	113.51	108.20
34	2	1533	C	O4'-C1'-N1	6.64	113.51	108.20
34	2	446	C	N3-C4-N4	6.64	122.65	118.00
34	2	1579	G	C5-C6-O6	-6.64	124.62	128.60
34	2	1279	C	O4'-C1'-N1	6.64	113.51	108.20
34	2	1739	G	C5-C6-O6	-6.64	124.62	128.60
11	K	149	TYR	CB-CG-CD2	-6.63	117.02	121.00
34	2	428	G	O4'-C1'-N9	6.63	113.51	108.20
34	2	616	G	C5-C6-O6	-6.63	124.62	128.60
34	2	1127	G	C5-C6-O6	-6.63	124.62	128.60
34	2	1449	C	C2-N1-C1'	6.63	126.10	118.80
34	2	238	G	C5-C6-O6	-6.63	124.62	128.60
34	2	1188	U	O4'-C1'-N1	6.63	113.50	108.20
34	2	1766	C	N3-C4-N4	6.63	122.64	118.00
34	2	1201	C	N3-C4-N4	6.63	122.64	118.00
34	2	854	A	C5-C6-N1	-6.63	114.39	117.70
34	2	1262	C	N3-C4-N4	6.63	122.64	118.00
34	2	1700	C	N3-C4-N4	6.63	122.64	118.00
34	2	1272	A	C5-C6-N6	-6.62	118.40	123.70
34	2	1331	G	N3-C2-N2	6.62	124.54	119.90
34	2	1646	A	C5-C6-N6	-6.62	118.40	123.70
34	2	1788	C	N3-C4-N4	6.62	122.64	118.00
34	2	301	C	N3-C4-N4	6.62	122.63	118.00
34	2	1842	U	O4'-C1'-N1	6.62	113.50	108.20
34	2	48	C	N3-C4-N4	6.62	122.63	118.00
41	3	64	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	1428	U	O4'-C1'-N1	6.62	113.49	108.20
34	2	1800	A	C5-C6-N6	-6.61	118.41	123.70
34	2	1288	C	O4'-C1'-N1	6.61	113.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	877	G	C5-C6-O6	-6.61	124.63	128.60
34	2	1377	G	C5-C6-O6	-6.61	124.63	128.60
34	2	1403	U	O4'-C1'-N1	6.61	113.49	108.20
34	2	1469	G	C5-C6-O6	-6.61	124.63	128.60
34	2	308	C	O4'-C1'-N1	6.61	113.49	108.20
34	2	317	G	C5-C6-O6	-6.61	124.64	128.60
34	2	362	U	O4'-C1'-N1	6.61	113.48	108.20
34	2	576	G	C5-C6-O6	-6.61	124.64	128.60
34	2	1048	A	C5-C6-N6	-6.61	118.42	123.70
34	2	1074	C	O4'-C1'-N1	6.61	113.49	108.20
34	2	1099	C	N3-C4-N4	6.61	122.63	118.00
34	2	1175	G	C5-C6-O6	-6.61	124.64	128.60
34	2	1317	G	C5-C6-O6	-6.61	124.64	128.60
34	2	370	G	C5-C6-O6	-6.61	124.64	128.60
34	2	442	G	C5-C6-O6	-6.61	124.64	128.60
34	2	1228	U	O4'-C1'-N1	6.61	113.48	108.20
34	2	1765	G	C5-C6-O6	-6.60	124.64	128.60
11	K	142	SER	C-N-CA	6.60	138.20	121.70
34	2	1738	G	C5-C6-O6	-6.60	124.64	128.60
1	1	23	C	N3-C4-N4	6.60	122.62	118.00
34	2	889	U	O4'-C1'-N1	6.59	113.48	108.20
34	2	1332	C	N3-C4-N4	6.59	122.61	118.00
34	2	1556	A	C4-C5-C6	6.59	120.30	117.00
34	2	190	A	C4-C5-C6	6.59	120.29	117.00
34	2	1262	C	O4'-C1'-N1	6.59	113.47	108.20
34	2	164	A	C5-C6-N6	-6.59	118.43	123.70
34	2	573	A	C5-C6-N6	-6.59	118.43	123.70
34	2	1518	C	N3-C4-N4	6.59	122.61	118.00
34	2	1357	G	C5-C6-O6	-6.58	124.65	128.60
34	2	231	C	N3-C4-N4	6.58	122.61	118.00
34	2	527	C	N3-C4-N4	6.58	122.61	118.00
34	2	575	C	N3-C4-N4	6.58	122.61	118.00
34	2	1216	A	C5-C6-N6	-6.58	118.43	123.70
34	2	1713	G	N3-C2-N2	6.58	124.51	119.90
34	2	497	G	C5-C6-O6	-6.58	124.65	128.60
34	2	851	G	C5-C6-O6	-6.58	124.65	128.60
34	2	1142	C	O4'-C1'-N1	6.58	113.47	108.20
34	2	1193	G	C5-C6-O6	-6.58	124.65	128.60
34	2	1197	U	O4'-C1'-N1	6.58	113.46	108.20
34	2	101	U	O4'-C1'-N1	6.58	113.46	108.20
34	2	469	C	N3-C4-N4	6.58	122.61	118.00
34	2	1570	G	O4'-C1'-N9	6.58	113.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1846	C	N3-C4-N4	6.58	122.61	118.00
34	2	104	A	C4-C5-C6	6.58	120.29	117.00
34	2	341	G	O4'-C1'-N9	6.58	113.46	108.20
34	2	419	C	N3-C4-N4	6.58	122.60	118.00
34	2	1854	A	C5-C6-N6	-6.58	118.44	123.70
34	2	455	A	C4-C5-C6	6.58	120.29	117.00
34	2	1439	C	O4'-C1'-N1	6.58	113.46	108.20
34	2	71	G	C5-C6-O6	-6.57	124.66	128.60
34	2	537	G	C5-C6-O6	-6.57	124.66	128.60
34	2	549	G	C5-C6-O6	-6.57	124.66	128.60
34	2	653	C	N3-C4-N4	6.57	122.60	118.00
34	2	1365	A	C4-C5-C6	6.57	120.28	117.00
34	2	12	U	O4'-C1'-N1	6.57	113.45	108.20
34	2	276	U	O4'-C1'-N1	6.57	113.45	108.20
34	2	637	U	O4'-C1'-N1	6.57	113.45	108.20
34	2	1126	G	C5-C6-O6	-6.57	124.66	128.60
34	2	1729	G	C5-C6-O6	-6.57	124.66	128.60
34	2	1168	U	O4'-C1'-N1	6.57	113.45	108.20
34	2	1270	G	C5-C6-O6	-6.57	124.66	128.60
34	2	968	A	C4-C5-C6	6.56	120.28	117.00
34	2	1525	U	O4'-C1'-N1	6.56	113.45	108.20
34	2	425	A	C5-C6-N6	-6.56	118.45	123.70
34	2	1609	A	C5-C6-N6	-6.56	118.45	123.70
34	2	1643	G	C5-C6-O6	-6.56	124.67	128.60
34	2	1677	C	N3-C4-N4	6.56	122.59	118.00
34	2	1240	U	O4'-C1'-N1	6.55	113.44	108.20
34	2	1139	A	C4-C5-C6	6.55	120.28	117.00
34	2	74	G	C5-C6-O6	-6.55	124.67	128.60
34	2	806	A	C4-C5-C6	6.55	120.28	117.00
34	2	1520	C	N3-C4-N4	6.55	122.58	118.00
34	2	1627	G	C5-C6-O6	-6.55	124.67	128.60
13	M	57	TYR	CB-CG-CD1	6.55	124.93	121.00
34	2	33	G	O4'-C1'-N9	6.55	113.44	108.20
34	2	80	G	P-O3'-C3'	6.55	127.56	119.70
34	2	280	G	C5-C6-O6	-6.55	124.67	128.60
34	2	1303	U	O4'-C1'-N1	6.55	113.44	108.20
1	1	56	C	O4'-C1'-N1	6.54	113.44	108.20
34	2	184	G	C5-C6-O6	-6.54	124.67	128.60
34	2	1305	C	N3-C4-N4	6.54	122.58	118.00
34	2	1836	C	N3-C4-N4	6.54	122.58	118.00
34	2	924	G	C5-C6-O6	-6.54	124.67	128.60
34	2	1219	A	P-O3'-C3'	-6.54	111.85	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	289	GLY	N-CA-C	6.54	129.45	113.10
34	2	328	G	C5-C6-O6	-6.54	124.68	128.60
34	2	1600	G	C5-C6-O6	-6.54	124.68	128.60
34	2	647	U	O4'-C1'-N1	6.54	113.43	108.20
34	2	959	A	C5-C6-N6	-6.54	118.47	123.70
34	2	186	G	O4'-C1'-N9	6.54	113.43	108.20
34	2	608	C	N3-C4-N4	6.54	122.58	118.00
34	2	1275	C	N3-C4-N4	6.54	122.58	118.00
34	2	182	C	O4'-C1'-N1	6.53	113.43	108.20
34	2	1448	A	C5-C6-N6	-6.53	118.47	123.70
37	j	21	SER	N-CA-CB	6.53	120.30	110.50
34	2	539	C	O4'-C1'-N1	6.53	113.43	108.20
34	2	1414	C	O4'-C1'-N1	6.53	113.43	108.20
34	2	1797	U	O4'-C1'-N1	6.53	113.42	108.20
34	2	281	U	O4'-C1'-N1	6.53	113.42	108.20
34	2	673	G	C5-C6-O6	-6.53	124.68	128.60
34	2	1174	U	O4'-C1'-N1	6.53	113.42	108.20
34	2	1250	C	O4'-C1'-N1	6.53	113.42	108.20
34	2	1274	A	C5-C6-N6	-6.53	118.47	123.70
38	k	408	ASN	C-N-CA	6.53	138.03	121.70
34	2	577	A	C4-C5-C6	6.53	120.26	117.00
34	2	1329	U	O4'-C1'-N1	6.53	113.42	108.20
34	2	1732	G	O4'-C1'-N9	6.53	113.42	108.20
34	2	410	G	C5-C6-O6	-6.53	124.69	128.60
34	2	1088	G	C5-C6-O6	-6.53	124.69	128.60
34	2	1293	U	O4'-C1'-N1	6.53	113.42	108.20
34	2	1622	C	N3-C4-N4	6.53	122.57	118.00
34	2	31	U	O4'-C1'-N1	6.52	113.42	108.20
34	2	1075	C	O4'-C1'-N1	6.52	113.42	108.20
34	2	1704	G	C5-C6-O6	-6.52	124.69	128.60
34	2	75	G	C5-C6-O6	-6.52	124.69	128.60
34	2	419	C	O4'-C1'-N1	6.52	113.42	108.20
34	2	4	C	O4'-C1'-N1	6.52	113.42	108.20
34	2	180	G	C5-C6-O6	-6.52	124.69	128.60
34	2	1742	C	N3-C4-N4	6.52	122.56	118.00
34	2	1796	C	N3-C4-N4	6.52	122.56	118.00
34	2	402	G	C5-C6-O6	-6.52	124.69	128.60
34	2	501	U	O4'-C1'-N1	6.52	113.41	108.20
34	2	1187	C	N3-C4-N4	6.52	122.56	118.00
34	2	1733	C	N3-C4-N4	6.52	122.56	118.00
34	2	811	U	O4'-C1'-N1	6.52	113.41	108.20
34	2	151	C	N3-C4-N4	6.51	122.56	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	907	C	N3-C4-N4	6.51	122.56	118.00
34	2	1049	C	N3-C4-N4	6.51	122.56	118.00
34	2	1457	G	C5-C6-O6	-6.51	124.69	128.60
34	2	1569	C	O4'-C1'-N1	6.51	113.41	108.20
41	3	52	A	C5-C6-N6	-6.51	118.49	123.70
34	2	1577	C	N3-C4-N4	6.51	122.56	118.00
34	2	589	A	C5-C6-N6	-6.51	118.49	123.70
34	2	933	C	N3-C4-N4	6.51	122.56	118.00
34	2	324	C	N3-C4-N4	6.51	122.56	118.00
34	2	840	U	O4'-C1'-N1	6.51	113.41	108.20
34	2	1417	A	C4-C5-C6	6.51	120.25	117.00
34	2	1268	C	N3-C4-N4	6.50	122.55	118.00
1	1	47	U	O4'-C1'-N1	6.50	113.40	108.20
34	2	800	U	O4'-C1'-N1	6.50	113.40	108.20
34	2	1419	C	O4'-C1'-N1	6.50	113.40	108.20
34	2	872	C	O4'-C1'-N1	6.50	113.40	108.20
34	2	1278	A	C4-C5-C6	6.50	120.25	117.00
40	R	37	TYR	CB-CG-CD2	-6.50	117.10	121.00
34	2	92	A	C4-C5-C6	6.50	120.25	117.00
34	2	1755	U	O4'-C1'-N1	6.50	113.40	108.20
1	1	26	G	C5-C6-O6	-6.49	124.70	128.60
34	2	1702	U	O4'-C1'-N1	6.49	113.39	108.20
34	2	275	C	C2-N1-C1'	6.49	125.94	118.80
34	2	1618	A	C4-C5-C6	6.49	120.25	117.00
34	2	549	G	O4'-C1'-N9	6.49	113.39	108.20
34	2	884	U	O4'-C1'-N1	6.49	113.39	108.20
34	2	1285	U	O4'-C1'-N1	6.49	113.39	108.20
1	1	19	G	C5-C6-O6	-6.49	124.71	128.60
9	I	145	PHE	CB-CG-CD2	-6.49	116.26	120.80
34	2	894	U	O4'-C1'-N1	6.49	113.39	108.20
34	2	977	A	C4-C5-C6	6.49	120.24	117.00
34	2	1464	C	N3-C4-N4	6.49	122.54	118.00
34	2	1801	C	N3-C4-N4	6.49	122.54	118.00
34	2	170	A	C4-C5-C6	6.48	120.24	117.00
34	2	1060	C	N3-C4-N4	6.48	122.54	118.00
34	2	50	A	C4-C5-C6	6.48	120.24	117.00
34	2	51	U	O4'-C1'-N1	6.48	113.39	108.20
34	2	848	G	C5-C6-O6	-6.48	124.71	128.60
34	2	1107	U	O4'-C1'-N1	6.48	113.39	108.20
34	2	1481	U	O4'-C1'-N1	6.48	113.39	108.20
34	2	1230	C	N3-C4-N4	6.48	122.53	118.00
34	2	1792	C	O4'-C1'-N1	6.48	113.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	313	C	N3-C4-N4	6.48	122.53	118.00
34	2	1222	G	C5-C6-O6	-6.48	124.71	128.60
34	2	1635	A	C4-C5-C6	6.48	120.24	117.00
34	2	1344	G	C5-C6-O6	-6.48	124.71	128.60
34	2	1054	A	C4-C5-C6	6.47	120.24	117.00
34	2	1177	A	C5-C6-N6	-6.47	118.52	123.70
34	2	1610	U	O4'-C1'-N1	6.47	113.38	108.20
34	2	1805	C	N3-C4-N4	6.47	122.53	118.00
34	2	1165	G	C5-C6-O6	-6.47	124.72	128.60
34	2	1408	C	N3-C4-N4	6.47	122.53	118.00
34	2	1515	G	C4-N9-C1'	6.47	134.91	126.50
11	K	149	TYR	CB-CG-CD1	6.47	124.88	121.00
35	A	269	PHE	CB-CG-CD1	6.47	125.33	120.80
34	2	308	C	N3-C4-N4	6.47	122.53	118.00
34	2	623	C	N3-C4-N4	6.47	122.53	118.00
34	2	962	U	O4'-C1'-N1	6.47	113.37	108.20
34	2	1210	A	C4-C5-C6	6.47	120.23	117.00
34	2	1492	U	O4'-C1'-N1	6.47	113.37	108.20
34	2	90	G	C5-C6-O6	-6.47	124.72	128.60
34	2	474	A	C4-C5-C6	6.47	120.23	117.00
34	2	1784	A	C4-C5-C6	6.47	120.23	117.00
34	2	1798	U	O4'-C1'-N1	6.47	113.37	108.20
1	1	54	A	C4-C5-C6	6.46	120.23	117.00
34	2	386	U	O4'-C1'-N1	6.46	113.37	108.20
34	2	1113	C	O4'-C1'-N1	6.46	113.37	108.20
34	2	1015	C	O4'-C1'-N1	6.46	113.37	108.20
34	2	227	A	C5-C6-N6	-6.46	118.53	123.70
34	2	988	A	C4-C5-C6	6.46	120.23	117.00
34	2	1068	U	O4'-C1'-N1	6.46	113.37	108.20
34	2	1843	G	C5-C6-O6	-6.46	124.73	128.60
34	2	1856	G	C5-C6-O6	-6.46	124.73	128.60
34	2	287	U	O4'-C1'-N1	6.46	113.36	108.20
34	2	1103	G	O4'-C1'-N9	6.46	113.36	108.20
34	2	70	G	C5-C6-O6	-6.45	124.73	128.60
34	2	103	A	C5-C6-N6	-6.45	118.54	123.70
34	2	214	A	C4-C5-C6	6.45	120.23	117.00
34	2	466	A	C5-C6-N6	-6.45	118.54	123.70
34	2	1620	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	1273	C	N3-C4-N4	6.45	122.51	118.00
34	2	1369	C	O4'-C1'-N1	6.45	113.36	108.20
34	2	211	U	O4'-C1'-N1	6.45	113.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	622	C	O4'-C1'-N1	6.45	113.36	108.20
34	2	839	C	N3-C4-N4	6.45	122.51	118.00
34	2	331	C	N3-C4-N4	6.44	122.51	118.00
34	2	1264	C	N3-C4-N4	6.44	122.51	118.00
34	2	1272	A	C4-C5-C6	6.44	120.22	117.00
34	2	1526	A	C5-C6-N1	-6.44	114.48	117.70
34	2	996	C	O4'-C1'-N1	6.44	113.35	108.20
34	2	1532	A	C4-C5-C6	6.44	120.22	117.00
34	2	1630	C	N3-C4-N4	6.44	122.51	118.00
38	k	567	ARG	NE-CZ-NH2	6.44	123.52	120.30
34	2	148	U	O4'-C1'-N1	6.44	113.35	108.20
1	1	38	A	C5-C6-N6	-6.43	118.55	123.70
34	2	380	C	N3-C4-N4	6.43	122.50	118.00
34	2	907	C	O4'-C1'-N1	6.43	113.35	108.20
34	2	1208	G	O4'-C1'-N9	6.43	113.35	108.20
34	2	1219	A	C4-C5-C6	6.43	120.22	117.00
34	2	1474	U	O4'-C1'-N1	6.43	113.34	108.20
34	2	521	A	C5-C6-N1	-6.43	114.49	117.70
34	2	1131	C	N3-C4-N4	6.43	122.50	118.00
34	2	1652	G	C5-C6-O6	-6.43	124.74	128.60
34	2	1375	A	C4-C5-C6	6.43	120.21	117.00
34	2	512	A	C4-C5-C6	6.43	120.21	117.00
34	2	862	U	O4'-C1'-N1	6.43	113.34	108.20
34	2	1467	C	N3-C4-N4	6.43	122.50	118.00
38	k	481	ASP	CB-CG-OD1	6.43	124.08	118.30
34	2	1342	U	O4'-C1'-N1	6.42	113.34	108.20
34	2	1382	A	C4-C5-C6	6.42	120.21	117.00
34	2	1297	A	O4'-C1'-N9	6.42	113.34	108.20
34	2	1308	G	N3-C2-N2	6.42	124.39	119.90
34	2	1560	C	N3-C4-N4	6.42	122.49	118.00
34	2	339	A	C5-C6-N6	-6.42	118.57	123.70
34	2	551	A	C4-C5-C6	6.42	120.21	117.00
34	2	816	U	O4'-C1'-N1	6.42	113.33	108.20
34	2	436	G	C5-C6-O6	-6.42	124.75	128.60
34	2	831	C	O4'-C1'-N1	6.42	113.33	108.20
34	2	902	U	O4'-C1'-N1	6.42	113.33	108.20
34	2	1859	C	O4'-C1'-N1	6.42	113.33	108.20
34	2	312	C	N3-C4-N4	6.41	122.49	118.00
34	2	1172	G	O4'-C1'-N9	6.41	113.33	108.20
41	3	36	A	C4-C5-C6	6.41	120.21	117.00
1	1	45	G	O4'-C1'-N9	6.41	113.33	108.20
34	2	1198	U	O4'-C1'-N1	6.41	113.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	348	C	N3-C4-N4	6.41	122.49	118.00
34	2	1298	G	C5-C6-O6	-6.41	124.75	128.60
34	2	1661	C	N3-C4-N4	6.41	122.49	118.00
34	2	119	U	O4'-C1'-N1	6.41	113.33	108.20
34	2	342	U	O4'-C1'-N1	6.41	113.32	108.20
34	2	829	C	N3-C4-N4	6.41	122.48	118.00
34	2	1548	C	O4'-C1'-N1	6.41	113.33	108.20
34	2	1128	C	N3-C4-N4	6.40	122.48	118.00
34	2	1645	A	C4-C5-C6	6.40	120.20	117.00
34	2	522	C	N3-C4-N4	6.40	122.48	118.00
34	2	799	C	N3-C4-N4	6.40	122.48	118.00
34	2	1352	G	C5-C6-O6	-6.40	124.76	128.60
1	1	14	C	N3-C4-N4	6.40	122.48	118.00
34	2	306	C	N3-C4-N4	6.40	122.48	118.00
34	2	460	G	O4'-C1'-N9	6.40	113.32	108.20
34	2	505	G	C5-C6-O6	-6.40	124.76	128.60
34	2	868	A	C4-C5-C6	6.40	120.20	117.00
34	2	1787	A	C4-C5-C6	6.40	120.20	117.00
34	2	530	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	1601	G	C5-C6-O6	-6.40	124.76	128.60
34	2	189	G	C5-C6-O6	-6.39	124.76	128.60
34	2	40	A	C4-C5-C6	6.39	120.20	117.00
34	2	1386	U	O4'-C1'-N1	6.39	113.31	108.20
34	2	569	C	N3-C4-N4	6.39	122.47	118.00
34	2	1049	C	O4'-C1'-N1	6.39	113.31	108.20
34	2	1138	G	C5-C6-O6	-6.39	124.77	128.60
34	2	1587	C	O4'-C1'-N1	6.39	113.31	108.20
34	2	1681	G	O4'-C1'-N9	6.39	113.31	108.20
34	2	1046	A	O4'-C1'-N9	6.39	113.31	108.20
34	2	1517	A	C4-C5-C6	6.39	120.19	117.00
34	2	112	U	O4'-C1'-N1	6.38	113.31	108.20
34	2	416	A	C4-C5-C6	6.38	120.19	117.00
34	2	829	C	O4'-C1'-N1	6.38	113.31	108.20
34	2	1140	A	C4-C5-C6	6.38	120.19	117.00
34	2	657	U	O4'-C1'-N1	6.38	113.30	108.20
34	2	1370	C	N3-C4-N4	6.38	122.47	118.00
38	k	455	ILE	CA-C-N	-6.38	103.16	117.20
34	2	175	A	O4'-C1'-N9	6.38	113.30	108.20
34	2	666	C	N3-C4-N4	6.38	122.47	118.00
34	2	1034	U	O4'-C1'-N1	6.38	113.30	108.20
34	2	1190	A	C5-C6-N1	-6.38	114.51	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1276	G	C5-C6-O6	-6.38	124.77	128.60
34	2	1648	U	O4'-C1'-N1	6.38	113.30	108.20
34	2	925	G	O4'-C1'-N9	6.38	113.30	108.20
34	2	1024	A	C4-C5-C6	6.38	120.19	117.00
34	2	1060	C	O4'-C1'-N1	6.38	113.30	108.20
34	2	1384	A	C4-C5-C6	6.38	120.19	117.00
34	2	1451	A	C5-C6-N1	-6.38	114.51	117.70
34	2	1680	U	O4'-C1'-N1	6.38	113.30	108.20
34	2	488	C	N3-C4-N4	6.37	122.46	118.00
34	2	524	G	O4'-C1'-N9	6.37	113.30	108.20
34	2	623	C	O4'-C1'-N1	6.37	113.30	108.20
34	2	1349	A	C5-C6-N6	-6.37	118.60	123.70
34	2	1589	A	C4-C5-C6	6.37	120.19	117.00
34	2	1044	G	N3-C2-N2	6.37	124.36	119.90
34	2	1064	G	C5-C6-O6	-6.37	124.78	128.60
34	2	544	A	C4-C5-C6	6.37	120.18	117.00
34	2	583	C	O4'-C1'-N1	6.37	113.30	108.20
34	2	1853	A	C4-C5-C6	6.37	120.18	117.00
34	2	230	C	N3-C4-N4	6.37	122.46	118.00
34	2	417	U	O4'-C1'-N1	6.37	113.29	108.20
34	2	834	G	C5-C6-O6	-6.37	124.78	128.60
34	2	937	C	N3-C4-N4	6.37	122.46	118.00
34	2	1603	U	O4'-C1'-N1	6.37	113.29	108.20
34	2	109	U	O4'-C1'-N1	6.36	113.29	108.20
34	2	1373	U	O4'-C1'-N1	6.36	113.29	108.20
34	2	64	A	C5-C6-N6	-6.36	118.61	123.70
34	2	893	U	O4'-C1'-N1	6.36	113.29	108.20
34	2	1665	C	N3-C4-N4	6.36	122.45	118.00
34	2	1825	A	C4-C5-C6	6.36	120.18	117.00
34	2	1827	C	N3-C4-N4	6.36	122.45	118.00
34	2	1630	C	O4'-C1'-N1	6.36	113.29	108.20
34	2	13	C	O4'-C1'-N1	6.36	113.29	108.20
34	2	405	A	C5-C6-N6	-6.36	118.61	123.70
34	2	599	U	O4'-C1'-N1	6.36	113.29	108.20
34	2	888	U	O4'-C1'-N1	6.35	113.28	108.20
34	2	350	A	C4-C5-C6	6.35	120.18	117.00
34	2	964	U	O4'-C1'-N1	6.35	113.28	108.20
34	2	1080	A	C4-C5-C6	6.35	120.18	117.00
34	2	171	A	N1-C6-N6	6.35	122.41	118.60
1	1	40	C	N3-C4-N4	6.35	122.44	118.00
34	2	365	U	O4'-C1'-N1	6.35	113.28	108.20
34	2	1295	A	C4-C5-C6	6.35	120.17	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	558	C	N3-C4-N4	6.35	122.44	118.00
34	2	825	C	N3-C4-N4	6.35	122.44	118.00
34	2	1557	C	O4'-C1'-N1	6.35	113.28	108.20
34	2	1372	A	C4-C5-C6	6.35	120.17	117.00
34	2	1071	C	N3-C4-N4	6.34	122.44	118.00
1	1	17	C	OP2-P-O3'	-6.34	91.25	105.20
34	2	1683	C	N3-C4-N4	6.34	122.44	118.00
34	2	106	C	N3-C4-N4	6.34	122.44	118.00
34	2	970	C	N3-C4-N4	6.34	122.44	118.00
34	2	82	G	C5-C6-O6	-6.34	124.80	128.60
34	2	341	G	C5-C6-O6	-6.33	124.80	128.60
34	2	580	A	C4-C5-C6	6.33	120.17	117.00
34	2	645	A	C4-C5-C6	6.33	120.17	117.00
34	2	1014	U	O4'-C1'-N1	6.33	113.27	108.20
34	2	78	C	O4'-C1'-N1	6.33	113.27	108.20
34	2	89	C	N3-C4-N4	6.33	122.43	118.00
34	2	1213	A	C4-C5-C6	6.33	120.17	117.00
34	2	1850	C	N3-C4-N4	6.33	122.43	118.00
34	2	164	A	C4-C5-C6	6.33	120.16	117.00
34	2	606	A	C4-C5-C6	6.33	120.16	117.00
34	2	67	C	O3'-P-O5'	-6.32	91.98	104.00
34	2	398	A	C4-C5-C6	6.32	120.16	117.00
34	2	883	U	O4'-C1'-N1	6.32	113.26	108.20
34	2	988	A	C5-C6-N6	-6.32	118.64	123.70
34	2	1494	A	C4-C5-C6	6.32	120.16	117.00
34	2	1181	C	N3-C4-N4	6.32	122.42	118.00
34	2	1516	C	N3-C4-N4	6.32	122.42	118.00
34	2	1552	C	O4'-C1'-N1	6.32	113.26	108.20
34	2	1712	C	N3-C4-N4	6.32	122.42	118.00
1	1	21	A	C4-C5-C6	6.32	120.16	117.00
34	2	392	C	N3-C4-N4	6.32	122.42	118.00
34	2	614	C	O4'-C1'-N1	6.32	113.25	108.20
34	2	408	A	C4-C5-C6	6.32	120.16	117.00
34	2	444	U	O4'-C1'-N1	6.32	113.25	108.20
34	2	984	C	N3-C4-N4	6.32	122.42	118.00
34	2	1111	U	O4'-C1'-N1	6.32	113.25	108.20
34	2	1686	U	O4'-C1'-N1	6.32	113.25	108.20
34	2	912	A	P-O3'-C3'	6.31	127.28	119.70
34	2	1118	A	C5-C6-N6	-6.31	118.65	123.70
34	2	447	C	N3-C4-N4	6.31	122.42	118.00
34	2	1646	A	C4-C5-C6	6.31	120.16	117.00
34	2	140	U	P-O3'-C3'	6.31	127.27	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1307	C	O4'-C1'-N1	6.31	113.25	108.20
34	2	563	U	O4'-C1'-N1	6.31	113.25	108.20
34	2	996	C	N3-C4-N4	6.31	122.42	118.00
34	2	46	A	C4-C5-C6	6.30	120.15	117.00
34	2	843	A	C4-C5-C6	6.30	120.15	117.00
34	2	1726	A	C4-C5-C6	6.30	120.15	117.00
34	2	921	G	C5-C6-O6	-6.30	124.82	128.60
34	2	428	G	C5-C6-O6	-6.30	124.82	128.60
34	2	433	U	O4'-C1'-N1	6.30	113.24	108.20
34	2	439	A	C4-C5-C6	6.30	120.15	117.00
34	2	675	A	O4'-C1'-N9	6.30	113.24	108.20
34	2	467	G	C5-C6-O6	-6.30	124.82	128.60
34	2	479	A	C5-C6-N6	-6.30	118.66	123.70
34	2	998	U	O4'-C1'-N1	6.30	113.24	108.20
34	2	1282	G	C5-C6-O6	-6.30	124.82	128.60
34	2	892	U	O4'-C1'-N1	6.30	113.24	108.20
34	2	299	G	C5-C6-O6	-6.30	124.82	128.60
34	2	618	A	C4-C5-C6	6.30	120.15	117.00
34	2	1532	A	C5-C6-N6	-6.30	118.66	123.70
34	2	1636	A	C5-C6-N6	-6.30	118.66	123.70
40	R	37	TYR	CB-CG-CD1	6.30	124.78	121.00
34	2	116	U	O4'-C1'-N1	6.29	113.24	108.20
34	2	11	A	C4-C5-C6	6.29	120.15	117.00
34	2	905	G	C5-C6-O6	-6.29	124.82	128.60
34	2	1073	A	C4-C5-C6	6.29	120.15	117.00
34	2	1157	U	O4'-C1'-N1	6.29	113.23	108.20
34	2	10	G	C5-C6-O6	-6.29	124.83	128.60
34	2	304	A	C4-C5-C6	6.29	120.15	117.00
34	2	366	A	C5-C6-N6	-6.29	118.67	123.70
34	2	234	C	O4'-C1'-N1	6.29	113.23	108.20
