



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:06 AM EST

PDB ID : 4V6K
EMDB ID : EMD-1849
Title : Structural insights into cognate vs. near-cognate discrimination during decoding.
Authors : Agirrezabala, X.; Schreiner, E.; Trabuco, L.G.; Lei, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.
Deposited on : 2011-01-07
Resolution : 8.25 Å(reported)
Based on initial model : 2I2V

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

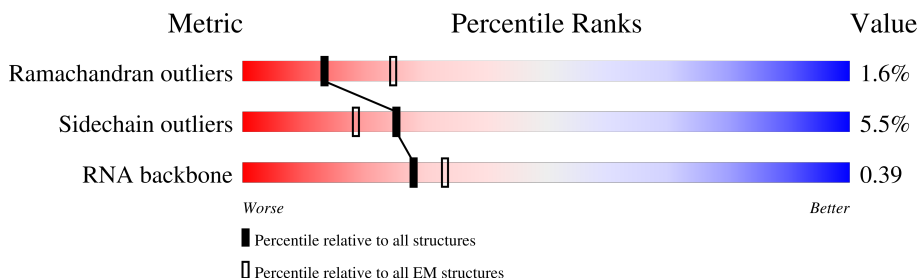
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.25 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AA	120	
2	AB	2904	
3	AC	234	
4	AD	273	
5	AE	209	
6	AF	201	
7	AG	179	
8	AH	177	

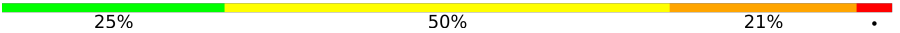
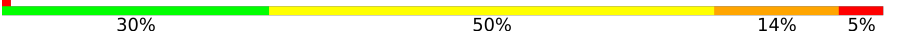
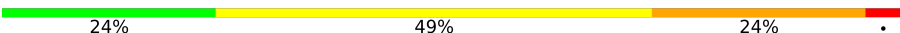
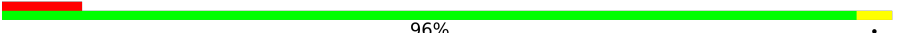











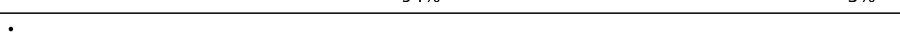

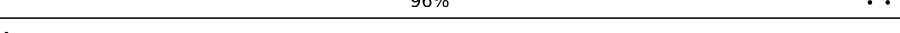

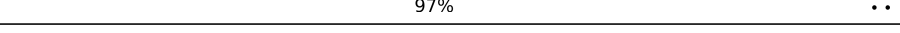
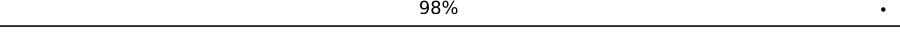
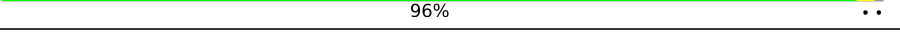


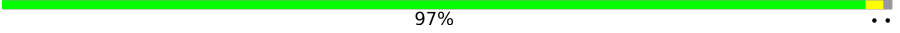
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Mol	Chain	Length	Quality of chain
9	AI	149	
10	AJ	142	
11	AK	142	
12	AL	123	
13	AM	144	
14	AN	136	
15	AO	127	
16	AP	117	
17	AQ	115	
18	AR	118	
19	AS	103	
20	AT	110	
21	AU	100	
22	AV	104	
23	AW	94	
24	AX	85	
25	AY	78	
26	AZ	63	
27	Aa	59	
28	Ab	70	
29	Ac	57	
30	Ad	55	
31	Ae	46	
32	Af	65	
33	Ag	38	

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Mol	Chain	Length	Quality of chain
34	BA	1542	
35	BB	76	
35	BE	76	
36	BC	393	
37	BD	24	
38	BF	241	
39	BG	233	
40	BH	206	
41	BI	167	
42	BJ	135	
43	BK	179	
44	BL	130	
45	BM	130	
46	BN	103	
47	BO	129	
48	BP	124	
49	BQ	118	
50	BR	101	
51	BS	89	
52	BT	82	
53	BU	84	
54	BV	75	
55	BW	92	
56	BX	87	
57	BY	71	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 153634 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 ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

- Molecule 2 is a RNA chain called ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	103	Total	C	N	O	S	0	0
			789	498	148	143			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AZ	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Aa	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ab	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ac	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ad	54	Total	C	N	O	S	0	0
			441	284	81	76			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ae	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Af	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ag	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 35 is a RNA chain called A/T-site tRNA Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	BB	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		
35	BE	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		

- Molecule 36 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BC	393	Total	C	N	O	S	0	0
			3036	1918	523	582	13		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BD	24	Total	C	N	O	P	0	0
			495	222	68	181	24		

- Molecule 38 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BF	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 39 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BG	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 40 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BH	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 41 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BI	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 42 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BJ	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 43 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BK	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 44 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BL	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 45 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BM	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 46 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BN	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BO	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 48 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BP	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 49 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BQ	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 50 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BR	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 51 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BS	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 52 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BT	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 53 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BU	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 54 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BV	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 55 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BW	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 56 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BX	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

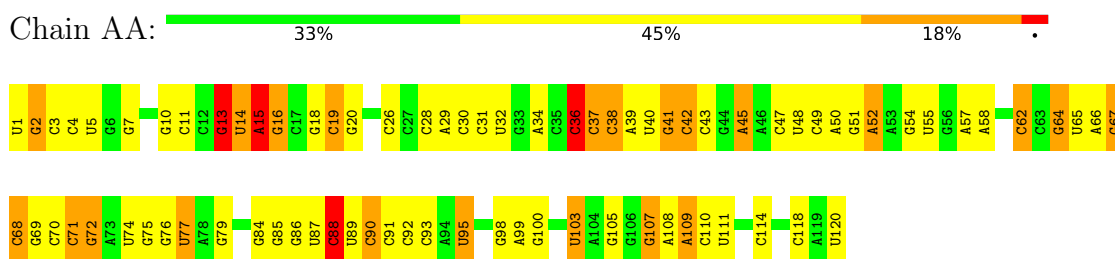
- Molecule 57 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BY	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

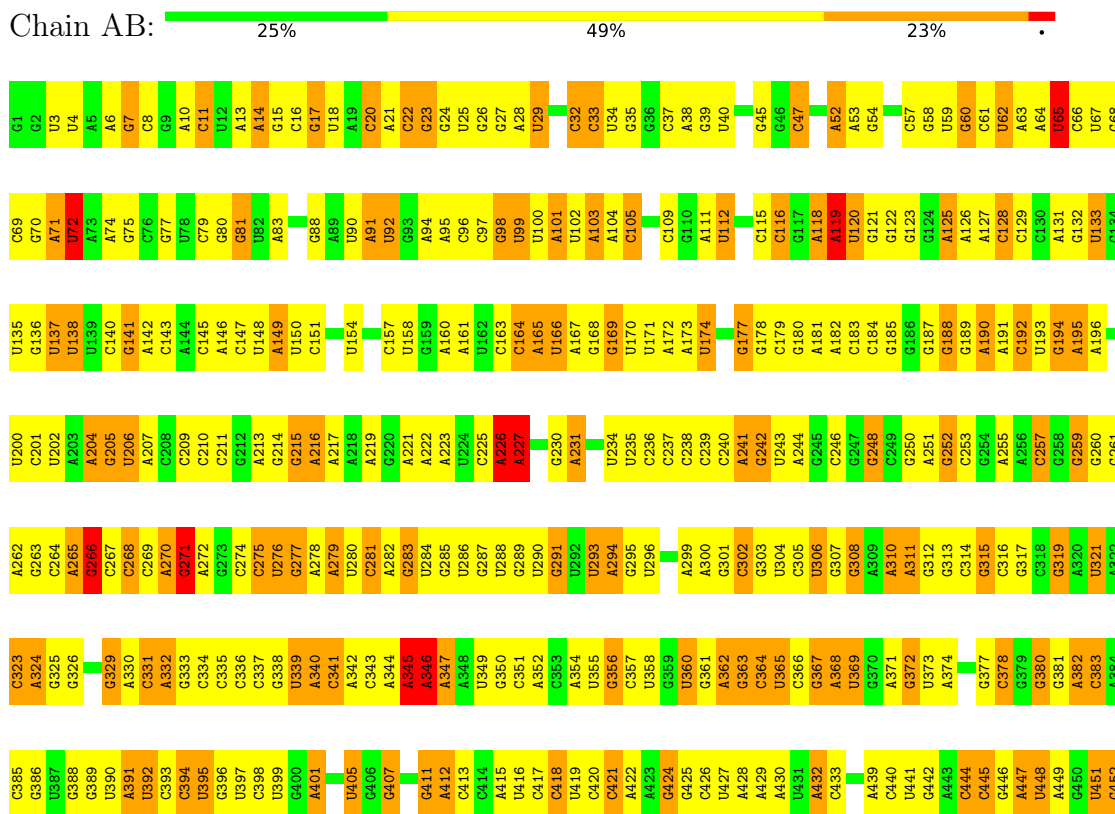
3 Residue-property plots

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

• Molecule 1: ribosomal RNA 5S

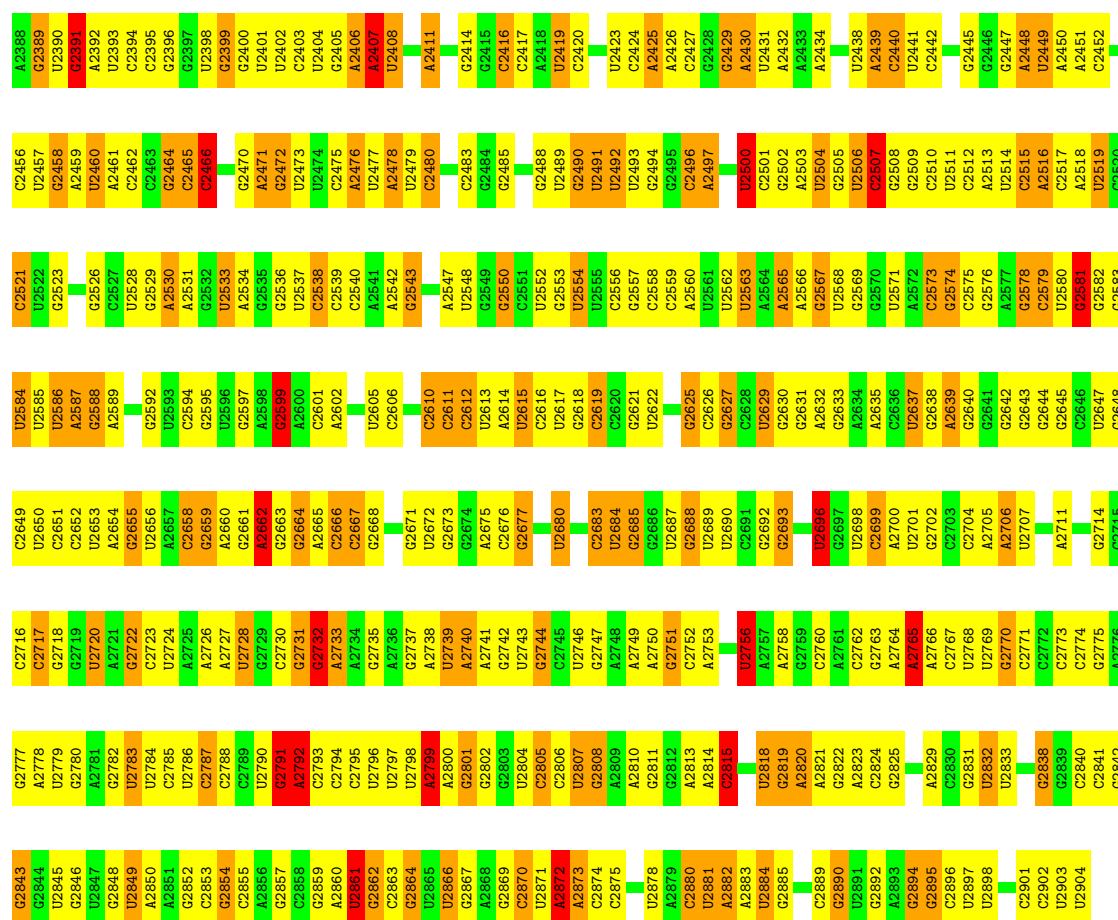


• Molecule 2: ribosomal RNA 23S

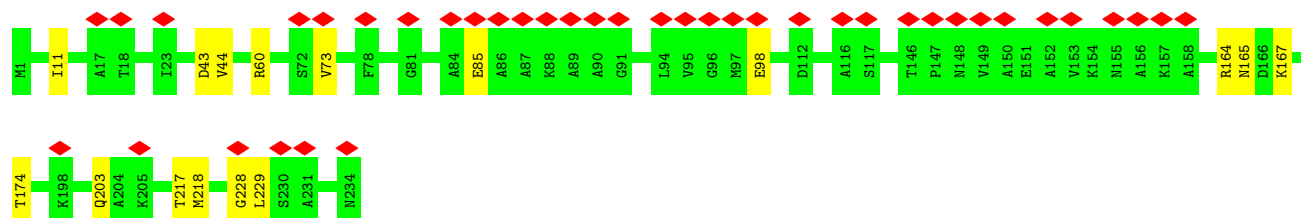


C1351	A1284	U1217	C1153	G1091	C964	C901	U839	G776	U714	G648	G579	C516	C456
U1352	A1285	G1218	G1154	C1092	C965	C902	C840	G777	A715	G649	U580	C517	C457
A1353	A1286	U1219	G1093	G1094	G966	C903	G841	G778	A716	C650	C581	U519	C458
G1355	A1287	G1220	U1159	U1094	U967	U906	U842	G779	C717	G651	A582	U518	C459
G1356	G1288	C1221	G1160	A1096	G968	G907	G843	G780	A718	C584	C584	U521	A460
G1357	G1289	U1222	C1161	A1097	G969	C908	A844	G781	C719	A654	C585	A522	C461
G1358	C1290	G1293	G1162	U1098	U970	U909	A845	A782	U720	G655	G585	C523	C462
A1359	C1291	U1224	G1163	A1098	G971	A909	U846	A783	A721	G656	C586	G524	G463
G1360	C1292	G1225	C1164	U1099	A972	A910	C848	G784	A722	U657	C587	U525	U464
G1361	G1165	A1226	G1036	G1037	G973	A911	C849	G785	G723	U658	C588	U526	G465
C1362	G1166	C1227	G1038	U1101	A974	C912	C850	G786	U724	G659	U589	G466	
C1363	C1167	G1228	A1039	G1038	A975	C913	C851	C787	G725	C660	A590	G527	A467
G1364	C1170	U1229	A1040	A1103	G976	G914	U852	A788	G726	A661	U591	A528	A468
A1365	C1171	G1230	G1041	C1104	G977	C915	C854	A789	A727	G662	A592	A529	G469
A1366	C1172	U1231	G1106	U1105	G978	G916	G855	G790	G728	G663	U593	G530	A470
A1367	G1299	G1232	G1107	A1108	A979	A917	G856	G791	G729	G664	U594	C531	A471
G1368	U1173	C1233	U1108	G1107	A980	A918	G857	A792	A730	U665	C595	A532	A472
G1369	A1301	U1234	A1046	U1108	A981	U919	G858	A793	C731	A666	U596	G533	A473
G1370	A1302	G1235	C1109	C1109	A982	A920	G859	A794	G732	U667	G597	U634	G474
C1371	G1303	A1236	G1110	G1110	A983	C921	U860	G795	G733	A688	U598	G535	C475
G1372	A1304	G1237	A1111	C1049	A984	C922	A861	C796	A734	G669	A599	G536	A476
A1373	C1305	G1238	G1112	C1052	C987	G923	G862	G797	C735	A670	G600	G537	A477
G1374	C1306	U1241	U1113	C1053	A988	G924	A863	G798	C736	C671	C601	A538	A478
U1375	A1307	C1242	G1114	A1054	G989	A925	G864	G801	C737	G672	A602	G539	A479
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G1377	U1183	A1244	C1117	G1056	C991	U931	C867	U803	A739	A674	G604	A541	C481
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A1382	U1188	U1249	G1122	U1061	A996	U934	U872	G898	G745	G681	G612	G547	C486
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A1395	U1198	U1263	G1134	G1071	C1005	C944	G881	C817	G756	C691	C623	C557	A497
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• Molecule 3: 50S ribosomal protein L1