34	2	467	G	O4'-C1'-N9	6.29	113.23	108.20
1	1	13	G	O4'-C1'-N9	6.29	113.23	108.20
34	2	861	A	C4-C5-C6	6.29	120.14	117.00
34	2	1020	A	C4-C5-C6	6.29	120.14	117.00
34	2	352	C	N3-C4-N4	6.29	122.40	118.00
34	2	361	A	C4-C5-C6	6.29	120.14	117.00
34	2	443	C	N3-C4-N4	6.29	122.40	118.00
34	2	1032	A	C4-C5-C6	6.29	120.14	117.00
34	2	1046	A	C4-C5-C6	6.29	120.14	117.00
34	2	1118	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	1465	A	C5-C6-N6	-6.29	118.67	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1541	G	C5-C6-O6	-6.29	124.83	128.60
34	2	914	U	O4'-C1'-N1	6.28	113.23	108.20
34	2	979	A	C4-C5-C6	6.28	120.14	117.00
34	2	1043	C	N3-C4-N4	6.28	122.40	118.00
34	2	1148	U	O4'-C1'-N1	6.28	113.23	108.20
34	2	614	C	N3-C4-N4	6.28	122.40	118.00
34	2	1030	A	C4-C5-C6	6.28	120.14	117.00
34	2	1369	C	N3-C4-N4	6.28	122.39	118.00
34	2	1791	U	O4'-C1'-N1	6.28	113.22	108.20
34	2	958	A	C4-C5-C6	6.28	120.14	117.00
34	2	1577	C	O4'-C1'-N1	6.28	113.22	108.20
34	2	120	U	O4'-C1'-N1	6.27	113.22	108.20
34	2	1453	U	O4'-C1'-N1	6.27	113.22	108.20
34	2	1245	C	O4'-C1'-N1	6.27	113.22	108.20
1	1	10	G	C5-C6-O6	-6.27	124.84	128.60
34	2	84	A	C4-C5-C6	6.27	120.13	117.00
34	2	414	C	N3-C4-N4	6.27	122.39	118.00
34	2	1052	U	O4'-C1'-N1	6.27	113.22	108.20
34	2	177	G	N3-C2-N2	6.27	124.29	119.90
34	2	220	C	N3-C4-N4	6.27	122.39	118.00
34	2	565	A	C4-C5-C6	6.27	120.13	117.00
34	2	582	C	O4'-C1'-N1	6.27	113.21	108.20
34	2	1444	A	C4-C5-C6	6.27	120.13	117.00
38	k	150	SER	C-N-CA	-6.27	106.03	121.70
34	2	1527	C	N3-C4-N4	6.26	122.39	118.00
34	2	1737	C	N3-C4-N4	6.26	122.39	118.00
34	2	489	G	C5-C6-O6	-6.26	124.84	128.60
34	2	915	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	1602	A	C4-C5-C6	6.26	120.13	117.00
34	2	858	A	C4-C5-C6	6.26	120.13	117.00
34	2	1169	A	C4-C5-C6	6.26	120.13	117.00
34	2	1375	A	C5-C6-N6	-6.26	118.69	123.70
34	2	1089	A	C4-C5-C6	6.26	120.13	117.00
34	2	667	G	C5-C6-O6	-6.26	124.85	128.60
34	2	329	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	1632	A	C4-C5-C6	6.25	120.13	117.00
34	2	676	U	O4'-C1'-N1	6.25	113.20	108.20
34	2	1115	A	C4-C5-C6	6.25	120.12	117.00
34	2	1828	A	C4-C5-C6	6.25	120.13	117.00
34	2	506	A	C4-C5-C6	6.25	120.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1656	A	C4-C5-C6	6.25	120.12	117.00
34	2	83	A	C4-C5-C6	6.25	120.12	117.00
34	2	479	A	C4-C5-C6	6.25	120.12	117.00
34	2	1261	A	C4-C5-C6	6.25	120.12	117.00
34	2	1596	A	C5-C6-N6	-6.25	118.70	123.70
34	2	1626	U	O4'-C1'-N1	6.25	113.20	108.20
34	2	927	C	N3-C4-N4	6.24	122.37	118.00
34	2	822	A	C5-C6-N1	-6.24	114.58	117.70
34	2	1826	A	C4-C5-C6	6.24	120.12	117.00
38	k	510	HIS	CA-C-N	6.24	130.93	117.20
1	1	50	A	O4'-C1'-N9	6.24	113.19	108.20
34	2	338	A	C4-C5-C6	6.24	120.12	117.00
34	2	1726	A	C5-C6-N6	-6.24	118.71	123.70
34	2	1170	U	OP1-P-O3'	6.24	118.92	105.20
34	2	1792	C	N3-C4-N4	6.24	122.37	118.00
34	2	388	A	C5-C6-N6	-6.24	118.71	123.70
34	2	659	A	C4-C5-C6	6.24	120.12	117.00
34	2	975	C	N3-C4-N4	6.24	122.36	118.00
34	2	1301	C	N3-C4-N4	6.24	122.36	118.00
34	2	1508	C	N3-C4-N4	6.24	122.36	118.00
34	2	1588	C	N3-C4-N4	6.24	122.36	118.00
34	2	485	U	O4'-C1'-N1	6.23	113.19	108.20
34	2	509	A	C5-C6-N1	-6.23	114.58	117.70
34	2	929	G	O4'-C1'-N9	6.23	113.19	108.20
34	2	852	C	N3-C4-N4	6.23	122.36	118.00
1	1	76	A	C4-C5-C6	6.23	120.11	117.00
34	2	372	C	O4'-C1'-N1	6.23	113.18	108.20
34	2	1003	C	N3-C4-N4	6.23	122.36	118.00
34	2	1058	A	C4-C5-C6	6.23	120.11	117.00
34	2	1022	C	N3-C4-N4	6.23	122.36	118.00
34	2	918	A	C4-C5-C6	6.22	120.11	117.00
34	2	1020	A	C5-C6-N6	-6.22	118.72	123.70
34	2	1621	C	N3-C4-N4	6.22	122.36	118.00
34	2	1224	A	C5-C6-N6	-6.22	118.72	123.70
34	2	195	C	O4'-C1'-N1	6.22	113.17	108.20
34	2	1236	A	C4-C5-C6	6.22	120.11	117.00
34	2	1713	G	C5-C6-O6	-6.22	124.87	128.60
1	1	2	A	O4'-C1'-N9	6.22	113.17	108.20
34	2	886	U	O4'-C1'-N1	6.22	113.17	108.20
1	1	62	C	N3-C4-N4	6.21	122.35	118.00
34	2	541	U	O4'-C1'-N1	6.21	113.17	108.20
34	2	1513	C	C2-N1-C1'	6.21	125.64	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1063	C	N3-C4-N4	6.21	122.35	118.00
34	2	1689	U	O4'-C1'-N1	6.21	113.17	108.20
34	2	99	A	C5-C6-N6	-6.21	118.73	123.70
34	2	986	A	C5-C6-N6	-6.21	118.73	123.70
34	2	1498	C	N3-C4-N4	6.21	122.35	118.00
34	2	967	G	C5-C6-O6	-6.21	124.87	128.60
34	2	1660	G	C5-C6-O6	-6.21	124.87	128.60
34	2	1673	A	C4-C5-C6	6.21	120.11	117.00
34	2	674	G	O4'-C1'-N9	6.21	113.17	108.20
34	2	1190	A	C5-C6-N6	-6.21	118.73	123.70
34	2	1479	A	C4-C5-C6	6.21	120.10	117.00
34	2	425	A	C4-C5-C6	6.21	120.10	117.00
34	2	1614	A	C4-C5-C6	6.21	120.10	117.00
34	2	987	G	C4-N9-C1'	6.21	134.57	126.50
34	2	1719	A	C4-C5-C6	6.21	120.10	117.00
34	2	545	A	C5-C6-N6	-6.20	118.74	123.70
34	2	807	A	C5-C6-N1	-6.20	114.60	117.70
34	2	1666	G	N3-C2-N2	6.20	124.24	119.90
34	2	1124	C	N3-C4-N4	6.20	122.34	118.00
34	2	1501	U	O4'-C1'-N1	6.20	113.16	108.20
34	2	483	A	C5-C6-N6	-6.20	118.74	123.70
34	2	1023	A	C5-C6-N1	-6.20	114.60	117.70
34	2	1340	A	C4-C5-C6	6.20	120.10	117.00
34	2	1450	A	C4-C5-C6	6.20	120.10	117.00
34	2	1663	U	O4'-C1'-N1	6.20	113.16	108.20
34	2	1783	G	C5-C6-O6	-6.20	124.88	128.60
34	2	630	A	C4-C5-C6	6.20	120.10	117.00
34	2	1470	A	C5-C6-N6	-6.20	118.74	123.70
34	2	1480	A	C4-C5-C6	6.20	120.10	117.00
34	2	1517	A	C5-C6-N1	-6.20	114.60	117.70
34	2	21	U	O4'-C1'-N1	6.20	113.16	108.20
34	2	1005	A	C5-C6-N6	-6.20	118.74	123.70
34	2	1378	A	C4-C5-C6	6.20	120.10	117.00
34	2	1385	C	N3-C4-N4	6.20	122.34	118.00
34	2	1398	A	C5-C6-N6	-6.20	118.74	123.70
1	1	66	C	N3-C4-N4	6.19	122.34	118.00
34	2	382	A	C5-C6-N6	-6.19	118.75	123.70
34	2	729	C	N3-C4-N4	6.19	122.33	118.00
34	2	1069	U	O4'-C1'-N1	6.19	113.15	108.20
34	2	1145	A	C5-C6-N6	-6.19	118.75	123.70
34	2	1613	C	N3-C4-N4	6.19	122.33	118.00
34	2	946	C	N3-C4-N4	6.19	122.33	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1313	U	O4'-C1'-N1	6.19	113.15	108.20
34	2	1711	C	N3-C4-N4	6.19	122.33	118.00
34	2	310	G	O4'-C1'-N9	6.19	113.15	108.20
34	2	1557	C	N3-C4-N4	6.19	122.33	118.00
34	2	1794	A	C4-C5-C6	6.19	120.09	117.00
34	2	1839	A	C4-C5-C6	6.19	120.09	117.00
34	2	1302	U	O4'-C1'-N1	6.18	113.15	108.20
34	2	1466	C	N3-C4-N4	6.18	122.33	118.00
34	2	366	A	C4-C5-C6	6.18	120.09	117.00
34	2	392	C	N3-C4-C5	-6.18	119.43	121.90
34	2	511	A	C4-C5-C6	6.18	120.09	117.00
34	2	825	C	O4'-C1'-N1	6.18	113.15	108.20
34	2	859	U	O4'-C1'-N1	6.18	113.15	108.20
34	2	1672	U	O4'-C1'-N1	6.18	113.15	108.20
34	2	1006	G	O4'-C1'-N9	6.18	113.14	108.20
34	2	1287	A	C4-C5-C6	6.18	120.09	117.00
34	2	1353	A	C5-C6-N1	-6.18	114.61	117.70
34	2	833	A	C4-C5-C6	6.18	120.09	117.00
34	2	912	A	C4-C5-C6	6.18	120.09	117.00
34	2	1132	U	O4'-C1'-N1	6.18	113.14	108.20
34	2	1625	A	C5-C6-N1	-6.18	114.61	117.70
1	1	33	C	O4'-C1'-N1	6.18	113.14	108.20
34	2	22	A	C5-C6-N6	-6.18	118.76	123.70
34	2	283	A	C4-C5-C6	6.18	120.09	117.00
1	1	24	G	O4'-C1'-N9	6.17	113.14	108.20
34	2	181	A	C4-C5-C6	6.17	120.09	117.00
34	2	288	A	C4-C5-C6	6.17	120.09	117.00
34	2	518	A	C5-C6-N6	-6.17	118.76	123.70
34	2	1109	A	C4-C5-C6	6.17	120.09	117.00
34	2	228	A	C4-C5-C6	6.17	120.09	117.00
34	2	232	A	C4-C5-C6	6.17	120.09	117.00
34	2	559	A	C4-C5-C6	6.17	120.09	117.00
34	2	858	A	C5-C6-N6	-6.17	118.76	123.70
34	2	1105	C	C6-N1-C1'	-6.17	113.39	120.80
34	2	35	C	N3-C4-N4	6.17	122.32	118.00
34	2	165	G	C5-C6-O6	-6.17	124.90	128.60
34	2	1145	A	C4-C5-C6	6.17	120.08	117.00
34	2	1431	C	O4'-C1'-N1	6.17	113.14	108.20
34	2	535	A	C5-C6-N6	-6.17	118.76	123.70
34	2	1668	U	O4'-C1'-N1	6.17	113.14	108.20
34	2	513	A	C4-C5-C6	6.17	120.08	117.00
34	2	565	A	C5-C6-N6	-6.17	118.77	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	826	A	C4-C5-C6	6.17	120.08	117.00
34	2	1226	C	N3-C4-N4	6.17	122.32	118.00
34	2	1328	A	C5-C6-N6	-6.17	118.77	123.70
34	2	1395	C	N3-C4-N4	6.17	122.32	118.00
34	2	32	U	O4'-C1'-N1	6.17	113.13	108.20
34	2	854	A	C4-C5-C6	6.17	120.08	117.00
34	2	1363	U	O4'-C1'-N1	6.17	113.13	108.20
34	2	1401	A	C5-C6-N6	-6.17	118.77	123.70
41	3	52	A	C4-C5-C6	6.17	120.08	117.00
34	2	595	A	C4-C5-C6	6.17	120.08	117.00
34	2	1083	A	C4-C5-C6	6.17	120.08	117.00
34	2	1089	A	C5-C6-N1	-6.17	114.62	117.70
34	2	1280	A	C5-C6-N6	-6.16	118.77	123.70
34	2	1775	A	C5-C6-N6	-6.16	118.77	123.70
34	2	121	U	O4'-C1'-N1	6.16	113.13	108.20
34	2	1687	U	O4'-C1'-N1	6.16	113.13	108.20
34	2	1703	C	N3-C4-C5	-6.16	119.44	121.90
34	2	487	C	N3-C4-N4	6.16	122.31	118.00
34	2	1299	C	C6-N1-C1'	-6.16	113.41	120.80
34	2	1585	C	N3-C4-N4	6.16	122.31	118.00
34	2	1650	C	N3-C4-N4	6.16	122.31	118.00
34	2	77	A	C4-C5-C6	6.16	120.08	117.00
34	2	168	C	N3-C4-N4	6.16	122.31	118.00
34	2	1803	A	C4-C5-C6	6.16	120.08	117.00
34	2	1829	A	C4-C5-C6	6.16	120.08	117.00
34	2	1078	A	C4-C5-C6	6.16	120.08	117.00
34	2	1380	C	N3-C4-N4	6.16	122.31	118.00
34	2	377	C	N3-C4-N4	6.16	122.31	118.00
34	2	1123	C	N3-C4-N4	6.16	122.31	118.00
34	2	1502	A	C4-C5-C6	6.16	120.08	117.00
34	2	330	C	N3-C4-N4	6.15	122.31	118.00
34	2	394	G	O4'-C1'-N9	6.15	113.12	108.20
34	2	1236	A	C5-C6-N6	-6.15	118.78	123.70
34	2	1578	C	O4'-C1'-N1	6.15	113.12	108.20
34	2	404	A	C5-C6-N6	-6.15	118.78	123.70
34	2	545	A	C4-C5-C6	6.15	120.08	117.00
34	2	944	C	N3-C4-N4	6.15	122.31	118.00
34	2	963	C	N3-C4-N4	6.15	122.31	118.00
34	2	1518	C	O4'-C1'-N1	6.15	113.12	108.20
34	2	1845	A	C4-C5-C6	6.15	120.08	117.00
1	1	41	C	N3-C4-N4	6.15	122.31	118.00
34	2	73	C	O4'-C1'-N1	6.15	113.12	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1479	A	O4'-C1'-N9	6.15	113.12	108.20
34	2	1860	A	C4-C5-C6	6.15	120.08	117.00
34	2	388	A	C4-C5-C6	6.15	120.07	117.00
34	2	1234	U	O4'-C1'-N1	6.15	113.12	108.20
34	2	1349	A	C4-C5-C6	6.15	120.07	117.00
34	2	1391	C	O4'-C1'-N1	6.15	113.12	108.20
34	2	1524	C	N3-C4-N4	6.15	122.30	118.00
34	2	1715	U	O4'-C1'-N1	6.15	113.12	108.20
34	2	1863	A	C5-C6-N6	-6.15	118.78	123.70
34	2	218	A	C4-C5-C6	6.14	120.07	117.00
34	2	347	C	N3-C4-N4	6.14	122.30	118.00
34	2	1554	C	N3-C4-N4	6.14	122.30	118.00
9	I	28	TYR	CB-CG-CD2	-6.14	117.31	121.00
34	2	809	A	C4-C5-C6	6.14	120.07	117.00
34	2	1097	U	O4'-C1'-N1	6.14	113.11	108.20
34	2	1378	A	C5-C6-N6	-6.14	118.79	123.70
34	2	85	A	C5-C6-N1	-6.14	114.63	117.70
34	2	1379	A	C4-C5-C6	6.14	120.07	117.00
34	2	1391	C	N3-C4-N4	6.14	122.30	118.00
34	2	1409	G	O4'-C1'-N9	6.14	113.11	108.20
34	2	486	C	N3-C4-N4	6.14	122.30	118.00
34	2	638	A	C4-C5-C6	6.14	120.07	117.00
34	2	238	G	O4'-C1'-N9	6.14	113.11	108.20
34	2	1495	U	O4'-C1'-N1	6.14	113.11	108.20
34	2	53	C	N3-C4-N4	6.13	122.29	118.00
34	2	195	C	N3-C4-C5	-6.13	119.45	121.90
34	2	398	A	C5-C6-N6	-6.13	118.79	123.70
34	2	882	A	C5-C6-N6	-6.13	118.79	123.70
34	2	1436	C	N3-C4-N4	6.13	122.29	118.00
1	1	76	A	C5-C6-N6	-6.13	118.80	123.70
34	2	361	A	C5-C6-N6	-6.13	118.80	123.70
34	2	1609	A	C4-C5-C6	6.13	120.07	117.00
34	2	1611	U	O4'-C1'-N1	6.13	113.11	108.20
34	2	4	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	566	A	C4-C5-C6	6.13	120.06	117.00
34	2	91	A	C4-C5-C6	6.13	120.06	117.00
34	2	240	C	O4'-C1'-N1	6.13	113.10	108.20
34	2	644	A	C4-C5-C6	6.13	120.06	117.00
34	2	976	A	C4-C5-C6	6.13	120.06	117.00
34	2	326	A	C4-C5-C6	6.13	120.06	117.00
34	2	662	A	C4-C5-C6	6.13	120.06	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1189	U	O4'-C1'-N1	6.13	113.10	108.20
34	2	1589	A	C5-C6-N6	-6.13	118.80	123.70
34	2	1413	C	N3-C4-N4	6.12	122.29	118.00
34	2	518	A	C4-C5-C6	6.12	120.06	117.00
34	2	225	C	O4'-C1'-N1	6.12	113.10	108.20
34	2	458	A	C4-C5-C6	6.12	120.06	117.00
34	2	490	A	C4-C5-C6	6.12	120.06	117.00
34	2	1255	A	C4-C5-C6	6.12	120.06	117.00
34	2	1513	C	N3-C4-C5	-6.12	119.45	121.90
34	2	1844	A	C5-C6-N1	-6.12	114.64	117.70
34	2	731	C	N3-C4-N4	6.12	122.28	118.00
34	2	835	C	C2-N1-C1'	6.12	125.53	118.80
34	2	1312	C	N3-C4-N4	6.12	122.28	118.00
34	2	1854	A	C4-C5-C6	6.12	120.06	117.00
34	2	449	C	N3-C4-N4	6.12	122.28	118.00
34	2	149	A	O4'-C1'-N9	6.12	113.09	108.20
34	2	983	A	C4-C5-C6	6.12	120.06	117.00
34	2	1104	G	O4'-C1'-N9	6.12	113.09	108.20
34	2	1604	C	N3-C4-C5	-6.11	119.45	121.90
34	2	490	A	C5-C6-N6	-6.11	118.81	123.70
34	2	1102	C	N3-C4-N4	6.11	122.28	118.00
1	1	69	U	O4'-C1'-N1	6.11	113.09	108.20
34	2	1209	C	N3-C4-N4	6.11	122.28	118.00
34	2	1333	C	N3-C4-N4	6.11	122.28	118.00
34	2	1596	A	C4-C5-C6	6.11	120.05	117.00
34	2	1659	A	C4-C5-C6	6.11	120.05	117.00
34	2	994	A	C5-C6-N1	-6.11	114.65	117.70
34	2	1366	A	C5-C6-N6	-6.11	118.81	123.70
34	2	1719	A	C5-C6-N6	-6.11	118.82	123.70
38	k	440	GLN	O-C-N	-6.11	112.93	122.70
34	2	42	A	C4-C5-C6	6.10	120.05	117.00
34	2	1407	G	C5-C6-O6	-6.10	124.94	128.60
34	2	1775	A	C4-C5-C6	6.10	120.05	117.00
34	2	516	A	O4'-C1'-N9	6.10	113.08	108.20
34	2	1350	G	C5-C6-O6	-6.10	124.94	128.60
34	2	1401	A	C4-C5-C6	6.10	120.05	117.00
34	2	554	A	C4-C5-C6	6.10	120.05	117.00
34	2	1237	A	C4-C5-C6	6.10	120.05	117.00
24	Z	41	PHE	CB-CG-CD1	6.10	125.07	120.80
34	2	215	U	O4'-C1'-N1	6.10	113.08	108.20
34	2	317	G	O4'-C1'-N9	6.10	113.08	108.20
34	2	340	C	N3-C4-N4	6.10	122.27	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	968	A	C5-C6-N1	-6.10	114.65	117.70
34	2	1141	A	C5-C6-N6	-6.10	118.82	123.70
34	2	98	C	N3-C4-N4	6.10	122.27	118.00
34	2	141	A	C5-C6-N6	-6.10	118.82	123.70
34	2	332	C	N3-C4-N4	6.10	122.27	118.00
34	2	1007	A	C4-C5-C6	6.10	120.05	117.00
34	2	1136	G	O4'-C1'-N9	6.10	113.08	108.20
34	2	1739	G	N3-C2-N2	6.10	124.17	119.90
34	2	1178	A	C5-C6-N1	-6.09	114.65	117.70
34	2	1222	G	N3-C2-N2	6.09	124.17	119.90
34	2	1540	A	C4-C5-C6	6.09	120.05	117.00
34	2	232	A	C5-C6-N6	-6.09	118.83	123.70
34	2	343	C	N3-C4-N4	6.09	122.26	118.00
34	2	1214	C	N3-C4-N4	6.09	122.26	118.00
34	2	1392	A	C4-C5-C6	6.09	120.05	117.00
34	2	1277	G	O4'-C1'-N9	6.09	113.07	108.20
34	2	1582	G	C5-C6-O6	-6.09	124.95	128.60
34	2	63	U	O4'-C1'-N1	6.09	113.07	108.20
34	2	205	G	C5-C6-O6	-6.09	124.95	128.60
34	2	395	G	O4'-C1'-N9	6.09	113.07	108.20
34	2	536	G	P-O3'-C3'	6.09	127.00	119.70
34	2	574	A	C5-C6-N6	-6.09	118.83	123.70
34	2	805	A	C4-C5-C6	6.09	120.04	117.00
34	2	1115	A	O4'-C1'-N9	6.09	113.07	108.20
34	2	1008	A	C4-C5-C6	6.08	120.04	117.00
34	2	1538	U	O4'-C1'-N1	6.08	113.07	108.20
34	2	182	C	N3-C4-N4	6.08	122.26	118.00
34	2	127	C	O4'-C1'-N1	6.08	113.06	108.20
34	2	1684	C	N3-C4-N4	6.08	122.26	118.00
34	2	1695	C	N3-C4-N4	6.08	122.26	118.00
34	2	904	A	C5-C6-N6	-6.08	118.84	123.70
12	L	159	PHE	CB-CG-CD1	6.08	125.06	120.80
34	2	882	A	C4-C5-C6	6.08	120.04	117.00
34	2	1120	C	N3-C4-N4	6.08	122.25	118.00
34	2	1551	A	C4-C5-C6	6.08	120.04	117.00
34	2	1629	A	C4-C5-C6	6.08	120.04	117.00
34	2	1038	A	C5-C6-N6	-6.08	118.84	123.70
34	2	476	A	C4-C5-C6	6.08	120.04	117.00
34	2	823	A	C4-C5-C6	6.08	120.04	117.00
34	2	26	U	O4'-C1'-N1	6.07	113.06	108.20
34	2	423	A	C5-C6-N1	-6.07	114.66	117.70
34	2	951	A	C4-C5-C6	6.07	120.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1337	C	N3-C4-N4	6.07	122.25	118.00
34	2	1482	A	C4-C5-C6	6.07	120.04	117.00
34	2	554	A	O4'-C1'-N9	6.07	113.06	108.20
34	2	584	A	C4-C5-C6	6.07	120.03	117.00
34	2	1176	C	N3-C4-N4	6.07	122.25	118.00
34	2	1694	A	C4-C5-C6	6.07	120.03	117.00
34	2	175	A	C4-C5-C6	6.07	120.03	117.00
34	2	463	A	C4-C5-C6	6.07	120.03	117.00
34	2	1079	A	C4-C5-C6	6.07	120.03	117.00
1	1	59	A	C4-C5-C6	6.07	120.03	117.00
34	2	405	A	C4-C5-C6	6.07	120.03	117.00
34	2	1242	A	C5-C6-N6	-6.07	118.85	123.70
34	2	1540	A	O4'-C1'-N9	6.07	113.05	108.20
34	2	1269	C	N3-C4-N4	6.06	122.25	118.00
34	2	107	A	C4-C5-C6	6.06	120.03	117.00
34	2	940	A	C5-C6-N1	-6.06	114.67	117.70
34	2	1807	A	C4-C5-C6	6.06	120.03	117.00
34	2	1644	U	O4'-C1'-N1	6.06	113.05	108.20
37	j	95	TYR	CB-CG-CD2	-6.06	117.36	121.00
34	2	152	U	O4'-C1'-N1	6.06	113.05	108.20
34	2	916	A	C5-C6-N1	-6.06	114.67	117.70
34	2	1249	A	C4-C5-C6	6.06	120.03	117.00
34	2	404	A	C4-C5-C6	6.05	120.03	117.00
34	2	959	A	C4-C5-C6	6.05	120.03	117.00
34	2	1029	G	N3-C2-N2	6.05	124.14	119.90
34	2	1161	G	O4'-C1'-N9	6.05	113.04	108.20
34	2	1835	C	N3-C4-N4	6.05	122.24	118.00
34	2	1056	A	O4'-C1'-N9	6.05	113.04	108.20
34	2	223	A	C4-C5-C6	6.05	120.03	117.00
34	2	327	C	N3-C4-N4	6.05	122.24	118.00
34	2	528	U	O4'-C1'-N1	6.05	113.04	108.20
34	2	880	C	N3-C4-N4	6.05	122.24	118.00
34	2	1274	A	C4-C5-C6	6.05	120.03	117.00
34	2	1862	U	C2-N1-C1'	6.05	124.96	117.70
34	2	169	U	O4'-C1'-N1	6.05	113.04	108.20
34	2	521	A	C4-C5-C6	6.05	120.03	117.00
34	2	423	A	C5-C6-N6	-6.05	118.86	123.70
34	2	643	A	C5-C6-N6	-6.05	118.86	123.70
34	2	589	A	C4-C5-C6	6.05	120.02	117.00
34	2	1045	A	C5-C6-N1	-6.05	114.68	117.70
34	2	354	A	C5-C6-N1	-6.04	114.68	117.70
34	2	459	A	C4-C5-C6	6.04	120.02	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	514	U	O4'-C1'-N1	6.04	113.04	108.20
34	2	453	C	O4'-C1'-N1	6.04	113.03	108.20
34	2	624	A	C4-C5-C6	6.04	120.02	117.00
34	2	1306	U	O4'-C1'-N1	6.04	113.03	108.20
34	2	1863	A	C4-C5-C6	6.04	120.02	117.00
34	2	643	A	C4-C5-C6	6.04	120.02	117.00
34	2	1669	G	N3-C2-N2	6.04	124.13	119.90
34	2	1053	C	C6-N1-C1'	-6.04	113.55	120.80
34	2	1179	A	C5-C6-N6	-6.04	118.87	123.70
34	2	1295	A	C5-C6-N6	-6.04	118.87	123.70
34	2	207	U	O4'-C1'-N1	6.04	113.03	108.20
34	2	640	A	C4-C5-C6	6.04	120.02	117.00
34	2	442	G	O4'-C1'-N9	6.04	113.03	108.20
34	2	1365	A	C5-C6-N6	-6.04	118.87	123.70
34	2	445	A	C4-C5-C6	6.04	120.02	117.00
34	2	940	A	C5-C6-N6	-6.04	118.87	123.70
34	2	1171	G	O4'-C1'-N9	6.04	113.03	108.20
34	2	1476	A	C4-C5-C6	6.04	120.02	117.00
34	2	1590	U	O4'-C1'-N1	6.04	113.03	108.20
34	2	1716	U	O4'-C1'-N1	6.04	113.03	108.20
34	2	798	A	C4-C5-C6	6.03	120.02	117.00
34	2	900	A	C4-C5-C6	6.03	120.02	117.00
34	2	1146	A	C4-C5-C6	6.03	120.02	117.00
34	2	1422	U	O4'-C1'-N1	6.03	113.03	108.20
34	2	909	A	C4-C5-C6	6.03	120.02	117.00
34	2	49	C	O4'-C1'-N1	6.03	113.02	108.20
34	2	339	A	C4-C5-C6	6.03	120.02	117.00
34	2	1636	A	C4-C5-C6	6.03	120.02	117.00
34	2	1031	A	C4-C5-C6	6.03	120.02	117.00
34	2	1693	C	N3-C4-N4	6.03	122.22	118.00
1	1	58	A	C5-C6-N6	-6.03	118.88	123.70
34	2	99	A	C4-C5-C6	6.03	120.01	117.00
34	2	297	C	O4'-C1'-N1	6.03	113.02	108.20
34	2	346	C	O4'-C1'-N1	6.03	113.02	108.20
34	2	1368	U	O4'-C1'-N1	6.03	113.02	108.20
34	2	1774	G	O4'-C1'-N9	6.03	113.02	108.20
34	2	629	C	N3-C4-N4	6.03	122.22	118.00
34	2	1073	A	C5-C6-N6	-6.03	118.88	123.70
34	2	1460	C	O4'-C1'-N1	6.03	113.02	108.20
34	2	1567	C	N3-C4-C5	-6.03	119.49	121.90
34	2	1607	G	O4'-C1'-N9	6.03	113.02	108.20
34	2	303	G	O4'-C1'-N9	6.02	113.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	340	C	O4'-C1'-N1	6.02	113.02	108.20
34	2	107	A	C5-C6-N6	-6.02	118.88	123.70
34	2	1076	A	C4-C5-C6	6.02	120.01	117.00
34	2	1227	C	N3-C4-N4	6.02	122.22	118.00
34	2	1247	A	C4-C5-C6	6.02	120.01	117.00
34	2	1431	C	N3-C4-N4	6.02	122.22	118.00
34	2	1639	C	N3-C4-N4	6.02	122.22	118.00
34	2	54	A	C4-C5-C6	6.02	120.01	117.00
34	2	1081	C	N3-C4-C5	-6.02	119.49	121.90
34	2	171	A	C4-C5-C6	6.02	120.01	117.00
34	2	992	A	C4-C5-C6	6.02	120.01	117.00
34	2	1691	C	O4'-C1'-N1	6.02	113.02	108.20
34	2	1734	C	N3-C4-N4	6.02	122.21	118.00
34	2	225	C	N3-C4-N4	6.02	122.21	118.00
34	2	1465	A	C4-C5-C6	6.02	120.01	117.00
34	2	333	A	C4-C5-C6	6.02	120.01	117.00
34	2	898	G	O4'-C1'-N9	6.02	113.01	108.20
34	2	900	A	C5-C6-N1	-6.02	114.69	117.70
34	2	326	A	C5-C6-N1	-6.01	114.69	117.70
34	2	450	A	C4-C5-C6	6.01	120.01	117.00
34	2	845	A	C4-C5-C6	6.01	120.01	117.00
34	2	1144	A	C4-C5-C6	6.01	120.01	117.00
34	2	1667	U	O4'-C1'-N1	6.01	113.01	108.20
34	2	20	G	O4'-C1'-N9	6.01	113.01	108.20
34	2	448	A	C5-C6-N6	-6.01	118.89	123.70
34	2	1735	C	N3-C4-C5	-6.01	119.50	121.90
34	2	630	A	C5-C6-N6	-6.01	118.89	123.70
34	2	812	A	C4-C5-C6	6.01	120.00	117.00
34	2	1800	A	C4-C5-C6	6.01	120.00	117.00
34	2	1264	C	O4'-C1'-N1	6.01	113.01	108.20
34	2	153	G	O4'-C1'-N9	6.01	113.00	108.20
34	2	1625	A	C4-C5-C6	6.01	120.00	117.00
34	2	1690	A	C4-C5-C6	6.01	120.00	117.00
34	2	346	C	N3-C4-N4	6.00	122.20	118.00
34	2	9	U	O4'-C1'-N1	6.00	113.00	108.20
34	2	922	A	C4-C5-C6	6.00	120.00	117.00
34	2	953	A	C4-C5-C6	6.00	120.00	117.00
34	2	1026	A	C4-C5-C6	6.00	120.00	117.00
34	2	1426	C	N3-C4-N4	6.00	122.20	118.00
34	2	1782	A	C4-C5-C6	6.00	120.00	117.00
37	j	19	ASN	C-N-CA	6.00	136.71	121.70
34	2	423	A	C4-C5-C6	6.00	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1005	A	O4'-C1'-N9	6.00	113.00	108.20
34	2	1291	A	C5-C6-N1	-6.00	114.70	117.70
34	2	2	A	C4-C5-C6	6.00	120.00	117.00
34	2	1177	A	C4-C5-C6	6.00	120.00	117.00
34	2	435	A	C4-C5-C6	6.00	120.00	117.00
34	2	1119	C	N3-C4-N4	6.00	122.20	118.00
34	2	1583	A	C4-C5-C6	6.00	120.00	117.00
34	2	960	A	O4'-C1'-N9	6.00	113.00	108.20
34	2	979	A	C5-C6-N6	-6.00	118.90	123.70
34	2	1194	G	C5-C6-O6	-5.99	125.00	128.60
34	2	1245	C	N3-C4-N4	5.99	122.19	118.00
34	2	1693	C	O4'-C1'-N1	5.99	112.99	108.20
34	2	850	A	C4-C5-C6	5.99	120.00	117.00
34	2	1067	G	P-O3'-C3'	5.99	126.89	119.70
34	2	1473	U	C2-N1-C1'	5.99	124.89	117.70
34	2	1001	G	O4'-C1'-N9	5.99	112.99	108.20
34	2	1212	C	O4'-C1'-N1	5.99	112.99	108.20
34	2	1256	A	C4-C5-C6	5.99	120.00	117.00
34	2	1398	A	C4-C5-C6	5.99	120.00	117.00
1	1	67	U	O4'-C1'-N1	5.99	112.99	108.20
34	2	638	A	C5-C6-N6	-5.99	118.91	123.70
34	2	1094	C	N3-C4-N4	5.99	122.19	118.00
34	2	1526	A	C5-C6-N6	-5.99	118.91	123.70
34	2	1754	G	O4'-C1'-N9	5.99	112.99	108.20
34	2	1101	G	O4'-C1'-N9	5.99	112.99	108.20
34	2	1196	A	C4-C5-C6	5.99	119.99	117.00
34	2	1534	U	O4'-C1'-N1	5.98	112.99	108.20
34	2	292	A	C4-C5-C6	5.98	119.99	117.00
34	2	976	A	C5-C6-N6	-5.98	118.92	123.70
34	2	984	C	O4'-C1'-N1	5.98	112.98	108.20
34	2	1574	A	C5-C6-N6	-5.98	118.92	123.70
34	2	664	C	N3-C4-C5	-5.98	119.51	121.90
34	2	918	A	C5-C6-N6	-5.98	118.92	123.70
34	2	493	C	N3-C4-N4	5.98	122.18	118.00
34	2	564	A	C4-C5-C6	5.98	119.99	117.00
34	2	1710	A	C4-C5-C6	5.98	119.99	117.00
34	2	1780	U	O4'-C1'-N1	5.98	112.98	108.20
34	2	1011	U	O4'-C1'-N1	5.97	112.98	108.20
34	2	1019	A	C4-C5-C6	5.97	119.99	117.00
34	2	1374	A	C4-C5-C6	5.97	119.99	117.00
34	2	288	A	C5-C6-N6	-5.97	118.92	123.70
34	2	445	A	C5-C6-N1	-5.97	114.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	502	A	C4-C5-C6	5.97	119.99	117.00
34	2	850	A	C5-C6-N1	-5.97	114.71	117.70
34	2	166	A	C4-C5-C6	5.97	119.98	117.00
34	2	516	A	C4-C5-C6	5.97	119.98	117.00
34	2	631	A	C5-C6-N6	-5.97	118.92	123.70
1	1	44	A	C4-C5-C6	5.97	119.98	117.00
34	2	1494	A	C5-C6-N1	-5.97	114.72	117.70
34	2	540	C	O4'-C1'-N1	5.97	112.97	108.20
34	2	896	C	N3-C4-C5	-5.97	119.51	121.90
1	1	73	A	C4-C5-C6	5.96	119.98	117.00
34	2	58	C	N3-C4-N4	5.96	122.17	118.00
1	1	26	G	O4'-C1'-N9	5.96	112.97	108.20
34	2	61	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	1472	A	C5-C6-N6	-5.96	118.93	123.70
34	2	1826	A	C5-C6-N1	-5.96	114.72	117.70
34	2	1461	A	C4-C5-C6	5.96	119.98	117.00
34	2	226	A	C4-C5-C6	5.96	119.98	117.00
34	2	1211	C	N3-C4-N4	5.96	122.17	118.00
34	2	1432	C	N3-C4-N4	5.96	122.17	118.00
34	2	1597	U	O4'-C1'-N1	5.96	112.97	108.20
34	2	195	C	N3-C4-N4	5.96	122.17	118.00
34	2	206	A	C5-C6-N1	-5.96	114.72	117.70
34	2	972	G	O4'-C1'-N9	5.96	112.97	108.20
34	2	1016	A	C5-C6-N6	-5.96	118.94	123.70
34	2	1289	A	C4-C5-C6	5.96	119.98	117.00
34	2	1470	A	C4-C5-C6	5.96	119.98	117.00
34	2	1659	A	C5-C6-N6	-5.96	118.94	123.70
34	2	1405	A	C4-C5-C6	5.96	119.98	117.00
34	2	1670	A	C5-C6-N6	-5.95	118.94	123.70
34	2	1441	U	O4'-C1'-N1	5.95	112.96	108.20
34	2	19	A	C4-C5-C6	5.95	119.98	117.00
34	2	430	G	O4'-C1'-N9	5.95	112.96	108.20
34	2	814	A	C4-C5-C6	5.95	119.97	117.00
34	2	897	G	C5-C6-O6	-5.95	125.03	128.60
34	2	943	G	O4'-C1'-N9	5.95	112.96	108.20
34	2	1553	C	N3-C4-N4	5.95	122.17	118.00
34	2	559	A	C5-C6-N6	-5.95	118.94	123.70
34	2	1146	A	C5-C6-N1	-5.95	114.73	117.70
34	2	1587	C	N3-C4-N4	5.95	122.16	118.00
34	2	1616	U	O4'-C1'-N1	5.95	112.96	108.20
1	1	56	C	N3-C4-C5	-5.95	119.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	24	C	N3-C4-C5	-5.95	119.52	121.90
34	2	141	A	C4-C5-C6	5.95	119.97	117.00
34	2	860	A	C4-C5-C6	5.95	119.97	117.00
34	2	1657	U	O4'-C1'-N1	5.95	112.96	108.20
35	A	33	TYR	CB-CG-CD1	5.95	124.57	121.00
34	2	45	A	C4-C5-C6	5.94	119.97	117.00
34	2	379	A	C5-C6-N6	-5.94	118.94	123.70
34	2	14	C	N3-C4-C5	-5.94	119.52	121.90
34	2	1038	A	C4-C5-C6	5.94	119.97	117.00
34	2	1127	G	O4'-C1'-N9	5.94	112.95	108.20
34	2	1250	C	N3-C4-N4	5.94	122.16	118.00
34	2	1448	A	C4-C5-C6	5.94	119.97	117.00
34	2	1533	C	N3-C4-C5	-5.94	119.52	121.90
34	2	475	A	C4-C5-C6	5.94	119.97	117.00
34	2	1067	G	O4'-C1'-N9	5.94	112.95	108.20
34	2	357	U	O4'-C1'-N1	5.94	112.95	108.20
34	2	582	C	N3-C4-N4	5.94	122.16	118.00
34	2	1081	C	N3-C4-N4	5.94	122.16	118.00
34	2	1219	A	C5-C6-N6	-5.94	118.95	123.70
34	2	934	A	C4-C5-C6	5.93	119.97	117.00
34	2	1224	A	C4-C5-C6	5.93	119.97	117.00
34	2	1434	A	C5-C6-N6	-5.93	118.95	123.70
34	2	463	A	C5-C6-N6	-5.93	118.95	123.70
34	2	857	A	C4-C5-C6	5.93	119.97	117.00
34	2	1218	G	O3'-P-O5'	-5.93	92.73	104.00
34	2	1443	G	O4'-C1'-N9	5.93	112.95	108.20
34	2	293	A	C5-C6-N1	-5.93	114.73	117.70
34	2	904	A	C5-C6-N1	-5.93	114.73	117.70
34	2	1255	A	C5-C6-N6	-5.93	118.96	123.70
1	1	35	A	C4-C5-C6	5.93	119.96	117.00
34	2	39	A	C4-C5-C6	5.93	119.96	117.00
34	2	1161	G	N1-C6-O6	5.93	123.46	119.90
34	2	1243	C	O4'-C1'-N1	5.93	112.94	108.20
34	2	335	U	O4'-C1'-N1	5.92	112.94	108.20
34	2	1785	A	C4-C5-C6	5.92	119.96	117.00
34	2	525	G	O4'-C1'-N9	5.92	112.94	108.20
34	2	1641	C	N3-C4-N4	5.92	122.15	118.00
34	2	986	A	C5-C6-N1	-5.92	114.74	117.70
34	2	1574	A	C4-C5-C6	5.92	119.96	117.00
34	2	1795	A	C4-C5-C6	5.92	119.96	117.00
34	2	1812	A	C4-C5-C6	5.92	119.96	117.00
34	2	201	G	O4'-C1'-N9	5.92	112.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	809	A	C5-C6-N6	-5.92	118.96	123.70
34	2	1472	A	P-O3'-C3'	5.92	126.80	119.70
34	2	1692	A	C5-C6-N6	-5.92	118.96	123.70
34	2	517	C	N3-C4-N4	5.92	122.14	118.00
34	2	1027	A	C5-C6-N1	-5.92	114.74	117.70
34	2	1451	A	C4-C5-C6	5.92	119.96	117.00
34	2	147	A	C5-C6-N6	-5.92	118.97	123.70
34	2	176	U	O4'-C1'-N1	5.92	112.93	108.20
34	2	808	A	O4'-C1'-N9	5.91	112.93	108.20
34	2	408	A	O4'-C1'-N9	5.91	112.93	108.20
34	2	511	A	C5-C6-N1	-5.91	114.75	117.70
34	2	1307	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	1600	G	N3-C2-N2	5.91	124.04	119.90
34	2	482	C	O4'-C1'-N1	5.91	112.93	108.20
34	2	1141	A	C5-C6-N1	-5.91	114.75	117.70
34	2	1584	A	C5-C6-N1	-5.91	114.75	117.70
34	2	188	U	O4'-C1'-N1	5.91	112.92	108.20
34	2	111	A	C4-C5-C6	5.91	119.95	117.00
34	2	631	A	C4-C5-C6	5.91	119.95	117.00
34	2	1090	C	N3-C4-N4	5.91	122.13	118.00
34	2	234	C	N3-C4-C5	-5.90	119.54	121.90
34	2	979	A	O4'-C1'-N9	5.90	112.92	108.20
34	2	1218	G	O4'-C1'-N9	5.90	112.92	108.20
34	2	1781	G	O4'-C1'-N9	5.90	112.92	108.20
34	2	72	C	N3-C4-N4	5.90	122.13	118.00
34	2	628	C	N3-C4-N4	5.90	122.13	118.00
34	2	1336	U	O4'-C1'-N1	5.90	112.92	108.20
34	2	1482	A	C5-C6-N6	-5.90	118.98	123.70
34	2	272	C	O4'-C1'-N1	5.90	112.92	108.20
34	2	545	A	C5-C6-N1	-5.90	114.75	117.70
1	1	15	A	C5-C6-N6	-5.90	118.98	123.70
34	2	381	C	N3-C4-N4	5.90	122.13	118.00
34	2	1844	A	C4-C5-C6	5.90	119.95	117.00
34	2	37	C	N3-C4-N4	5.89	122.13	118.00
34	2	498	A	C4-C5-C6	5.89	119.95	117.00
34	2	535	A	C4-C5-C6	5.89	119.95	117.00
34	2	1249	A	C5-C6-N6	-5.89	118.98	123.70
34	2	85	A	C4-C5-C6	5.89	119.94	117.00
34	2	159	A	C4-C5-C6	5.89	119.94	117.00
34	2	1082	G	O4'-C1'-N9	5.89	112.91	108.20
34	2	853	U	O4'-C1'-N1	5.89	112.91	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	510	A	C5-C6-N6	-5.89	118.99	123.70
34	2	1004	A	C5-C6-N6	-5.89	118.99	123.70
34	2	1105	C	N3-C4-N4	5.89	122.12	118.00
34	2	356	U	O4'-C1'-N1	5.88	112.91	108.20
34	2	1096	A	C4-C5-C6	5.88	119.94	117.00
34	2	871	A	C4-C5-C6	5.88	119.94	117.00
1	1	74	C	N3-C4-N4	5.88	122.12	118.00
34	2	661	A	C4-C5-C6	5.88	119.94	117.00
34	2	593	C	O4'-C1'-N1	5.88	112.90	108.20
34	2	1746	C	O4'-C1'-N1	5.88	112.90	108.20
34	2	554	A	C5-C6-N6	-5.88	119.00	123.70
34	2	821	A	C4-C5-C6	5.88	119.94	117.00
34	2	1048	A	C4-C5-C6	5.88	119.94	117.00
34	2	588	G	O4'-C1'-N9	5.88	112.90	108.20
34	2	1170	U	N3-C4-O4	5.88	123.51	119.40
34	2	1291	A	C4-C5-C6	5.88	119.94	117.00
34	2	1468	C	N3-C4-N4	5.88	122.11	118.00
34	2	1651	G	O4'-C1'-N9	5.88	112.90	108.20
34	2	1661	C	N3-C4-C5	-5.88	119.55	121.90
34	2	70	G	O4'-C1'-N9	5.88	112.90	108.20
34	2	1414	C	N3-C4-N4	5.88	122.11	118.00
34	2	27	A	C5-C6-N6	-5.87	119.00	123.70
34	2	390	C	N3-C4-N4	5.87	122.11	118.00
34	2	896	C	N3-C4-N4	5.87	122.11	118.00
34	2	953	A	C5-C6-N1	-5.87	114.76	117.70
34	2	1642	A	C4-C5-C6	5.87	119.94	117.00
34	2	64	A	C4-C5-C6	5.87	119.94	117.00
34	2	382	A	C4-C5-C6	5.87	119.94	117.00
34	2	513	A	O4'-C1'-N9	5.87	112.90	108.20
34	2	1543	G	O4'-C1'-N9	5.87	112.90	108.20
34	2	103	A	C4-C5-C6	5.87	119.93	117.00
34	2	609	A	C4-C5-C6	5.87	119.93	117.00
34	2	1008	A	C5-C6-N6	-5.87	119.00	123.70
34	2	1051	A	C4-C5-C6	5.87	119.93	117.00
34	2	1430	C	N3-C4-N4	5.87	122.11	118.00
34	2	333	A	C5-C6-N1	-5.87	114.77	117.70
34	2	376	C	N3-C4-N4	5.87	122.11	118.00
34	2	855	G	O4'-C1'-N9	5.87	112.89	108.20
34	2	899	A	C4-C5-C6	5.87	119.93	117.00
34	2	1674	A	C5-C6-N6	-5.87	119.01	123.70
34	2	1476	A	C5-C6-N6	-5.86	119.01	123.70
34	2	1435	A	C4-C5-C6	5.86	119.93	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	475	A	C5-C6-N6	-5.86	119.01	123.70
34	2	651	U	O4'-C1'-N1	5.86	112.89	108.20
34	2	1640	C	N3-C4-N4	5.86	122.10	118.00
1	1	30	G	O4'-C1'-N9	5.86	112.89	108.20
1	1	42	A	O4'-C1'-N9	5.86	112.89	108.20
34	2	229	A	C5-C6-N1	-5.86	114.77	117.70
34	2	523	A	C4-C5-C6	5.86	119.93	117.00
34	2	947	C	N3-C4-N4	5.86	122.10	118.00
34	2	1022	C	O4'-C1'-N1	5.86	112.89	108.20
34	2	27	A	C4-C5-C6	5.85	119.93	117.00
34	2	474	A	C5-C6-N1	-5.85	114.77	117.70
34	2	481	C	N3-C4-N4	5.85	122.10	118.00
34	2	1839	A	C5-C6-N6	-5.85	119.02	123.70
34	2	1195	A	C4-C5-C6	5.85	119.93	117.00
34	2	510	A	C4-C5-C6	5.85	119.92	117.00
34	2	868	A	C5-C6-N6	-5.85	119.02	123.70
34	2	1439	C	N3-C4-N4	5.85	122.09	118.00
10	J	63	PHE	CB-CG-CD1	5.85	124.89	120.80
34	2	1139	A	C5-C6-N6	-5.85	119.02	123.70
34	2	50	A	C5-C6-N6	-5.85	119.02	123.70
34	2	237	G	OP2-P-O3'	5.85	118.06	105.20
34	2	1710	A	C5-C6-N6	-5.85	119.02	123.70
4	D	84	PHE	CB-CG-CD1	5.84	124.89	120.80
34	2	978	G	O4'-C1'-N9	5.84	112.88	108.20
34	2	1789	G	O4'-C1'-N9	5.84	112.88	108.20
38	k	267	ARG	NE-CZ-NH2	5.84	123.22	120.30
34	2	516	A	C5-C6-N1	-5.84	114.78	117.70
35	A	33	TYR	CB-CG-CD2	-5.84	117.50	121.00
34	2	221	A	C4-C5-C6	5.84	119.92	117.00
34	2	407	C	N3-C4-N4	5.84	122.09	118.00
34	2	1204	A	C4-C5-C6	5.84	119.92	117.00
34	2	1691	C	N3-C4-C5	-5.84	119.56	121.90
34	2	65	C	N3-C4-N4	5.84	122.09	118.00
34	2	1410	A	C5-C6-N1	-5.84	114.78	117.70
1	1	2	A	C4-C5-C6	5.84	119.92	117.00
34	2	509	A	C4-C5-C6	5.84	119.92	117.00
38	k	481	ASP	CB-CG-OD2	-5.84	113.05	118.30
34	2	1507	U	O4'-C1'-N1	5.83	112.87	108.20
34	2	307	G	O4'-C1'-N9	5.83	112.87	108.20
34	2	1004	A	C4-C5-C6	5.83	119.92	117.00
34	2	1031	A	C5-C6-N6	-5.83	119.03	123.70
34	2	40	A	C5-C6-N6	-5.83	119.03	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	459	A	O4'-C1'-N9	5.83	112.86	108.20
34	2	1235	U	O4'-C1'-N1	5.83	112.86	108.20
34	2	1406	C	N3-C4-N4	5.83	122.08	118.00
34	2	1482	A	O4'-C1'-N9	5.83	112.86	108.20
34	2	1703	C	N3-C4-N4	5.83	122.08	118.00
34	2	146	G	O4'-C1'-N9	5.83	112.86	108.20
34	2	609	A	C5-C6-N1	-5.83	114.79	117.70
34	2	865	A	C4-C5-C6	5.83	119.92	117.00
34	2	631	A	C5-C6-N1	-5.83	114.79	117.70
34	2	309	A	C4-C5-C6	5.83	119.91	117.00
34	2	877	G	O4'-C1'-N9	5.83	112.86	108.20
34	2	275	C	O4'-C1'-N1	5.82	112.86	108.20
34	2	1344	G	O4'-C1'-N9	5.82	112.86	108.20
34	2	454	A	C4-C5-C6	5.82	119.91	117.00
34	2	1721	G	O4'-C1'-N9	5.82	112.86	108.20
1	1	15	A	C4-C5-C6	5.82	119.91	117.00
34	2	185	C	N3-C4-C5	-5.82	119.57	121.90
34	2	458	A	C5-C6-N6	-5.82	119.04	123.70
34	2	835	C	O4'-C1'-N1	5.82	112.86	108.20
34	2	869	G	P-O3'-C3'	5.82	126.68	119.70
34	2	923	C	N3-C4-N4	5.82	122.07	118.00
34	2	1026	A	C5-C6-N6	-5.82	119.04	123.70
34	2	1387	C	N3-C4-N4	5.82	122.07	118.00
34	2	496	G	O4'-C1'-N9	5.82	112.86	108.20
34	2	60	A	C4-C5-C6	5.82	119.91	117.00
34	2	857	A	C5-C6-N6	-5.82	119.05	123.70
34	2	899	A	C5-C6-N1	-5.82	114.79	117.70
34	2	228	A	C5-C6-N1	-5.82	114.79	117.70
34	2	548	G	O4'-C1'-N9	5.82	112.85	108.20
34	2	1016	A	C5-C6-N1	-5.81	114.79	117.70
34	2	1808	G	N3-C2-N2	5.81	123.97	119.90
34	2	1154	G	O4'-C1'-N9	5.81	112.85	108.20
34	2	142	C	N3-C4-N4	5.81	122.07	118.00
34	2	677	C	N3-C4-N4	5.81	122.07	118.00
34	2	969	C	N3-C4-C5	-5.81	119.58	121.90
41	3	40	C	O3'-P-O5'	5.81	115.04	104.00
34	2	379	A	C4-C5-C6	5.81	119.90	117.00
34	2	551	A	O4'-C1'-N9	5.81	112.85	108.20
34	2	584	A	C5-C6-N1	-5.81	114.80	117.70
34	2	1035	C	N3-C4-N4	5.81	122.07	118.00
34	2	1248	C	N3-C4-N4	5.81	122.06	118.00
34	2	1771	G	O4'-C1'-N9	5.81	112.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	804	A	C4-C5-C6	5.81	119.90	117.00
34	2	819	U	O4'-C1'-N1	5.81	112.84	108.20
34	2	142	C	C2-N1-C1'	5.80	125.18	118.80
34	2	1356	U	O4'-C1'-N1	5.80	112.84	108.20
34	2	1782	A	C5-C6-N6	-5.80	119.06	123.70
34	2	166	A	C5-C6-N1	-5.80	114.80	117.70
34	2	796	U	O4'-C1'-N1	5.80	112.84	108.20
34	2	958	A	C5-C6-N6	-5.80	119.06	123.70
34	2	1086	C	N3-C4-N4	5.80	122.06	118.00
34	2	502	A	C5-C6-N1	-5.80	114.80	117.70
34	2	1216	A	C4-C5-C6	5.80	119.90	117.00
34	2	1185	A	C5-C6-N1	-5.80	114.80	117.70
34	2	805	A	C5-C6-N6	-5.80	119.06	123.70
34	2	1673	A	C5-C6-N6	-5.80	119.06	123.70
34	2	1857	A	C4-C5-C6	5.80	119.90	117.00
1	1	59	A	C5-C6-N1	-5.79	114.80	117.70
34	2	934	A	C5-C6-N1	-5.79	114.80	117.70
34	2	234	C	N3-C4-N4	5.79	122.06	118.00
34	2	399	C	N3-C4-N4	5.79	122.06	118.00
34	2	510	A	O4'-C1'-N9	5.79	112.83	108.20
34	2	966	G	O4'-C1'-N9	5.79	112.83	108.20
34	2	1019	A	C5-C6-N6	-5.79	119.07	123.70
34	2	1690	A	C5-C6-N6	-5.79	119.06	123.70
34	2	512	A	C5-C6-N1	-5.79	114.80	117.70
34	2	1297	A	C5-C6-N1	-5.79	114.81	117.70
34	2	1499	C	N3-C4-N4	5.79	122.05	118.00
34	2	1670	A	C4-C5-C6	5.79	119.89	117.00
34	2	462	C	N3-C4-C5	-5.79	119.58	121.90
34	2	1564	A	C5-C6-N6	-5.79	119.07	123.70
34	2	1727	G	O4'-C1'-N9	5.79	112.83	108.20
34	2	1839	A	O4'-C1'-N9	5.78	112.83	108.20
34	2	159	A	C5-C6-N1	-5.78	114.81	117.70
34	2	1204	A	C5-C6-N6	-5.78	119.08	123.70
41	3	37	C	N3-C4-N4	5.78	122.05	118.00
34	2	533	C	N3-C4-C5	-5.78	119.59	121.90
34	2	658	A	C4-C5-C6	5.78	119.89	117.00
34	2	1433	C	N3-C4-N4	5.78	122.04	118.00
34	2	1807	A	C5-C6-N1	-5.78	114.81	117.70
34	2	314	U	O4'-C1'-N1	5.78	112.82	108.20
34	2	509	A	C5-C6-N6	-5.78	119.08	123.70
34	2	812	A	C5-C6-N6	-5.78	119.08	123.70
34	2	1526	A	C4-C5-C6	5.78	119.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1654	U	O4'-C1'-N1	5.78	112.82	108.20
34	2	900	A	O4'-C1'-N9	5.77	112.82	108.20
34	2	448	A	C4-C5-C6	5.77	119.89	117.00
34	2	815	G	O4'-C1'-N9	5.77	112.82	108.20
34	2	851	G	O4'-C1'-N9	5.77	112.82	108.20
31	g	101	PHE	CB-CG-CD1	5.77	124.84	120.80
34	2	1201	C	N3-C4-C5	-5.77	119.59	121.90
34	2	1503	G	O4'-C1'-N9	5.77	112.82	108.20
34	2	179	C	N3-C4-N4	5.77	122.04	118.00
34	2	1074	C	N3-C4-N4	5.77	122.04	118.00
34	2	1719	A	C5-C6-N1	-5.77	114.81	117.70
34	2	660	A	C5-C6-N6	-5.77	119.08	123.70
34	2	1674	A	C4-C5-C6	5.77	119.88	117.00
1	1	38	A	C4-C5-C6	5.76	119.88	117.00
34	2	865	A	C5-C6-N6	-5.76	119.09	123.70
34	2	1860	A	C5-C6-N6	-5.76	119.09	123.70
34	2	364	G	C5-C6-O6	-5.76	125.14	128.60
34	2	1247	A	C5-C6-N6	-5.76	119.09	123.70
34	2	1710	A	C5-C6-N1	-5.76	114.82	117.70
1	1	29	G	O4'-C1'-N9	5.76	112.81	108.20
34	2	54	A	C5-C6-N6	-5.76	119.09	123.70
34	2	667	G	N3-C2-N2	5.76	123.93	119.90
34	2	25	A	C5-C6-N6	-5.76	119.09	123.70
34	2	1027	A	C4-C5-C6	5.76	119.88	117.00
34	2	1437	U	O4'-C1'-N1	5.76	112.81	108.20
34	2	1569	C	N3-C4-C5	-5.76	119.60	121.90
34	2	1569	C	N3-C4-N4	5.76	122.03	118.00
34	2	1179	A	C4-C5-C6	5.75	119.88	117.00
34	2	422	G	O4'-C1'-N9	5.75	112.80	108.20
34	2	1211	C	N3-C4-C5	-5.75	119.60	121.90
34	2	22	A	C4-C5-C6	5.75	119.88	117.00
34	2	383	U	O4'-C1'-N1	5.75	112.80	108.20
34	2	633	A	C4-C5-C6	5.75	119.88	117.00
34	2	1841	G	O4'-C1'-N9	5.75	112.80	108.20
34	2	1698	C	N3-C4-C5	-5.75	119.60	121.90
34	2	353	A	C5-C6-N1	-5.75	114.83	117.70
34	2	986	A	C4-C5-C6	5.75	119.87	117.00
34	2	1722	G	O4'-C1'-N9	5.75	112.80	108.20
34	2	1051	A	C5-C6-N1	-5.75	114.83	117.70
34	2	1522	C	N3-C4-N4	5.75	122.02	118.00
34	2	1159	C	N3-C4-C5	-5.74	119.60	121.90
34	2	1811	G	O4'-C1'-N9	5.74	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	223	A	C5-C6-N6	-5.74	119.11	123.70
34	2	483	A	C4-C5-C6	5.74	119.87	117.00
34	2	595	A	C5-C6-N1	-5.74	114.83	117.70
34	2	19	A	C5-C6-N1	-5.74	114.83	117.70
34	2	455	A	C5-C6-N6	-5.74	119.11	123.70
34	2	1205	A	C4-C5-C6	5.74	119.87	117.00
34	2	369	C	N3-C4-N4	5.74	122.02	118.00
34	2	584	A	C5-C6-N6	-5.74	119.11	123.70
34	2	801	U	O4'-C1'-N1	5.74	112.79	108.20
34	2	909	A	C5-C6-N6	-5.74	119.11	123.70
34	2	1144	A	O4'-C1'-N9	5.74	112.79	108.20
34	2	1379	A	C5-C6-N6	-5.74	119.11	123.70
34	2	1056	A	C4-C5-C6	5.74	119.87	117.00
34	2	293	A	C4-C5-C6	5.74	119.87	117.00
34	2	492	C	N3-C4-N4	5.74	122.02	118.00
34	2	1096	A	C5-C6-N1	-5.74	114.83	117.70
34	2	1485	A	C5-C6-N6	-5.74	119.11	123.70
34	2	1691	C	N3-C4-N4	5.74	122.02	118.00
34	2	1184	A	C5-C6-N1	-5.73	114.83	117.70
34	2	1472	A	O4'-C1'-N9	5.73	112.79	108.20
1	1	2	A	C5-C6-N1	-5.73	114.83	117.70
34	2	1016	A	C4-C5-C6	5.73	119.87	117.00
34	2	1515	G	C8-N9-C1'	-5.73	119.55	127.00
34	2	11	A	C5-C6-N6	-5.73	119.11	123.70
34	2	495	G	O4'-C1'-N9	5.73	112.78	108.20
34	2	1424	G	O4'-C1'-N9	5.73	112.78	108.20
34	2	1485	A	C4-C5-C6	5.73	119.86	117.00
34	2	68	A	C4-C5-C6	5.73	119.86	117.00