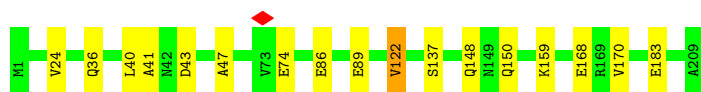


• Molecule 4: 50S ribosomal protein L2

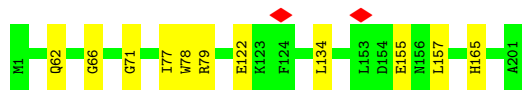


• Molecule 5: 50S ribosomal protein L3

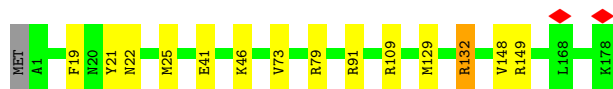




- Molecule 6: 50S ribosomal protein L4



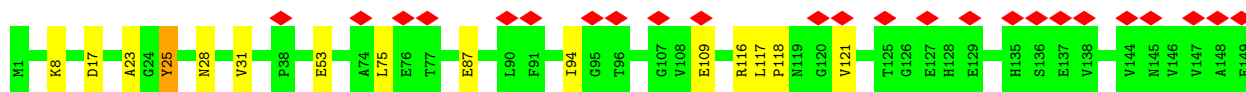
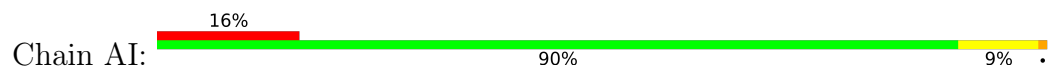
- Molecule 7: 50S ribosomal protein L5



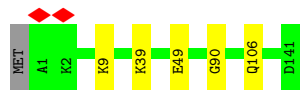
- Molecule 8: 50S ribosomal protein L6



- Molecule 9: 50S ribosomal protein L9



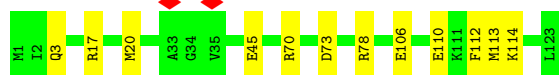
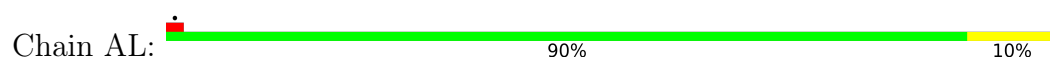
- Molecule 10: 50S ribosomal protein L11



- Molecule 11: 50S ribosomal protein L13



- Molecule 12: 50S ribosomal protein L14



- Molecule 13: 50S ribosomal protein L15



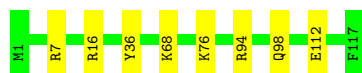
- Molecule 14: 50S ribosomal protein L16



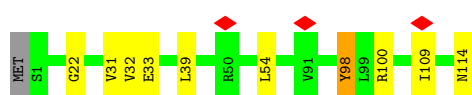
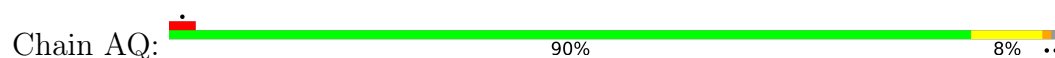
- Molecule 15: 50S ribosomal protein L17



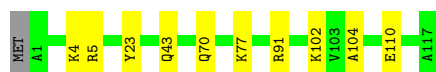
- Molecule 16: 50S ribosomal protein L18



- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20



- Molecule 19: 50S ribosomal protein L21

Chain AS:  90% 10%



- Molecule 20: 50S ribosomal protein L22

Chain AT:  95% 5%



- Molecule 21: 50S ribosomal protein L23

Chain AU:  93% 7%



- Molecule 22: 50S ribosomal protein L24

Chain AV:  95% 5%



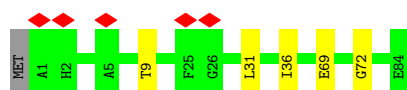
- Molecule 23: 50S ribosomal protein L25

Chain AW:  91% 9%



- Molecule 24: 50S ribosomal protein L27

Chain AX:  6% 93% 6%




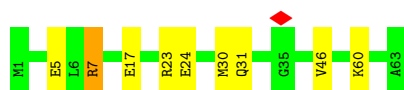
- Molecule 25: 50S ribosomal protein L28

Chain AY:  96% 4%



- Molecule 26: 50S ribosomal protein L29

Chain AZ:  86% 13%




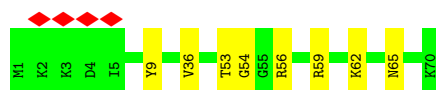
- Molecule 27: 50S ribosomal protein L30

Chain Aa:  92% 7%




- Molecule 28: 50S ribosomal protein L31

Chain Ab:  6% 89% 11%



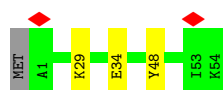
- Molecule 29: 50S ribosomal protein L32

Chain Ac:  88% 11%




- Molecule 30: 50S ribosomal protein L33

Chain Ad:  93% 5%



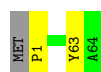
- Molecule 31: 50S ribosomal protein L34

Chain Ae:  87% 13%



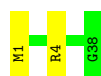
- Molecule 32: 50S ribosomal protein L35

Chain Af:  95%



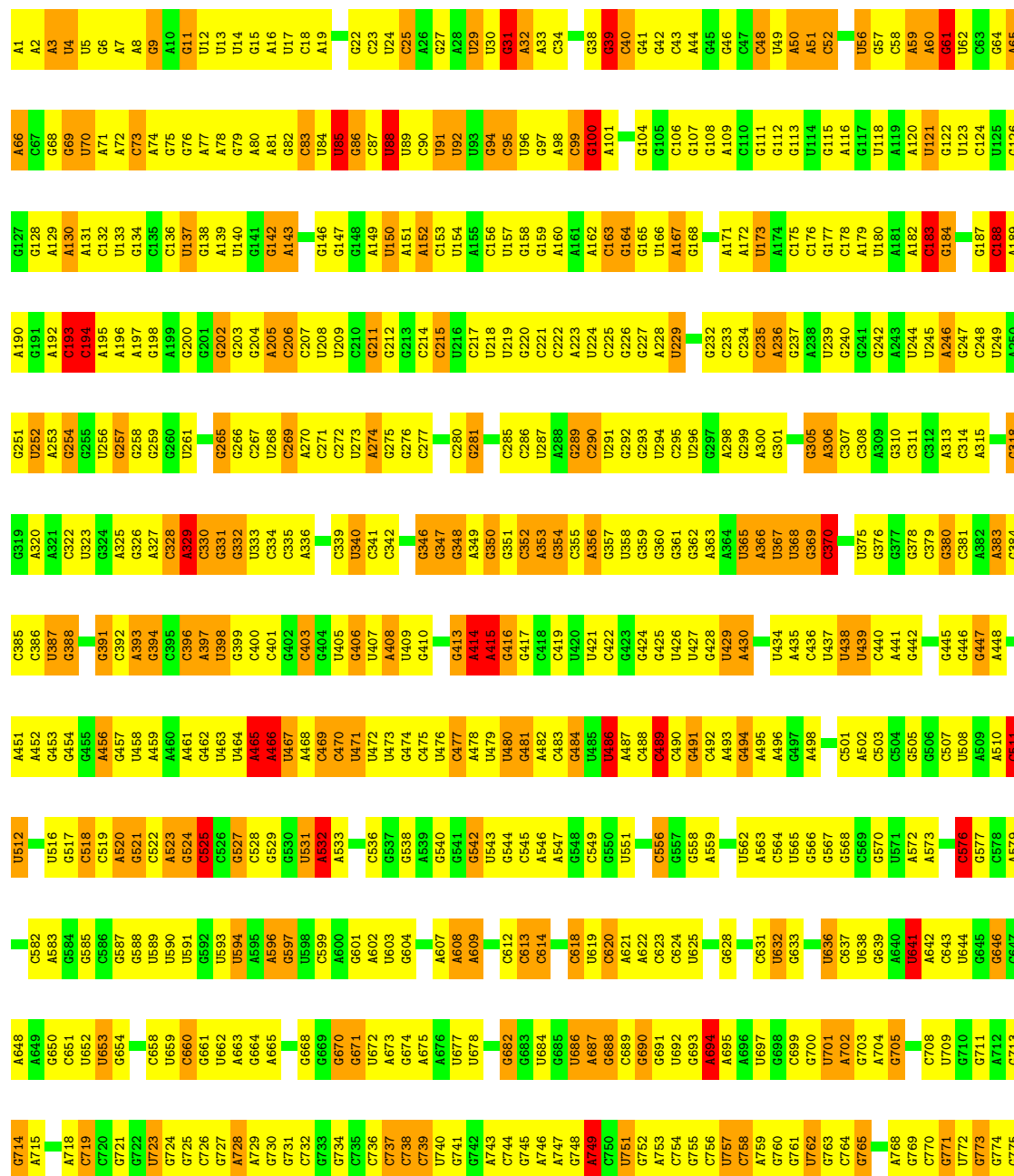
• Molecule 33: 50S ribosomal protein L36

Chain Ag:  95% 5%

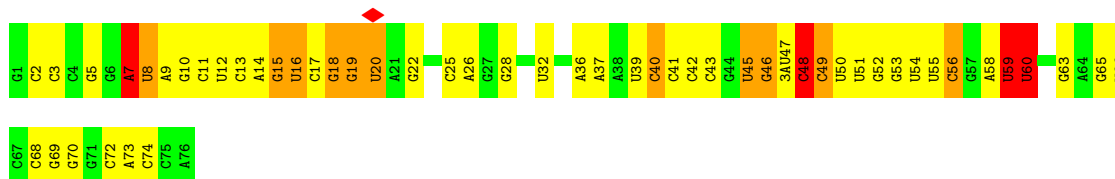


• Molecule 34: 16S ribosomal RNA

Chain BA:  25% 50% 21%

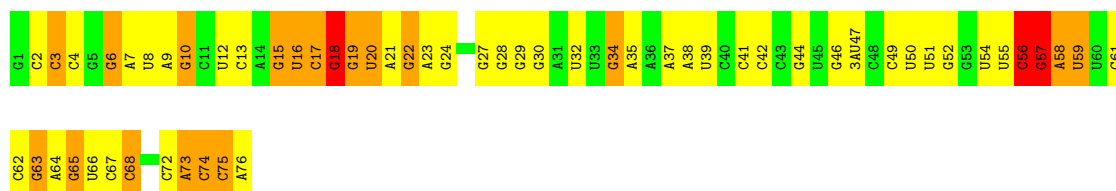


- Molecule 35: A/T-site tRNA Phe



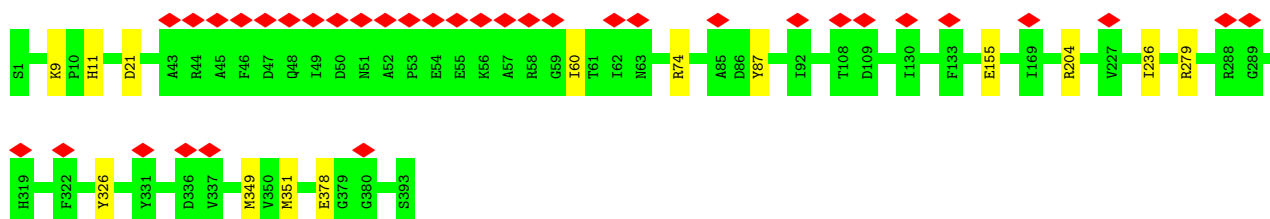
- Molecule 35: A/T-site tRNA Phe

Chain BE: 



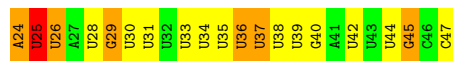
- Molecule 36: Elongation factor Tu 2

Chain BC: 



- Molecule 37: mRNA

Chain BD: 



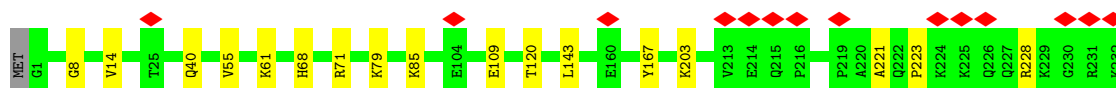
- Molecule 38: 30S ribosomal protein S2

Chain BF: 



- Molecule 39: 30S ribosomal protein S3

Chain BG: 

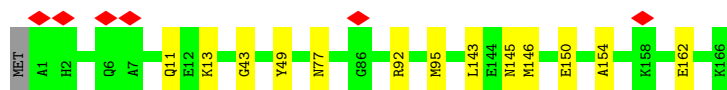


- Molecule 40: 30S ribosomal protein S4

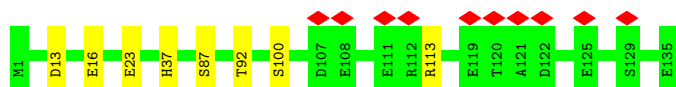
Chain BH: 



• Molecule 41: 30S ribosomal protein S5

Chain BI:  92% 8%

• Molecule 42: 30S ribosomal protein S6

Chain BJ:  7% 94% 6%

• Molecule 43: 30S ribosomal protein S7

Chain BK:  93% 7%

• Molecule 44: 30S ribosomal protein S8

Chain BL:  93% 6%

• Molecule 45: 30S ribosomal protein S9

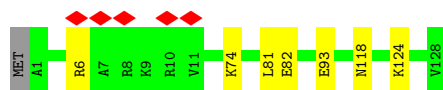
Chain BM:  90% 9%

• Molecule 46: 30S ribosomal protein S10

Chain BN:  86% 14%

• Molecule 47: 30S ribosomal protein S11

Chain BO:  94% 5%



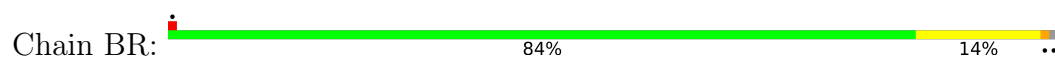
- Molecule 48: 30S ribosomal protein S12



- Molecule 49: 30S ribosomal protein S13



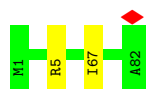
- Molecule 50: 30S ribosomal protein S14



- Molecule 51: 30S ribosomal protein S15




- Molecule 52: 30S ribosomal protein S16



- Molecule 53: 30S ribosomal protein S17



- Molecule 54: 30S ribosomal protein S18

Chain BV:  87% 9% ..



- Molecule 55: 30S ribosomal protein S19

Chain BW:  5% 92% 5% ..




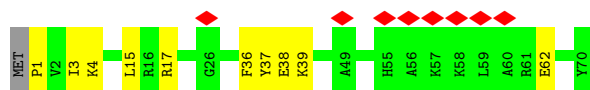
- Molecule 56: 30S ribosomal protein S20

Chain BX:  97% ..



- Molecule 57: 30S ribosomal protein S21

Chain BY:  11% 85% 14% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	359223	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	299.406	Depositor
Minimum map value	-102.404	Depositor
Average map value	5.380	Depositor
Map value standard deviation	28.487	Depositor
Recommended contour level	32.4	Depositor
Map size (\AA)	375, 375, 375	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	1.5, 1.5, 1.5	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 7MG, 1MG, 3TD, 6MZ, 2MG, 5MC, 2MA, CH, 3AU, 5MU, OMG, MIA, OMC, OMU, 4OC, 4SU, MA6, PSU, UR3

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	AA	1.18	0/2869	2.04	104/4474 (2.3%)
2	AB	1.17	0/69257	1.96	2261/108040 (2.1%)
3	AC	0.56	0/1748	0.96	1/2355 (0.0%)
4	AD	0.60	0/2131	1.07	1/2863 (0.0%)
5	AE	0.58	0/1586	1.02	0/2134
6	AF	0.57	0/1571	0.99	0/2113
7	AG	0.65	0/1444	1.10	4/1937 (0.2%)
8	AH	0.59	0/1343	1.02	0/1816
9	AI	0.57	0/1122	1.01	1/1515 (0.1%)
10	AJ	0.57	0/1046	0.92	0/1410
11	AK	0.63	0/1152	0.99	0/1551
12	AL	0.57	0/956	1.00	0/1279
13	AM	0.60	0/1062	1.01	0/1413
14	AN	0.63	0/1093	1.05	1/1460 (0.1%)
15	AO	0.61	0/1021	1.03	0/1364
16	AP	0.60	0/910	1.00	0/1219
17	AQ	0.61	0/929	1.06	0/1242
18	AR	0.67	0/960	1.02	1/1278 (0.1%)
19	AS	0.62	0/829	1.01	0/1107
20	AT	0.52	0/864	0.96	0/1156
21	AU	0.55	0/794	0.99	0/1060
22	AV	0.56	0/797	1.03	0/1062
23	AW	0.60	0/766	0.97	0/1025
24	AX	0.64	0/642	1.09	0/848
25	AY	0.64	0/635	1.06	0/848
26	AZ	0.56	0/510	1.10	1/677 (0.1%)
27	Aa	0.54	0/453	0.98	0/605
28	Ab	0.63	0/559	1.17	2/745 (0.3%)
29	Ac	0.59	0/450	1.05	0/599
30	Ad	0.61	0/448	1.00	0/594
31	Ae	0.63	0/380	1.11	1/498 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Af	0.58	0/513	1.01	1/676 (0.1%)
33	Ag	0.53	0/303	1.00	0/397
34	BA	1.17	1/36769 (0.0%)	1.96	1171/57354 (2.0%)
35	BB	1.23	0/1580	1.96	45/2459 (1.8%)
35	BE	1.20	0/1580	2.05	59/2459 (2.4%)
36	BC	0.61	0/3092	0.96	1/4183 (0.0%)
37	BD	1.30	0/548	1.88	16/848 (1.9%)
38	BF	0.60	0/1904	1.00	0/2565
39	BG	0.60	0/1852	1.04	0/2490
40	BH	0.63	0/1665	1.02	0/2227
41	BI	0.56	0/1239	1.00	1/1664 (0.1%)
42	BJ	0.61	0/1121	1.05	0/1509
43	BK	0.62	0/1422	1.04	1/1908 (0.1%)
44	BL	0.58	0/989	0.97	0/1326
45	BM	0.65	0/1048	1.03	0/1394
46	BN	0.59	0/835	1.08	0/1127
47	BO	0.61	0/982	1.00	0/1323
48	BP	0.61	0/969	1.09	0/1300
49	BQ	0.57	0/919	1.01	0/1226
50	BR	0.63	0/817	1.14	1/1088 (0.1%)
51	BS	0.58	0/724	1.00	1/966 (0.1%)
52	BT	0.63	0/659	1.04	0/884
53	BU	0.58	0/681	0.99	0/913
54	BV	0.71	0/637	1.06	0/851
55	BW	0.60	0/744	1.02	3/995 (0.3%)
56	BX	0.55	0/676	0.91	0/895
57	BY	0.69	0/598	1.17	1/792 (0.1%)
All	All	1.03	1/165193 (0.0%)	1.75	3679/246106 (1.5%)