34	2	1655	C	N3-C4-C5	-5.73	119.61	121.90
1	1	10	G	C4-N9-C1'	5.73	133.95	126.50
34	2	1366	A	C4-C5-C6	5.73	119.86	117.00
34	2	664	C	N3-C4-N4	5.73	122.01	118.00
1	1	44	A	C5-C6-N1	-5.72	114.84	117.70
34	2	566	A	C5-C6-N1	-5.72	114.84	117.70
34	2	1083	A	C5-C6-N6	-5.72	119.12	123.70
34	2	1088	G	O4'-C1'-N9	5.72	112.78	108.20
34	2	1699	C	N3-C4-N4	5.72	122.01	118.00
34	2	1723	U	O4'-C1'-N1	5.72	112.78	108.20
34	2	59	U	O4'-C1'-N1	5.72	112.78	108.20
34	2	1738	G	N3-C2-N2	5.72	123.91	119.90
34	2	1658	A	C4-C5-C6	5.72	119.86	117.00
1	1	73	A	C5-C6-N6	-5.72	119.12	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	295	C	O4'-C1'-N1	5.72	112.78	108.20
34	2	1227	C	N3-C4-C5	-5.72	119.61	121.90
34	2	1183	G	N3-C2-N2	5.72	123.90	119.90
34	2	13	C	N3-C4-C5	-5.72	119.61	121.90
34	2	290	A	C4-C5-C6	5.72	119.86	117.00
34	2	1246	A	C5-C6-N6	-5.72	119.13	123.70
34	2	1351	C	N3-C4-C5	-5.72	119.61	121.90
34	2	1502	A	C5-C6-N1	-5.72	114.84	117.70
34	2	1696	C	N3-C4-C5	-5.72	119.61	121.90
34	2	1086	C	N3-C4-C5	-5.71	119.61	121.90
34	2	572	U	O4'-C1'-N1	5.71	112.77	108.20
34	2	1382	A	C5-C6-N6	-5.71	119.13	123.70
34	2	1456	C	N3-C4-C5	-5.71	119.62	121.90
34	2	871	A	C5-C6-N6	-5.71	119.13	123.70
34	2	1076	A	C5-C6-N6	-5.71	119.13	123.70
34	2	1175	G	N3-C2-N2	5.71	123.90	119.90
34	2	1444	A	C5-C6-N6	-5.71	119.13	123.70
34	2	1821	U	O4'-C1'-N1	5.71	112.77	108.20
34	2	218	A	C5-C6-N1	-5.71	114.85	117.70
34	2	1276	G	O4'-C1'-N9	5.71	112.77	108.20
34	2	1449	C	C6-N1-C1'	-5.71	113.95	120.80
34	2	450	A	C5-C6-N6	-5.71	119.14	123.70
41	3	38	C	N3-C4-N4	5.71	121.99	118.00
1	1	5	A	O4'-C1'-N9	5.70	112.76	108.20
34	2	382	A	O4'-C1'-N9	5.70	112.76	108.20
34	2	633	A	C5-C6-N1	-5.70	114.85	117.70
34	2	1165	G	N3-C2-N2	5.70	123.89	119.90
34	2	1300	U	O4'-C1'-N1	5.70	112.76	108.20
34	2	99	A	O4'-C1'-N9	5.70	112.76	108.20
34	2	181	A	C5-C6-N1	-5.70	114.85	117.70
34	2	429	A	C4-C5-C6	5.70	119.85	117.00
1	1	56	C	N3-C4-N4	5.70	121.99	118.00
34	2	1410	A	O4'-C1'-N9	5.70	112.76	108.20
34	2	158	A	C4-C5-C6	5.70	119.85	117.00
34	2	974	G	O4'-C1'-N9	5.70	112.76	108.20
34	2	1140	A	C5-C6-N1	-5.70	114.85	117.70
34	2	1606	G	O4'-C1'-N9	5.70	112.76	108.20
34	2	272	C	C5-C4-N4	-5.69	116.22	120.20
34	2	891	G	O4'-C1'-N9	5.69	112.75	108.20
34	2	1415	C	N3-C4-N4	5.69	121.98	118.00
34	2	1592	C	N3-C4-N4	5.69	121.98	118.00
34	2	24	C	N3-C4-N4	5.69	121.98	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	117	C	N3-C4-N4	5.69	121.98	118.00
34	2	1536	G	O4'-C1'-N9	5.69	112.75	108.20
34	2	289	G	O4'-C1'-N9	5.69	112.75	108.20
34	2	302	C	N3-C4-N4	5.69	121.98	118.00
1	1	20	A	C4-C5-C6	5.69	119.84	117.00
34	2	866	A	C4-C5-C6	5.69	119.84	117.00
34	2	953	A	C5-C6-N6	-5.69	119.15	123.70
34	2	1050	G	O4'-C1'-N9	5.69	112.75	108.20
34	2	675	A	C4-C5-C6	5.68	119.84	117.00
34	2	905	G	O4'-C1'-N9	5.68	112.75	108.20
34	2	38	A	C4-C5-C6	5.68	119.84	117.00
34	2	284	C	O4'-C1'-N1	5.68	112.75	108.20
34	2	401	G	O4'-C1'-N9	5.68	112.75	108.20
34	2	437	A	C5-C6-N1	-5.68	114.86	117.70
34	2	459	A	C5-C6-N1	-5.68	114.86	117.70
34	2	76	U	O4'-C1'-N1	5.68	112.75	108.20
34	2	619	A	C5-C6-N6	-5.68	119.16	123.70
34	2	1429	C	N3-C4-N4	5.68	121.98	118.00
34	2	240	C	N3-C4-N4	5.68	121.98	118.00
34	2	644	A	C5-C6-N6	-5.68	119.16	123.70
34	2	1130	G	O4'-C1'-N9	5.68	112.74	108.20
34	2	1810	G	O4'-C1'-N9	5.68	112.74	108.20
34	2	275	C	N3-C4-C5	-5.68	119.63	121.90
34	2	416	A	C5-C6-N6	-5.68	119.16	123.70
34	2	868	A	O4'-C1'-N9	5.68	112.74	108.20
34	2	1075	C	N3-C4-N4	5.68	121.97	118.00
34	2	11	A	C5-C6-N1	-5.68	114.86	117.70
1	1	20	A	C5-C6-N6	-5.67	119.16	123.70
34	2	67	C	N3-C4-N4	5.67	121.97	118.00
34	2	971	G	O4'-C1'-N9	5.67	112.74	108.20
4	D	155	TYR	CB-CG-CD2	-5.67	117.60	121.00
34	2	951	A	O4'-C1'-N9	5.67	112.74	108.20
34	2	1193	G	O4'-C1'-N9	5.67	112.74	108.20
34	2	1206	G	O4'-C1'-N9	5.67	112.74	108.20
34	2	226	A	C5-C6-N1	-5.67	114.86	117.70
34	2	329	A	C5-C6-N6	-5.67	119.16	123.70
34	2	425	A	C5-C6-N1	-5.67	114.86	117.70
34	2	640	A	C5-C6-N1	-5.67	114.86	117.70
34	2	1205	A	C5-C6-N6	-5.67	119.16	123.70
34	2	1113	C	N3-C4-N4	5.67	121.97	118.00
34	2	108	G	O4'-C1'-N9	5.67	112.73	108.20
34	2	280	G	O4'-C1'-N9	5.67	112.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	319	G	O4'-C1'-N9	5.67	112.73	108.20
34	2	458	A	C5-C6-N1	-5.67	114.86	117.70
34	2	484	C	N3-C4-N4	5.67	121.97	118.00
34	2	587	G	O4'-C1'-N9	5.67	112.73	108.20
1	1	32	C	N3-C4-N4	5.67	121.97	118.00
34	2	174	C	N3-C4-N4	5.67	121.97	118.00
34	2	302	C	O4'-C1'-N1	5.67	112.73	108.20
34	2	577	A	C5-C6-N1	-5.67	114.87	117.70
34	2	983	A	C5-C6-N6	-5.67	119.17	123.70
34	2	1530	U	O4'-C1'-N1	5.66	112.73	108.20
34	2	22	A	C5-C6-N1	-5.66	114.87	117.70
34	2	526	A	C4-C5-C6	5.66	119.83	117.00
34	2	890	G	O4'-C1'-N9	5.66	112.73	108.20
34	2	1483	A	C4-C5-C6	5.66	119.83	117.00
34	2	1488	U	O4'-C1'-N1	5.66	112.73	108.20
34	2	1604	C	N3-C4-N4	5.66	121.96	118.00
34	2	1698	C	N3-C4-N4	5.66	121.96	118.00
34	2	1696	C	N3-C4-N4	5.66	121.96	118.00
34	2	29	G	O4'-C1'-N9	5.66	112.72	108.20
34	2	61	A	C5-C6-N1	-5.66	114.87	117.70
34	2	284	C	N3-C4-N4	5.66	121.96	118.00
34	2	536	G	O4'-C1'-N9	5.65	112.72	108.20
34	2	807	A	C4-C5-C6	5.65	119.83	117.00
34	2	297	C	N3-C4-N4	5.65	121.96	118.00
34	2	502	A	C5-C6-N6	-5.65	119.18	123.70
34	2	1192	A	C5-C6-N1	-5.65	114.88	117.70
34	2	1279	C	N3-C4-N4	5.65	121.96	118.00
34	2	350	A	OP1-P-O3'	5.65	117.63	105.20
34	2	658	A	C5-C6-N6	-5.65	119.18	123.70
34	2	1254	A	C4-C5-C6	5.65	119.82	117.00
1	1	48	C	N3-C4-C5	-5.65	119.64	121.90
34	2	1190	A	C4-C5-C6	5.65	119.82	117.00
34	2	158	A	C5-C6-N6	-5.64	119.18	123.70
34	2	1129	A	C4-C5-C6	5.64	119.82	117.00
34	2	1317	G	O4'-C1'-N9	5.64	112.72	108.20
34	2	1245	C	N3-C4-C5	-5.64	119.64	121.90
34	2	1456	C	N3-C4-N4	5.64	121.95	118.00
34	2	1309	A	C4-C5-C6	5.64	119.82	117.00
34	2	1289	A	C5-C6-N1	-5.64	114.88	117.70
34	2	1652	G	O4'-C1'-N9	5.64	112.71	108.20
34	2	1340	A	C5-C6-N6	-5.64	119.19	123.70
34	2	1421	G	C5-C6-O6	-5.64	125.22	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	75	C	N3-C4-N4	5.63	121.94	118.00
34	2	77	A	C5-C6-N1	-5.63	114.88	117.70
34	2	426	G	O4'-C1'-N9	5.63	112.71	108.20
41	3	36	A	C5-C6-N6	-5.63	119.19	123.70
12	L	159	PHE	CB-CG-CD2	-5.63	116.86	120.80
34	2	114	G	O4'-C1'-N9	5.63	112.71	108.20
34	2	654	A	C5-C6-N1	-5.63	114.89	117.70
34	2	662	A	C5-C6-N6	-5.63	119.20	123.70
34	2	1100	G	O4'-C1'-N9	5.63	112.70	108.20
34	2	1135	C	N3-C4-C5	-5.63	119.65	121.90
34	2	191	C	O4'-C1'-N1	5.63	112.70	108.20
34	2	1372	A	C5-C6-N6	-5.63	119.20	123.70
34	2	1399	C	N3-C4-N4	5.63	121.94	118.00
34	2	603	C	N3-C4-N4	5.63	121.94	118.00
34	2	1397	A	C4-C5-C6	5.63	119.81	117.00
34	2	1511	G	O4'-C1'-N9	5.63	112.70	108.20
34	2	359	C	N3-C4-N4	5.63	121.94	118.00
34	2	1026	A	C5-C6-N1	-5.63	114.89	117.70
34	2	1126	G	O4'-C1'-N9	5.63	112.70	108.20
34	2	1564	A	C5-C6-N1	-5.63	114.89	117.70
34	2	1735	C	N3-C4-N4	5.63	121.94	118.00
34	2	1859	C	N3-C4-N4	5.63	121.94	118.00
34	2	1475	G	O4'-C1'-N9	5.62	112.70	108.20
34	2	1567	C	N3-C4-N4	5.62	121.94	118.00
34	2	1692	A	C5-C6-N1	-5.62	114.89	117.70
34	2	316	C	N3-C4-N4	5.62	121.94	118.00
34	2	510	A	C5-C6-N1	-5.62	114.89	117.70
34	2	170	A	C5-C6-N1	-5.62	114.89	117.70
34	2	182	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	993	A	C5-C6-N6	-5.62	119.20	123.70
34	2	1548	C	N3-C4-N4	5.62	121.93	118.00
34	2	1795	A	O4'-C1'-N9	5.62	112.70	108.20
34	2	470	G	O4'-C1'-N9	5.62	112.69	108.20
34	2	512	A	C5-C6-N6	-5.62	119.21	123.70
34	2	1196	A	C5-C6-N6	-5.62	119.21	123.70
34	2	1331	G	O4'-C1'-N9	5.62	112.69	108.20
34	2	1449	C	N3-C4-N4	5.62	121.93	118.00
13	M	70	TYR	CB-CG-CD2	-5.61	117.63	121.00
34	2	603	C	N3-C4-C5	-5.61	119.66	121.90
34	2	624	A	C5-C6-N6	-5.61	119.21	123.70
34	2	650	C	N3-C4-C5	-5.61	119.66	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1191	A	O4'-C1'-N9	5.61	112.69	108.20
34	2	618	A	C5-C6-N1	-5.61	114.90	117.70
34	2	1080	A	C5-C6-N1	-5.61	114.90	117.70
34	2	1310	U	C2-N1-C1'	5.61	124.43	117.70
34	2	1812	A	C5-C6-N1	-5.61	114.90	117.70
34	2	16	G	N3-C2-N2	5.61	123.82	119.90
34	2	90	G	O4'-C1'-N9	5.61	112.68	108.20
34	2	218	A	O4'-C1'-N9	5.61	112.69	108.20
34	2	321	C	N3-C4-C5	-5.61	119.66	121.90
34	2	354	A	C4-C5-C6	5.61	119.80	117.00
34	2	630	A	C5-C6-N1	-5.61	114.90	117.70
34	2	638	A	C5-C6-N1	-5.60	114.90	117.70
34	2	275	C	N3-C4-N4	5.60	121.92	118.00
34	2	277	U	O4'-C1'-N1	5.60	112.68	108.20
34	2	476	A	C5-C6-N6	-5.60	119.22	123.70
34	2	826	A	C5-C6-N6	-5.60	119.22	123.70
34	2	1075	C	N3-C4-C5	-5.60	119.66	121.90
34	2	1442	A	C4-C5-C6	5.60	119.80	117.00
34	2	1542	C	N3-C4-C5	-5.60	119.66	121.90
34	2	1246	A	C4-C5-C6	5.60	119.80	117.00
34	2	1729	G	N3-C2-N2	5.60	123.82	119.90
1	1	35	A	C5-C6-N6	-5.60	119.22	123.70
34	2	221	A	C5-C6-N1	-5.60	114.90	117.70
34	2	1155	G	O4'-C1'-N9	5.60	112.68	108.20
34	2	1212	C	N3-C4-N4	5.60	121.92	118.00
34	2	1714	A	O4'-C1'-N9	5.60	112.68	108.20
32	n	65	TYR	CB-CG-CD2	-5.60	117.64	121.00
34	2	98	C	O4'-C1'-N1	5.60	112.68	108.20
34	2	628	C	N3-C4-C5	-5.60	119.66	121.90
34	2	1195	A	C5-C6-N1	-5.60	114.90	117.70
34	2	1221	U	O4'-C1'-N1	5.60	112.68	108.20
34	2	1364	U	O4'-C1'-N1	5.60	112.68	108.20
34	2	1799	G	O4'-C1'-N9	5.60	112.68	108.20
34	2	904	A	C4-C5-C6	5.60	119.80	117.00
34	2	491	C	N3-C4-C5	-5.59	119.66	121.90
34	2	807	A	C5-C6-N6	-5.59	119.22	123.70
34	2	1280	A	C4-C5-C6	5.59	119.80	117.00
34	2	1384	A	C5-C6-N6	-5.59	119.22	123.70
34	2	1787	A	O4'-C1'-N9	5.59	112.67	108.20
34	2	830	C	N3-C4-N4	5.59	121.91	118.00
34	2	1179	A	C5-C6-N1	-5.59	114.90	117.70
34	2	1575	A	C5-C6-N1	-5.59	114.91	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	205	ASP	CB-CG-OD1	5.59	123.33	118.30
41	3	37	C	N3-C4-C5	-5.59	119.66	121.90
34	2	38	A	C5-C6-N6	-5.59	119.23	123.70
34	2	91	A	C5-C6-N6	-5.59	119.23	123.70
34	2	613	G	O4'-C1'-N9	5.59	112.67	108.20
34	2	922	A	O4'-C1'-N9	5.59	112.67	108.20
34	2	1483	A	C5-C6-N6	-5.59	119.23	123.70
35	A	82	TYR	CB-CG-CD2	-5.59	117.65	121.00
34	2	861	A	C5-C6-N6	-5.59	119.23	123.70
34	2	1216	A	O4'-C1'-N9	5.59	112.67	108.20
1	1	48	C	N3-C4-N4	5.59	121.91	118.00
34	2	283	A	C5-C6-N6	-5.59	119.23	123.70
34	2	418	U	C2-N1-C1'	5.59	124.40	117.70
34	2	1134	C	N3-C4-N4	5.59	121.91	118.00
34	2	1159	C	N3-C4-N4	5.59	121.91	118.00
34	2	1714	A	C5-C6-N6	-5.59	119.23	123.70
34	2	1845	A	C5-C6-N6	-5.59	119.23	123.70
1	1	20	A	C5-C6-N1	-5.58	114.91	117.70
1	1	61	C	N3-C4-N4	5.58	121.91	118.00
34	2	645	A	C5-C6-N6	-5.58	119.23	123.70
34	2	1478	C	N3-C4-N4	5.58	121.91	118.00
34	2	1528	A	C4-C5-C6	5.58	119.79	117.00
34	2	1656	A	C5-C6-N6	-5.58	119.23	123.70
34	2	1655	C	N3-C4-N4	5.58	121.91	118.00
34	2	13	C	N3-C4-N4	5.58	121.91	118.00
34	2	624	A	C5-C6-N1	-5.58	114.91	117.70
34	2	1121	C	N3-C4-N4	5.58	121.91	118.00
34	2	1586	C	N3-C4-N4	5.58	121.91	118.00
34	2	1618	A	C5-C6-N6	-5.58	119.24	123.70
34	2	1812	A	O4'-C1'-N9	5.58	112.66	108.20
34	2	3	C	N3-C4-N4	5.58	121.90	118.00
34	2	576	G	O4'-C1'-N9	5.58	112.66	108.20
34	2	1060	C	N3-C4-C5	-5.58	119.67	121.90
1	1	14	C	N3-C4-C5	-5.58	119.67	121.90
34	2	860	A	C5-C6-N6	-5.57	119.24	123.70
34	2	980	C	N3-C4-C5	-5.57	119.67	121.90
34	2	102	A	C5-C6-N1	-5.57	114.92	117.70
34	2	397	G	C4-N9-C1'	5.57	133.74	126.50
34	2	580	A	O4'-C1'-N9	5.57	112.66	108.20
34	2	1072	G	O4'-C1'-N9	5.57	112.66	108.20
34	2	46	A	C5-C6-N1	-5.57	114.92	117.70
34	2	583	C	N3-C4-N4	5.57	121.90	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1080	A	C5-C6-N6	-5.57	119.25	123.70
34	2	1278	A	C5-C6-N6	-5.57	119.25	123.70
40	R	15	PHE	CB-CG-CD1	5.57	124.70	120.80
34	2	175	A	C5-C6-N6	-5.57	119.25	123.70
34	2	438	A	C4-C5-C6	5.57	119.78	117.00
34	2	544	A	C5-C6-N1	-5.57	114.92	117.70
34	2	1129	A	C5-C6-N6	-5.57	119.25	123.70
34	2	275	C	C6-N1-C1'	-5.56	114.12	120.80
34	2	1095	G	O4'-C1'-N9	5.56	112.65	108.20
34	2	2	A	C5-C6-N6	-5.56	119.25	123.70
34	2	594	A	C5-C6-N1	-5.56	114.92	117.70
34	2	969	C	N3-C4-N4	5.56	121.89	118.00
34	2	1533	C	N3-C4-N4	5.56	121.89	118.00
34	2	807	A	O4'-C1'-N9	5.56	112.65	108.20
34	2	1433	C	N3-C4-C5	-5.56	119.68	121.90
34	2	67	C	C6-N1-C2	-5.56	118.08	120.30
34	2	429	A	C5-C6-N6	-5.56	119.25	123.70
34	2	453	C	N3-C4-N4	5.56	121.89	118.00
34	2	544	A	C5-C6-N6	-5.56	119.25	123.70
34	2	922	A	C5-C6-N6	-5.56	119.25	123.70
34	2	940	A	C4-C5-C6	5.56	119.78	117.00
34	2	455	A	C5-C6-N1	-5.55	114.92	117.70
1	1	68	C	O4'-C1'-N1	5.55	112.64	108.20
34	2	675	A	C5-C6-N6	-5.55	119.26	123.70
1	1	35	A	C5-C6-N1	-5.55	114.92	117.70
34	2	68	A	C5-C6-N1	-5.55	114.92	117.70
34	2	1419	C	N3-C4-N4	5.55	121.89	118.00
34	2	1502	A	C5-C6-N6	-5.55	119.26	123.70
34	2	677	C	N3-C4-C5	-5.55	119.68	121.90
34	2	729	C	N3-C4-C5	-5.55	119.68	121.90
34	2	835	C	N3-C4-C5	-5.55	119.68	121.90
34	2	1619	U	C2-N1-C1'	5.55	124.36	117.70
34	2	50	A	C5-C6-N1	-5.55	114.93	117.70
34	2	72	C	N3-C4-C5	-5.55	119.68	121.90
34	2	440	C	N3-C4-N4	5.55	121.88	118.00
34	2	1158	C	N3-C4-N4	5.55	121.88	118.00
34	2	1186	A	C5-C6-N1	-5.55	114.93	117.70
34	2	1840	G	O4'-C1'-N9	5.55	112.64	108.20
34	2	993	A	C5-C6-N1	-5.54	114.93	117.70
34	2	1815	U	P-O3'-C3'	5.54	126.35	119.70
34	2	1382	A	C5-C6-N1	-5.54	114.93	117.70
34	2	117	C	N3-C4-C5	-5.54	119.68	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	343	C	N3-C4-C5	-5.54	119.68	121.90
34	2	669	A	C4-C5-C6	5.54	119.77	117.00
34	2	1054	A	C5-C6-N6	-5.54	119.27	123.70
34	2	1112	C	N3-C4-N4	5.54	121.88	118.00
34	2	1237	A	C5-C6-N1	-5.54	114.93	117.70
41	3	40	C	N3-C4-C5	-5.54	119.68	121.90
34	2	166	A	O4'-C1'-N9	5.54	112.63	108.20
34	2	993	A	C4-C5-C6	5.54	119.77	117.00
34	2	1541	G	O4'-C1'-N9	5.54	112.63	108.20
1	1	32	C	N3-C4-C5	-5.54	119.69	121.90
1	1	55	U	O4'-C1'-N1	5.54	112.63	108.20
34	2	491	C	N3-C4-N4	5.54	121.88	118.00
34	2	574	A	C4-C5-C6	5.54	119.77	117.00
34	2	580	A	C5-C6-N6	-5.54	119.27	123.70
34	2	901	C	N3-C4-C5	-5.54	119.69	121.90
34	2	1444	A	C5-C6-N1	-5.54	114.93	117.70
34	2	1290	G	O4'-C1'-N9	5.54	112.63	108.20
34	2	1400	U	O4'-C1'-N1	5.54	112.63	108.20
34	2	304	A	C5-C6-N1	-5.54	114.93	117.70
34	2	453	C	N3-C4-C5	-5.54	119.69	121.90
34	2	560	C	N3-C4-N4	5.54	121.88	118.00
34	2	820	C	N3-C4-N4	5.54	121.88	118.00
34	2	873	C	N3-C4-N4	5.54	121.88	118.00
34	2	958	A	C5-C6-N1	-5.54	114.93	117.70
34	2	1697	G	O4'-C1'-N9	5.54	112.63	108.20
34	2	1784	A	O4'-C1'-N9	5.54	112.63	108.20
34	2	178	C	N3-C4-C5	-5.53	119.69	121.90
34	2	450	A	C5-C6-N1	-5.53	114.93	117.70
34	2	1260	C	N3-C4-N4	5.53	121.87	118.00
34	2	1678	C	N3-C4-N4	5.53	121.87	118.00
34	2	1320	G	O4'-C1'-N9	5.53	112.62	108.20
34	2	290	A	C5-C6-N1	-5.53	114.94	117.70
34	2	389	C	N3-C4-N4	5.53	121.87	118.00
34	2	573	A	O4'-C1'-N9	5.53	112.62	108.20
34	2	833	A	C5-C6-N6	-5.53	119.28	123.70
34	2	866	A	C5-C6-N6	-5.53	119.28	123.70
34	2	1435	A	O4'-C1'-N9	5.53	112.62	108.20
34	2	1551	A	C5-C6-N6	-5.53	119.28	123.70
34	2	1844	A	O4'-C1'-N9	5.53	112.62	108.20
34	2	560	C	N3-C4-C5	-5.53	119.69	121.90
34	2	605	C	N3-C4-C5	-5.53	119.69	121.90
34	2	823	A	C5-C6-N6	-5.53	119.28	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	831	C	N3-C4-N4	5.53	121.87	118.00
34	2	1015	C	N3-C4-C5	-5.53	119.69	121.90
34	2	1575	A	C4-C5-C6	5.53	119.76	117.00
34	2	1596	A	C5-C6-N1	-5.53	114.94	117.70
34	2	482	C	N3-C4-N4	5.52	121.87	118.00
34	2	1286	G	O4'-C1'-N9	5.52	112.62	108.20
1	1	28	U	O4'-C1'-N1	5.52	112.62	108.20
34	2	330	C	N3-C4-C5	-5.52	119.69	121.90
34	2	959	A	C5-C6-N1	-5.52	114.94	117.70
34	2	1205	A	C5-C6-N1	-5.52	114.94	117.70
34	2	1719	A	O4'-C1'-N9	5.52	112.62	108.20
1	1	38	A	O4'-C1'-N9	5.52	112.62	108.20
34	2	1066	A	O4'-C1'-N9	5.52	112.61	108.20
34	2	1092	G	O4'-C1'-N9	5.52	112.62	108.20
34	2	1434	A	C4-C5-C6	5.52	119.76	117.00
1	1	75	C	N3-C4-C5	-5.52	119.69	121.90
34	2	25	A	C4-C5-C6	5.52	119.76	117.00
34	2	381	C	N3-C4-C5	-5.52	119.69	121.90
34	2	1284	U	O4'-C1'-N1	5.52	112.61	108.20
34	2	429	A	C5-C6-N1	-5.51	114.94	117.70
34	2	448	A	C5-C6-N1	-5.51	114.94	117.70
34	2	912	A	C5-C6-N1	-5.51	114.94	117.70
34	2	1137	G	O4'-C1'-N9	5.51	112.61	108.20
34	2	1659	A	O4'-C1'-N9	5.51	112.61	108.20
34	2	535	A	O4'-C1'-N9	5.51	112.61	108.20
34	2	1410	A	C4-C5-C6	5.51	119.76	117.00
24	Z	41	PHE	CB-CG-CD2	-5.51	116.94	120.80
34	2	315	C	N3-C4-N4	5.51	121.86	118.00
34	2	1105	C	N3-C4-C5	-5.51	119.69	121.90
34	2	1365	A	C5-C6-N1	-5.51	114.94	117.70
34	2	1578	C	N3-C4-C5	-5.51	119.69	121.90
34	2	1807	A	O4'-C1'-N9	5.51	112.61	108.20
1	1	18	G	C4'-C3'-O3'	5.51	124.02	113.00
34	2	1334	G	O4'-C1'-N9	5.51	112.61	108.20
34	2	1563	C	N3-C4-N4	5.51	121.86	118.00
34	2	149	A	C4-C5-C6	5.51	119.75	117.00
34	2	1149	C	N3-C4-N4	5.51	121.86	118.00
10	J	63	PHE	CB-CG-CD2	-5.51	116.94	120.80
34	2	798	A	C5-C6-N6	-5.51	119.29	123.70
34	2	845	A	C5-C6-N6	-5.51	119.30	123.70
34	2	949	C	N3-C4-N4	5.50	121.85	118.00
34	2	1163	G	O4'-C1'-N9	5.50	112.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	292	A	C5-C6-N6	-5.50	119.30	123.70
34	2	1078	A	C5-C6-N6	-5.50	119.30	123.70
34	2	1328	A	C4-C5-C6	5.50	119.75	117.00
34	2	1770	G	O4'-C1'-N9	5.50	112.60	108.20
41	3	51	C	N3-C4-N4	5.50	121.85	118.00
34	2	67	C	O4'-C1'-N1	5.50	112.60	108.20
34	2	78	C	N3-C4-C5	-5.50	119.70	121.90
34	2	1548	C	P-O3'-C3'	5.50	126.30	119.70
34	2	340	C	N3-C4-C5	-5.50	119.70	121.90
34	2	391	A	C4-C5-C6	5.50	119.75	117.00
34	2	1185	A	O4'-C1'-N9	5.50	112.60	108.20
34	2	179	C	N3-C4-C5	-5.50	119.70	121.90
34	2	445	A	C5-C6-N6	-5.50	119.30	123.70
34	2	1243	C	N3-C4-N4	5.50	121.85	118.00
34	2	1287	A	C5-C6-N6	-5.50	119.30	123.70
34	2	1563	C	N3-C4-C5	-5.50	119.70	121.90
34	2	1693	C	N3-C4-C5	-5.50	119.70	121.90
34	2	23	G	O4'-C1'-N9	5.50	112.60	108.20
34	2	490	A	C5-C6-N1	-5.50	114.95	117.70
34	2	661	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	1120	C	N3-C4-C5	-5.49	119.70	121.90
34	2	1551	A	C5-C6-N1	-5.49	114.95	117.70
34	2	912	A	C5-C6-N6	-5.49	119.31	123.70
34	2	1614	A	C5-C6-N1	-5.49	114.95	117.70
34	2	454	A	C5-C6-N6	-5.49	119.31	123.70
34	2	809	A	O4'-C1'-N9	5.49	112.59	108.20
34	2	920	G	O4'-C1'-N9	5.49	112.59	108.20
34	2	958	A	O4'-C1'-N9	5.49	112.59	108.20
34	2	1614	A	C5-C6-N6	-5.49	119.31	123.70
1	1	58	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	901	C	N3-C4-N4	5.49	121.84	118.00
34	2	945	G	O4'-C1'-N9	5.49	112.59	108.20
34	2	1083	A	C5-C6-N1	-5.49	114.96	117.70
34	2	1659	A	C5-C6-N1	-5.49	114.96	117.70
34	2	515	A	C4-C5-C6	5.49	119.74	117.00
34	2	45	A	C5-C6-N6	-5.49	119.31	123.70
34	2	80	G	O4'-C1'-N9	5.49	112.59	108.20
34	2	526	A	O4'-C1'-N9	5.49	112.59	108.20
34	2	196	U	O4'-C1'-N1	5.48	112.59	108.20
34	2	166	A	C5-C6-N6	-5.48	119.31	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	283	A	C5-C6-N1	-5.48	114.96	117.70
34	2	1215	C	N3-C4-N4	5.48	121.84	118.00
34	2	1483	A	O4'-C1'-N9	5.48	112.59	108.20
41	3	40	C	N3-C4-N4	5.48	121.84	118.00
34	2	297	C	N3-C4-C5	-5.48	119.71	121.90
34	2	533	C	N3-C4-N4	5.48	121.84	118.00
34	2	593	C	N3-C4-N4	5.48	121.84	118.00
34	2	660	A	C4-C5-C6	5.48	119.74	117.00
34	2	1396	U	O4'-C1'-N1	5.48	112.58	108.20
34	2	288	A	C5-C6-N1	-5.48	114.96	117.70
34	2	1360	U	C6-N1-C1'	-5.48	113.53	121.20
1	1	59	A	C5-C6-N6	-5.48	119.32	123.70
34	2	1679	C	N3-C4-N4	5.48	121.83	118.00
34	2	1752	G	O4'-C1'-N9	5.48	112.58	108.20
34	2	1472	A	C5-C6-N1	-5.48	114.96	117.70
34	2	580	A	C5-C6-N1	-5.47	114.96	117.70
34	2	1540	A	C5-C6-N6	-5.47	119.32	123.70
41	3	50	C	N3-C4-N4	5.47	121.83	118.00
34	2	189	G	N3-C2-N2	5.47	123.73	119.90
34	2	828	G	O4'-C1'-N9	5.47	112.58	108.20
34	2	926	C	N3-C4-N4	5.47	121.83	118.00
34	2	980	C	N3-C4-N4	5.47	121.83	118.00
34	2	1257	C	N3-C4-N4	5.47	121.83	118.00
34	2	1258	C	N3-C4-C5	-5.47	119.71	121.90
38	k	128	LYS	C-N-CD	5.47	139.89	128.40
34	2	323	G	O4'-C1'-N9	5.47	112.58	108.20
34	2	960	A	C5-C6-N1	-5.47	114.96	117.70
34	2	566	A	C5-C6-N6	-5.47	119.33	123.70
34	2	845	A	O4'-C1'-N9	5.47	112.58	108.20
34	2	1273	C	N3-C4-C5	-5.47	119.71	121.90
34	2	1297	A	C5-C6-N6	-5.47	119.33	123.70
34	2	1699	C	N3-C4-C5	-5.47	119.71	121.90
34	2	1242	A	C5-C6-N1	-5.47	114.97	117.70
34	2	1399	C	N3-C4-C5	-5.47	119.71	121.90
34	2	860	A	C5-C6-N1	-5.46	114.97	117.70
34	2	977	A	O4'-C1'-N9	5.46	112.57	108.20
34	2	473	C	N3-C4-N4	5.46	121.82	118.00
34	2	650	C	N3-C4-N4	5.46	121.82	118.00
34	2	924	G	O4'-C1'-N9	5.46	112.57	108.20
34	2	1411	C	N3-C4-N4	5.46	121.82	118.00
34	2	1549	C	N3-C4-N4	5.46	121.82	118.00
34	2	1576	C	N3-C4-N4	5.46	121.82	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1476	A	C5-C6-N1	-5.46	114.97	117.70
1	1	76	A	C5-C6-N1	-5.46	114.97	117.70
34	2	85	A	C5-C6-N6	-5.46	119.33	123.70
34	2	185	C	N3-C4-N4	5.46	121.82	118.00
34	2	519	A	C4-C5-C6	5.46	119.73	117.00
34	2	643	A	C5-C6-N1	-5.46	114.97	117.70
34	2	814	A	C5-C6-N6	-5.46	119.33	123.70
34	2	882	A	C5-C6-N1	-5.46	114.97	117.70
34	2	956	U	O4'-C1'-N1	5.46	112.57	108.20
34	2	1412	C	N3-C4-N4	5.46	121.82	118.00
34	2	1450	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	590	G	O4'-C1'-N9	5.46	112.56	108.20
34	2	994	A	C5-C6-N6	-5.46	119.33	123.70
34	2	1641	C	N3-C4-C5	-5.46	119.72	121.90
34	2	1583	A	C5-C6-N6	-5.46	119.34	123.70
38	k	137	PRO	C-N-CD	5.46	139.86	128.40
34	2	435	A	C5-C6-N6	-5.45	119.34	123.70
34	2	831	C	N3-C4-C5	-5.45	119.72	121.90
34	2	1056	A	C5-C6-N6	-5.45	119.34	123.70
34	2	1093	G	O4'-C1'-N9	5.45	112.56	108.20
34	2	1176	C	N3-C4-C5	-5.45	119.72	121.90
34	2	1529	C	O4'-C1'-N1	5.45	112.56	108.20
34	2	1257	C	N3-C4-C5	-5.45	119.72	121.90
34	2	1566	G	O4'-C1'-N9	5.45	112.56	108.20
34	2	96	C	N3-C4-N4	5.45	121.81	118.00
34	2	1340	A	C5-C6-N1	-5.45	114.97	117.70
34	2	1628	A	C5-C6-N1	-5.45	114.97	117.70
34	2	1692	A	C4-C5-C6	5.45	119.72	117.00
1	1	44	A	C5-C6-N6	-5.45	119.34	123.70
34	2	377	C	N3-C4-C5	-5.45	119.72	121.90
34	2	631	A	O4'-C1'-N9	5.45	112.56	108.20
34	2	1195	A	C5-C6-N6	-5.45	119.34	123.70
34	2	1204	A	C5-C6-N1	-5.45	114.97	117.70
34	2	1430	C	N3-C4-C5	-5.45	119.72	121.90
34	2	1548	C	N3-C4-C5	-5.45	119.72	121.90
34	2	515	A	C5-C6-N1	-5.45	114.98	117.70
34	2	605	C	N3-C4-N4	5.45	121.81	118.00
34	2	633	A	C5-C6-N6	-5.45	119.34	123.70
34	2	1399	C	O4'-C1'-N1	5.45	112.56	108.20
38	k	136	ASP	C-N-CD	5.45	139.84	128.40
34	2	25	A	C5-C6-N1	-5.45	114.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	111	A	C5-C6-N1	-5.45	114.98	117.70
34	2	284	C	N3-C4-C5	-5.45	119.72	121.90
34	2	1510	G	O4'-C1'-N9	5.45	112.56	108.20
34	2	846	C	N3-C4-N4	5.44	121.81	118.00
34	2	228	A	C5-C6-N6	-5.44	119.35	123.70
34	2	507	C	N3-C4-C5	-5.44	119.72	121.90
34	2	1793	G	N3-C2-N2	5.44	123.71	119.90
34	2	508	G	O4'-C1'-N9	5.44	112.55	108.20
34	2	1552	C	N3-C4-C5	-5.44	119.72	121.90
38	k	176	ILE	C-N-CD	5.44	139.82	128.40
34	2	270	G	O4'-C1'-N9	5.44	112.55	108.20
34	2	354	A	C5-C6-N6	-5.44	119.35	123.70
34	2	466	A	O4'-C1'-N9	5.44	112.55	108.20
34	2	1480	A	C5-C6-N6	-5.44	119.35	123.70
34	2	56	G	O4'-C1'-N9	5.44	112.55	108.20
34	2	997	A	C5-C6-N1	-5.44	114.98	117.70
34	2	1008	A	O4'-C1'-N9	5.44	112.55	108.20
34	2	1857	A	O4'-C1'-N9	5.44	112.55	108.20
34	2	1200	A	O4'-C1'-N9	5.44	112.55	108.20
34	2	806	A	C5-C6-N1	-5.43	114.98	117.70
34	2	1347	G	O4'-C1'-N9	5.43	112.55	108.20
34	2	557	C	N3-C4-N4	5.43	121.80	118.00
34	2	835	C	N3-C4-N4	5.43	121.80	118.00
34	2	861	A	C5-C6-N1	-5.43	114.98	117.70
34	2	976	A	O4'-C1'-N9	5.43	112.55	108.20
34	2	1007	A	O4'-C1'-N9	5.43	112.55	108.20
34	2	1226	C	N3-C4-C5	-5.43	119.73	121.90
34	2	1753	G	O4'-C1'-N9	5.43	112.55	108.20
34	2	1795	A	C5-C6-N6	-5.43	119.35	123.70
34	2	1256	A	C5-C6-N1	-5.43	114.98	117.70
34	2	83	A	C5-C6-N1	-5.43	114.98	117.70
34	2	573	A	C4-C5-C6	5.43	119.72	117.00
34	2	1418	G	N3-C2-N2	5.43	123.70	119.90
34	2	110	U	O4'-C1'-N1	5.43	112.54	108.20
34	2	440	C	N3-C4-C5	-5.43	119.73	121.90
34	2	338	A	C5-C6-N1	-5.43	114.99	117.70
34	2	367	G	O4'-C1'-N9	5.43	112.54	108.20
34	2	550	A	C5-C6-N1	-5.43	114.99	117.70
34	2	659	A	C5-C6-N1	-5.43	114.99	117.70
34	2	865	A	O4'-C1'-N9	5.43	112.54	108.20
34	2	27	A	O4'-C1'-N9	5.42	112.54	108.20
34	2	1260	C	N3-C4-C5	-5.42	119.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	89	ARG	NE-CZ-NH1	5.42	123.01	120.30
34	2	290	A	C5-C6-N6	-5.42	119.36	123.70
34	2	1129	A	C5-C6-N1	-5.42	114.99	117.70
34	2	1258	C	N3-C4-N4	5.42	121.80	118.00
34	2	1359	C	N3-C4-C5	-5.42	119.73	121.90
34	2	118	C	N3-C4-N4	5.42	121.79	118.00
34	2	178	C	N3-C4-N4	5.42	121.79	118.00
34	2	989	G	O4'-C1'-N9	5.42	112.53	108.20
34	2	997	A	C4-C5-C6	5.42	119.71	117.00
34	2	1477	G	O4'-C1'-N9	5.42	112.53	108.20
34	2	1766	C	P-O3'-C3'	-5.42	113.20	119.70
34	2	4	C	N3-C4-C5	-5.41	119.73	121.90
34	2	45	A	C5-C6-N1	-5.41	114.99	117.70
34	2	955	G	N3-C2-N2	5.41	123.69	119.90
34	2	1782	A	C5-C6-N1	-5.41	114.99	117.70
34	2	1786	G	O4'-C1'-N9	5.41	112.53	108.20
34	2	294	C	N3-C4-N4	5.41	121.79	118.00
34	2	606	A	C5-C6-N1	-5.41	115.00	117.70
34	2	841	G	O4'-C1'-N9	5.41	112.53	108.20
34	2	476	A	C5-C6-N1	-5.41	115.00	117.70
34	2	645	A	C5-C6-N1	-5.41	115.00	117.70
34	2	1450	A	C5-C6-N1	-5.41	115.00	117.70
34	2	940	A	O4'-C1'-N9	5.41	112.53	108.20
34	2	1435	A	C5-C6-N6	-5.41	119.38	123.70
34	2	111	A	C5-C6-N6	-5.41	119.38	123.70
34	2	183	G	O4'-C1'-N9	5.41	112.53	108.20
34	2	511	A	O4'-C1'-N9	5.41	112.52	108.20
34	2	915	A	C5-C6-N6	-5.41	119.38	123.70
34	2	1010	G	O4'-C1'-N9	5.41	112.52	108.20
32	n	65	TYR	CB-CG-CD1	5.40	124.24	121.00
34	2	1377	G	O4'-C1'-N9	5.40	112.52	108.20
34	2	1859	C	N3-C4-C5	-5.40	119.74	121.90
34	2	73	C	N3-C4-N4	5.40	121.78	118.00
34	2	351	U	OP2-P-O3'	5.40	117.08	105.20
34	2	993	A	O4'-C1'-N9	5.40	112.52	108.20
34	2	77	A	C5-C6-N6	-5.40	119.38	123.70
34	2	1031	A	O4'-C1'-N9	5.40	112.52	108.20
34	2	1504	A	C4-C5-C6	5.40	119.70	117.00
41	3	38	C	N3-C4-C5	-5.40	119.74	121.90
34	2	139	C	N3-C4-C5	-5.40	119.74	121.90
34	2	551	A	C5-C6-N6	-5.40	119.38	123.70
34	2	562	U	O4'-C1'-N1	5.40	112.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	2	A	C5-C6-N1	-5.40	115.00	117.70
34	2	826	A	C5-C6-N1	-5.40	115.00	117.70
34	2	1461	A	C5-C6-N6	-5.40	119.38	123.70
34	2	1632	A	C5-C6-N1	-5.40	115.00	117.70
34	2	1113	C	N3-C4-C5	-5.40	119.74	121.90
34	2	19	A	C5-C6-N6	-5.39	119.38	123.70
34	2	421	G	O4'-C1'-N9	5.39	112.52	108.20
34	2	492	C	N3-C4-C5	-5.39	119.74	121.90
34	2	1279	C	N3-C4-C5	-5.39	119.74	121.90
34	2	1812	A	C5-C6-N6	-5.39	119.38	123.70
1	1	60	A	C5-C6-N1	-5.39	115.00	117.70
9	I	28	TYR	CB-CG-CD1	5.39	124.23	121.00
34	2	82	G	N3-C2-N2	5.39	123.67	119.90
34	2	821	A	C5-C6-N6	-5.39	119.39	123.70
34	2	988	A	C5-C6-N1	-5.39	115.00	117.70
34	2	1019	A	C5-C6-N1	-5.39	115.00	117.70
34	2	1144	A	C5-C6-N6	-5.39	119.39	123.70
34	2	1468	C	N3-C4-C5	-5.39	119.74	121.90
34	2	127	C	N3-C4-N4	5.39	121.77	118.00
34	2	1829	A	C5-C6-N6	-5.39	119.39	123.70
34	2	61	A	C5-C6-N6	-5.39	119.39	123.70
34	2	408	A	C5-C6-N6	-5.39	119.39	123.70
34	2	1307	C	N3-C4-C5	-5.39	119.75	121.90
34	2	1639	C	N3-C4-C5	-5.39	119.74	121.90
34	2	551	A	C5-C6-N1	-5.39	115.01	117.70
34	2	1467	C	N3-C4-C5	-5.39	119.75	121.90
34	2	84	A	C5-C6-N6	-5.39	119.39	123.70
34	2	104	A	C5-C6-N1	-5.39	115.01	117.70
34	2	303	G	P-O3'-C3'	5.39	126.16	119.70
34	2	926	C	N3-C4-C5	-5.38	119.75	121.90
34	2	976	A	C5-C6-N1	-5.38	115.01	117.70
34	2	1186	A	O4'-C1'-N9	5.38	112.51	108.20
34	2	1442	A	C5-C6-N1	-5.38	115.01	117.70
34	2	1705	C	N3-C4-N4	5.38	121.77	118.00
34	2	1740	A	C5-C6-N6	-5.38	119.39	123.70
34	2	14	C	N3-C4-N4	5.38	121.77	118.00
30	f	135	HIS	CA-CB-CG	5.38	122.75	113.60
34	2	316	C	N3-C4-C5	-5.38	119.75	121.90
34	2	550	A	C4-C5-C6	5.38	119.69	117.00
34	2	49	C	N3-C4-C5	-5.38	119.75	121.90
34	2	94	G	O4'-C1'-N9	5.38	112.50	108.20
34	2	354	A	O4'-C1'-N9	5.38	112.50	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1241	G	O4'-C1'-N9	5.38	112.50	108.20
34	2	145	G	O4'-C1'-N9	5.38	112.50	108.20
34	2	1144	A	C5-C6-N1	-5.38	115.01	117.70
1	1	12	C	N3-C4-C5	-5.38	119.75	121.90
34	2	125	C	N3-C4-N4	5.38	121.76	118.00
34	2	1362	G	O4'-C1'-N9	5.38	112.50	108.20
34	2	1618	A	C5-C6-N1	-5.38	115.01	117.70
34	2	494	G	O4'-C1'-N9	5.38	112.50	108.20
34	2	806	A	C5-C6-N6	-5.38	119.40	123.70
34	2	660	A	C5-C6-N1	-5.37	115.01	117.70
34	2	921	G	O4'-C1'-N9	5.37	112.50	108.20
34	2	1783	G	N3-C2-N2	5.37	123.66	119.90
34	2	805	A	C5-C6-N1	-5.37	115.01	117.70
34	2	1287	A	C5-C6-N1	-5.37	115.02	117.70
34	2	1397	A	C5-C6-N6	-5.37	119.40	123.70
34	2	1602	A	O4'-C1'-N9	5.37	112.50	108.20
34	2	516	A	C5-C6-N6	-5.37	119.40	123.70
5	E	175	SER	N-CA-CB	5.37	118.55	110.50
34	2	830	C	N3-C4-C5	-5.37	119.75	121.90
34	2	1039	G	O4'-C1'-N9	5.37	112.49	108.20
34	2	1414	C	N3-C4-C5	-5.37	119.75	121.90
34	2	1435	A	C5-C6-N1	-5.37	115.02	117.70
34	2	1795	A	C5-C6-N1	-5.37	115.02	117.70
34	2	1860	A	C5-C6-N1	-5.37	115.02	117.70
34	2	1243	C	N3-C4-C5	-5.37	119.75	121.90
34	2	159	A	C5-C6-N6	-5.37	119.41	123.70
34	2	1078	A	C5-C6-N1	-5.37	115.02	117.70
34	2	158	A	C5-C6-N1	-5.36	115.02	117.70
34	2	218	A	C5-C6-N6	-5.36	119.41	123.70
34	2	654	A	C5-C6-N6	-5.36	119.41	123.70
34	2	42	A	C5-C6-N1	-5.36	115.02	117.70
34	2	836	C	N3-C4-N4	5.36	121.75	118.00
34	2	236	C	N3-C4-C5	-5.36	119.76	121.90
34	2	1081	C	O4'-C1'-N1	5.36	112.49	108.20
34	2	1283	A	C5-C6-N1	-5.36	115.02	117.70
34	2	1552	C	N3-C4-N4	5.36	121.75	118.00
34	2	1694	A	C5-C6-N1	-5.36	115.02	117.70
34	2	221	A	O4'-C1'-N9	5.36	112.49	108.20
34	2	1196	A	C5-C6-N1	-5.36	115.02	117.70
34	2	35	C	N3-C4-C5	-5.36	119.76	121.90
34	2	521	A	O4'-C1'-N9	5.36	112.49	108.20
34	2	669	A	O4'-C1'-N9	5.36	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	798	A	C5-C6-N1	-5.36	115.02	117.70
34	2	1158	C	N3-C4-C5	-5.36	119.76	121.90
34	2	1576	C	N3-C4-C5	-5.36	119.76	121.90
34	2	511	A	C5-C6-N6	-5.36	119.42	123.70
34	2	845	A	C5-C6-N1	-5.35	115.02	117.70
34	2	808	A	C4-C5-C6	5.35	119.67	117.00
34	2	1053	C	N3-C4-C5	-5.35	119.76	121.90
34	2	1420	G	O4'-C1'-N9	5.35	112.48	108.20
34	2	1658	A	C5-C6-N6	-5.35	119.42	123.70
34	2	3	C	N3-C4-C5	-5.35	119.76	121.90
34	2	150	A	C4-C5-C6	5.35	119.67	117.00
34	2	928	G	O4'-C1'-N9	5.35	112.48	108.20
34	2	1051	A	C5-C6-N6	-5.35	119.42	123.70
34	2	1054	A	C5-C6-N1	-5.35	115.03	117.70
34	2	1134	C	N3-C4-C5	-5.35	119.76	121.90
34	2	1248	C	N3-C4-C5	-5.35	119.76	121.90
34	2	366	A	O4'-C1'-N9	5.35	112.48	108.20
34	2	221	A	C5-C6-N6	-5.34	119.42	123.70
34	2	659	A	C5-C6-N6	-5.34	119.42	123.70
34	2	809	A	C5-C6-N1	-5.34	115.03	117.70
34	2	1537	C	N3-C4-N4	5.34	121.74	118.00
34	2	1419	C	N3-C4-C5	-5.34	119.76	121.90
34	2	435	A	O4'-C1'-N9	5.34	112.47	108.20
34	2	654	A	C4-C5-C6	5.34	119.67	117.00
34	2	1745	C	C5-C4-N4	-5.34	116.46	120.20
34	2	1215	C	N3-C4-C5	-5.34	119.76	121.90
34	2	1348	G	O4'-C1'-N9	5.34	112.47	108.20
34	2	1484	C	O4'-C1'-N1	5.34	112.47	108.20
34	2	1746	C	C5-C4-N4	-5.34	116.46	120.20
34	2	400	G	O4'-C1'-N9	5.34	112.47	108.20
34	2	654	A	O4'-C1'-N9	5.34	112.47	108.20
34	2	850	A	O4'-C1'-N9	5.34	112.47	108.20
34	2	1115	A	C5-C6-N6	-5.34	119.43	123.70
34	2	104	A	O4'-C1'-N9	5.34	112.47	108.20
34	2	328	G	O4'-C1'-N9	5.34	112.47	108.20
34	2	390	C	N3-C4-C5	-5.34	119.77	121.90
34	2	1047	G	O4'-C1'-N9	5.34	112.47	108.20
34	2	1066	A	C5-C6-N1	-5.34	115.03	117.70
34	2	1184	A	O4'-C1'-N9	5.34	112.47	108.20
34	2	1844	A	C5-C6-N6	-5.34	119.43	123.70
34	2	1522	C	N3-C4-C5	-5.33	119.77	121.90
34	2	174	C	N3-C4-C5	-5.33	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	197	U	C6-N1-C1'	-5.33	113.73	121.20
34	2	564	A	C5-C6-N1	-5.33	115.03	117.70
34	2	1114	C	N3-C4-N4	5.33	121.73	118.00
34	2	1726	A	C5-C6-N1	-5.33	115.03	117.70
1	1	15	A	C5-C6-N1	-5.33	115.03	117.70
34	2	404	A	C5-C6-N1	-5.33	115.03	117.70
34	2	1087	C	N3-C4-C5	-5.33	119.77	121.90
34	2	1089	A	C5-C6-N6	-5.33	119.44	123.70
34	2	1478	C	N3-C4-C5	-5.33	119.77	121.90
34	2	302	C	N3-C4-C5	-5.33	119.77	121.90
34	2	1695	C	O4'-C1'-N1	5.33	112.46	108.20
34	2	52	G	O4'-C1'-N9	5.33	112.46	108.20
34	2	463	A	O4'-C1'-N9	5.33	112.46	108.20
34	2	1448	A	C5-C6-N1	-5.33	115.04	117.70
34	2	1640	C	N3-C4-C5	-5.33	119.77	121.90
34	2	64	A	C5-C6-N1	-5.33	115.04	117.70
34	2	338	A	O4'-C1'-N9	5.33	112.46	108.20
34	2	42	A	C5-C6-N6	-5.33	119.44	123.70
34	2	493	C	N3-C4-C5	-5.33	119.77	121.90
34	2	1102	C	N3-C4-C5	-5.33	119.77	121.90
34	2	408	A	C5-C6-N1	-5.32	115.04	117.70
34	2	812	A	C5-C6-N1	-5.32	115.04	117.70
34	2	1773	G	O4'-C1'-N9	5.32	112.46	108.20
34	2	466	A	C4-C5-C6	5.32	119.66	117.00
34	2	915	A	C5-C6-N1	-5.32	115.04	117.70
34	2	1718	G	O4'-C1'-N9	5.32	112.46	108.20
34	2	484	C	N3-C4-C5	-5.32	119.77	121.90
34	2	1018	U	C2-N1-C1'	5.32	124.08	117.70
34	2	73	C	N3-C4-C5	-5.32	119.77	121.90
34	2	868	A	C5-C6-N1	-5.32	115.04	117.70
34	2	1043	C	N3-C4-C5	-5.32	119.77	121.90
34	2	1146	A	C5-C6-N6	-5.32	119.44	123.70
34	2	1589	A	C5-C6-N1	-5.32	115.04	117.70
34	2	1635	A	C5-C6-N1	-5.32	115.04	117.70
34	2	91	A	C5-C6-N1	-5.32	115.04	117.70
34	2	618	A	C5-C6-N6	-5.32	119.45	123.70
34	2	670	G	O4'-C1'-N9	5.32	112.45	108.20
34	2	1694	A	C5-C6-N6	-5.32	119.45	123.70
34	2	67	C	N3-C4-C5	-5.31	119.77	121.90
34	2	473	C	N3-C4-C5	-5.31	119.77	121.90
34	2	214	A	C5-C6-N1	-5.31	115.04	117.70
34	2	1216	A	C5-C6-N1	-5.31	115.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	122	G	O4'-C1'-N9	5.31	112.45	108.20
34	2	373	G	O4'-C1'-N9	5.31	112.45	108.20
34	2	1829	A	C5-C6-N1	-5.31	115.04	117.70
34	2	142	C	C6-N1-C1'	-5.31	114.43	120.80
34	2	351	U	O4'-C1'-N1	5.31	112.45	108.20
34	2	450	A	O4'-C1'-N9	5.31	112.45	108.20
34	2	625	G	O4'-C1'-N9	5.31	112.45	108.20
34	2	1195	A	O4'-C1'-N9	5.31	112.45	108.20
34	2	1374	A	C5-C6-N6	-5.31	119.45	123.70
34	2	1565	G	O4'-C1'-N9	5.31	112.45	108.20
41	3	36	A	C5-C6-N1	-5.31	115.05	117.70
34	2	295	C	N3-C4-N4	5.31	121.72	118.00
34	2	833	A	C5-C6-N1	-5.31	115.05	117.70
34	2	985	C	N3-C4-C5	-5.31	119.78	121.90
34	2	1324	G	O4'-C1'-N9	5.31	112.45	108.20
34	2	1479	A	C5-C6-N6	-5.31	119.45	123.70
34	2	1528	A	C5-C6-N1	-5.31	115.05	117.70
34	2	1540	A	C5-C6-N1	-5.31	115.05	117.70
34	2	60	A	C5-C6-N1	-5.31	115.05	117.70
34	2	199	G	O4'-C1'-N9	5.31	112.44	108.20
34	2	1140	A	O4'-C1'-N9	5.31	112.44	108.20
34	2	16	G	O4'-C1'-N9	5.30	112.44	108.20
34	2	398	A	C5-C6-N1	-5.30	115.05	117.70
34	2	992	A	C5-C6-N6	-5.30	119.46	123.70
34	2	1338	U	O4'-C1'-N1	5.30	112.44	108.20
34	2	227	A	O4'-C1'-N9	5.30	112.44	108.20
34	2	1048	A	C5-C6-N1	-5.30	115.05	117.70
34	2	1214	C	N3-C4-C5	-5.30	119.78	121.90
34	2	1524	C	N3-C4-C5	-5.30	119.78	121.90
34	2	609	A	C5-C6-N6	-5.30	119.46	123.70
34	2	661	A	C5-C6-N6	-5.30	119.46	123.70
34	2	827	G	O4'-C1'-N9	5.30	112.44	108.20
34	2	1446	G	O4'-C1'-N9	5.30	112.44	108.20
34	2	1019	A	O4'-C1'-N9	5.30	112.44	108.20
34	2	62	G	O4'-C1'-N9	5.30	112.44	108.20
34	2	850	A	C5-C6-N6	-5.30	119.46	123.70
34	2	1008	A	C5-C6-N1	-5.30	115.05	117.70
34	2	1038	A	C5-C6-N1	-5.30	115.05	117.70
34	2	1731	G	O4'-C1'-N9	5.30	112.44	108.20
1	1	74	C	N3-C4-C5	-5.29	119.78	121.90
30	f	150	PHE	CB-CG-CD1	5.29	124.51	120.80
34	2	1254	A	C5-C6-N1	-5.29	115.05	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1482	A	C5-C6-N1	-5.29	115.05	117.70
34	2	1803	A	C5-C6-N1	-5.29	115.05	117.70
34	2	84	A	C5-C6-N1	-5.29	115.05	117.70
34	2	513	A	C5-C6-N1	-5.29	115.05	117.70
34	2	1267	C	N3-C4-N4	5.29	121.70	118.00
34	2	675	A	C5-C6-N1	-5.29	115.05	117.70
34	2	1114	C	N3-C4-C5	-5.29	119.78	121.90
34	2	1740	A	C5-C6-N1	-5.29	115.05	117.70
34	2	1372	A	C5-C6-N1	-5.29	115.06	117.70
34	2	1578	C	N3-C4-N4	5.29	121.70	118.00
34	2	223	A	C5-C6-N1	-5.29	115.06	117.70
34	2	295	C	N3-C4-C5	-5.29	119.78	121.90
34	2	540	C	N3-C4-C5	-5.29	119.78	121.90
34	2	899	A	C5-C6-N6	-5.29	119.47	123.70
34	2	1413	C	N3-C4-C5	-5.29	119.78	121.90
34	2	1863	A	C5-C6-N1	-5.29	115.06	117.70
27	c	79	PHE	CB-CG-CD1	5.29	124.50	120.80
34	2	407	C	N3-C4-C5	-5.29	119.78	121.90
34	2	1714	A	C5-C6-N1	-5.29	115.06	117.70
34	2	814	A	C5-C6-N1	-5.29	115.06	117.70
34	2	1032	A	C5-C6-N1	-5.29	115.06	117.70
34	2	1115	A	C5-C6-N1	-5.29	115.06	117.70
34	2	1379	A	C5-C6-N1	-5.29	115.06	117.70
34	2	139	C	N3-C4-N4	5.28	121.70	118.00
34	2	329	A	C5-C6-N1	-5.28	115.06	117.70
34	2	454	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	804	A	C5-C6-N6	-5.28	119.47	123.70
34	2	1378	A	C5-C6-N1	-5.28	115.06	117.70
34	2	1845	A	C5-C6-N1	-5.28	115.06	117.70
41	3	50	C	N3-C4-C5	-5.28	119.79	121.90
34	2	908	C	N3-C4-N4	5.28	121.70	118.00
35	A	82	TYR	CB-CG-CD1	5.28	124.17	121.00
34	2	910	U	O4'-C1'-N1	5.28	112.42	108.20
34	2	1465	A	C5-C6-N1	-5.28	115.06	117.70
34	2	1625	A	C5-C6-N6	-5.28	119.47	123.70
34	2	557	C	N3-C4-C5	-5.28	119.79	121.90
34	2	1800	A	O4'-C1'-N9	5.28	112.42	108.20
1	1	2	A	C5-C6-N6	-5.28	119.48	123.70
34	2	363	G	O4'-C1'-N9	5.28	112.42	108.20
34	2	1212	C	N3-C4-C5	-5.28	119.79	121.90
34	2	320	G	O4'-C1'-N9	5.28	112.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	863	G	O4'-C1'-N9	5.28	112.42	108.20
34	2	1330	G	C5-C6-O6	-5.28	125.44	128.60
34	2	1586	C	N3-C4-C5	-5.28	119.79	121.90
34	2	804	A	O4'-C1'-N9	5.27	112.42	108.20
34	2	1015	C	N3-C4-N4	5.27	121.69	118.00
34	2	1111	U	C6-N1-C1'	-5.27	113.82	121.20
41	3	64	A	C5-C6-N1	-5.27	115.06	117.70
34	2	226	A	C5-C6-N6	-5.27	119.48	123.70
34	2	299	G	O4'-C1'-N9	5.27	112.42	108.20
34	2	535	A	C5-C6-N1	-5.27	115.06	117.70
34	2	814	A	O4'-C1'-N9	5.27	112.42	108.20
34	2	949	C	N3-C4-C5	-5.27	119.79	121.90
34	2	1237	A	C5-C6-N6	-5.27	119.48	123.70
34	2	1513	C	C6-N1-C1'	-5.27	114.47	120.80
34	2	38	A	C5-C6-N1	-5.27	115.07	117.70
34	2	506	A	C5-C6-N6	-5.27	119.48	123.70
34	2	652	G	N1-C6-O6	5.27	123.06	119.90
34	2	27	A	C5-C6-N1	-5.27	115.07	117.70
34	2	142	C	N3-C4-C5	-5.27	119.79	121.90
34	2	165	G	C4-N9-C1'	5.27	133.35	126.50