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	AA	0	27
2	AB	0	821
3	AC	0	2
5	AE	0	3
6	AF	0	1
8	AH	0	2
9	AI	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	AK	0	2
15	AO	0	1
17	AQ	0	1
18	AR	0	1
28	Ab	0	1
30	Ad	0	1
31	Ae	0	2
34	BA	0	473
35	BB	0	12
35	BE	0	15
37	BD	0	4
38	BF	0	1
39	BG	0	2
40	BH	0	2
41	BI	0	3
42	BJ	0	1
43	BK	0	2
45	BM	0	2
47	BO	0	1
48	BP	0	1
50	BR	0	1
54	BV	0	1
55	BW	0	1
57	BY	0	3
All	All	0	1392

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BA	1535	C	P-O5'	5.14	1.64	1.59

All (3679) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	13	G	O4'-C1'-N9	15.20	120.36	108.20
2	AB	736	C	O4'-C1'-N1	14.43	119.74	108.20
34	BA	465	A	O4'-C1'-N9	13.60	119.08	108.20
2	AB	2832	U	O4'-C1'-N1	12.97	118.58	108.20
34	BA	1152	A	O4'-C1'-N9	12.96	118.57	108.20
1	AA	49	C	O4'-C1'-N1	12.84	118.47	108.20
1	AA	30	C	O4'-C1'-N1	12.65	118.32	108.20
2	AB	2092	U	O4'-C1'-N1	12.43	118.14	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1078	U	O4'-C1'-N1	12.33	118.06	108.20
2	AB	784	G	O4'-C1'-N9	12.14	117.91	108.20
2	AB	1535	A	O4'-C1'-N9	12.04	117.83	108.20
2	AB	2147	A	O4'-C1'-N9	11.81	117.64	108.20
2	AB	1730	C	O4'-C1'-N1	11.50	117.40	108.20
2	AB	1294	U	O4'-C1'-N1	11.35	117.28	108.20
2	AB	323	C	O4'-C1'-N1	11.31	117.25	108.20
2	AB	1701	A	O4'-C1'-N9	11.31	117.25	108.20
2	AB	100	U	O4'-C1'-N1	11.30	117.24	108.20
34	BA	1322	C	O4'-C1'-N1	11.10	117.08	108.20
2	AB	382	A	O4'-C1'-N9	11.09	117.07	108.20
34	BA	792	A	O4'-C1'-N9	11.03	117.02	108.20
2	AB	372	G	O4'-C1'-N9	10.99	116.99	108.20
34	BA	1212	U	O4'-C1'-N1	10.98	116.99	108.20
2	AB	1808	A	O4'-C1'-N9	10.90	116.92	108.20
34	BA	225	C	O4'-C1'-N1	10.85	116.88	108.20
2	AB	1870	C	O4'-C1'-N1	10.84	116.87	108.20
2	AB	2903	U	O4'-C1'-N1	10.77	116.81	108.20
2	AB	2742	G	O4'-C1'-N9	10.72	116.77	108.20
2	AB	2147	A	C1'-O4'-C4'	-10.71	101.33	109.90
2	AB	362	A	O4'-C1'-N9	10.70	116.76	108.20
2	AB	2667	C	O4'-C1'-N1	10.62	116.70	108.20
2	AB	740	C	O4'-C1'-N1	10.62	116.69	108.20
2	AB	2610	C	O4'-C1'-N1	10.59	116.67	108.20
2	AB	316	C	O4'-C1'-N1	10.55	116.64	108.20
2	AB	2666	C	O4'-C1'-N1	10.53	116.63	108.20
2	AB	2276	G	O4'-C1'-N9	10.52	116.62	108.20
2	AB	2637	U	O4'-C1'-N1	10.45	116.56	108.20
2	AB	346	A	O4'-C1'-N9	10.41	116.53	108.20
2	AB	277	G	C1'-O4'-C4'	-10.40	101.58	109.90
2	AB	169	G	O4'-C1'-N9	10.36	116.49	108.20
34	BA	899	C	O3'-P-O5'	-10.35	84.33	104.00
34	BA	1193	G	O4'-C1'-N9	10.34	116.47	108.20
34	BA	593	U	O4'-C1'-N1	10.29	116.43	108.20
34	BA	1435	G	O4'-C1'-N9	10.25	116.40	108.20
2	AB	302	C	O4'-C1'-N1	10.24	116.39	108.20
2	AB	1552	A	O4'-C1'-N9	10.23	116.39	108.20
2	AB	1209	U	O4'-C1'-N1	10.20	116.36	108.20
2	AB	1081	U	O4'-C1'-N1	10.19	116.35	108.20
34	BA	274	A	O4'-C1'-N9	10.17	116.33	108.20
2	AB	105	C	O4'-C1'-N1	10.13	116.31	108.20
2	AB	1195	G	O4'-C1'-N9	10.08	116.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	835	U	O4'-C1'-N1	10.05	116.24	108.20
34	BA	664	G	O4'-C1'-N9	10.04	116.23	108.20
2	AB	351	C	O4'-C1'-N1	10.01	116.21	108.20
2	AB	1981	A	O4'-C1'-N9	9.98	116.18	108.20
2	AB	1967	C	O4'-C1'-N1	9.96	116.17	108.20
35	BB	25	C	O4'-C1'-N1	9.95	116.16	108.20
2	AB	1016	G	O4'-C1'-N9	9.94	116.15	108.20
2	AB	2213	U	O4'-C1'-N1	9.93	116.15	108.20
2	AB	1185	G	O4'-C1'-N9	9.91	116.13	108.20
1	AA	118	C	O4'-C1'-N1	9.91	116.13	108.20
34	BA	244	U	O4'-C1'-N1	9.91	116.13	108.20
34	BA	1457	G	O4'-C1'-N9	9.91	116.13	108.20
2	AB	2518	A	O4'-C1'-N9	9.91	116.12	108.20
2	AB	550	C	O4'-C1'-N1	9.87	116.09	108.20
35	BE	17	C	O4'-C1'-N1	9.85	116.08	108.20
2	AB	1542	U	O4'-C1'-N1	9.84	116.07	108.20
2	AB	1647	U	O4'-C1'-N1	9.80	116.04	108.20
2	AB	339	U	O4'-C1'-N1	9.79	116.03	108.20
34	BA	396	C	O4'-C1'-N1	9.78	116.02	108.20
2	AB	1714	U	O4'-C1'-N1	9.75	116.00	108.20
2	AB	1901	A	O4'-C1'-N9	9.70	115.96	108.20
2	AB	1477	A	C5'-C4'-O4'	9.70	120.73	109.10
2	AB	1703	G	O4'-C1'-N9	9.69	115.95	108.20
2	AB	1026	G	O4'-C1'-N9	9.65	115.92	108.20
2	AB	206	U	O4'-C1'-N1	9.64	115.91	108.20
34	BA	277	C	O4'-C1'-N1	9.64	115.91	108.20
34	BA	811	C	O4'-C1'-N1	9.64	115.91	108.20
34	BA	488	C	O4'-C1'-N1	9.62	115.89	108.20
2	AB	744	U	O4'-C1'-N1	9.61	115.89	108.20
34	BA	834	U	O4'-C1'-N1	9.61	115.89	108.20
2	AB	876	C	O4'-C1'-N1	9.58	115.86	108.20
34	BA	936	C	O4'-C1'-N1	9.58	115.86	108.20
34	BA	532	A	O4'-C1'-N9	9.56	115.85	108.20
2	AB	512	G	O4'-C1'-N9	9.54	115.83	108.20
2	AB	614	A	O4'-C1'-N9	9.54	115.83	108.20
2	AB	1443	U	O4'-C1'-N1	9.53	115.82	108.20
34	BA	214	C	O4'-C1'-N1	9.52	115.81	108.20
34	BA	379	C	O4'-C1'-N1	9.51	115.81	108.20
34	BA	1540	U	O4'-C1'-N1	9.51	115.81	108.20
34	BA	1071	C	O4'-C1'-N1	9.49	115.79	108.20
34	BA	29	U	O4'-C1'-N1	9.49	115.79	108.20
34	BA	158	G	O4'-C1'-N9	9.46	115.77	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	52	A	O4'-C1'-N9	9.46	115.77	108.20
2	AB	1245	G	O4'-C1'-N9	9.46	115.77	108.20
34	BA	770	C	O4'-C1'-N1	9.46	115.76	108.20
34	BA	842	U	O4'-C1'-N1	9.44	115.75	108.20
34	BA	890	G	O4'-C1'-N9	9.40	115.72	108.20
1	AA	93	C	O4'-C1'-N1	9.39	115.71	108.20
2	AB	546	U	O4'-C1'-N1	9.38	115.70	108.20
2	AB	2707	U	O4'-C1'-N1	9.35	115.68	108.20
2	AB	1293	C	O4'-C1'-N1	9.33	115.67	108.20
2	AB	1520	U	O4'-C1'-N1	9.33	115.66	108.20
2	AB	2684	U	O4'-C1'-N1	9.32	115.66	108.20
2	AB	354	A	O4'-C1'-N9	9.32	115.65	108.20
34	BA	465	A	C1'-O4'-C4'	-9.31	102.45	109.90
7	AG	132	ARG	NE-CZ-NH2	9.31	124.95	120.30
34	BA	1232	U	O4'-C1'-N1	9.30	115.64	108.20
2	AB	2465	C	O4'-C1'-N1	9.26	115.61	108.20
2	AB	268	C	O4'-C1'-N1	9.26	115.61	108.20
2	AB	2098	U	O4'-C1'-N1	9.26	115.61	108.20
2	AB	1729	U	O4'-C1'-N1	9.25	115.60	108.20
2	AB	1394	U	C5'-C4'-C3'	-9.24	101.21	116.00
2	AB	39	G	O4'-C1'-N9	9.22	115.58	108.20
2	AB	1816	C	O4'-C1'-N1	9.22	115.58	108.20
34	BA	408	A	O4'-C1'-N9	9.22	115.58	108.20
2	AB	921	C	O4'-C1'-N1	9.20	115.56	108.20
2	AB	1102	C	O4'-C1'-N1	9.18	115.55	108.20
2	AB	276	U	O4'-C1'-N1	9.18	115.54	108.20
2	AB	1409	U	O4'-C1'-N1	9.18	115.54	108.20
2	AB	70	G	O4'-C1'-N9	9.16	115.53	108.20
34	BA	1449	C	O4'-C1'-N1	9.16	115.53	108.20
2	AB	321	U	O4'-C1'-N1	9.15	115.52	108.20
2	AB	2226	C	O4'-C1'-N1	9.15	115.52	108.20
34	BA	798	U	O4'-C1'-N1	9.15	115.52	108.20
1	AA	68	C	O4'-C1'-N1	9.14	115.51	108.20
2	AB	2212	A	O4'-C1'-N9	9.13	115.51	108.20
34	BA	1414	U	O4'-C1'-N1	9.13	115.50	108.20
2	AB	945	A	O4'-C1'-N9	9.12	115.50	108.20
2	AB	2864	G	C5'-C4'-C3'	-9.12	101.41	116.00
34	BA	862	C	O4'-C1'-N1	9.12	115.50	108.20
2	AB	2138	G	O4'-C1'-N9	9.11	115.49	108.20
2	AB	1639	C	O4'-C1'-N1	9.10	115.48	108.20
2	AB	306	U	O4'-C1'-N1	9.10	115.48	108.20
2	AB	2739	U	O4'-C1'-N1	9.10	115.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1931	U	O4'-C1'-N1	9.09	115.47	108.20
34	BA	245	U	O4'-C1'-N1	9.04	115.43	108.20
34	BA	375	U	O4'-C1'-N1	9.04	115.43	108.20
2	AB	1578	U	O4'-C1'-N1	9.03	115.42	108.20
34	BA	1541	U	O4'-C1'-N1	9.03	115.43	108.20
2	AB	1849	G	O4'-C1'-N9	9.02	115.42	108.20
2	AB	2188	U	O4'-C1'-N1	9.02	115.42	108.20
2	AB	2855	C	O4'-C1'-N1	9.02	115.42	108.20
34	BA	332	G	O4'-C1'-N9	9.01	115.41	108.20
2	AB	2652	C	O4'-C1'-N1	9.00	115.40	108.20
2	AB	1648	U	O4'-C1'-N1	8.97	115.38	108.20
2	AB	616	A	C5'-C4'-C3'	-8.96	101.66	116.00
2	AB	908	C	O4'-C1'-N1	8.96	115.37	108.20
2	AB	1304	A	O4'-C1'-N9	8.96	115.37	108.20
2	AB	1539	U	O4'-C1'-N1	8.96	115.37	108.20
2	AB	1763	G	O4'-C1'-N9	8.96	115.36	108.20
2	AB	1181	U	O4'-C1'-N1	8.94	115.35	108.20
2	AB	510	C	O4'-C1'-N1	8.92	115.33	108.20
2	AB	1774	C	O4'-C1'-N1	8.92	115.33	108.20
2	AB	365	U	O4'-C1'-N1	8.91	115.33	108.20
2	AB	1444	G	O4'-C1'-N9	8.91	115.33	108.20
34	BA	1141	C	O4'-C1'-N1	8.91	115.33	108.20
2	AB	407	G	O4'-C1'-N9	8.90	115.32	108.20
2	AB	2793	C	O4'-C1'-N1	8.89	115.31	108.20
2	AB	2559	C	O4'-C1'-N1	8.89	115.31	108.20
34	BA	1444	U	O4'-C1'-N1	8.87	115.30	108.20
2	AB	1374	G	O4'-C1'-N9	8.87	115.30	108.20
2	AB	2051	A	O4'-C1'-N9	8.86	115.29	108.20
37	BD	26	U	O4'-C1'-N1	8.85	115.28	108.20
2	AB	2264	C	O4'-C1'-N1	8.84	115.28	108.20
34	BA	90	C	O4'-C1'-N1	8.84	115.27	108.20
34	BA	353	A	O4'-C1'-N9	8.84	115.27	108.20
1	AA	11	C	O4'-C1'-N1	8.83	115.27	108.20
2	AB	279	A	O3'-P-O5'	-8.83	87.22	104.00
2	AB	116	C	O4'-C1'-N1	8.82	115.26	108.20
2	AB	2102	G	O4'-C1'-N9	8.81	115.25	108.20
2	AB	1041	G	O4'-C1'-N9	8.81	115.25	108.20
2	AB	2664	G	C8-N9-C4	-8.81	102.88	106.40
2	AB	236	C	O4'-C1'-N1	8.79	115.23	108.20
34	BA	163	C	O4'-C1'-N1	8.79	115.23	108.20
2	AB	1777	U	O4'-C1'-N1	8.78	115.22	108.20
2	AB	1941	C	O4'-C1'-N1	8.77	115.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1067	A	O4'-C1'-N9	8.76	115.20	108.20
2	AB	975	A	C5'-C4'-O4'	8.75	119.60	109.10
34	BA	705	G	O4'-C1'-N9	8.75	115.20	108.20
34	BA	812	G	O4'-C1'-N9	8.74	115.19	108.20
34	BA	1364	U	O4'-C1'-N1	8.74	115.20	108.20
2	AB	1434	A	O4'-C1'-N9	8.74	115.19	108.20
34	BA	69	G	O4'-C1'-N9	8.73	115.19	108.20
2	AB	125	A	C1'-O4'-C4'	-8.70	102.94	109.90
2	AB	2215	C	C5'-C4'-O4'	8.69	119.53	109.10
2	AB	718	A	O4'-C1'-N9	8.69	115.15	108.20
34	BA	1454	G	O4'-C1'-N9	8.69	115.15	108.20
34	BA	1266	G	O4'-C1'-N9	8.68	115.14	108.20
2	AB	1868	C	O4'-C1'-N1	8.68	115.14	108.20
34	BA	815	A	O4'-C1'-C2'	-8.67	97.13	105.80
2	AB	2140	G	O4'-C1'-N9	8.67	115.14	108.20
2	AB	2751	G	O4'-C1'-N9	8.66	115.13	108.20
2	AB	405	U	O4'-C1'-N1	8.66	115.13	108.20
2	AB	1318	U	O4'-C1'-N1	8.66	115.13	108.20
2	AB	870	U	O4'-C1'-N1	8.65	115.12	108.20
2	AB	2391	G	O4'-C1'-N9	8.64	115.11	108.20
34	BA	461	A	O4'-C1'-N9	8.64	115.11	108.20
2	AB	148	U	O4'-C1'-N1	8.64	115.11	108.20