34	2	873	C	N3-C4-C5	-5.27	119.79	121.90
34	2	979	A	C5-C6-N1	-5.27	115.07	117.70
22	X	10	ASP	N-CA-CB	5.26	120.08	110.60
34	2	127	C	N3-C4-C5	-5.26	119.79	121.90
34	2	290	A	O4'-C1'-N9	5.26	112.41	108.20
34	2	826	A	O4'-C1'-N9	5.26	112.41	108.20
34	2	1196	A	O4'-C1'-N9	5.26	112.41	108.20
34	2	1571	G	O4'-C1'-N9	5.26	112.41	108.20
1	1	57	G	O4'-C1'-N9	5.26	112.41	108.20
34	2	1374	A	C5-C6-N1	-5.26	115.07	117.70
1	1	52	G	O4'-C1'-N9	5.26	112.41	108.20
34	2	19	A	O4'-C1'-N9	5.26	112.41	108.20
34	2	405	A	C5-C6-N1	-5.26	115.07	117.70
34	2	948	G	O4'-C1'-N9	5.26	112.41	108.20
34	2	1288	C	N3-C4-N4	5.26	121.68	118.00
34	2	1384	A	C5-C6-N1	-5.26	115.07	117.70
34	2	644	A	C5-C6-N1	-5.25	115.07	117.70
34	2	1064	G	N3-C2-N2	5.25	123.58	119.90
34	2	1129	A	O4'-C1'-N9	5.25	112.40	108.20
34	2	1857	A	C5-C6-N6	-5.25	119.50	123.70
1	1	39	C	O4'-C1'-N1	5.25	112.40	108.20
34	2	438	A	C5-C6-N6	-5.25	119.50	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	54	A	C5-C6-N1	-5.25	115.07	117.70
34	2	206	A	O4'-C1'-N9	5.25	112.40	108.20
34	2	538	C	N3-C4-C5	-5.25	119.80	121.90
34	2	636	G	O4'-C1'-N9	5.25	112.40	108.20
34	2	987	G	C8-N9-C1'	-5.25	120.17	127.00
34	2	1375	A	C5-C6-N1	-5.25	115.08	117.70
34	2	503	G	O4'-C1'-N9	5.25	112.40	108.20
34	2	60	A	C5-C6-N6	-5.25	119.50	123.70
34	2	655	G	O4'-C1'-N9	5.25	112.40	108.20
34	2	866	A	C5-C6-N1	-5.25	115.08	117.70
34	2	1096	A	C5-C6-N6	-5.25	119.50	123.70
34	2	1782	A	O4'-C1'-N9	5.25	112.40	108.20
34	2	1109	A	C5-C6-N1	-5.25	115.08	117.70
34	2	1231	G	O4'-C1'-N9	5.25	112.40	108.20
34	2	1776	G	O4'-C1'-N9	5.25	112.40	108.20
34	2	1807	A	C5-C6-N6	-5.25	119.50	123.70
34	2	415	G	O4'-C1'-N9	5.24	112.40	108.20
34	2	1316	G	O4'-C1'-N9	5.24	112.39	108.20
34	2	1612	G	N3-C2-N2	5.24	123.57	119.90
41	3	36	A	O4'-C1'-N9	5.24	112.39	108.20
34	2	78	C	N3-C4-N4	5.24	121.67	118.00
34	2	205	G	N3-C2-N2	5.24	123.57	119.90
35	A	100	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	1	11	G	O4'-C1'-N9	5.24	112.39	108.20
34	2	595	A	C5-C6-N6	-5.24	119.51	123.70
34	2	970	C	N3-C4-C5	-5.24	119.80	121.90
34	2	1020	A	C5-C6-N1	-5.24	115.08	117.70
34	2	1031	A	C5-C6-N1	-5.24	115.08	117.70
34	2	382	A	C5-C6-N1	-5.24	115.08	117.70
34	2	1123	C	N3-C4-C5	-5.24	119.80	121.90
34	2	1314	G	O4'-C1'-N9	5.24	112.39	108.20
38	k	388	PHE	CB-CG-CD1	5.24	124.47	120.80
34	2	435	A	C5-C6-N1	-5.24	115.08	117.70
34	2	601	G	O4'-C1'-N9	5.24	112.39	108.20
34	2	591	G	O4'-C1'-N9	5.24	112.39	108.20
34	2	1076	A	C5-C6-N1	-5.24	115.08	117.70
34	2	1162	G	O4'-C1'-N9	5.23	112.39	108.20
34	2	1192	A	O4'-C1'-N9	5.23	112.39	108.20
1	1	17	C	O4'-C1'-N1	5.23	112.39	108.20
34	2	338	A	C5-C6-N6	-5.23	119.51	123.70
34	2	389	C	N3-C4-C5	-5.23	119.81	121.90
34	2	472	G	N3-C2-N2	5.23	123.56	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	547	U	O4'-C1'-N1	5.23	112.39	108.20
34	2	798	A	O4'-C1'-N9	5.23	112.39	108.20
34	2	1186	A	C5-C6-N6	-5.23	119.52	123.70
34	2	369	C	N3-C4-C5	-5.23	119.81	121.90
34	2	662	A	C5-C6-N1	-5.23	115.08	117.70
34	2	1147	G	O4'-C1'-N9	5.23	112.38	108.20
34	2	1182	U	C1'-O4'-C4'	5.23	114.08	109.90
34	2	157	U	O4'-C1'-N1	5.23	112.38	108.20
34	2	820	C	N3-C4-C5	-5.23	119.81	121.90
34	2	857	A	C5-C6-N1	-5.23	115.09	117.70
34	2	1261	A	C5-C6-N1	-5.23	115.09	117.70
41	3	51	C	N3-C4-C5	-5.23	119.81	121.90
34	2	824	G	O4'-C1'-N9	5.23	112.38	108.20
34	2	1646	A	C5-C6-N1	-5.23	115.09	117.70
34	2	1705	C	N3-C4-C5	-5.23	119.81	121.90
3	C	139	TYR	CB-CG-CD2	-5.22	117.86	121.00
34	2	619	A	C5-C6-N1	-5.22	115.09	117.70
34	2	985	C	N3-C4-N4	5.22	121.66	118.00
34	2	1632	A	C5-C6-N6	-5.22	119.52	123.70
34	2	80	G	O3'-P-O5'	5.22	113.92	104.00
34	2	576	G	N3-C2-N2	5.22	123.56	119.90
34	2	1479	A	C5-C6-N1	-5.22	115.09	117.70
34	2	1613	C	N3-C4-C5	-5.22	119.81	121.90
34	2	1675	G	O4'-C1'-N9	5.22	112.38	108.20
34	2	371	C	N3-C4-N4	5.22	121.66	118.00
34	2	564	A	C5-C6-N6	-5.22	119.52	123.70
34	2	1030	A	O4'-C1'-N9	5.22	112.38	108.20
38	k	516	PHE	CB-CG-CD1	5.22	124.45	120.80
34	2	1542	C	N3-C4-N4	5.22	121.65	118.00
34	2	1549	C	N3-C4-C5	-5.22	119.81	121.90
34	2	1673	A	C5-C6-N1	-5.22	115.09	117.70
34	2	429	A	O4'-C1'-N9	5.21	112.37	108.20
34	2	502	A	O4'-C1'-N9	5.21	112.37	108.20
34	2	565	A	C5-C6-N1	-5.21	115.09	117.70
34	2	658	A	C5-C6-N1	-5.21	115.09	117.70
34	2	847	C	N3-C4-N4	5.21	121.65	118.00
34	2	1166	A	C4-C5-C6	5.21	119.61	117.00
34	2	1264	C	N3-C4-C5	-5.21	119.81	121.90
34	2	1275	C	N3-C4-C5	-5.21	119.81	121.90
34	2	1530	U	C2-N1-C1'	5.21	123.96	117.70
1	1	8	G	O4'-C1'-N9	5.21	112.37	108.20
34	2	951	A	C5-C6-N1	-5.21	115.09	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1717	G	O4'-C1'-N9	5.21	112.37	108.20
34	2	232	A	C5-C6-N1	-5.21	115.09	117.70
34	2	306	C	N3-C4-C5	-5.21	119.82	121.90
34	2	1690	A	C5-C6-N1	-5.21	115.09	117.70
34	2	40	A	C5-C6-N1	-5.21	115.10	117.70
34	2	167	G	O4'-C1'-N9	5.21	112.37	108.20
34	2	240	C	N3-C4-C5	-5.21	119.82	121.90
34	2	813	G	N3-C2-N2	5.21	123.54	119.90
34	2	1527	C	N3-C4-C5	-5.21	119.82	121.90
34	2	6	G	O4'-C1'-N9	5.20	112.36	108.20
34	2	899	A	O4'-C1'-N9	5.20	112.36	108.20
34	2	1025	G	O4'-C1'-N9	5.20	112.36	108.20
34	2	1480	A	C5-C6-N1	-5.20	115.10	117.70
34	2	1184	A	C5-C6-N6	-5.20	119.54	123.70
34	2	1372	A	O4'-C1'-N9	5.20	112.36	108.20
34	2	1532	A	O4'-C1'-N9	5.20	112.36	108.20
34	2	546	U	O4'-C1'-N1	5.20	112.36	108.20
34	2	1609	A	C5-C6-N1	-5.20	115.10	117.70
34	2	99	A	C5-C6-N1	-5.20	115.10	117.70
34	2	1539	C	C5-C4-N4	-5.20	116.56	120.20
34	2	1730	A	C5-C6-N1	-5.20	115.10	117.70
1	1	73	A	C5-C6-N1	-5.20	115.10	117.70
34	2	107	A	C5-C6-N1	-5.20	115.10	117.70
34	2	1059	C	N3-C4-N4	5.20	121.64	118.00
34	2	1405	A	O4'-C1'-N9	5.20	112.36	108.20
34	2	1312	C	N3-C4-C5	-5.19	119.82	121.90
34	2	53	C	N3-C4-C5	-5.19	119.82	121.90
34	2	545	A	P-O3'-C3'	5.19	125.93	119.70
34	2	1140	A	C5-C6-N6	-5.19	119.55	123.70
34	2	1670	A	C5-C6-N1	-5.19	115.10	117.70
34	2	80	G	OP2-P-O3'	-5.19	93.78	105.20
34	2	1180	G	O4'-C1'-N9	5.19	112.35	108.20
34	2	175	A	C5-C6-N1	-5.19	115.11	117.70
34	2	509	A	O4'-C1'-N9	5.19	112.35	108.20
34	2	1024	A	C5-C6-N1	-5.19	115.11	117.70
34	2	918	A	O4'-C1'-N9	5.19	112.35	108.20
34	2	1442	A	C5-C6-N6	-5.19	119.55	123.70
34	2	78	C	C2-N1-C1'	5.19	124.50	118.80
34	2	953	A	O4'-C1'-N9	5.19	112.35	108.20
34	2	1038	A	O4'-C1'-N9	5.18	112.35	108.20
34	2	1058	A	C5-C6-N1	-5.18	115.11	117.70
34	2	1274	A	C5-C6-N1	-5.18	115.11	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1149	C	N3-C4-C5	-5.18	119.83	121.90
34	2	1491	G	O4'-C1'-N9	5.18	112.35	108.20
34	2	77	A	O4'-C1'-N9	5.18	112.34	108.20
34	2	1327	C	N3-C4-N4	5.18	121.63	118.00
34	2	118	C	N3-C4-C5	-5.18	119.83	121.90
34	2	353	A	C4-C5-C6	5.18	119.59	117.00
34	2	677	C	O4'-C1'-N1	5.18	112.34	108.20
34	2	846	C	N3-C4-C5	-5.18	119.83	121.90
34	2	1431	C	N3-C4-C5	-5.18	119.83	121.90
34	2	526	A	C5-C6-N6	-5.17	119.56	123.70
34	2	446	C	N3-C4-C5	-5.17	119.83	121.90
34	2	519	A	C5-C6-N1	-5.17	115.11	117.70
34	2	402	G	O4'-C1'-N9	5.17	112.34	108.20
34	2	458	A	O4'-C1'-N9	5.17	112.34	108.20
34	2	908	C	N3-C4-C5	-5.17	119.83	121.90
34	2	1164	G	O4'-C1'-N9	5.17	112.34	108.20
34	2	416	A	C5-C6-N1	-5.17	115.11	117.70
34	2	1058	A	C5-C6-N6	-5.17	119.56	123.70
34	2	388	A	C5-C6-N1	-5.17	115.12	117.70
34	2	656	U	O4'-C1'-N1	5.17	112.33	108.20
34	2	1087	C	N3-C4-N4	5.17	121.62	118.00
34	2	1401	A	O4'-C1'-N9	5.17	112.33	108.20
34	2	1470	A	C5-C6-N1	-5.17	115.12	117.70
34	2	1809	A	C5-C6-N6	-5.17	119.57	123.70
34	2	326	A	C5-C6-N6	-5.17	119.57	123.70
34	2	1295	A	C5-C6-N1	-5.17	115.12	117.70
34	2	1847	C	N3-C4-N4	5.17	121.62	118.00
34	2	835	C	C6-N1-C1'	-5.16	114.60	120.80
34	2	1078	A	O4'-C1'-N9	5.16	112.33	108.20
34	2	1330	G	O4'-C1'-N9	5.16	112.33	108.20
34	2	1361	G	O4'-C1'-N9	5.16	112.33	108.20
34	2	1544	U	O4'-C1'-N1	5.16	112.33	108.20
34	2	1785	A	O4'-C1'-N9	5.16	112.33	108.20
38	k	551	LEU	CB-CG-CD2	5.16	119.78	111.00
34	2	235	C	C5-C4-N4	-5.16	116.59	120.20
34	2	84	A	O4'-C1'-N9	5.16	112.33	108.20
34	2	919	G	O4'-C1'-N9	5.16	112.33	108.20
34	2	1411	C	N3-C4-C5	-5.16	119.84	121.90
34	2	1557	C	N3-C4-C5	-5.16	119.84	121.90
34	2	292	A	C5-C6-N1	-5.16	115.12	117.70
34	2	359	C	N3-C4-C5	-5.16	119.84	121.90
34	2	1262	C	N3-C4-C5	-5.16	119.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	181	A	C5-C6-N6	-5.15	119.58	123.70
34	2	1825	A	C5-C6-N1	-5.15	115.12	117.70
34	2	915	A	O4'-C1'-N9	5.15	112.32	108.20
34	2	1730	A	C5-C6-N6	-5.15	119.58	123.70
34	2	1793	G	O4'-C1'-N9	5.15	112.32	108.20
34	2	1803	A	O4'-C1'-N9	5.15	112.32	108.20
41	3	64	A	C5-C6-N6	-5.15	119.58	123.70
34	2	10	G	N3-C2-N2	5.15	123.51	119.90
34	2	293	A	C5-C6-N6	-5.15	119.58	123.70
34	2	1434	A	O4'-C1'-N9	5.15	112.32	108.20
34	2	1321	G	O4'-C1'-N9	5.15	112.32	108.20
34	2	1337	C	O4'-C1'-N1	5.15	112.32	108.20
34	2	1449	C	N3-C4-C5	-5.15	119.84	121.90
34	2	1701	G	O4'-C1'-N9	5.15	112.32	108.20
34	2	1805	C	N3-C4-C5	-5.15	119.84	121.90
34	2	1117	G	O4'-C1'-N9	5.15	112.32	108.20
34	2	1832	U	O4'-C1'-N1	5.14	112.31	108.20
34	2	1837	G	O4'-C1'-N9	5.14	112.32	108.20
34	2	463	A	C5-C6-N1	-5.14	115.13	117.70
34	2	1247	A	C5-C6-N1	-5.14	115.13	117.70
34	2	202	U	O4'-C1'-N1	5.14	112.31	108.20
34	2	445	A	O4'-C1'-N9	5.14	112.31	108.20
34	2	623	C	N3-C4-C5	-5.14	119.84	121.90
34	2	804	A	C5-C6-N1	-5.14	115.13	117.70
34	2	1508	C	N3-C4-C5	-5.14	119.84	121.90
34	2	1845	A	O4'-C1'-N9	5.14	112.31	108.20
34	2	518	A	C5-C6-N1	-5.14	115.13	117.70
34	2	836	C	N3-C4-C5	-5.14	119.85	121.90
34	2	1322	U	C2-N1-C1'	5.14	123.86	117.70
34	2	160	U	O4'-C1'-N1	5.13	112.31	108.20
34	2	593	C	N3-C4-C5	-5.13	119.85	121.90
34	2	854	A	C5-C6-N6	-5.13	119.59	123.70
34	2	932	G	O4'-C1'-N9	5.13	112.31	108.20
34	2	938	G	N3-C2-N2	5.13	123.49	119.90
34	2	1219	A	O4'-C1'-N9	5.13	112.31	108.20
34	2	1568	G	O4'-C1'-N9	5.13	112.31	108.20
34	2	1630	C	N3-C4-C5	-5.13	119.85	121.90
34	2	1636	A	C5-C6-N1	-5.13	115.13	117.70
34	2	871	A	C5-C6-N1	-5.13	115.13	117.70
34	2	1509	G	O4'-C1'-N9	5.13	112.31	108.20
1	1	22	G	O4'-C1'-N9	5.13	112.31	108.20
34	2	1066	A	C5-C6-N6	-5.13	119.59	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1432	C	O4'-C1'-N1	5.13	112.31	108.20
34	2	1664	G	O4'-C1'-N9	5.13	112.30	108.20
34	2	1751	G	O4'-C1'-N9	5.13	112.31	108.20
13	M	70	TYR	CB-CG-CD1	5.13	124.08	121.00
1	1	23	C	N3-C4-C5	-5.13	119.85	121.90
34	2	967	G	N3-C2-N2	5.13	123.49	119.90
34	2	1333	C	N3-C4-C5	-5.13	119.85	121.90
34	2	1629	A	O4'-C1'-N9	5.13	112.30	108.20
34	2	318	U	O4'-C1'-N1	5.13	112.30	108.20
34	2	371	C	N3-C4-C5	-5.13	119.85	121.90
34	2	372	C	N3-C4-C5	-5.13	119.85	121.90
34	2	427	G	O4'-C1'-N9	5.13	112.30	108.20
34	2	583	C	N3-C4-C5	-5.13	119.85	121.90
34	2	609	A	O4'-C1'-N9	5.13	112.30	108.20
34	2	644	A	O4'-C1'-N9	5.12	112.30	108.20
34	2	1674	A	C5-C6-N1	-5.12	115.14	117.70
34	2	141	A	P-O3'-C3'	5.12	125.85	119.70
34	2	545	A	O4'-C1'-N9	5.12	112.30	108.20
34	2	968	A	C5-C6-N6	-5.12	119.60	123.70
34	2	673	G	O4'-C1'-N9	5.12	112.30	108.20
34	2	333	A	O4'-C1'-N9	5.12	112.30	108.20
34	2	965	U	O4'-C1'-N1	5.12	112.30	108.20
34	2	1291	A	C5-C6-N6	-5.12	119.61	123.70
34	2	1499	C	N3-C4-C5	-5.12	119.85	121.90
34	2	1537	C	N3-C4-C5	-5.12	119.85	121.90
34	2	371	C	O4'-C1'-N1	5.12	112.29	108.20
34	2	164	A	O4'-C1'-N9	5.12	112.29	108.20
34	2	589	A	O4'-C1'-N9	5.12	112.29	108.20
34	2	922	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	1407	G	O4'-C1'-N9	5.12	112.29	108.20
36	B	194	LYS	N-CA-CB	5.12	119.81	110.60
37	j	95	TYR	C-N-CA	5.12	134.49	121.70
34	2	333	A	C5-C6-N6	-5.11	119.61	123.70
31	g	101	PHE	CB-CG-CD2	-5.11	117.22	120.80
34	2	58	C	N3-C4-C5	-5.11	119.86	121.90
34	2	1394	G	O4'-C1'-N9	5.11	112.28	108.20
34	2	1483	A	C5-C6-N1	-5.11	115.15	117.70
34	2	91	A	O4'-C1'-N9	5.11	112.28	108.20
34	2	985	C	O4'-C1'-N1	5.10	112.28	108.20
34	2	1647	G	O4'-C1'-N9	5.10	112.28	108.20
34	2	1744	G	O4'-C1'-N9	5.10	112.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	372	C	N3-C4-N4	5.10	121.57	118.00
34	2	379	A	O4'-C1'-N9	5.10	112.28	108.20
34	2	7	G	O4'-C1'-N9	5.10	112.28	108.20
34	2	1056	A	C5-C6-N1	-5.10	115.15	117.70
34	2	1851	G	O4'-C1'-N9	5.10	112.28	108.20
34	2	559	A	C5-C6-N1	-5.10	115.15	117.70
34	2	1353	A	C5-C6-N6	-5.10	119.62	123.70
34	2	1376	C	N3-C4-C5	-5.10	119.86	121.90
1	1	73	A	O4'-C1'-N9	5.10	112.28	108.20
34	2	288	A	O4'-C1'-N9	5.10	112.28	108.20
34	2	566	A	O4'-C1'-N9	5.10	112.28	108.20
34	2	1305	C	N3-C4-C5	-5.10	119.86	121.90
34	2	1337	C	N3-C4-C5	-5.10	119.86	121.90
34	2	1451	A	C5-C6-N6	-5.10	119.62	123.70
34	2	483	A	O4'-C1'-N9	5.10	112.28	108.20
34	2	1131	C	N3-C4-C5	-5.10	119.86	121.90
34	2	1166	A	O4'-C1'-N9	5.10	112.28	108.20
34	2	448	A	O4'-C1'-N9	5.09	112.28	108.20
34	2	992	A	C5-C6-N1	-5.09	115.15	117.70
34	2	1380	C	N3-C4-C5	-5.09	119.86	121.90
34	2	1850	C	N3-C4-C5	-5.09	119.86	121.90
34	2	39	A	O4'-C1'-N9	5.09	112.27	108.20
34	2	823	A	O4'-C1'-N9	5.09	112.27	108.20
34	2	856	G	O4'-C1'-N9	5.09	112.27	108.20
34	2	1032	A	O4'-C1'-N9	5.09	112.27	108.20
34	2	1457	G	N3-C2-N2	5.09	123.46	119.90
34	2	65	C	N3-C4-C5	-5.09	119.86	121.90
34	2	431	C	N3-C4-C5	-5.09	119.86	121.90
34	2	1299	C	N3-C4-C5	-5.09	119.86	121.90
34	2	39	A	C5-C6-N1	-5.09	115.16	117.70
34	2	92	A	C5-C6-N1	-5.09	115.16	117.70
34	2	410	G	O4'-C1'-N9	5.08	112.27	108.20
34	2	900	A	C5-C6-N6	-5.08	119.63	123.70
34	2	909	A	C5-C6-N1	-5.08	115.16	117.70
34	2	960	A	C5-C6-N6	-5.08	119.63	123.70
34	2	1135	C	N3-C4-N4	5.08	121.56	118.00
1	1	38	A	C5-C6-N1	-5.08	115.16	117.70
34	2	1261	A	C5-C6-N6	-5.08	119.64	123.70
34	2	1287	A	O4'-C1'-N9	5.08	112.26	108.20
34	2	151	C	N3-C4-C5	-5.08	119.87	121.90
34	2	1004	A	C5-C6-N1	-5.08	115.16	117.70
34	2	1521	G	O4'-C1'-N9	5.08	112.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1592	C	N3-C4-C5	-5.08	119.87	121.90
34	2	649	G	O4'-C1'-N9	5.08	112.26	108.20
34	2	1327	C	N3-C4-C5	-5.08	119.87	121.90
34	2	1822	C	N3-C4-C5	-5.08	119.87	121.90
34	2	337	G	O4'-C1'-N9	5.07	112.26	108.20
34	2	437	A	C5-N7-C8	5.07	106.44	103.90
34	2	934	A	C5-C6-N6	-5.07	119.64	123.70
34	2	1229	G	O4'-C1'-N9	5.07	112.26	108.20
34	2	1303	U	C5-C4-O4	-5.07	122.86	125.90
34	2	934	A	O4'-C1'-N9	5.07	112.26	108.20
34	2	1170	U	C6-N1-C1'	-5.07	114.10	121.20
34	2	1278	A	C5-C6-N1	-5.07	115.16	117.70
34	2	1608	G	O4'-C1'-N9	5.07	112.26	108.20
34	2	1777	C	N3-C4-N4	5.07	121.55	118.00
34	2	1824	U	O4'-C1'-N1	5.07	112.26	108.20
34	2	1469	G	O4'-C1'-N9	5.07	112.25	108.20
34	2	1371	G	O4'-C1'-N9	5.07	112.25	108.20
34	2	1426	C	N3-C4-C5	-5.07	119.87	121.90
34	2	229	A	C5-C6-N6	-5.07	119.65	123.70
34	2	1383	G	O4'-C1'-N9	5.07	112.25	108.20
34	2	1494	A	C5-C6-N6	-5.07	119.65	123.70
36	B	279	LYS	C-N-CD	5.07	139.04	128.40
34	2	1381	G	O4'-C1'-N9	5.06	112.25	108.20
34	2	1487	G	O4'-C1'-N9	5.06	112.25	108.20
34	2	171	A	C5-C6-N1	-5.06	115.17	117.70
34	2	1224	A	C5-C6-N1	-5.06	115.17	117.70
34	2	1734	C	N3-C4-C5	-5.06	119.88	121.90
34	2	1549	C	O4'-C1'-N1	5.06	112.25	108.20
34	2	1216	A	P-O3'-C3'	5.06	125.77	119.70
34	2	1266	G	O4'-C1'-N9	5.06	112.25	108.20
34	2	1497	C	N3-C4-C5	-5.06	119.88	121.90
34	2	1583	A	C5-C6-N1	-5.06	115.17	117.70
34	2	102	A	C5-C6-N6	-5.06	119.66	123.70
34	2	849	C	N3-C4-N4	5.06	121.54	118.00
1	1	74	C	O4'-C1'-N1	5.06	112.25	108.20
34	2	1410	A	C5-C6-N6	-5.06	119.66	123.70
34	2	1849	G	O4'-C1'-N9	5.06	112.24	108.20
34	2	482	C	N3-C4-C5	-5.05	119.88	121.90
34	2	968	A	O4'-C1'-N9	5.05	112.24	108.20
34	2	994	A	O4'-C1'-N9	5.05	112.24	108.20
34	2	1583	A	O4'-C1'-N9	5.05	112.24	108.20
34	2	1397	A	C5-C6-N1	-5.05	115.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	339	A	C5-C6-N1	-5.05	115.17	117.70
34	2	431	C	N3-C4-N4	5.05	121.54	118.00
34	2	1246	A	C5-C6-N1	-5.05	115.17	117.70
34	2	48	C	N3-C4-C5	-5.05	119.88	121.90
34	2	438	A	C5-C6-N1	-5.05	115.18	117.70
34	2	479	A	C5-C6-N1	-5.05	115.18	117.70
34	2	483	A	C5-C6-N1	-5.05	115.18	117.70
34	2	805	A	O4'-C1'-N9	5.05	112.24	108.20
34	2	1178	A	O4'-C1'-N9	5.05	112.24	108.20
34	2	1826	A	C5-C6-N6	-5.05	119.66	123.70
34	2	1839	A	C5-C6-N1	-5.05	115.18	117.70
34	2	615	G	N3-C2-N2	5.04	123.43	119.90
34	2	1048	A	O4'-C1'-N9	5.04	112.24	108.20
34	2	957	G	O4'-C1'-N9	5.04	112.23	108.20
34	2	1181	C	N3-C4-C5	-5.04	119.88	121.90
34	2	1777	C	O4'-C1'-N1	5.04	112.23	108.20
34	2	125	C	N3-C4-C5	-5.04	119.88	121.90
34	2	615	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	858	A	O4'-C1'-N9	5.04	112.23	108.20
34	2	907	C	N3-C4-C5	-5.04	119.88	121.90
34	2	1213	A	C5-C6-N1	-5.04	115.18	117.70
34	2	1384	A	O4'-C1'-N9	5.04	112.23	108.20
34	2	1777	C	N3-C4-C5	-5.04	119.88	121.90
34	2	40	A	O4'-C1'-N9	5.04	112.23	108.20
34	2	523	A	C5-C6-N6	-5.04	119.67	123.70
34	2	843	A	O4'-C1'-N9	5.04	112.23	108.20
34	2	1046	A	C5-C6-N1	-5.04	115.18	117.70
34	2	1236	A	C5-C6-N1	-5.04	115.18	117.70
34	2	620	U	O4'-C1'-N1	5.04	112.23	108.20
34	2	847	C	N3-C4-C5	-5.04	119.89	121.90
34	2	938	G	O4'-C1'-N9	5.04	112.23	108.20
34	2	1432	C	N3-C4-C5	-5.04	119.89	121.90
34	2	58	C	O4'-C1'-N1	5.03	112.23	108.20
34	2	1650	C	N3-C4-C5	-5.03	119.89	121.90
34	2	1784	A	C5-C6-N1	-5.03	115.18	117.70
34	2	1045	A	C5-C6-N6	-5.03	119.68	123.70
34	2	1601	G	N3-C2-N2	5.03	123.42	119.90
34	2	293	A	O4'-C1'-N9	5.03	112.22	108.20
34	2	897	G	O4'-C1'-N9	5.03	112.22	108.20
34	2	1142	C	C5-C4-N4	-5.03	116.68	120.20
34	2	316	C	O4'-C1'-N1	5.03	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2	1036	G	O4'-C1'-N9	5.03	112.22	108.20
34	2	311	C	O4'-C1'-N1	5.02	112.22	108.20
34	2	44	U	O4'-C1'-N1	5.02	112.22	108.20
34	2	1027	A	O4'-C1'-N9	5.02	112.22	108.20
1	1	40	C	N3-C4-C5	-5.02	119.89	121.90
34	2	1742	C	N3-C4-C5	-5.02	119.89	121.90
34	2	1857	A	C5-C6-N1	-5.02	115.19	117.70
34	2	1299	C	N3-C4-N4	5.02	121.51	118.00
34	2	1516	C	O4'-C1'-N1	5.02	112.21	108.20
34	2	1649	G	O4'-C1'-N9	5.02	112.21	108.20
34	2	1110	U	O4'-C1'-N1	5.02	112.21	108.20
34	2	1004	A	O4'-C1'-N9	5.01	112.21	108.20
34	2	574	A	C5-C6-N1	-5.01	115.19	117.70
34	2	984	C	N3-C4-C5	-5.01	119.89	121.90
34	2	1712	C	N3-C4-C5	-5.01	119.89	121.90
34	2	366	A	C5-C6-N1	-5.01	115.19	117.70
34	2	874	G	O4'-C1'-N9	5.01	112.21	108.20
34	2	1585	C	N3-C4-C5	-5.01	119.89	121.90
34	2	279	G	O4'-C1'-N9	5.01	112.21	108.20
34	2	799	C	N3-C4-C5	-5.01	119.90	121.90
34	2	1835	C	N3-C4-C5	-5.01	119.90	121.90
34	2	823	A	C5-C6-N1	-5.01	115.20	117.70
34	2	1024	A	O4'-C1'-N9	5.01	112.21	108.20
34	2	1341	G	O4'-C1'-N9	5.01	112.20	108.20
34	2	1587	C	N3-C4-C5	-5.01	119.90	121.90
34	2	564	A	O4'-C1'-N9	5.00	112.20	108.20
34	2	1523	G	O4'-C1'-N9	5.00	112.20	108.20
34	2	1532	A	C5-C6-N1	-5.00	115.20	117.70
34	2	42	A	O4'-C1'-N9	5.00	112.20	108.20
34	2	79	A	C4'-C3'-C2'	-5.00	97.60	102.60
34	2	1272	A	C5-C6-N1	-5.00	115.20	117.70
34	2	1628	A	C5-C6-N6	-5.00	119.70	123.70
34	2	1809	A	C5-C6-N1	-5.00	115.20	117.70

All (4) chirality outliers are listed below:

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

All (144) 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	1105	C	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
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	1626	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	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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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

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	206/209 (99%)	177 (86%)	21 (10%)	8 (4%)	2	14
4	D	213/264 (81%)	191 (90%)	16 (8%)	6 (3%)	4	21
5	E	224/226 (99%)	208 (93%)	14 (6%)	2 (1%)	14	49
6	F	225/243 (93%)	202 (90%)	14 (6%)	9 (4%)	2	14
7	G	261/263 (99%)	233 (89%)	24 (9%)	4 (2%)	8	36
8	H	189/191 (99%)	169 (89%)	17 (9%)	3 (2%)	8	34
9	I	235/237 (99%)	209 (89%)	22 (9%)	4 (2%)	7	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	188/192 (98%)	161 (86%)	18 (10%)	9 (5%)	2	11
11	K	204/206 (99%)	178 (87%)	20 (10%)	6 (3%)	3	20
12	L	180/182 (99%)	167 (93%)	11 (6%)	2 (1%)	12	44
13	M	96/98 (98%)	74 (77%)	16 (17%)	6 (6%)	1	6
14	N	156/158 (99%)	130 (83%)	22 (14%)	4 (3%)	4	23
15	O	122/132 (92%)	105 (86%)	13 (11%)	4 (3%)	3	18
16	P	148/150 (99%)	130 (88%)	11 (7%)	7 (5%)	2	11
17	Q	134/151 (89%)	118 (88%)	13 (10%)	3 (2%)	5	27
18	S	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	37
19	T	124/135 (92%)	112 (90%)	8 (6%)	4 (3%)	3	19
20	V	139/141 (99%)	128 (92%)	8 (6%)	3 (2%)	5	27
21	W	102/119 (86%)	93 (91%)	9 (9%)	0	100	100
22	X	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	24
23	Y	127/130 (98%)	117 (92%)	6 (5%)	4 (3%)	3	19
24	Z	140/143 (98%)	128 (91%)	8 (6%)	4 (3%)	3	20
25	a	124/133 (93%)	104 (84%)	10 (8%)	10 (8%)	1	3
26	b	97/115 (84%)	90 (93%)	5 (5%)	2 (2%)	5	28
27	c	82/84 (98%)	69 (84%)	9 (11%)	4 (5%)	2	10
28	d	62/69 (90%)	57 (92%)	4 (6%)	1 (2%)	8	34
29	e	51/56 (91%)	40 (78%)	7 (14%)	4 (8%)	1	4
30	f	69/71 (97%)	51 (74%)	12 (17%)	6 (9%)	0	3
31	g	311/313 (99%)	273 (88%)	33 (11%)	5 (2%)	8	34
32	n	73/124 (59%)	69 (94%)	3 (4%)	1 (1%)	9	37
33	i	57/133 (43%)	49 (86%)	7 (12%)	1 (2%)	7	32
35	A	264/284 (93%)	233 (88%)	25 (10%)	6 (2%)	5	26
36	B	420/422 (100%)	352 (84%)	48 (11%)	20 (5%)	2	11
37	j	107/111 (96%)	64 (60%)	27 (25%)	16 (15%)	0	0
38	k	577/595 (97%)	431 (75%)	95 (16%)	51 (9%)	0	3
39	U	141/152 (93%)	123 (87%)	12 (8%)	6 (4%)	2	13
40	R	138/145 (95%)	107 (78%)	18 (13%)	13 (9%)	0	2
All	All	6228/6625 (94%)	5362 (86%)	624 (10%)	242 (4%)	4	14

All (242) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	191	ARG
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
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

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Mol	Chain	Res	Type
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
3	C	46	ILE
4	D	82	ARG
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
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
30	f	98	VAL
36	B	63	VAL

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Mol	Chain	Res	Type
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	42	LEU
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
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
26	b	62	TYR

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Mol	Chain	Res	Type
27	c	83	GLN
28	d	52	GLU
29	e	24	CYS
31	g	13	GLY
31	g	161	SER
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	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
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

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Mol	Chain	Res	Type
19	T	84	TYR
22	X	28	ASP
24	Z	53	GLU
25	a	9	THR
26	b	11	ALA
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
40	R	140	ARG
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
27	c	75	GLU
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
38	k	379	GLY
39	U	141	ARG

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Mol	Chain	Res	Type
39	U	148	VAL
40	R	38	SER
40	R	74	GLU
40	R	130	ARG
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
3	C	3	GLY
7	G	152	PRO
13	M	3	MET
14	N	26	GLY
27	c	38	PRO
38	k	99	ILE
38	k	100	PRO
38	k	137	PRO
4	D	79	VAL
6	F	196	GLY
10	J	45	ILE
23	Y	29	PRO
31	g	275	ILE
38	k	177	PRO
38	k	237	ILE
9	I	67	VAL
40	R	129	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	l	24/24 (100%)	23 (96%)	1 (4%)	25	59
3	C	174/175 (99%)	173 (99%)	1 (1%)	84	93
4	D	196/231 (85%)	196 (100%)	0	100	100
5	E	187/187 (100%)	184 (98%)	3 (2%)	58	82
6	F	190/202 (94%)	187 (98%)	3 (2%)	58	82
7	G	225/225 (100%)	225 (100%)	0	100	100
8	H	161/161 (100%)	159 (99%)	2 (1%)	67	86
9	I	207/207 (100%)	206 (100%)	1 (0%)	86	94
10	J	170/172 (99%)	170 (100%)	0	100	100
11	K	177/177 (100%)	176 (99%)	1 (1%)	84	93
12	L	157/157 (100%)	155 (99%)	2 (1%)	65	85
13	M	89/89 (100%)	89 (100%)	0	100	100
14	N	142/142 (100%)	136 (96%)	6 (4%)	25	59
15	O	104/108 (96%)	100 (96%)	4 (4%)	28	62
16	P	130/130 (100%)	126 (97%)	4 (3%)	35	68
17	Q	106/119 (89%)	105 (99%)	1 (1%)	75	89
18	S	117/117 (100%)	115 (98%)	2 (2%)	56	81
19	T	114/121 (94%)	114 (100%)	0	100	100
20	V	113/113 (100%)	113 (100%)	0	100	100
21	W	94/107 (88%)	93 (99%)	1 (1%)	70	87
22	X	67/67 (100%)	67 (100%)	0	100	100
23	Y	112/113 (99%)	112 (100%)	0	100	100
24	Z	114/115 (99%)	113 (99%)	1 (1%)	75	89
25	a	108/115 (94%)	101 (94%)	7 (6%)	14	43
26	b	87/99 (88%)	87 (100%)	0	100	100
27	c	76/76 (100%)	76 (100%)	0	100	100
28	d	57/62 (92%)	57 (100%)	0	100	100
29	e	47/49 (96%)	45 (96%)	2 (4%)	25	58
30	f	64/64 (100%)	63 (98%)	1 (2%)	58	82
31	g	272/272 (100%)	271 (100%)	1 (0%)	89	95
32	n	66/102 (65%)	65 (98%)	1 (2%)	60	83
33	i	49/106 (46%)	47 (96%)	2 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	A	238/255 (93%)	231 (97%)	7 (3%)	37	70
36	B	354/354 (100%)	328 (93%)	26 (7%)	11	39
37	j	92/93 (99%)	68 (74%)	24 (26%)	0	2
38	k	523/523 (100%)	466 (89%)	57 (11%)	5	22
39	U	125/132 (95%)	120 (96%)	5 (4%)	27	61
40	R	126/130 (97%)	119 (94%)	7 (6%)	17	49
All	All	5454/5691 (96%)	5281 (97%)	173 (3%)	36	67

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	l	2	ARG
3	C	209	GLU
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
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

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Mol	Chain	Res	Type
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
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
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

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Mol	Chain	Res	Type
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
37	j	72	ASN
37	j	82	ARG
37	j	90	ASP
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
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
38	k	549	GLN
38	k	578	ASN
38	k	593	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	13 (17%)	3 (4%)
34	2	1736/1863 (93%)	242 (13%)	7 (0%)
41	3	41/42 (97%)	26 (63%)	1 (2%)
All	All	1851/1980 (93%)	281 (15%)	11 (0%)

All (281) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	1106	G
34	2	1112	C
34	2	1113	C
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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 (11) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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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	1270	G
34	2	1716	U
34	2	1857	A
41	3	39	U

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

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	$\# Z > 2$
1	T6A	1	37	1	27,34,35	1.05	2 (7%)	29,49,52	2.65	9 (31%)
34	C4J	2	1244	34	24,29,30	0.79	1 (4%)	29,42,45	1.03	1 (3%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	37	T6A	C5-C4	2.52	1.47	1.40
1	1	37	T6A	O4'-C1'	2.28	1.44	1.41
34	2	1244	C4J	C1'-C5	-2.11	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	8.51	136.12	121.94
1	1	37	T6A	C2-N1-C6	7.08	122.66	116.59
1	1	37	T6A	C14-C12-C13	3.70	116.49	110.19
1	1	37	T6A	N3-C2-N1	-3.61	123.03	128.68
34	2	1244	C4J	C4-N3-C2	-3.41	121.15	125.46
1	1	37	T6A	N6-C6-N1	3.08	122.85	118.72
1	1	37	T6A	O10-C10-N6	-2.93	118.66	123.62
1	1	37	T6A	C4-C5-N7	-2.77	106.51	109.40
1	1	37	T6A	C14-C12-N11	2.70	118.64	111.72
1	1	37	T6A	N6-C10-N11	2.07	116.65	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	$\# Z > 2$
44	GNP	k	704	43	29,34,34	1.76	6 (20%)	33,54,54	2.15	6 (18%)
42	SF4	k	701	38	0,12,12	-	-	-		
44	GNP	k	705	-	29,34,34	1.77	6 (20%)	33,54,54	2.17	6 (18%)
42	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
44	GNP	k	704	43	-	6/14/38/38	0/3/3/3
42	SF4	k	701	38	-	-	0/6/5/5
44	GNP	k	705	-	-	5/14/38/38	0/3/3/3
42	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)
44	k	705	GNP	PG-O2G	-4.54	1.44	1.56
44	k	704	GNP	PG-O2G	-4.53	1.44	1.56
44	k	704	GNP	C6-N1	4.07	1.40	1.33
44	k	705	GNP	PB-O2B	-4.02	1.45	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	k	705	GNP	C6-N1	3.86	1.39	1.33
44	k	704	GNP	PB-O2B	-3.74	1.46	1.56
44	k	705	GNP	C5-C6	3.17	1.46	1.41
44	k	704	GNP	C5-C6	3.13	1.46	1.41
44	k	704	GNP	C8-N7	-2.74	1.29	1.34
44	k	705	GNP	C8-N7	-2.73	1.29	1.34
44	k	704	GNP	C2-N1	2.60	1.40	1.35
44	k	705	GNP	C2-N1	2.41	1.39	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	704	GNP	C5-C6-N1	-7.90	112.63	123.43
44	k	705	GNP	C5-C6-N1	-7.88	112.65	123.43
44	k	705	GNP	C2-N1-C6	6.08	125.59	115.93
44	k	704	GNP	C2-N1-C6	6.01	125.47	115.93
44	k	705	GNP	N3-C2-N1	-3.76	122.21	127.22
44	k	704	GNP	N3-C2-N1	-3.74	122.24	127.22
44	k	704	GNP	O2G-PG-O3G	-2.56	100.82	107.64
44	k	705	GNP	O2G-PG-O3G	-2.51	100.96	107.64
44	k	705	GNP	C4-C5-C6	-2.51	118.40	120.80
44	k	704	GNP	C4-C5-C6	-2.38	118.52	120.80
44	k	704	GNP	O3G-PG-O1G	-2.16	108.02	113.45
44	k	705	GNP	O3G-PG-O1G	-2.11	108.14	113.45

There are no chirality outliers.

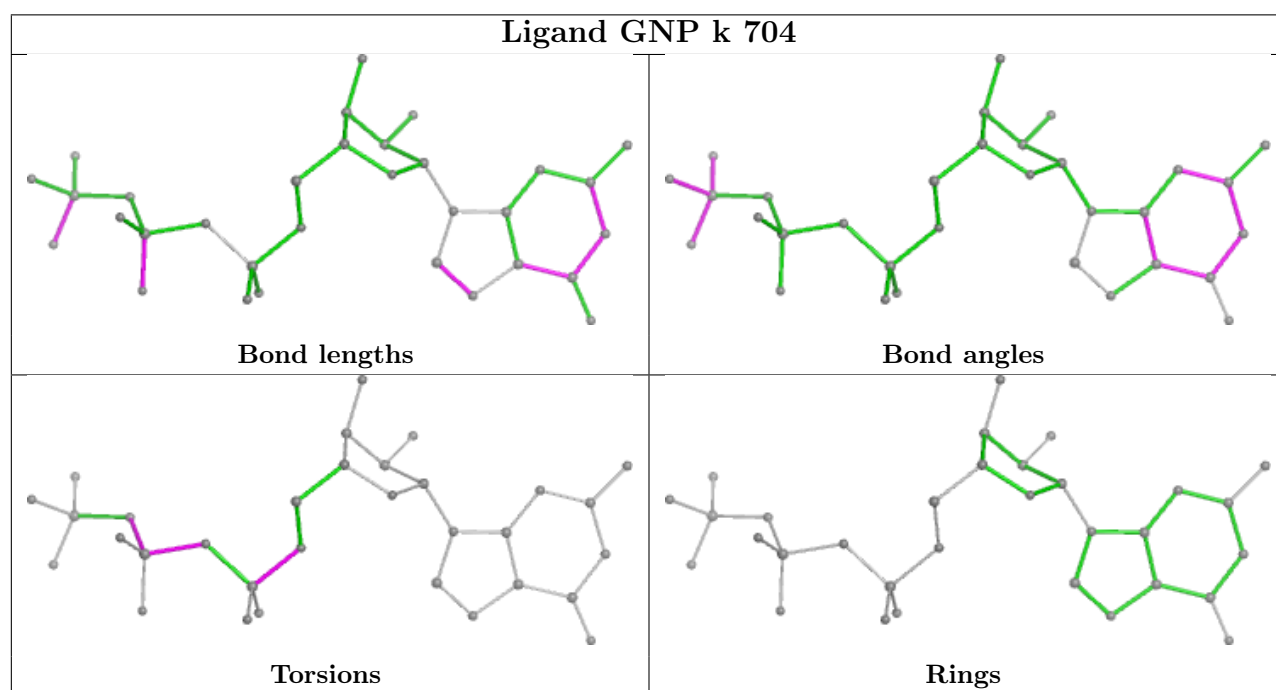
All (11) torsion outliers are listed below:

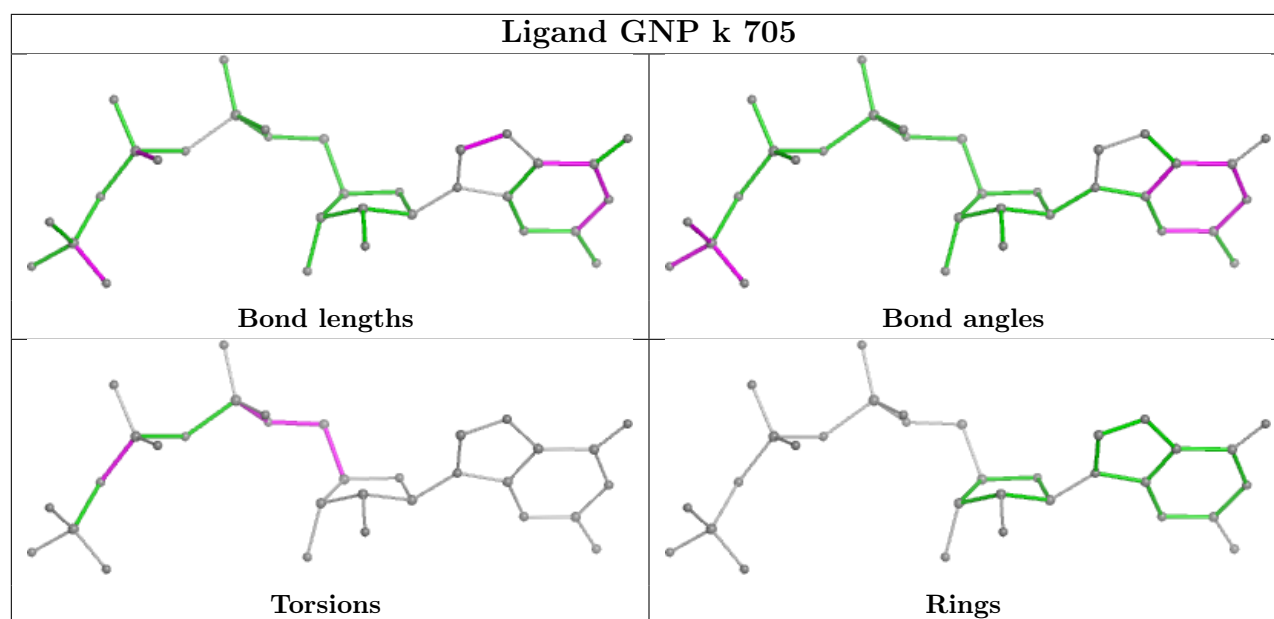
Mol	Chain	Res	Type	Atoms
44	k	704	GNP	PG-N3B-PB-O1B
44	k	704	GNP	PG-N3B-PB-O3A
44	k	704	GNP	PA-O3A-PB-O1B
44	k	704	GNP	PA-O3A-PB-O2B
44	k	705	GNP	PG-N3B-PB-O1B
44	k	705	GNP	C5'-O5'-PA-O3A
44	k	705	GNP	C5'-O5'-PA-O2A
44	k	704	GNP	C5'-O5'-PA-O3A
44	k	705	GNP	C4'-C5'-O5'-PA
44	k	705	GNP	O4'-C4'-C5'-O5'
44	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:

Mol	Chain	Number of breaks
38	k	23
34	2	4
1	1	2
39	U	1
25	a	1
41	3	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	k	518:VAL	C	519:GLU	N	2.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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	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	3	39:U	O3'	40:C	P	1.39
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	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
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

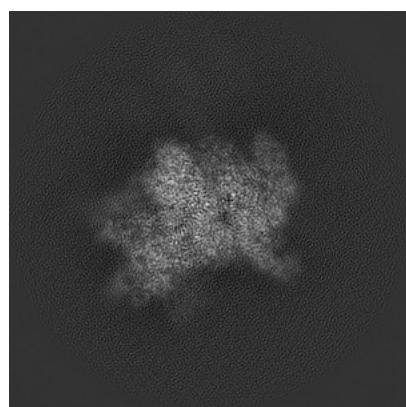
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10760. These allow visual inspection of the internal detail of the map and identification of artifacts.