34	BA	658	C	O4'-C1'-N1	8.64	115.11	108.20
2	AB	471	A	O4'-C1'-N9	8.63	115.10	108.20
2	AB	490	C	O4'-C1'-N1	8.62	115.10	108.20
2	AB	2197	U	O4'-C1'-N1	8.62	115.10	108.20
34	BA	677	U	O4'-C1'-N1	8.62	115.09	108.20
34	BA	472	U	O4'-C1'-N1	8.60	115.08	108.20
34	BA	870	U	O4'-C1'-N1	8.59	115.07	108.20
2	AB	1658	C	O4'-C1'-N1	8.58	115.06	108.20
34	BA	1105	A	O4'-C1'-N9	8.58	115.06	108.20
34	BA	1139	G	O4'-C1'-N9	8.58	115.06	108.20
2	AB	1832	C	O4'-C1'-N1	8.57	115.05	108.20
2	AB	934	U	O4'-C1'-N1	8.56	115.05	108.20
35	BE	51	U	O4'-C1'-N1	8.56	115.05	108.20
2	AB	2538	C	O4'-C1'-N1	8.56	115.05	108.20
2	AB	2773	C	O4'-C1'-N1	8.56	115.05	108.20
2	AB	2672	U	O4'-C1'-N1	8.56	115.05	108.20
34	BA	387	U	O4'-C1'-N1	8.55	115.04	108.20
2	AB	1986	C	C5'-C4'-O4'	8.54	119.34	109.10
34	BA	1425	U	O4'-C1'-N1	8.54	115.03	108.20
2	AB	92	U	O4'-C1'-N1	8.54	115.03	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1463	C	O4'-C1'-N1	8.53	115.03	108.20
2	AB	598	U	O4'-C1'-N1	8.52	115.02	108.20
34	BA	955	U	O4'-C1'-N1	8.52	115.02	108.20
2	AB	1851	U	O4'-C1'-N1	8.52	115.02	108.20
2	AB	277	G	P-O3'-C3'	8.50	129.90	119.70
2	AB	1649	G	C5'-C4'-O4'	8.50	119.30	109.10
2	AB	415	A	O4'-C1'-N9	8.49	114.99	108.20
2	AB	1933	G	O4'-C1'-N9	8.48	114.98	108.20
2	AB	2798	U	O4'-C1'-N1	8.48	114.98	108.20
1	AA	13	G	N9-C1'-C2'	-8.47	102.68	112.00
2	AB	1882	U	O4'-C1'-N1	8.47	114.97	108.20
2	AB	1784	A	O4'-C1'-N9	8.46	114.97	108.20
2	AB	1244	A	O4'-C1'-N9	8.46	114.97	108.20
2	AB	1943	U	O4'-C1'-N1	8.44	114.95	108.20
2	AB	1512	C	O4'-C1'-N1	8.43	114.94	108.20
2	AB	331	C	O4'-C1'-N1	8.42	114.93	108.20
2	AB	2175	C	O3'-P-O5'	-8.41	88.03	104.00
2	AB	2807	U	O4'-C1'-N1	8.41	114.92	108.20
2	AB	16	C	O4'-C1'-N1	8.40	114.92	108.20
2	AB	366	C	O4'-C1'-N1	8.40	114.92	108.20
2	AB	2396	G	O4'-C1'-N9	8.40	114.92	108.20
34	BA	1299	A	O4'-C1'-N9	8.40	114.92	108.20
34	BA	1377	A	C5'-C4'-O4'	8.40	119.18	109.10
34	BA	419	C	O4'-C1'-N1	8.39	114.91	108.20
34	BA	465	A	C5'-C4'-O4'	8.39	119.17	109.10
2	AB	319	G	O4'-C1'-N9	8.38	114.90	108.20
2	AB	1588	G	O3'-P-O5'	-8.38	88.08	104.00
2	AB	1720	U	O4'-C1'-N1	8.38	114.90	108.20
2	AB	2020	A	C5'-C4'-O4'	8.38	119.15	109.10
2	AB	2581	G	O4'-C1'-N9	8.38	114.90	108.20
2	AB	458	G	O4'-C1'-N9	8.37	114.90	108.20
34	BA	1315	U	C5'-C4'-O4'	8.37	119.14	109.10
2	AB	288	U	O4'-C1'-N1	8.36	114.89	108.20
2	AB	991	C	O4'-C1'-N1	8.36	114.88	108.20
34	BA	1478	U	O4'-C1'-N1	8.36	114.89	108.20
2	AB	737	C	O4'-C1'-N1	8.35	114.88	108.20
2	AB	1476	U	O4'-C1'-N1	8.35	114.88	108.20
34	BA	711	G	O4'-C1'-N9	8.34	114.87	108.20
2	AB	1372	U	O4'-C1'-N1	8.34	114.87	108.20
2	AB	2244	U	O4'-C1'-N1	8.34	114.87	108.20
34	BA	507	C	O4'-C1'-N1	8.33	114.86	108.20
34	BA	267	C	O4'-C1'-N1	8.32	114.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BE	22	G	O4'-C1'-N9	8.31	114.85	108.20
34	BA	126	G	O4'-C1'-N9	8.31	114.85	108.20
34	BA	1075	U	O4'-C1'-N1	8.31	114.85	108.20
34	BA	1372	U	O4'-C1'-N1	8.31	114.84	108.20
34	BA	567	G	O4'-C1'-N9	8.29	114.83	108.20
2	AB	2784	U	O4'-C1'-N1	8.29	114.83	108.20
34	BA	99	C	O4'-C1'-N1	8.29	114.83	108.20
34	BA	409	U	O4'-C1'-N1	8.28	114.83	108.20
2	AB	2032	G	O4'-C1'-N9	8.28	114.82	108.20
34	BA	78	A	O4'-C1'-N9	8.28	114.82	108.20
2	AB	1742	U	O4'-C1'-N1	8.27	114.81	108.20
34	BA	899	C	O4'-C1'-N1	8.26	114.81	108.20
34	BA	1255	G	O4'-C1'-N9	8.26	114.81	108.20
2	AB	1493	C	O4'-C1'-N1	8.26	114.80	108.20
2	AB	2655	G	O4'-C1'-N9	8.26	114.80	108.20
34	BA	453	G	O4'-C1'-N9	8.25	114.80	108.20
2	AB	1709	U	C5'-C4'-O4'	8.24	118.99	109.10
2	AB	2147	A	C5'-C4'-O4'	8.24	118.99	109.10
2	AB	1088	A	O4'-C1'-N9	8.24	114.79	108.20
2	AB	720	U	C5'-C4'-O4'	8.24	118.99	109.10
2	AB	1417	C	O4'-C1'-N1	8.24	114.79	108.20
2	AB	1526	C	O4'-C1'-N1	8.24	114.79	108.20
34	BA	1136	C	O4'-C1'-N1	8.24	114.79	108.20
2	AB	2473	U	O4'-C1'-N1	8.23	114.78	108.20
2	AB	2126	A	O4'-C1'-N9	8.23	114.78	108.20
34	BA	518	C	O4'-C1'-N1	8.22	114.78	108.20
2	AB	1886	U	O4'-C1'-N1	8.21	114.77	108.20
34	BA	702	A	O4'-C1'-N9	8.21	114.77	108.20
34	BA	268	U	C5'-C4'-O4'	8.21	118.95	109.10
2	AB	960	A	O4'-C1'-N9	-8.20	101.64	108.20
2	AB	865	C	O4'-C1'-N1	8.20	114.76	108.20
34	BA	25	C	O4'-C1'-N1	8.18	114.74	108.20
34	BA	384	G	O4'-C1'-N9	8.18	114.74	108.20
2	AB	63	A	O4'-C1'-N9	8.17	114.74	108.20
2	AB	2579	C	O4'-C1'-N1	8.17	114.74	108.20
34	BA	723	U	O4'-C1'-N1	8.17	114.73	108.20
2	AB	551	G	O4'-C1'-N9	8.16	114.73	108.20
35	BB	19	G	N3-C4-C5	-8.16	124.52	128.60
2	AB	1914	C	O4'-C1'-N1	8.16	114.73	108.20
2	AB	2321	U	O4'-C1'-N1	8.16	114.73	108.20
2	AB	65	U	O4'-C1'-N1	8.16	114.73	108.20
2	AB	2509	G	O4'-C1'-N9	8.15	114.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	59	U	O4'-C1'-N1	8.15	114.72	108.20
2	AB	517	C	O4'-C1'-N1	8.14	114.72	108.20
34	BA	1172	C	O4'-C1'-N1	8.14	114.71	108.20
34	BA	1409	C	O4'-C1'-N1	8.14	114.71	108.20
2	AB	295	G	O4'-C1'-N9	8.13	114.71	108.20
2	AB	880	G	O4'-C1'-N9	8.13	114.71	108.20
2	AB	776	G	O4'-C1'-N9	8.13	114.70	108.20
2	AB	971	G	O4'-C1'-N9	8.13	114.70	108.20
2	AB	32	C	O4'-C1'-N1	8.12	114.70	108.20
2	AB	1167	C	O4'-C1'-N1	8.12	114.70	108.20
34	BA	212	G	O4'-C1'-N9	8.12	114.69	108.20
2	AB	1798	U	O4'-C1'-N1	8.12	114.69	108.20
2	AB	345	A	C1'-O4'-C4'	-8.11	103.41	109.90
2	AB	1405	U	O4'-C1'-N1	8.11	114.69	108.20
2	AB	2843	G	O4'-C1'-N9	8.11	114.69	108.20
2	AB	1153	C	O4'-C1'-N1	8.10	114.68	108.20
2	AB	2404	U	O4'-C1'-N1	8.09	114.67	108.20
2	AB	2406	A	O4'-C1'-N9	8.09	114.67	108.20
2	AB	2438	U	O4'-C1'-N1	8.08	114.67	108.20
2	AB	1695	G	O4'-C1'-N9	8.08	114.67	108.20
2	AB	2265	U	O4'-C1'-N1	8.08	114.67	108.20
34	BA	85	U	O4'-C1'-N1	8.08	114.66	108.20
2	AB	1370	C	O4'-C1'-N1	8.07	114.66	108.20
34	BA	1281	C	O4'-C1'-N1	8.07	114.66	108.20
2	AB	2699	C	O4'-C1'-N1	8.07	114.66	108.20
2	AB	141	G	C5'-C4'-C3'	-8.07	103.09	116.00
34	BA	294	U	O4'-C1'-N1	8.07	114.65	108.20
2	AB	279	A	O4'-C1'-N9	8.06	114.65	108.20
2	AB	627	A	O4'-C1'-N9	8.06	114.65	108.20
34	BA	143	A	O4'-C1'-N9	8.06	114.65	108.20
2	AB	1549	A	O4'-C1'-N9	8.06	114.65	108.20
2	AB	1920	C	O4'-C1'-N1	8.05	114.64	108.20
2	AB	765	C	O4'-C1'-N1	8.05	114.64	108.20
34	BA	311	C	O4'-C1'-N1	8.04	114.63	108.20
34	BA	844	G	O4'-C1'-N9	8.04	114.63	108.20
2	AB	841	G	C5'-C4'-O4'	8.03	118.74	109.10
2	AB	158	U	O4'-C1'-N1	8.03	114.63	108.20
2	AB	291	G	O4'-C1'-N9	8.03	114.63	108.20
2	AB	1724	G	C8-N9-C4	-8.03	103.19	106.40
2	AB	1115	G	O4'-C1'-N9	8.02	114.62	108.20
2	AB	1767	G	O4'-C1'-N9	8.02	114.62	108.20
2	AB	2750	A	O4'-C1'-N9	8.02	114.61	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1506	U	O4'-C1'-N1	8.01	114.61	108.20
1	AA	36	C	O4'-C1'-N1	8.01	114.61	108.20
2	AB	1177	G	C5'-C4'-O4'	8.01	118.71	109.10
2	AB	1101	U	O4'-C1'-N1	8.01	114.61	108.20
2	AB	2901	C	O4'-C1'-N1	8.00	114.60	108.20
2	AB	1002	G	O4'-C1'-N9	8.00	114.60	108.20
34	BA	301	G	O4'-C1'-N9	8.00	114.60	108.20
2	AB	1887	C	O4'-C1'-N1	8.00	114.60	108.20
34	BA	1097	C	O4'-C1'-N1	7.99	114.59	108.20
34	BA	31	G	O4'-C1'-N9	7.99	114.59	108.20
2	AB	2178	C	O4'-C1'-N1	7.98	114.59	108.20
34	BA	1040	U	O4'-C1'-N1	7.98	114.59	108.20
34	BA	1258	G	O4'-C1'-N9	7.97	114.58	108.20
34	BA	465	A	C5'-C4'-C3'	-7.97	103.24	116.00
34	BA	675	A	O4'-C1'-N9	7.97	114.58	108.20
2	AB	246	C	O4'-C1'-N1	7.97	114.57	108.20
2	AB	2582	G	C8-N9-C4	-7.97	103.21	106.40
2	AB	193	U	O4'-C1'-N1	7.96	114.57	108.20
2	AB	961	C	O4'-C1'-N1	7.96	114.57	108.20
2	AB	1758	U	O4'-C1'-N1	7.96	114.57	108.20
2	AB	1484	U	O4'-C1'-N1	7.95	114.56	108.20
34	BA	150	U	O4'-C1'-N1	7.95	114.56	108.20
34	BA	860	A	O4'-C1'-N9	7.95	114.56	108.20
2	AB	856	G	C5'-C4'-O4'	7.95	118.64	109.10
34	BA	192	A	O4'-C1'-N9	7.94	114.55	108.20
2	AB	1275	A	O4'-C1'-N9	7.94	114.55	108.20
2	AB	2182	U	O4'-C1'-N1	7.94	114.55	108.20
2	AB	433	C	O4'-C1'-N1	7.93	114.55	108.20
34	BA	151	A	O4'-C1'-N9	7.93	114.55	108.20
34	BA	1315	U	C5'-C4'-C3'	-7.93	103.30	116.00
2	AB	128	C	O4'-C1'-N1	7.93	114.54	108.20
2	AB	618	G	O4'-C1'-N9	7.92	114.54	108.20
2	AB	2220	U	O4'-C1'-N1	7.91	114.52	108.20
34	BA	256	U	O4'-C1'-N1	7.91	114.53	108.20
2	AB	1118	C	O4'-C1'-N1	7.90	114.52	108.20
2	AB	2020	A	O4'-C1'-N9	7.90	114.52	108.20
2	AB	2310	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	95	U	O4'-C1'-N1	7.90	114.52	108.20
34	BA	1	A	O4'-C1'-N9	7.90	114.52	108.20
2	AB	2632	A	O4'-C1'-N9	7.89	114.52	108.20
34	BA	845	A	O4'-C1'-N9	7.89	114.52	108.20
35	BE	42	C	O4'-C1'-N1	7.89	114.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1196	C	O4'-C1'-N1	7.89	114.52	108.20
2	AB	266	G	C8-N9-C4	-7.89	103.24	106.40
34	BA	512	U	O4'-C1'-N1	7.89	114.51	108.20
34	BA	937	A	O4'-C1'-N9	7.89	114.51	108.20
34	BA	1480	A	O4'-C1'-N9	7.89	114.51	108.20
2	AB	1058	U	O4'-C1'-N1	7.88	114.50	108.20
35	BE	13	C	O4'-C1'-N1	7.88	114.50	108.20
2	AB	1985	C	O4'-C1'-N1	7.88	114.50	108.20
34	BA	930	C	O4'-C1'-N1	7.88	114.50	108.20
34	BA	1474	U	O4'-C1'-N1	7.88	114.50	108.20
34	BA	841	C	C6-N1-C2	-7.87	117.15	120.30
34	BA	1351	U	O4'-C1'-N1	7.87	114.49	108.20
34	BA	342	C	O4'-C1'-N1	7.86	114.49	108.20
2	AB	2110	G	O4'-C1'-N9	7.86	114.48	108.20
2	AB	891	G	O4'-C1'-N9	7.85	114.48	108.20
2	AB	1186	G	C5'-C4'-C3'	-7.85	103.44	116.00
2	AB	2882	A	C5'-C4'-O4'	7.85	118.52	109.10
2	AB	2374	C	O4'-C1'-N1	7.85	114.48	108.20
34	BA	562	U	O4'-C1'-N1	7.84	114.47	108.20
2	AB	519	U	O4'-C1'-N1	7.84	114.47	108.20
34	BA	594	U	O4'-C1'-N1	7.84	114.47	108.20
2	AB	336	C	O4'-C1'-N1	7.84	114.47	108.20
34	BA	904	U	O4'-C1'-N1	7.83	114.47	108.20