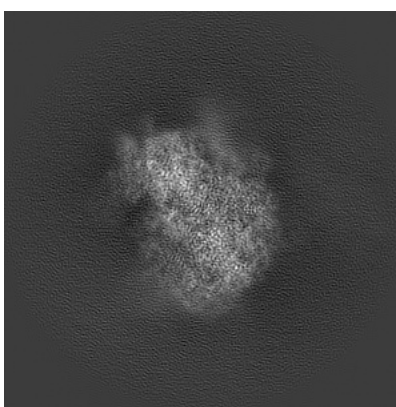
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

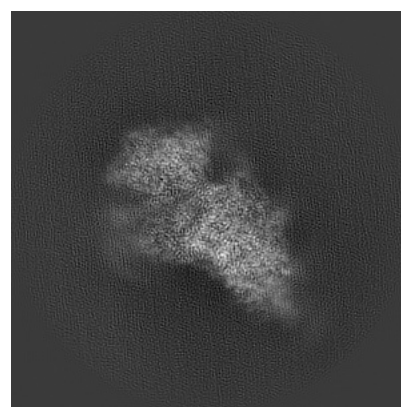
6.1.1 Primary map



X



Y

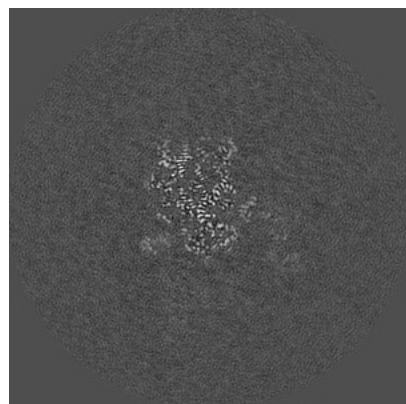


Z

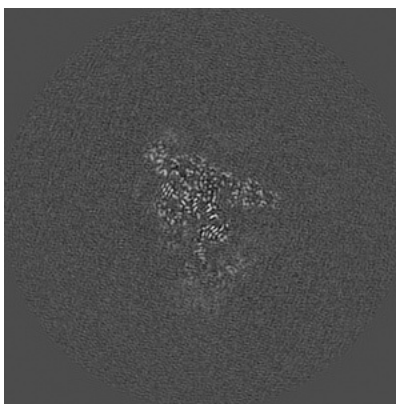
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

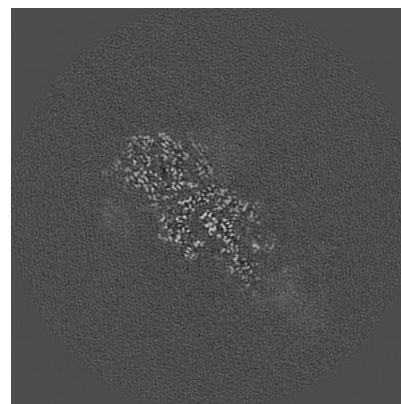
6.2.1 Primary map



X Index: 192



Y Index: 192

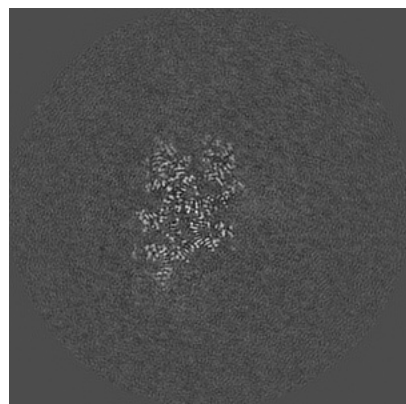


Z Index: 192

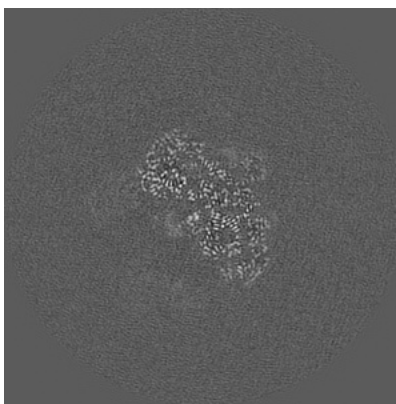
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

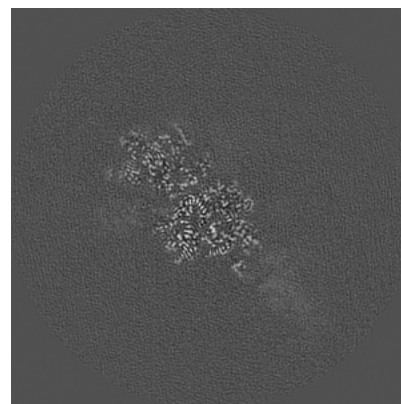
6.3.1 Primary map



X Index: 205



Y Index: 161

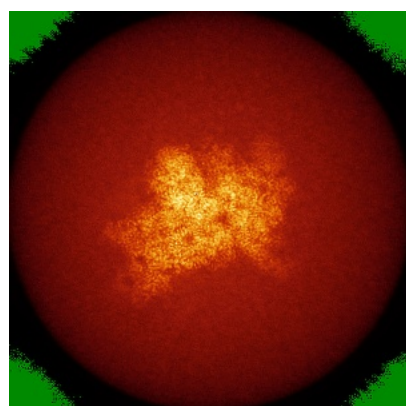


Z Index: 199

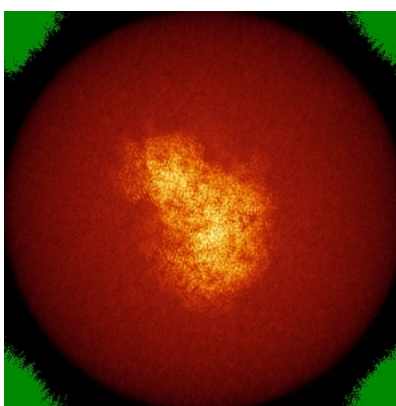
The images above show the largest variance slices of the map in three orthogonal directions.

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

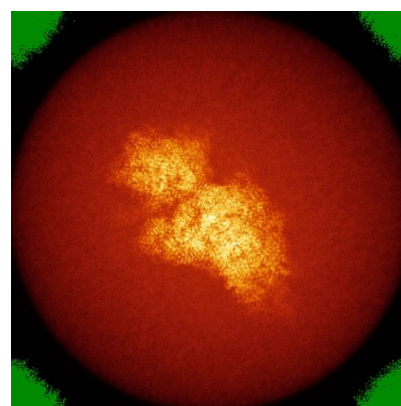
6.4.1 Primary map



X



Y

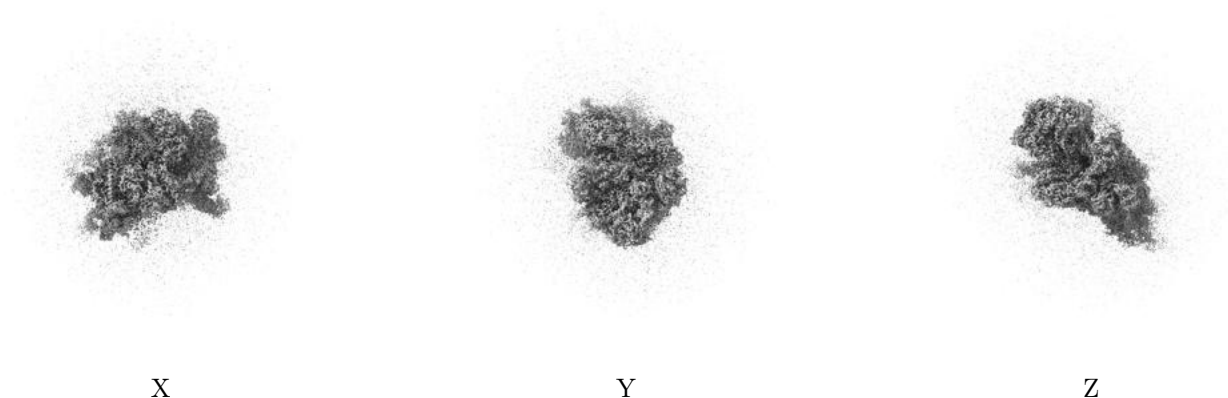


Z

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.

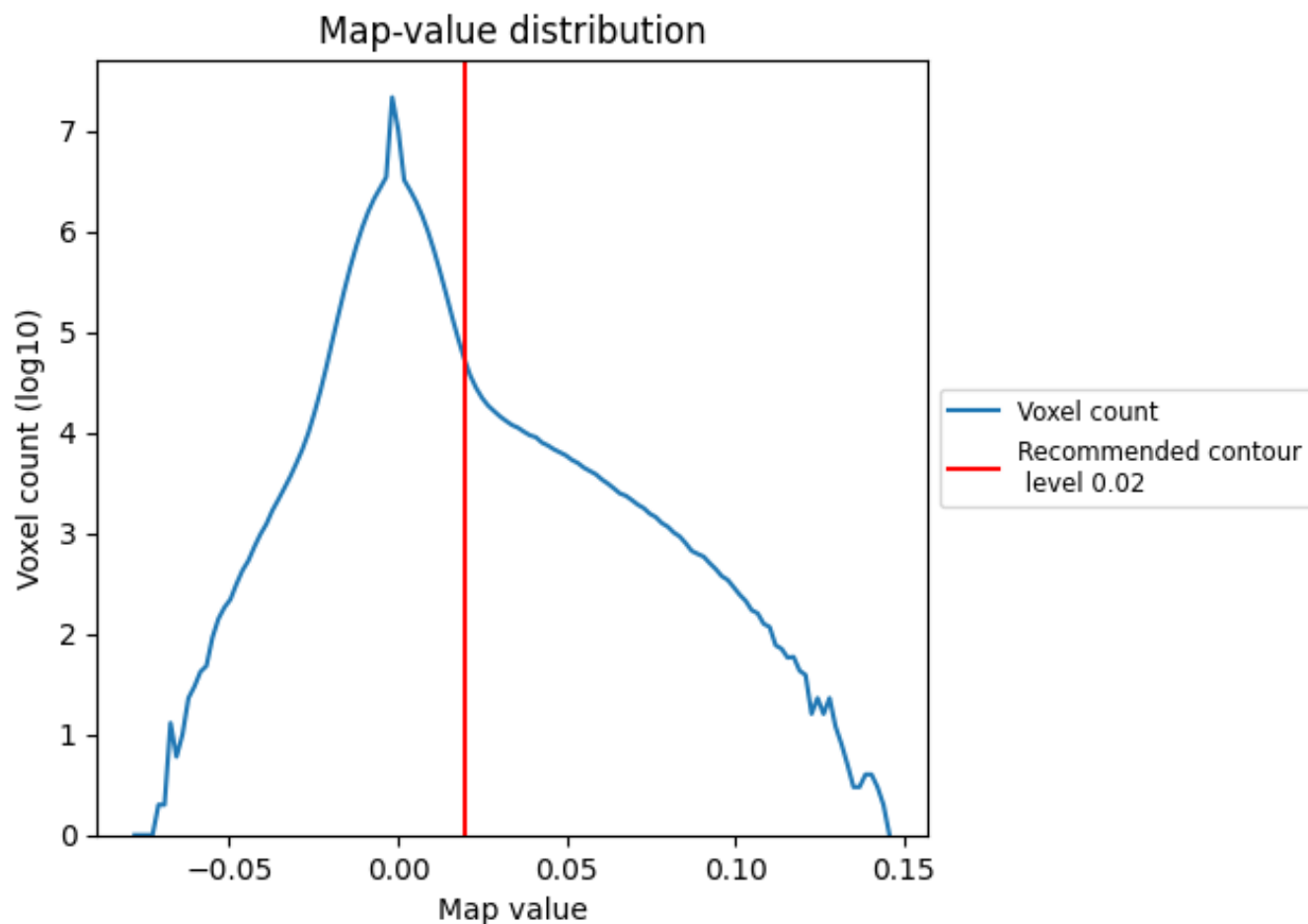
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

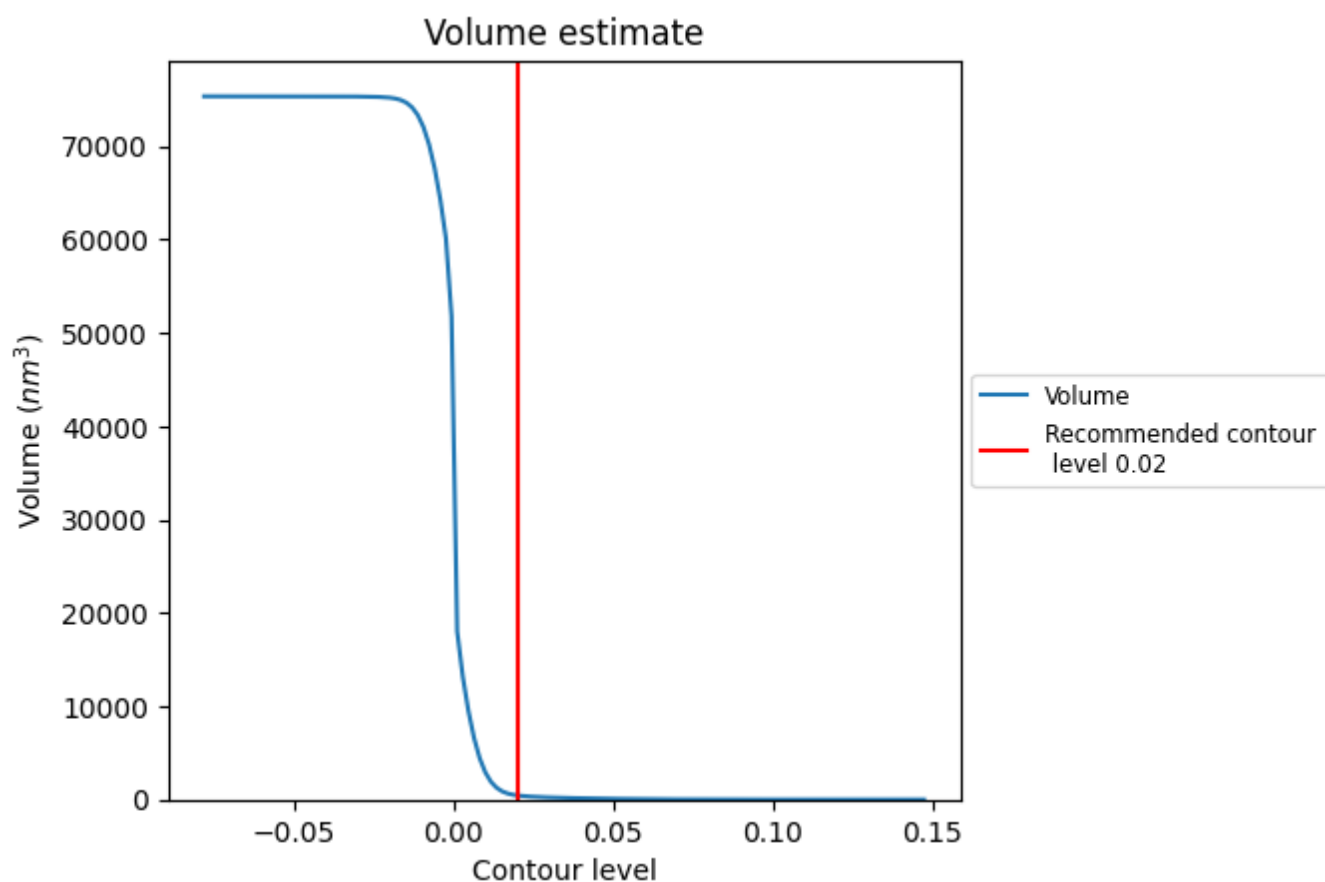
This section contains the results of statistical analysis of the map.

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.

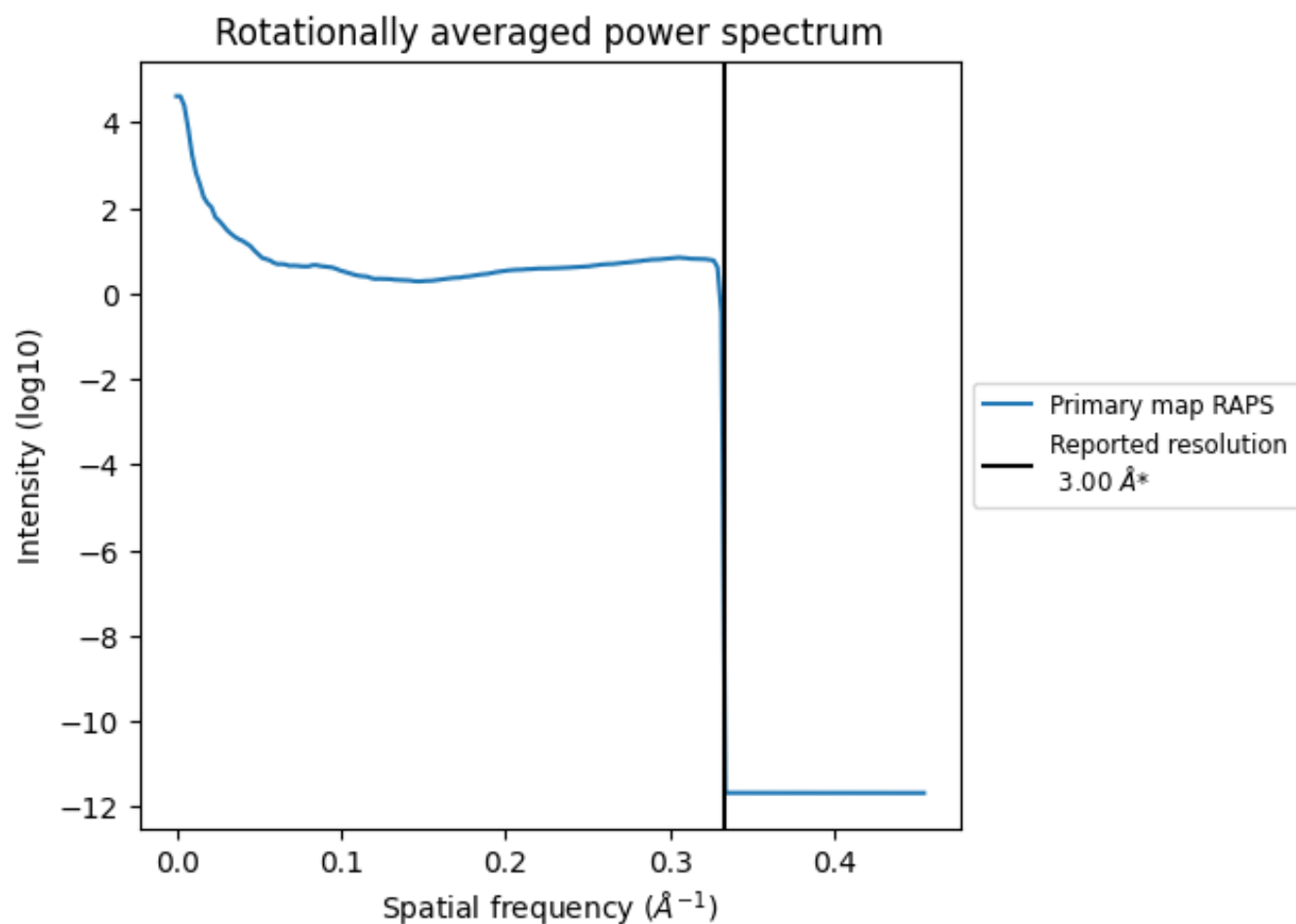
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 449 nm³; this corresponds to an approximate mass of 406 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 0.333 Å⁻¹

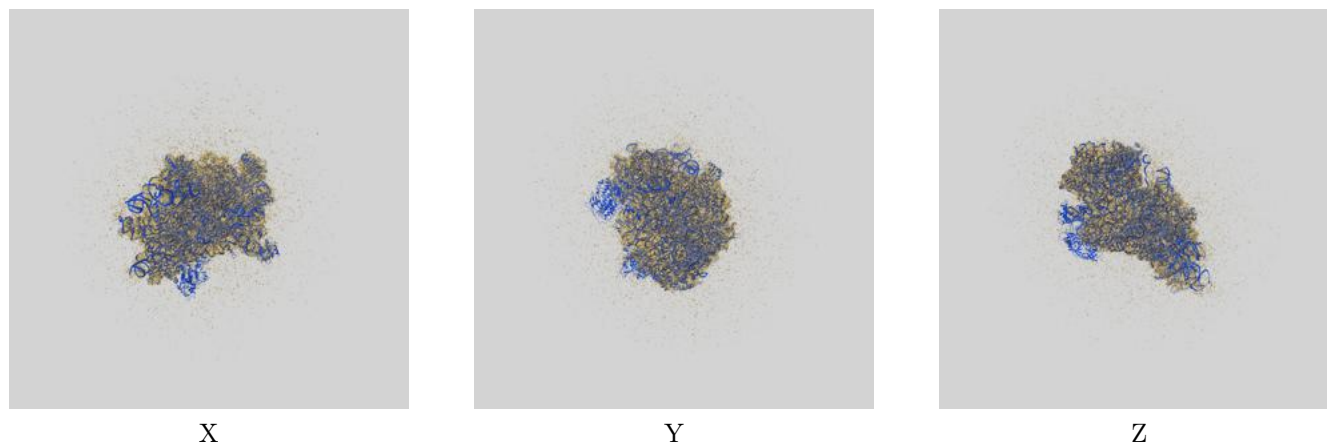
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

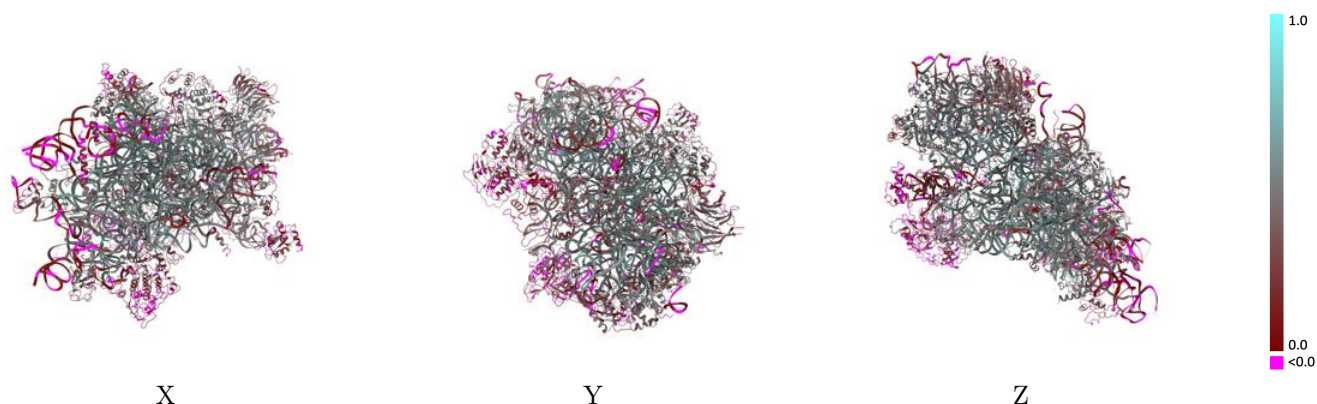
This section contains information regarding the fit between EMDB map EMD-10760 and PDB model 6YAL. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



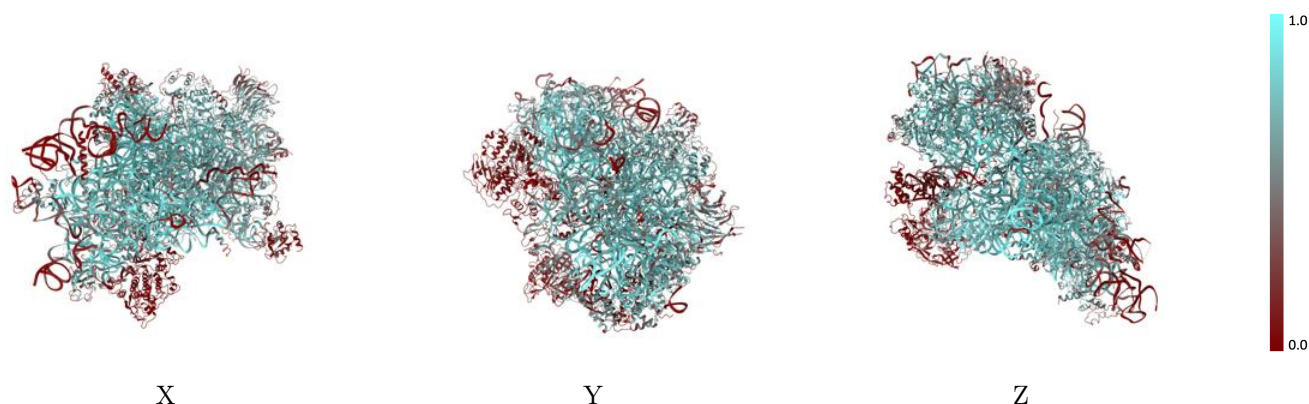
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



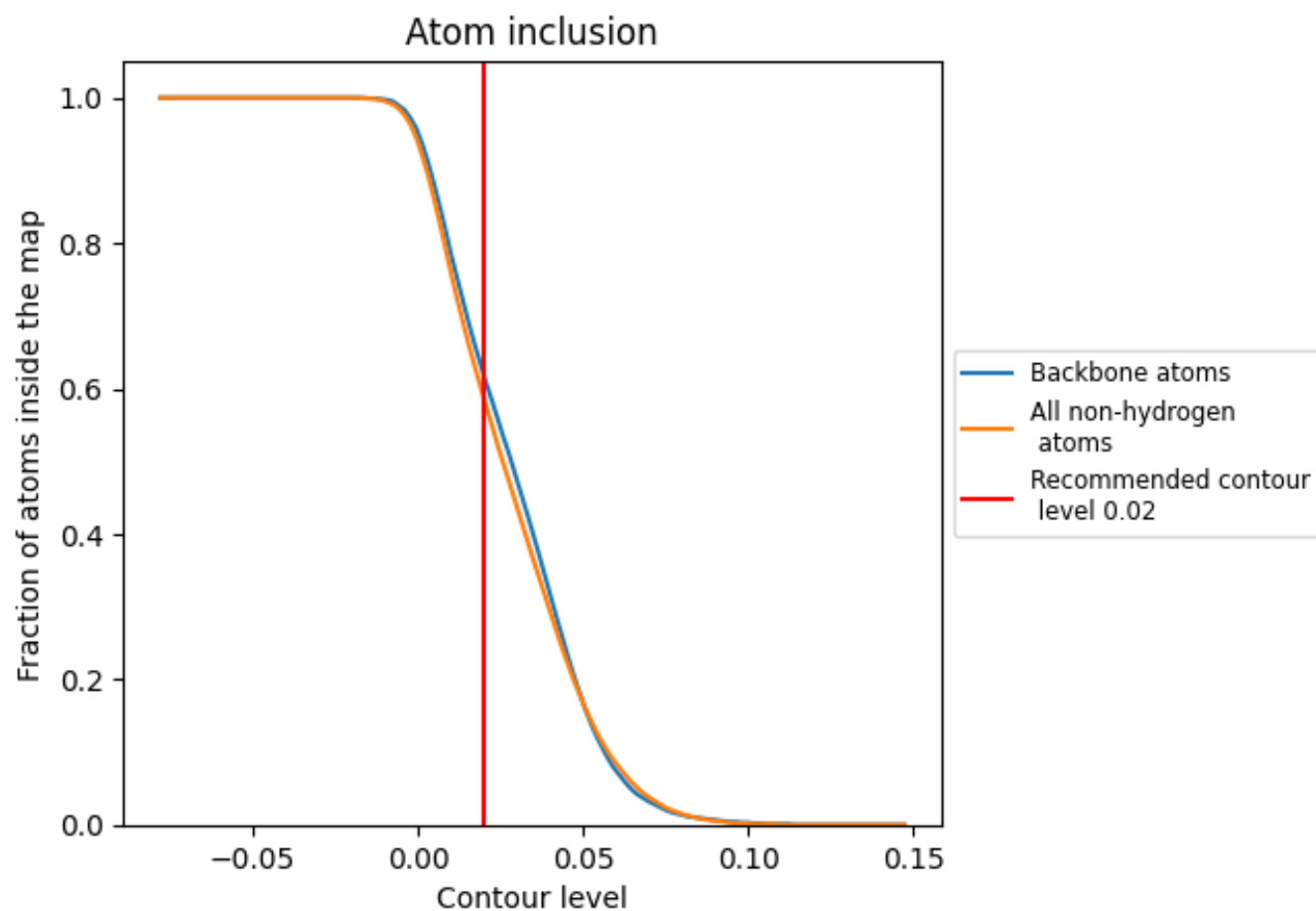
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 59% 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	 0.5860	 0.3790
1	 0.2280	 0.1570
2	 0.7700	 0.4650
3	 0.1330	 0.1270
A	 0.0440	 0.0980
B	 0.0020	 0.0100
C	 0.6800	 0.4320
D	 0.6480	 0.4170
E	 0.7120	 0.4660
F	 0.5430	 0.3560
G	 0.6900	 0.4550
H	 0.6310	 0.4090
I	 0.5000	 0.3310
J	 0.3730	 0.2690
K	 0.5910	 0.3850
L	 0.6780	 0.4330
M	 0.5200	 0.3330
N	 0.6270	 0.4100
O	 0.1320	 0.1360
P	 0.6790	 0.4410
Q	 0.6600	 0.4160
R	 0.4990	 0.3280
S	 0.6850	 0.4480
T	 0.5250	 0.3300
U	 0.5770	 0.3850
V	 0.6740	 0.4310
W	 0.5440	 0.3660
X	 0.6580	 0.4160
Y	 0.7660	 0.4940
Z	 0.7490	 0.4730
a	 0.6380	 0.4020
b	 0.7120	 0.4570
c	 0.5580	 0.3600
d	 0.5450	 0.3650
e	 0.5480	 0.2680



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Chain	Atom inclusion	Q-score
f	 0.1480	 0.1270
g	 0.4910	 0.3590
i	 0.4630	 0.3140
j	 0.2020	 0.2240
k	 0.0400	 0.1780
l	 0.5750	 0.3940
n	 0.4600	 0.3510