34	BA	73	C	O4'-C1'-N1	7.83	114.47	108.20
2	AB	1909	C	O4'-C1'-N1	7.83	114.46	108.20
2	AB	2769	U	O4'-C1'-N1	7.83	114.46	108.20
2	AB	1871	A	C3'-C2'-C1'	7.82	107.76	101.50
2	AB	1998	A	O4'-C1'-N9	7.82	114.46	108.20
2	AB	1148	U	O4'-C1'-N1	7.82	114.46	108.20
2	AB	1349	C	O4'-C1'-N1	7.82	114.46	108.20
2	AB	1079	C	O4'-C1'-N1	7.82	114.46	108.20
34	BA	65	A	O4'-C1'-N9	7.82	114.45	108.20
2	AB	1191	G	O4'-C1'-N9	7.81	114.45	108.20
34	BA	206	C	O4'-C1'-N1	7.81	114.45	108.20
35	BB	11	C	C5'-C4'-O4'	7.81	118.47	109.10
34	BA	359	G	O4'-C1'-N9	7.81	114.45	108.20
2	AB	651	G	O4'-C1'-N9	7.80	114.44	108.20
2	AB	1938	A	O4'-C1'-N9	7.80	114.44	108.20
2	AB	1509	A	O4'-C1'-N9	7.80	114.44	108.20
2	AB	2426	A	O4'-C1'-N9	7.80	114.44	108.20
34	BA	971	G	C5'-C4'-C3'	-7.79	103.53	116.00
2	AB	1097	U	O4'-C1'-N1	7.79	114.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	651	C	C5'-C4'-O4'	7.79	118.45	109.10
2	AB	803	U	O4'-C1'-N1	7.79	114.43	108.20
34	BA	898	G	O4'-C1'-N9	7.79	114.43	108.20
35	BB	49	C	O4'-C1'-N1	7.79	114.43	108.20
2	AB	1883	U	O4'-C1'-N1	7.79	114.43	108.20
2	AB	2825	G	O4'-C1'-N9	7.79	114.43	108.20
34	BA	1328	C	O4'-C1'-N1	7.78	114.43	108.20
2	AB	418	C	O4'-C1'-N1	7.78	114.42	108.20
2	AB	2470	G	O4'-C1'-N9	7.78	114.43	108.20
34	BA	211	G	N3-C4-C5	-7.78	124.71	128.60
2	AB	1282	U	O4'-C1'-N1	7.78	114.42	108.20
34	BA	1528	U	O4'-C1'-N1	7.78	114.42	108.20
2	AB	898	C	O4'-C1'-N1	7.77	114.42	108.20
2	AB	984	A	C1'-O4'-C4'	-7.77	103.69	109.90
34	BA	1202	U	O4'-C1'-N1	7.76	114.41	108.20
34	BA	972	C	O4'-C1'-N1	7.76	114.41	108.20
1	AA	70	C	O4'-C1'-N1	7.75	114.40	108.20
2	AB	2103	C	O4'-C1'-N1	7.75	114.40	108.20
35	BE	41	C	O4'-C1'-N1	7.75	114.40	108.20
2	AB	2001	C	O4'-C1'-N1	7.75	114.40	108.20
2	AB	2240	U	O4'-C1'-N1	7.75	114.40	108.20
2	AB	2164	C	O4'-C1'-N1	7.74	114.39	108.20
2	AB	341	C	O4'-C1'-N1	7.74	114.39	108.20
2	AB	2743	U	O4'-C1'-N1	7.74	114.39	108.20
2	AB	2762	C	O4'-C1'-N1	7.74	114.39	108.20
34	BA	1165	U	O4'-C1'-N1	7.74	114.39	108.20
34	BA	96	U	O4'-C1'-N1	7.74	114.39	108.20
2	AB	324	A	C5'-C4'-C3'	-7.73	103.63	116.00
1	AA	120	U	O4'-C1'-N1	7.73	114.39	108.20
2	AB	1351	C	O4'-C1'-N1	7.73	114.39	108.20
2	AB	878	A	O4'-C1'-N9	7.73	114.39	108.20
2	AB	1670	C	O4'-C1'-N1	7.73	114.39	108.20
2	AB	1895	C	O4'-C1'-N1	7.73	114.39	108.20
2	AB	1300	G	O4'-C1'-N9	7.73	114.38	108.20
2	AB	2795	C	O4'-C1'-N1	7.73	114.38	108.20
34	BA	1121	U	O4'-C1'-N1	7.73	114.38	108.20
2	AB	504	A	O4'-C1'-N9	7.73	114.38	108.20
34	BA	287	U	O4'-C1'-N1	7.73	114.38	108.20
2	AB	1166	G	O4'-C1'-N9	7.72	114.38	108.20
2	AB	2181	U	O4'-C1'-N1	7.72	114.38	108.20
34	BA	1471	U	O4'-C1'-N1	7.71	114.37	108.20
2	AB	1902	C	O4'-C1'-N1	7.71	114.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	984	A	O4'-C1'-C2'	-7.71	98.09	105.80
34	BA	83	C	O4'-C1'-N1	7.71	114.37	108.20
34	BA	465	A	O4'-C1'-C2'	-7.71	98.09	105.80
34	BA	1066	C	O4'-C1'-N1	7.71	114.36	108.20
2	AB	1423	G	O4'-C1'-N9	7.70	114.36	108.20
2	AB	305	C	C5'-C4'-C3'	-7.70	103.69	116.00
34	BA	1017	U	O4'-C1'-N1	7.69	114.36	108.20
2	AB	2370	G	O4'-C1'-N9	7.69	114.35	108.20
2	AB	277	G	C5'-C4'-O4'	7.69	118.33	109.10
2	AB	57	C	O4'-C1'-N1	7.68	114.34	108.20
2	AB	613	A	C3'-C2'-C1'	-7.68	95.36	101.50
34	BA	490	C	O4'-C1'-N1	7.68	114.34	108.20
34	BA	1223	C	C5'-C4'-C3'	-7.68	103.71	116.00
2	AB	1605	C	O4'-C1'-N1	7.68	114.34	108.20
2	AB	1053	C	O4'-C1'-N1	7.68	114.34	108.20
2	AB	2430	A	O4'-C1'-N9	7.68	114.34	108.20
2	AB	66	C	O4'-C1'-N1	7.67	114.33	108.20
2	AB	1606	C	O4'-C1'-N1	7.67	114.33	108.20
2	AB	216	A	O4'-C1'-N9	7.66	114.33	108.20
2	AB	349	U	O4'-C1'-N1	7.66	114.33	108.20
2	AB	1227	G	O4'-C1'-N9	7.66	114.33	108.20
2	AB	2723	C	O4'-C1'-N1	7.65	114.32	108.20
2	AB	1288	G	O4'-C1'-N9	7.65	114.32	108.20
2	AB	2612	C	O4'-C1'-N1	7.65	114.32	108.20
34	BA	1294	G	O4'-C1'-N9	7.65	114.32	108.20
2	AB	797	G	O4'-C1'-N9	7.64	114.31	108.20
2	AB	972	A	O4'-C1'-N9	7.64	114.31	108.20
34	BA	258	G	O4'-C1'-N9	7.64	114.31	108.20
2	AB	1853	A	O4'-C1'-N9	7.63	114.30	108.20
2	AB	899	A	O4'-C1'-N9	7.63	114.30	108.20
2	AB	259	G	O4'-C1'-N9	7.62	114.30	108.20
2	AB	1290	C	O4'-C1'-N1	7.62	114.30	108.20
2	AB	1485	U	O4'-C1'-N1	7.62	114.30	108.20
2	AB	593	U	O4'-C1'-N1	7.62	114.30	108.20
2	AB	1144	A	O4'-C1'-N9	7.62	114.29	108.20
2	AB	1173	U	O4'-C1'-N1	7.61	114.29	108.20
2	AB	1880	U	C5'-C4'-O4'	7.61	118.23	109.10
2	AB	702	U	O4'-C1'-N1	7.61	114.29	108.20
2	AB	1736	U	O4'-C1'-N1	7.60	114.28	108.20
2	AB	1402	U	O4'-C1'-N1	7.59	114.27	108.20
2	AB	38	A	O4'-C1'-N9	7.59	114.27	108.20
2	AB	1177	G	C5'-C4'-C3'	-7.59	103.85	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	783	C	C5'-C4'-O4'	7.59	118.21	109.10
34	BA	406	G	C5'-C4'-O4'	7.59	118.21	109.10
34	BA	672	U	O4'-C1'-N1	7.59	114.27	108.20
2	AB	60	G	O4'-C1'-N9	7.59	114.27	108.20
2	AB	1425	G	O4'-C1'-N9	7.58	114.27	108.20
37	BD	33	U	O4'-C1'-N1	7.58	114.27	108.20
2	AB	1837	C	O4'-C1'-N1	7.58	114.27	108.20
34	BA	970	C	C5'-C4'-O4'	7.58	118.20	109.10
2	AB	2794	C	O4'-C1'-N1	7.58	114.26	108.20
2	AB	2507	C	O4'-C1'-N1	7.58	114.26	108.20
2	AB	1183	U	O4'-C1'-N1	7.57	114.26	108.20
2	AB	2751	G	C1'-O4'-C4'	-7.57	103.85	109.90
2	AB	1769	U	O4'-C1'-N1	7.56	114.25	108.20
2	AB	1185	G	C1'-O4'-C4'	-7.55	103.86	109.90
34	BA	1538	C	C5'-C4'-C3'	7.55	128.08	116.00
2	AB	355	U	O4'-C1'-N1	7.55	114.24	108.20
2	AB	1361	G	O4'-C1'-N9	7.54	114.23	108.20
2	AB	644	A	O4'-C1'-N9	7.54	114.23	108.20
2	AB	473	G	C5'-C4'-O4'	7.54	118.15	109.10
1	AA	86	G	O4'-C1'-N9	7.54	114.23	108.20
2	AB	1612	C	O4'-C1'-N1	7.53	114.22	108.20
1	AA	89	U	O4'-C1'-N1	7.53	114.22	108.20
2	AB	2099	U	O4'-C1'-N1	7.53	114.22	108.20
2	AB	2123	G	O4'-C1'-N9	7.53	114.22	108.20
2	AB	1182	G	O4'-C1'-N9	7.53	114.22	108.20
2	AB	2696	U	C5'-C4'-O4'	7.53	118.13	109.10
34	BA	1410	A	O4'-C1'-N9	7.52	114.22	108.20
2	AB	603	A	O4'-C1'-N9	7.52	114.22	108.20
2	AB	2687	U	O4'-C1'-N1	7.52	114.21	108.20
2	AB	185	G	O4'-C1'-N9	7.51	114.21	108.20
2	AB	2362	C	O4'-C1'-N1	7.51	114.21	108.20
34	BA	670	G	O4'-C1'-N9	7.51	114.21	108.20
34	BA	880	C	O4'-C1'-N1	7.51	114.21	108.20
2	AB	191	A	O4'-C1'-N9	7.51	114.21	108.20
34	BA	52	C	O4'-C1'-N1	7.51	114.21	108.20
34	BA	558	G	O4'-C1'-N9	7.50	114.20	108.20
2	AB	252	G	O4'-C1'-N9	7.50	114.20	108.20
34	BA	809	G	O4'-C1'-N9	7.50	114.20	108.20
2	AB	1728	C	O4'-C1'-N1	7.50	114.20	108.20
2	AB	877	A	O4'-C1'-N9	7.49	114.19	108.20
2	AB	2391	G	C1'-O4'-C4'	-7.49	103.91	109.90
2	AB	518	G	C5'-C4'-O4'	7.49	118.08	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2556	C	O4'-C1'-N1	7.49	114.19	108.20
34	BA	1323	G	C5'-C4'-O4'	7.49	118.08	109.10
34	BA	793	U	O4'-C1'-N1	7.48	114.19	108.20
34	BA	133	U	O4'-C1'-N1	7.48	114.19	108.20
34	BA	1205	U	O4'-C1'-N1	7.48	114.18	108.20
35	BE	62	C	O4'-C1'-N1	7.47	114.18	108.20
34	BA	453	G	C8-N9-C4	-7.47	103.41	106.40
2	AB	2025	C	O4'-C1'-N1	7.47	114.17	108.20
34	BA	942	G	O4'-C1'-N9	7.46	114.17	108.20
34	BA	621	A	C5'-C4'-O4'	7.46	118.05	109.10
2	AB	1242	U	O4'-C1'-N1	7.46	114.16	108.20
34	BA	273	U	O4'-C1'-N1	7.45	114.16	108.20
2	AB	683	U	O4'-C1'-N1	7.45	114.16	108.20
2	AB	2558	C	O4'-C1'-N1	7.45	114.16	108.20
34	BA	469	C	O4'-C1'-N1	7.45	114.16	108.20
34	BA	1223	C	C4'-C3'-C2'	-7.45	95.15	102.60
2	AB	1706	C	O4'-C1'-N1	7.45	114.16	108.20
34	BA	956	U	O4'-C1'-N1	7.45	114.16	108.20
34	BA	1500	A	O4'-C1'-N9	7.45	114.16	108.20
2	AB	1878	G	O4'-C1'-N9	7.44	114.15	108.20
2	AB	2293	G	O4'-C1'-N9	7.43	114.15	108.20
2	AB	343	C	O4'-C1'-N1	7.43	114.15	108.20
34	BA	620	C	C5'-C4'-O4'	7.43	118.01	109.10
2	AB	25	U	O4'-C1'-N1	7.42	114.14	108.20
2	AB	2066	C	O4'-C1'-N1	7.42	114.14	108.20
2	AB	2852	G	O4'-C1'-N9	7.42	114.14	108.20
2	AB	1841	U	O4'-C1'-N1	7.42	114.13	108.20
34	BA	682	G	O4'-C1'-N9	7.42	114.14	108.20
34	BA	1225	A	O4'-C1'-N9	-7.42	102.27	108.20
2	AB	15	G	C8-N9-C4	-7.41	103.44	106.40
34	BA	1470	U	O4'-C1'-N1	7.41	114.13	108.20
2	AB	877	A	C8-N9-C4	-7.41	102.84	105.80
2	AB	1326	U	O4'-C1'-N1	7.41	114.12	108.20
34	BA	739	C	O4'-C1'-N1	7.40	114.12	108.20
2	AB	23	G	O4'-C1'-N9	7.40	114.12	108.20
34	BA	773	G	O4'-C1'-N9	7.40	114.12	108.20
2	AB	109	C	O4'-C1'-N1	7.40	114.12	108.20
2	AB	2885	G	C5'-C4'-C3'	-7.39	104.17	116.00
2	AB	2364	C	O4'-C1'-N1	7.39	114.11	108.20
2	AB	719	C	O4'-C1'-N1	7.39	114.11	108.20
2	AB	613	A	O4'-C1'-N9	7.39	114.11	108.20
2	AB	848	C	O4'-C1'-N1	7.39	114.11	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	156	C	O4'-C1'-N1	7.39	114.11	108.20
2	AB	951	C	O4'-C1'-N1	7.38	114.11	108.20
2	AB	2688	G	O4'-C1'-N9	7.38	114.11	108.20
2	AB	1573	G	O4'-C1'-N9	7.38	114.10	108.20
34	BA	348	G	O4'-C1'-N9	7.38	114.10	108.20
34	BA	782	A	O4'-C1'-N9	7.38	114.10	108.20
34	BA	1460	C	O4'-C1'-N1	7.38	114.10	108.20
2	AB	2733	A	O4'-C1'-N9	7.38	114.10	108.20
2	AB	475	C	O4'-C1'-N1	7.37	114.09	108.20
2	AB	2073	C	O4'-C1'-N1	7.37	114.09	108.20
34	BA	1455	G	O4'-C1'-N9	7.37	114.09	108.20
2	AB	1982	U	C5'-C4'-O4'	7.36	117.94	109.10
2	AB	1487	U	O4'-C1'-N1	7.36	114.09	108.20
2	AB	1569	A	O4'-C1'-N9	7.36	114.09	108.20
2	AB	1621	U	O4'-C1'-N1	7.36	114.09	108.20
34	BA	1320	C	C5'-C4'-O4'	7.36	117.93	109.10
2	AB	906	U	O4'-C1'-N1	7.35	114.08	108.20
2	AB	1638	C	O4'-C1'-N1	7.35	114.08	108.20
34	BA	383	A	O4'-C1'-N9	7.35	114.08	108.20
2	AB	1477	A	C5'-C4'-C3'	-7.35	104.24	116.00
34	BA	361	G	O4'-C1'-N9	7.35	114.08	108.20
35	BB	19	G	C8-N9-C4	-7.35	103.46	106.40
2	AB	211	C	O4'-C1'-N1	7.34	114.07	108.20
2	AB	1384	A	O4'-C1'-N9	-7.34	102.33	108.20
2	AB	1221	C	O4'-C1'-N1	7.34	114.07	108.20
2	AB	2079	U	O4'-C1'-N1	7.34	114.07	108.20
34	BA	815	A	C1'-O4'-C4'	-7.34	104.03	109.90
34	BA	1069	C	O4'-C1'-N1	7.34	114.07	108.20
2	AB	2007	U	O4'-C1'-N1	7.34	114.07	108.20
34	BA	458	U	O4'-C1'-N1	7.34	114.07	108.20
34	BA	1443	C	O4'-C1'-N1	7.34	114.07	108.20
34	BA	1218	C	O4'-C1'-N1	7.34	114.07	108.20
34	BA	1065	U	O4'-C1'-N1	7.33	114.07	108.20
2	AB	2229	U	O4'-C1'-N1	7.33	114.07	108.20
2	AB	2805	C	O4'-C1'-N1	7.33	114.07	108.20
2	AB	1162	G	O4'-C1'-N9	7.33	114.06	108.20
2	AB	1172	C	O4'-C1'-N1	7.33	114.06	108.20
2	AB	2086	U	O4'-C1'-N1	7.33	114.07	108.20
2	AB	1347	A	O4'-C1'-N9	7.33	114.06	108.20
2	AB	664	G	O4'-C1'-N9	7.32	114.06	108.20
34	BA	290	C	C5'-C4'-O4'	7.32	117.89	109.10
2	AB	416	U	C5'-C4'-O4'	7.32	117.89	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	946	C	O4'-C1'-N1	7.32	114.05	108.20
2	AB	984	A	C4'-C3'-C2'	-7.31	95.29	102.60
2	AB	225	C	O4'-C1'-N1	7.31	114.05	108.20
2	AB	452	G	O4'-C1'-N9	7.31	114.05	108.20
2	AB	1295	C	O4'-C1'-N1	7.31	114.05	108.20
2	AB	135	U	O4'-C1'-N1	7.30	114.04	108.20
34	BA	543	U	O4'-C1'-N1	7.30	114.04	108.20
34	BA	1025	U	O4'-C1'-N1	7.30	114.04	108.20
34	BA	1132	C	O4'-C1'-N1	7.30	114.04	108.20
2	AB	700	G	N9-C1'-C2'	-7.30	103.97	112.00
2	AB	984	A	O4'-C4'-C3'	7.30	111.94	106.10
2	AB	1112	G	C5'-C4'-O4'	7.29	117.86	109.10
2	AB	1061	U	C3'-C2'-C1'	-7.29	95.67	101.50
2	AB	2841	C	O4'-C1'-N1	7.29	114.03	108.20
2	AB	2139	U	O4'-C1'-N1	7.29	114.03	108.20
34	BA	1091	U	C5'-C4'-O4'	7.28	117.84	109.10
2	AB	1573	G	C8-N9-C4	-7.28	103.49	106.40
2	AB	1686	C	O4'-C1'-N1	7.28	114.03	108.20
1	AA	111	U	O4'-C1'-N1	7.28	114.02	108.20
2	AB	919	U	O4'-C1'-N1	7.28	114.02	108.20
2	AB	1801	A	O4'-C1'-N9	7.28	114.02	108.20
2	AB	120	U	O4'-C1'-N1	7.27	114.02	108.20
2	AB	811	U	O4'-C1'-N1	7.27	114.01	108.20
2	AB	930	G	O4'-C1'-N9	7.26	114.01	108.20
2	AB	168	G	O4'-C1'-N9	7.26	114.01	108.20
2	AB	1309	G	O4'-C1'-N9	7.26	114.01	108.20
2	AB	2792	A	C5'-C4'-C3'	-7.26	104.39	116.00
34	BA	900	A	C8-N9-C4	-7.26	102.90	105.80
34	BA	585	G	C5'-C4'-O4'	7.25	117.80	109.10
2	AB	257	C	O4'-C1'-N1	7.24	114.00	108.20
34	BA	1279	G	O4'-C1'-N9	7.24	114.00	108.20
2	AB	2456	C	O4'-C1'-N1	7.24	113.99	108.20
34	BA	678	U	O4'-C1'-N1	7.24	113.99	108.20
2	AB	2582	G	N3-C4-C5	-7.23	124.98	128.60
2	AB	733	G	C5'-C4'-O4'	7.23	117.78	109.10
2	AB	748	G	C5'-C4'-O4'	7.23	117.78	109.10
2	AB	2775	G	C8-N9-C4	-7.23	103.51	106.40
34	BA	1462	C	O4'-C1'-N1	7.23	113.98	108.20
2	AB	1271	G	O4'-C1'-N9	7.23	113.98	108.20
34	BA	386	C	C5'-C4'-O4'	7.23	117.77	109.10
2	AB	834	G	C8-N9-C4	-7.22	103.51	106.40
2	AB	1045	C	O4'-C1'-N1	7.22	113.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1231	U	O4'-C1'-N1	7.22	113.98	108.20
2	AB	1396	U	O4'-C1'-N1	7.22	113.98	108.20
34	BA	401	C	O4'-C1'-N1	7.22	113.98	108.20
2	AB	1146	C	O4'-C1'-N1	7.22	113.98	108.20
2	AB	2466	C	O4'-C1'-N1	7.22	113.98	108.20
34	BA	202	G	O4'-C1'-N9	7.22	113.98	108.20
2	AB	1233	C	O4'-C1'-N1	7.22	113.97	108.20
34	BA	397	A	O4'-C1'-N9	7.22	113.97	108.20
34	BA	24	U	O4'-C1'-N1	7.21	113.97	108.20
2	AB	399	U	O4'-C1'-N1	7.21	113.97	108.20
34	BA	1448	C	O4'-C1'-N1	7.21	113.97	108.20
2	AB	817	C	O4'-C1'-N1	7.20	113.96	108.20
2	AB	1575	C	O4'-C1'-N1	7.20	113.96	108.20
2	AB	2586	U	O4'-C1'-N1	7.20	113.96	108.20
2	AB	160	A	O4'-C1'-N9	7.20	113.96	108.20
2	AB	772	C	O4'-C1'-N1	7.20	113.96	108.20
34	BA	1432	G	O4'-C1'-N9	7.20	113.96	108.20
2	AB	1177	G	N3-C4-C5	-7.19	125.01	128.60
2	AB	489	G	O4'-C1'-N9	7.18	113.95	108.20
34	BA	327	A	C1'-O4'-C4'	-7.18	104.16	109.90
34	BA	690	G	O4'-C1'-N9	7.18	113.94	108.20
34	BA	1216	A	O4'-C1'-N9	7.18	113.94	108.20
2	AB	2659	G	O4'-C1'-N9	7.17	113.94	108.20
2	AB	58	G	O4'-C1'-N9	7.17	113.94	108.20
34	BA	1522	U	O4'-C1'-N1	7.17	113.93	108.20
2	AB	1316	U	O4'-C1'-N1	7.17	113.93	108.20
2	AB	2633	G	O4'-C1'-N9	7.17	113.93	108.20
2	AB	970	U	O4'-C1'-N1	7.16	113.93	108.20
2	AB	1653	G	C8-N9-C4	-7.16	103.54	106.40
34	BA	415	A	O4'-C1'-N9	7.16	113.92	108.20
2	AB	1541	C	O4'-C1'-N1	7.15	113.92	108.20
1	AA	107	G	C8-N9-C4	-7.15	103.54	106.40
2	AB	853	C	O4'-C1'-N1	7.15	113.92	108.20
2	AB	889	C	O4'-C1'-N1	7.15	113.92	108.20
34	BA	614	C	O4'-C1'-N1	7.15	113.92	108.20
34	BA	818	G	O4'-C1'-C2'	-7.15	98.65	105.80
34	BA	962	C	C5'-C4'-O4'	7.15	117.68	109.10
2	AB	2200	C	O4'-C1'-N1	7.15	113.92	108.20
2	AB	913	U	O4'-C1'-N1	7.15	113.92	108.20
2	AB	2651	C	O4'-C1'-N1	7.15	113.92	108.20
34	BA	1326	U	O4'-C1'-N1	7.15	113.92	108.20
34	BA	1479	C	O4'-C1'-N1	7.15	113.92	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	208	U	O4'-C1'-N1	7.15	113.92	108.20
2	AB	1827	U	O4'-C1'-N1	7.14	113.91	108.20
2	AB	1025	G	O4'-C1'-N9	7.14	113.91	108.20
34	BA	489	C	C5'-C4'-O4'	7.14	117.67	109.10
2	AB	591	U	O4'-C1'-N1	7.14	113.91	108.20
2	AB	2693	G	O4'-C1'-N9	7.13	113.91	108.20
2	AB	2223	G	O4'-C1'-N9	7.13	113.90	108.20
2	AB	487	C	O4'-C1'-N1	7.13	113.90	108.20
2	AB	2698	U	O4'-C1'-N1	7.13	113.90	108.20
2	AB	2172	U	P-O3'-C3'	7.12	128.25	119.70
2	AB	2342	C	O4'-C1'-N1	7.12	113.90	108.20
2	AB	892	A	O4'-C1'-N9	7.12	113.89	108.20
2	AB	29	U	O4'-C1'-N1	7.11	113.89	108.20
2	AB	1052	C	O4'-C1'-N1	7.11	113.89	108.20
2	AB	2479	U	O4'-C1'-N1	7.11	113.89	108.20
2	AB	2890	G	O4'-C1'-N9	7.11	113.89	108.20
2	AB	1537	G	O4'-C1'-N9	7.10	113.88	108.20
2	AB	1080	A	O4'-C1'-N9	7.10	113.88	108.20
2	AB	1657	U	O4'-C1'-N1	7.10	113.88	108.20
2	AB	1696	G	O4'-C1'-N9	7.09	113.88	108.20
2	AB	271	G	O4'-C1'-N9	7.09	113.88	108.20
2	AB	2015	A	O4'-C1'-N9	7.09	113.87	108.20
34	BA	1061	G	O4'-C1'-N9	7.09	113.87	108.20
34	BA	952	U	O4'-C1'-N1	7.09	113.87	108.20
2	AB	1193	G	O4'-C1'-N9	7.08	113.87	108.20
2	AB	2058	A	P-O3'-C3'	7.08	128.20	119.70
34	BA	178	C	O4'-C1'-N1	7.08	113.87	108.20
34	BA	941	G	O4'-C1'-N9	7.08	113.86	108.20
34	BA	52	C	C1'-O4'-C4'	-7.08	104.24	109.90
2	AB	2112	G	C8-N9-C4	-7.08	103.57	106.40
34	BA	1467	C	O4'-C1'-N1	7.08	113.86	108.20
34	BA	992	U	O4'-C1'-N1	7.07	113.86	108.20
2	AB	2195	U	O4'-C1'-N1	7.07	113.86	108.20
34	BA	198	G	C5'-C4'-O4'	7.07	117.58	109.10
2	AB	1946	U	O4'-C1'-N1	7.07	113.86	108.20
2	AB	345	A	O4'-C1'-N9	7.07	113.85	108.20
2	AB	1299	G	O4'-C1'-N9	7.07	113.85	108.20
2	AB	2866	U	O4'-C1'-N1	7.07	113.85	108.20
34	BA	1007	U	O4'-C1'-N1	7.07	113.85	108.20
2	AB	1097	U	N1-C1'-C2'	-7.06	104.23	112.00
2	AB	1843	C	O4'-C1'-N1	7.06	113.85	108.20
34	BA	1045	C	O4'-C1'-N1	7.06	113.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BE	56	C	O4'-C1'-N1	7.06	113.85	108.20
2	AB	2054	A	C5'-C4'-C3'	-7.06	104.71	116.00
34	BA	865	A	O4'-C1'-N9	7.05	113.84	108.20
34	BA	1355	G	O4'-C1'-N9	7.05	113.84	108.20
2	AB	1577	C	C5'-C4'-O4'	7.05	117.56	109.10
2	AB	304	U	O4'-C1'-N1	7.05	113.84	108.20
2	AB	1145	C	O4'-C1'-N1	7.05	113.84	108.20
2	AB	264	C	O4'-C1'-N1	7.04	113.83	108.20
34	BA	609	A	C8-N9-C4	-7.04	102.98	105.80
34	BA	909	A	O4'-C1'-N9	7.04	113.83	108.20
2	AB	1217	U	O4'-C1'-N1	7.04	113.83	108.20
2	AB	1580	A	C5'-C4'-C3'	-7.04	104.74	116.00
35	BB	5	G	O4'-C1'-N9	7.03	113.83	108.20
34	BA	1279	G	C3'-C2'-C1'	7.03	107.13	101.50
2	AB	1482	G	O4'-C1'-N9	7.03	113.82	108.20
2	AB	2791	G	O4'-C1'-N9	7.03	113.82	108.20
34	BA	121	U	C3'-C2'-C1'	7.03	107.12	101.50
2	AB	290	U	C5'-C4'-O4'	7.03	117.53	109.10
2	AB	974	G	O4'-C1'-N9	7.02	113.82	108.20
2	AB	769	U	O4'-C1'-N1	7.02	113.82	108.20
2	AB	1761	C	O4'-C1'-N1	7.02	113.81	108.20
34	BA	137	U	O4'-C1'-N1	7.02	113.81	108.20
34	BA	886	G	O4'-C1'-N9	7.02	113.81	108.20
34	BA	1234	C	O4'-C1'-N1	7.02	113.81	108.20
35	BE	50	U	O4'-C1'-N1	7.02	113.81	108.20
2	AB	226	A	C5'-C4'-O4'	7.02	117.52	109.10
2	AB	424	G	O4'-C1'-N9	7.01	113.81	108.20
2	AB	445	C	O4'-C1'-N1	7.01	113.81	108.20
2	AB	874	G	O4'-C1'-N9	7.01	113.81	108.20
2	AB	548	G	N3-C4-C5	-7.01	125.09	128.60
2	AB	2649	C	O4'-C1'-N1	7.01	113.81	108.20
34	BA	646	G	O4'-C1'-N9	7.01	113.81	108.20
34	BA	1464	U	O4'-C1'-N1	7.01	113.81	108.20
2	AB	701	G	O4'-C1'-N9	7.01	113.81	108.20
2	AB	281	C	O4'-C1'-N1	7.01	113.81	108.20
2	AB	2358	A	O4'-C1'-N9	7.01	113.81	108.20
2	AB	2662	A	O4'-C1'-N9	7.01	113.81	108.20
34	BA	851	G	O4'-C1'-N9	7.00	113.80	108.20
2	AB	1874	C	O4'-C1'-N1	7.00	113.80	108.20
55	BW	77	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	AB	1845	G	O4'-C1'-N9	7.00	113.80	108.20
34	BA	631	C	O4'-C1'-N1	7.00	113.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1083	U	O4'-C1'-N1	6.99	113.80	108.20
34	BA	1094	G	O4'-C1'-N9	6.99	113.79	108.20
2	AB	502	A	O4'-C1'-N9	6.99	113.79	108.20
2	AB	552	U	O4'-C1'-N1	6.99	113.79	108.20
34	BA	270	A	O4'-C1'-N9	6.99	113.79	108.20
34	BA	778	G	O4'-C1'-N9	6.99	113.79	108.20
34	BA	1190	G	O4'-C1'-N9	6.99	113.79	108.20
2	AB	673	C	O4'-C1'-N1	6.99	113.79	108.20
2	AB	1956	U	C5'-C4'-O4'	6.99	117.48	109.10
34	BA	1169	A	O4'-C1'-N9	6.99	113.79	108.20
34	BA	1147	C	O4'-C1'-N1	6.98	113.79	108.20
2	AB	774	G	C8-N9-C4	-6.98	103.61	106.40
2	AB	913	U	O4'-C4'-C3'	6.98	111.68	106.10
34	BA	803	G	C8-N9-C4	-6.98	103.61	106.40
34	BA	1061	G	C8-N9-C4	-6.98	103.61	106.40
2	AB	357	C	O4'-C1'-N1	6.98	113.78	108.20
34	BA	1536	C	C1'-O4'-C4'	-6.98	104.32	109.90
1	AA	47	C	O4'-C1'-N1	6.97	113.78	108.20
2	AB	658	U	O4'-C1'-N1	6.97	113.78	108.20
2	AB	965	C	O4'-C1'-N1	6.97	113.78	108.20
2	AB	1188	U	O4'-C1'-N1	6.97	113.77	108.20
35	BE	29	G	C5'-C4'-O4'	6.97	117.46	109.10
2	AB	548	G	C2-N3-C4	6.96	115.38	111.90
2	AB	599	A	O4'-C1'-N9	6.96	113.77	108.20
34	BA	650	G	O4'-C1'-N9	6.96	113.77	108.20
2	AB	385	C	O4'-C1'-N1	6.96	113.77	108.20
2	AB	2416	C	O4'-C1'-N1	6.96	113.77	108.20
2	AB	1906	G	O4'-C1'-N9	6.96	113.76	108.20
2	AB	1678	A	O4'-C1'-N9	6.95	113.76	108.20
34	BA	1453	G	O4'-C1'-N9	6.95	113.76	108.20
2	AB	2489	U	O4'-C1'-N1	6.95	113.76	108.20
34	BA	142	G	C5'-C4'-O4'	6.95	117.44	109.10
35	BE	67	C	O4'-C1'-N1	6.95	113.76	108.20
2	AB	556	A	O4'-C1'-N9	6.95	113.76	108.20
2	AB	396	G	C8-N9-C4	-6.95	103.62	106.40
2	AB	2339	C	C5'-C4'-O4'	6.94	117.43	109.10
2	AB	231	A	O4'-C1'-N9	6.94	113.75	108.20
2	AB	555	G	C8-N9-C4	-6.94	103.62	106.40
37	BD	38	U	O4'-C1'-N1	6.94	113.75	108.20
34	BA	2	A	C5'-C4'-C3'	-6.94	104.90	116.00
34	BA	759	A	O4'-C1'-N9	6.94	113.75	108.20
1	AA	28	C	O4'-C1'-N1	6.94	113.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1414	C	O4'-C1'-N1	6.94	113.75	108.20
34	BA	1539	C	P-O3'-C3'	6.94	128.03	119.70
2	AB	1529	G	O4'-C1'-N9	6.93	113.75	108.20
34	BA	59	A	C5'-C4'-O4'	6.93	117.42	109.10
2	AB	1015	U	O4'-C1'-N1	6.93	113.75	108.20
34	BA	623	C	O4'-C1'-N1	6.93	113.75	108.20
2	AB	1629	U	O4'-C1'-N1	6.93	113.75	108.20
34	BA	1090	U	O4'-C1'-N1	6.93	113.74	108.20
35	BB	40	C	O4'-C1'-N1	6.93	113.74	108.20
2	AB	2751	G	P-O3'-C3'	6.93	128.01	119.70
37	BD	36	U	O4'-C1'-N1	6.93	113.74	108.20
34	BA	1356	G	O4'-C1'-N9	6.92	113.74	108.20
35	BE	68	C	O4'-C1'-N1	6.92	113.74	108.20
2	AB	2811	G	O4'-C1'-N9	6.92	113.74	108.20
34	BA	92	U	O4'-C1'-N1	6.92	113.74	108.20
2	AB	814	C	O4'-C1'-N1	6.92	113.73	108.20
34	BA	524	G	C3'-C2'-C1'	6.92	107.03	101.50
34	BA	524	G	O4'-C1'-N9	6.92	113.73	108.20
34	BA	619	U	C5'-C4'-C3'	-6.92	104.93	116.00
2	AB	278	A	P-O3'-C3'	6.92	128.00	119.70
34	BA	219	U	O4'-C1'-N1	6.92	113.73	108.20
34	BA	327	A	C5'-C4'-O4'	6.92	117.40	109.10
34	BA	1099	G	O4'-C1'-N9	6.92	113.73	108.20
2	AB	834	G	N3-C4-C5	-6.92	125.14	128.60
2	AB	2026	U	O4'-C1'-N1	6.92	113.73	108.20
34	BA	308	C	O4'-C1'-N1	6.91	113.73	108.20
2	AB	1572	A	C5'-C4'-O4'	6.91	117.39	109.10
2	AB	2337	G	C5'-C4'-O4'	6.91	117.39	109.10
34	BA	1307	U	O4'-C1'-N1	6.91	113.73	108.20
2	AB	2818	U	O4'-C1'-N1	6.91	113.72	108.20
2	AB	2011	U	O4'-C1'-N1	6.90	113.72	108.20
2	AB	2861	U	O4'-C1'-N1	6.90	113.72	108.20
2	AB	1499	C	O4'-C1'-N1	6.90	113.72	108.20
34	BA	1051	C	O4'-C1'-N1	6.90	113.72	108.20
2	AB	1218	G	O4'-C1'-N9	6.90	113.72	108.20
2	AB	1877	A	O4'-C1'-N9	6.90	113.72	108.20
2	AB	784	G	C1'-O4'-C4'	-6.89	104.38	109.90
2	AB	953	G	O4'-C1'-N9	6.89	113.72	108.20
2	AB	1177	G	C8-N9-C4	-6.89	103.64	106.40
34	BA	824	G	C5'-C4'-O4'	6.89	117.37	109.10
34	BA	1117	A	C5'-C4'-O4'	6.89	117.37	109.10
34	BA	1137	C	C5'-C4'-C3'	-6.89	104.97	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	112	U	O4'-C1'-N1	6.89	113.71	108.20
34	BA	837	U	O4'-C1'-N1	6.89	113.71	108.20
2	AB	280	U	O4'-C1'-N1	6.89	113.71	108.20
2	AB	2760	C	C5'-C4'-O4'	6.89	117.36	109.10
35	BE	12	U	C5'-C4'-O4'	6.89	117.36	109.10
34	BA	1361	G	O4'-C1'-N9	6.88	113.71	108.20
34	BA	1021	A	O4'-C1'-N9	6.88	113.71	108.20
34	BA	1388	C	O4'-C1'-N1	6.88	113.71	108.20
2	AB	2359	C	O4'-C1'-N1	6.88	113.70	108.20
34	BA	1499	A	C5'-C4'-O4'	6.88	117.36	109.10
2	AB	774	G	O4'-C1'-N9	6.88	113.70	108.20
2	AB	2207	C	O4'-C1'-N1	6.88	113.70	108.20
34	BA	887	G	O4'-C1'-N9	6.88	113.70	108.20
2	AB	80	G	O4'-C1'-N9	6.87	113.70	108.20
34	BA	1495	U	O4'-C1'-N1	6.87	113.70	108.20
2	AB	1887	C	C4'-C3'-C2'	6.87	109.47	102.60
1	AA	90	C	C1'-O4'-C4'	-6.87	104.41	109.90
34	BA	1225	A	C5'-C4'-O4'	6.86	117.33	109.10
34	BA	621	A	C5'-C4'-C3'	-6.86	105.02	116.00
34	BA	923	A	O4'-C1'-N9	6.86	113.69	108.20
2	AB	1584	U	O4'-C1'-N1	6.86	113.69	108.20
1	AA	41	G	O4'-C1'-N9	6.86	113.69	108.20
2	AB	1993	U	O4'-C1'-N1	6.86	113.69	108.20
2	AB	2730	C	O4'-C1'-N1	6.86	113.69	108.20
34	BA	88	U	O4'-C1'-N1	6.86	113.68	108.20
34	BA	475	C	O4'-C1'-N1	6.86	113.68	108.20
34	BA	1377	A	C1'-O4'-C4'	-6.86	104.42	109.90
2	AB	1100	C	O4'-C1'-N1	6.85	113.68	108.20
34	BA	1117	A	C5'-C4'-C3'	-6.85	105.03	116.00
35	BE	19	G	O4'-C1'-N9	6.85	113.68	108.20
2	AB	1676	A	O4'-C1'-N9	6.85	113.68	108.20
2	AB	2044	C	O4'-C1'-N1	6.85	113.68	108.20
2	AB	2215	C	C5'-C4'-C3'	-6.85	105.04	116.00
2	AB	2548	U	O4'-C1'-N1	6.85	113.68	108.20
2	AB	2125	G	O4'-C1'-N9	6.85	113.68	108.20
2	AB	2519	U	O4'-C1'-N1	6.84	113.67	108.20
34	BA	1401	G	N3-C4-C5	-6.84	125.18	128.60
2	AB	601	C	O4'-C1'-N1	6.84	113.67	108.20
2	AB	1886	U	C1'-O4'-C4'	-6.84	104.43	109.90
2	AB	1357	C	O4'-C1'-N1	6.83	113.67	108.20
2	AB	1691	C	O4'-C1'-N1	6.83	113.67	108.20
2	AB	662	G	O4'-C1'-N9	6.83	113.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2126	A	O3'-P-O5'	-6.83	91.03	104.00
34	BA	1028	C	O4'-C1'-N1	6.83	113.66	108.20
35	BE	66	U	O4'-C1'-N1	6.83	113.66	108.20
1	AA	95	U	C5'-C4'-O4'	6.82	117.29	109.10
34	BA	757	U	O4'-C1'-N1	6.82	113.66	108.20
35	BB	52	G	O4'-C1'-N9	6.82	113.66	108.20
2	AB	1013	C	O4'-C1'-N1	6.82	113.66	108.20
34	BA	830	G	C5'-C4'-O4'	6.82	117.28	109.10
34	BA	703	G	O4'-C1'-N9	6.82	113.65	108.20
34	BA	901	A	O4'-C1'-N9	6.82	113.66	108.20
35	BE	64	A	O4'-C1'-N9	6.81	113.65	108.20
2	AB	2496	C	O4'-C1'-N1	6.81	113.65	108.20
2	AB	1642	G	O4'-C1'-N9	6.81	113.65	108.20
34	BA	414	A	C8-N9-C4	-6.81	103.08	105.80
1	AA	69	G	O4'-C1'-N9	6.81	113.65	108.20
34	BA	582	C	O4'-C1'-N1	6.81	113.65	108.20
34	BA	1382	C	O4'-C1'-N1	6.81	113.64	108.20
2	AB	2257	U	O4'-C1'-N1	6.80	113.64	108.20
2	AB	2702	G	C5'-C4'-C3'	-6.80	105.11	116.00
2	AB	312	G	C5'-C4'-O4'	6.80	117.26	109.10
2	AB	2124	G	C5'-C4'-O4'	6.80	117.26	109.10
2	AB	700	G	O4'-C1'-N9	6.80	113.64	108.20
35	BB	13	C	O4'-C1'-N1	6.79	113.64	108.20
34	BA	1003	G	O4'-C1'-N9	6.79	113.64	108.20
34	BA	72	A	C5'-C4'-O4'	6.79	117.25	109.10
2	AB	1673	G	O4'-C1'-N9	6.79	113.63	108.20
2	AB	1747	U	O4'-C1'-N1	6.79	113.63	108.20
2	AB	2018	G	O4'-C1'-N9	6.79	113.63	108.20
34	BA	628	G	O4'-C1'-N9	6.79	113.63	108.20
34	BA	737	C	O4'-C1'-N1	6.79	113.63	108.20
2	AB	2872	A	C5'-C4'-O4'	6.78	117.24	109.10
2	AB	2129	C	N1-C2-O2	6.78	122.97	118.90
2	AB	285	G	O4'-C1'-N9	6.78	113.62	108.20
2	AB	583	G	O4'-C1'-N9	6.78	113.62	108.20
34	BA	60	A	P-O3'-C3'	6.78	127.84	119.70
34	BA	828	U	O4'-C1'-N1	6.78	113.62	108.20
34	BA	888	G	O4'-C1'-N9	6.78	113.62	108.20
2	AB	2109	U	O4'-C1'-N1	6.78	113.62	108.20
2	AB	494	G	O4'-C1'-N9	6.78	113.62	108.20
2	AB	826	U	O4'-C1'-N1	6.78	113.62	108.20
2	AB	2045	C	O4'-C1'-N1	6.78	113.62	108.20
2	AB	27	G	O4'-C1'-N9	6.77	113.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	559	G	C5'-C4'-O4'	6.77	117.22	109.10
2	AB	2403	C	O4'-C1'-N1	6.77	113.61	108.20
34	BA	405	U	O4'-C1'-N1	6.76	113.61	108.20
1	AA	32	U	O4'-C1'-N1	6.76	113.61	108.20
2	AB	35	G	N3-C4-C5	-6.76	125.22	128.60
34	BA	1170	A	C5'-C4'-O4'	6.76	117.21	109.10
2	AB	21	A	O4'-C1'-N9	6.76	113.61	108.20
2	AB	1710	G	C5'-C4'-O4'	6.75	117.21	109.10
2	AB	2107	G	O4'-C1'-N9	6.75	113.60	108.20
34	BA	528	C	O4'-C1'-N1	6.75	113.60	108.20
2	AB	1860	G	C8-N9-C4	-6.75	103.70	106.40
34	BA	1172	C	C5'-C4'-C3'	-6.75	105.20	116.00
2	AB	2062	A	O3'-P-O5'	-6.75	91.18	104.00
34	BA	1413	A	O4'-C1'-N9	6.75	113.60	108.20
34	BA	467	U	O4'-C1'-N1	6.74	113.59	108.20
2	AB	1986	C	O4'-C1'-N1	6.74	113.59	108.20
2	AB	296	U	O4'-C1'-N1	6.74	113.59	108.20
2	AB	2792	A	C5'-C4'-O4'	6.74	117.19	109.10
2	AB	594	U	O4'-C1'-N1	6.74	113.59	108.20
2	AB	1213	A	C5'-C4'-O4'	6.74	117.19	109.10
1	AA	85	G	O4'-C1'-N9	6.74	113.59	108.20
2	AB	244	A	O4'-C1'-N9	6.74	113.59	108.20
2	AB	538	A	O4'-C1'-N9	6.74	113.59	108.20
2	AB	1049	C	O4'-C1'-N1	6.74	113.59	108.20
2	AB	2106	U	O4'-C1'-N1	6.74	113.59	108.20
2	AB	241	A	O4'-C1'-N9	6.73	113.59	108.20
34	BA	328	C	N1-C2-O2	6.73	122.94	118.90
2	AB	869	G	O4'-C1'-N9	6.73	113.58	108.20
34	BA	235	C	O4'-C1'-N1	6.73	113.58	108.20
34	BA	803	G	N3-C4-C5	-6.73	125.23	128.60
34	BA	391	G	O4'-C1'-N9	6.73	113.58	108.20
2	AB	920	A	O4'-C1'-N9	6.73	113.58	108.20
2	AB	419	U	O4'-C1'-N1	6.72	113.58	108.20
34	BA	1221	G	O4'-C1'-N9	6.72	113.58	108.20
2	AB	1297	C	O4'-C1'-N1	6.72	113.58	108.20
34	BA	638	U	C5'-C4'-O4'	6.72	117.16	109.10
2	AB	195	A	C5'-C4'-O4'	6.72	117.16	109.10
2	AB	1833	C	O4'-C1'-N1	6.72	113.58	108.20
2	AB	1916	A	O4'-C1'-N9	6.72	113.58	108.20
2	AB	2732	G	O4'-C1'-N9	6.72	113.57	108.20
34	BA	173	U	O4'-C1'-N1	6.72	113.57	108.20
2	AB	464	U	O4'-C1'-N1	6.71	113.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1084	G	C8-N9-C4	-6.71	103.72	106.40
34	BA	1533	C	O3'-P-O5'	6.71	116.76	104.00
34	BA	1109	C	O4'-C1'-N1	6.71	113.57	108.20
2	AB	834	G	N7-C8-N9	6.71	116.45	113.10
2	AB	230	G	C4'-C3'-C2'	-6.71	95.89	102.60
2	AB	1069	A	O4'-C1'-N9	6.71	113.57	108.20
2	AB	2716	C	C5'-C4'-O4'	6.71	117.15	109.10
34	BA	39	G	O4'-C1'-N9	6.71	113.57	108.20
34	BA	221	C	O4'-C1'-N1	6.71	113.57	108.20
1	AA	34	A	C5'-C4'-O4'	6.71	117.15	109.10
2	AB	395	U	O4'-C1'-N1	6.71	113.56	108.20
34	BA	1015	G	O4'-C1'-N9	6.71	113.56	108.20
2	AB	1991	U	O4'-C1'-N1	6.70	113.56	108.20
2	AB	2819	G	C5'-C4'-C3'	-6.70	105.28	116.00
28	Ab	9	TYR	CB-CG-CD1	-6.70	116.98	121.00
34	BA	157	U	O4'-C1'-N1	6.70	113.56	108.20
34	BA	1283	U	O4'-C1'-N1	6.70	113.56	108.20
2	AB	827	U	P-O3'-C3'	6.70	127.74	119.70
2	AB	2838	G	C5'-C4'-O4'	6.70	117.14	109.10
34	BA	859	G	C5'-C4'-O4'	6.70	117.14	109.10
34	BA	1235	U	O4'-C1'-N1	6.70	113.56	108.20
2	AB	183	C	O4'-C1'-N1	6.70	113.56	108.20
2	AB	1261	C	O4'-C1'-N1	6.70	113.56	108.20
2	AB	2692	G	C4'-C3'-C2'	-6.70	95.90	102.60
34	BA	1131	G	C5'-C4'-O4'	6.70	117.14	109.10
2	AB	694	U	O4'-C1'-N1	6.70	113.56	108.20
2	AB	1863	G	C5'-C4'-O4'	6.70	117.14	109.10
34	BA	907	A	C5'-C4'-C3'	-6.70	105.29	116.00
1	AA	67	G	C8-N9-C4	-6.69	103.72	106.40
2	AB	2353	G	O4'-C1'-N9	6.69	113.55	108.20
2	AB	2594	C	O4'-C1'-N1	6.69	113.55	108.20
32	Af	1	PRO	CA-N-CD	-6.69	102.13	111.50
34	BA	291	U	O4'-C1'-N1	6.69	113.55	108.20
2	AB	2206	C	O4'-C1'-N1	6.69	113.55	108.20
34	BA	1271	A	C5'-C4'-C3'	-6.69	105.30	116.00
34	BA	1346	A	O4'-C1'-N9	6.69	113.55	108.20
34	BA	536	C	O4'-C1'-N1	6.68	113.55	108.20
34	BA	1312	G	C5'-C4'-O4'	6.68	117.12	109.10
2	AB	2802	G	O4'-C1'-N9	6.68	113.55	108.20
2	AB	209	C	O4'-C1'-N1	6.68	113.54	108.20
2	AB	1562	U	O4'-C1'-N1	6.68	113.54	108.20
34	BA	988	G	O4'-C1'-N9	6.68	113.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	51	A	O4'-C1'-N9	6.68	113.54	108.20
2	AB	2790	U	O4'-C4'-C3'	6.68	111.44	106.10
2	AB	2732	G	C5'-C4'-C3'	-6.67	105.32	116.00
34	BA	477	C	O4'-C1'-N1	6.67	113.54	108.20
34	BA	736	C	C5'-C4'-O4'	6.67	117.11	109.10
2	AB	459	U	O4'-C1'-N1	6.67	113.54	108.20
2	AB	2005	A	O4'-C1'-N9	6.67	113.54	108.20
2	AB	96	C	O4'-C1'-N1	6.67	113.54	108.20
2	AB	121	G	O4'-C1'-N9	6.67	113.54	108.20
34	BA	804	U	O4'-C1'-N1	6.67	113.54	108.20
34	BA	1225	A	N9-C1'-C2'	6.67	122.67	114.00
34	BA	659	U	O4'-C1'-N1	6.67	113.54	108.20
34	BA	848	C	O4'-C1'-N1	6.67	113.53	108.20
2	AB	2236	U	O4'-C1'-N1	6.67	113.53	108.20
34	BA	551	U	O4'-C1'-N1	6.67	113.53	108.20
35	BB	42	C	O4'-C1'-N1	6.67	113.53	108.20
2	AB	2298	A	C5'-C4'-C3'	-6.67	105.34	116.00
34	BA	1192	C	O4'-C1'-N1	6.66	113.53	108.20
34	BA	951	G	C8-N9-C4	-6.66	103.74	106.40
35	BB	56	C	O4'-C1'-N1	6.66	113.53	108.20
2	AB	832	U	O4'-C1'-N1	6.66	113.53	108.20
2	AB	967	U	O4'-C1'-N1	6.66	113.53	108.20
34	BA	612	C	O4'-C1'-N1	6.65	113.52	108.20
2	AB	1006	C	O4'-C1'-N1	6.65	113.52	108.20
2	AB	1070	A	C3'-C2'-C1'	6.65	106.82	101.50
2	AB	1159	U	O4'-C1'-N1	6.65	113.52	108.20
2	AB	360	U	O4'-C1'-N1	6.64	113.52	108.20
2	AB	806	C	O4'-C1'-N1	6.64	113.52	108.20
34	BA	414	A	O3'-P-O5'	-6.64	91.38	104.00
2	AB	1935	G	O4'-C1'-N9	6.64	113.51	108.20
34	BA	180	U	O4'-C1'-N1	6.64	113.51	108.20
2	AB	2089	C	O4'-C1'-N1	6.64	113.51	108.20
2	AB	278	A	C8-N9-C4	-6.63	103.15	105.80
2	AB	325	G	O4'-C1'-N9	6.63	113.51	108.20
2	AB	791	C	O4'-C1'-N1	6.63	113.51	108.20
2	AB	1588	G	O4'-C1'-N9	6.63	113.51	108.20
2	AB	1847	A	O4'-C4'-C3'	6.63	111.41	106.10
34	BA	52	C	C5'-C4'-O4'	6.63	117.06	109.10
34	BA	147	G	C8-N9-C4	-6.63	103.75	106.40
2	AB	1990	C	O4'-C1'-N1	6.63	113.50	108.20
2	AB	1727	C	C5'-C4'-O4'	6.63	117.05	109.10
34	BA	933	G	N3-C4-C5	-6.63	125.29	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1571	A	O4'-C1'-N9	6.62	113.50	108.20
34	BA	246	A	C5'-C4'-O4'	6.62	117.05	109.10
2	AB	1331	G	C8-N9-C4	-6.62	103.75	106.40
2	AB	1951	U	P-O3'-C3'	6.62	127.65	119.70
1	AA	92	C	O4'-C1'-N1	6.62	113.50	108.20
2	AB	885	C	O4'-C1'-N1	6.62	113.50	108.20
34	BA	498	A	C8-N9-C4	-6.62	103.15	105.80
2	AB	1378	A	O4'-C1'-N9	6.62	113.50	108.20
2	AB	20	C	O4'-C1'-N1	6.62	113.50	108.20
34	BA	613	C	O4'-C1'-N1	6.62	113.49	108.20
35	BB	22	G	O4'-C1'-N9	6.62	113.49	108.20
2	AB	1859	U	O4'-C1'-N1	6.61	113.49	108.20
34	BA	132	C	O4'-C1'-N1	6.61	113.49	108.20
34	BA	1530	G	O4'-C1'-N9	6.61	113.49	108.20
2	AB	1976	U	O4'-C1'-N1	6.61	113.49	108.20
2	AB	1989	G	O4'-C1'-N9	6.61	113.49	108.20
34	BA	91	U	C5'-C4'-O4'	6.61	117.03	109.10
2	AB	361	G	P-O3'-C3'	6.61	127.63	119.70
34	BA	97	G	C8-N9-C4	-6.60	103.76	106.40
2	AB	655	A	P-O3'-C3'	6.60	127.62	119.70
2	AB	350	G	O4'-C1'-N9	6.60	113.48	108.20
34	BA	694	A	O4'-C1'-N9	6.60	113.48	108.20
2	AB	672	C	O4'-C1'-N1	6.60	113.48	108.20
2	AB	1422	G	C5'-C4'-O4'	6.60	117.02	109.10
2	AB	1516	G	O4'-C1'-N9	6.60	113.48	108.20
2	AB	188	G	O4'-C1'-N9	6.60	113.48	108.20
34	BA	653	U	C3'-C2'-C1'	6.60	106.78	101.50
2	AB	1881	C	O4'-C1'-N1	6.59	113.47	108.20
2	AB	2896	C	C5'-C4'-O4'	6.59	117.01	109.10
35	BE	18	G	O4'-C1'-N9	6.59	113.48	108.20
34	BA	1430	A	O4'-C1'-N9	6.59	113.47	108.20
34	BA	118	U	O4'-C1'-N1	6.59	113.47	108.20
2	AB	137	U	O4'-C1'-N1	6.59	113.47	108.20
2	AB	788	A	O4'-C1'-N9	6.58	113.47	108.20
34	BA	160	A	O4'-C1'-N9	6.58	113.47	108.20
34	BA	861	G	C8-N9-C4	-6.58	103.77	106.40
34	BA	857	C	O4'-C1'-N1	6.58	113.46	108.20
2	AB	67	U	O4'-C1'-N1	6.58	113.46	108.20
34	BA	341	C	O4'-C1'-N1	6.58	113.46	108.20
34	BA	603	U	O4'-C1'-N1	6.58	113.46	108.20
34	BA	310	G	C8-N9-C4	-6.58	103.77	106.40
34	BA	747	A	O4'-C1'-N9	6.58	113.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	333	G	N3-C4-C5	-6.57	125.31	128.60
34	BA	1010	U	O4'-C1'-N1	6.57	113.46	108.20
2	AB	1460	U	O4'-C1'-N1	6.57	113.46	108.20
2	AB	2395	C	O4'-C1'-N1	6.57	113.46	108.20
34	BA	1103	C	O4'-C1'-N1	6.57	113.46	108.20
2	AB	2208	C	O4'-C1'-N1	6.57	113.45	108.20
2	AB	2067	G	O4'-C4'-C3'	6.56	111.35	106.10
34	BA	1104	G	C5'-C4'-O4'	6.56	116.98	109.10
34	BA	1409	C	C5'-C4'-C3'	-6.56	105.50	116.00
2	AB	1109	C	O4'-C1'-N1	6.56	113.45	108.20
34	BA	58	C	O4'-C1'-N1	6.56	113.45	108.20
35	BE	7	A	O4'-C1'-N9	6.56	113.44	108.20
2	AB	2523	G	C5'-C4'-O4'	6.55	116.97	109.10
1	AA	19	C	O4'-C1'-N1	6.55	113.44	108.20
2	AB	544	C	P-O3'-C3'	6.55	127.56	119.70
2	AB	2247	A	C5'-C4'-C3'	-6.55	105.52	116.00
34	BA	1006	G	O4'-C1'-N9	6.55	113.44	108.20
2	AB	424	G	N9-C1'-C2'	-6.55	104.80	112.00
2	AB	2758	A	C5'-C4'-O4'	6.55	116.96	109.10
2	AB	2804	U	O4'-C1'-N1	6.55	113.44	108.20
2	AB	234	U	O4'-C1'-N1	6.55	113.44	108.20
1	AA	42	C	O4'-C1'-N1	6.55	113.44	108.20
2	AB	831	G	O4'-C1'-N9	6.55	113.44	108.20
34	BA	379	C	C4'-C3'-C2'	-6.55	96.05	102.60
34	BA	671	G	O4'-C1'-N9	6.54	113.43	108.20
1	AA	71	C	O4'-C1'-N1	6.54	113.43	108.20
34	BA	57	G	C8-N9-C4	-6.54	103.78	106.40
34	BA	403	C	O4'-C1'-N1	6.54	113.43	108.20
34	BA	772	U	O4'-C1'-N1	6.54	113.43	108.20
34	BA	990	C	O4'-C1'-N1	6.54	113.43	108.20
2	AB	1310	G	C5'-C4'-C3'	-6.54	105.54	116.00
2	AB	1913	A	O4'-C1'-N9	6.54	113.43	108.20
2	AB	1291	C	O4'-C1'-N1	6.53	113.43	108.20
35	BB	60	U	O4'-C1'-N1	6.53	113.43	108.20
2	AB	2720	U	O4'-C1'-N1	6.53	113.42	108.20
2	AB	2819	G	C5'-C4'-O4'	6.53	116.94	109.10
34	BA	792	A	C1'-O4'-C4'	-6.53	104.67	109.90
34	BA	1304	G	O4'-C1'-N9	6.53	113.43	108.20
2	AB	394	C	O4'-C1'-N1	6.53	113.42	108.20
2	AB	166	U	O4'-C1'-N1	6.53	113.42	108.20
2	AB	2392	A	C8-N9-C4	-6.53	103.19	105.80
2	AB	999	U	O4'-C1'-N1	6.53	113.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1057	A	O4'-C1'-N9	6.52	113.42	108.20
35	BE	59	U	O4'-C1'-N1	6.52	113.42	108.20
34	BA	248	C	O4'-C1'-N1	6.52	113.42	108.20
2	AB	852	U	O4'-C1'-N1	6.52	113.42	108.20
2	AB	1035	U	O4'-C1'-N1	6.52	113.42	108.20
2	AB	1097	U	C5'-C4'-O4'	6.52	116.92	109.10
2	AB	2668	G	O4'-C1'-N9	6.52	113.41	108.20
2	AB	2820	A	O4'-C1'-N9	6.51	113.41	108.20
34	BA	271	C	C5'-C4'-O4'	6.51	116.92	109.10
2	AB	2043	C	O4'-C1'-N1	6.51	113.41	108.20
34	BA	1037	C	O4'-C1'-N1	6.51	113.41	108.20
34	BA	1273	C	O4'-C1'-N1	6.51	113.41	108.20
1	AA	74	U	O4'-C1'-N1	6.50	113.40	108.20
2	AB	2760	C	C5'-C4'-C3'	-6.50	105.59	116.00
35	BB	3	C	O4'-C1'-N1	6.50	113.40	108.20
2	AB	283	G	O4'-C1'-N9	6.50	113.40	108.20
2	AB	1105	U	O4'-C1'-N1	6.50	113.40	108.20
2	AB	1730	C	N1-C2-O2	6.50	122.80	118.90
2	AB	1913	A	O4'-C1'-C2'	-6.50	99.30	105.80
1	AA	91	C	O4'-C1'-N1	6.49	113.39	108.20
2	AB	352	A	O4'-C1'-N9	6.49	113.39	108.20
2	AB	954	G	C5'-C4'-O4'	6.49	116.89	109.10
2	AB	897	C	O4'-C1'-N1	6.49	113.39	108.20
2	AB	2039	U	O4'-C1'-N1	6.49	113.39	108.20
2	AB	2299	U	O4'-C1'-N1	6.49	113.39	108.20
2	AB	2747	G	O4'-C1'-N9	6.49	113.39	108.20
34	BA	484	G	O4'-C1'-N9	6.49	113.39	108.20
1	AA	98	G	C5'-C4'-O4'	6.49	116.88	109.10
2	AB	1907	G	O4'-C1'-N9	6.49	113.39	108.20
2	AB	2343	U	O4'-C1'-N1	6.49	113.39	108.20
2	AB	2543	G	N3-C4-C5	-6.49	125.36	128.60
34	BA	246	A	C5'-C4'-C3'	-6.48	105.63	116.00
34	BA	850	U	O4'-C1'-N1	6.48	113.38	108.20
2	AB	2500	U	O4'-C1'-N1	6.48	113.38	108.20
2	AB	528	A	O4'-C1'-N9	6.47	113.38	108.20
2	AB	1348	C	O4'-C1'-N1	6.47	113.38	108.20
34	BA	242	G	O4'-C1'-N9	6.47	113.38	108.20
2	AB	2515	C	O4'-C1'-N1	6.47	113.38	108.20
2	AB	2097	A	O4'-C1'-N9	6.47	113.37	108.20
34	BA	194	C	C2-N3-C4	6.47	123.13	119.90
2	AB	94	A	O4'-C1'-N9	6.46	113.37	108.20
2	AB	201	C	O4'-C1'-N1	6.46	113.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	492	C	O4'-C1'-N1	6.46	113.37	108.20
34	BA	1110	A	O4'-C1'-N9	6.46	113.37	108.20
2	AB	26	G	O4'-C1'-N9	6.45	113.36	108.20
34	BA	1009	U	O4'-C1'-N1	6.45	113.36	108.20
34	BA	1153	G	O4'-C1'-N9	6.45	113.36	108.20
2	AB	1402	U	C5'-C4'-O4'	6.45	116.84	109.10
2	AB	2849	U	O4'-C1'-N1	6.45	113.36	108.20
34	BA	632	U	O4'-C1'-N1	6.45	113.36	108.20
34	BA	314	C	O4'-C1'-N1	6.45	113.36	108.20
34	BA	1408	A	C5'-C4'-O4'	6.44	116.83	109.10
2	AB	157	C	O4'-C1'-N1	6.44	113.35	108.20
34	BA	6	G	C5'-C4'-C3'	-6.44	105.69	116.00
34	BA	1270	G	O4'-C1'-N9	6.44	113.35	108.20
2	AB	569	U	O4'-C1'-N1	6.44	113.35	108.20
34	BA	296	U	C5'-C4'-C3'	-6.44	105.70	116.00
34	BA	360	G	O4'-C1'-N9	6.44	113.35	108.20
34	BA	741	G	O4'-C1'-N9	6.44	113.35	108.20
2	AB	441	U	O4'-C1'-N1	6.44	113.35	108.20
2	AB	1662	U	O4'-C1'-N1	6.44	113.35	108.20
2	AB	2085	U	O4'-C1'-N1	6.44	113.35	108.20
2	AB	1641	A	C5'-C4'-C3'	-6.44	105.70	116.00
2	AB	2751	G	C2'-C3'-O3'	6.44	124.00	113.70
2	AB	1844	C	O4'-C1'-N1	6.44	113.35	108.20
34	BA	123	U	O4'-C1'-N1	6.43	113.35	108.20
34	BA	1458	G	O4'-C1'-N9	6.43	113.35	108.20
2	AB	192	C	O4'-C1'-N1	6.43	113.34	108.20
2	AB	611	C	O4'-C1'-N1	6.43	113.35	108.20
2	AB	2314	A	C5'-C4'-C3'	-6.43	105.71	116.00
2	AB	200	U	O4'-C1'-N1	6.43	113.34	108.20
34	BA	220	G	N3-C4-C5	-6.43	125.39	128.60
34	BA	369	G	O4'-C1'-N9	6.43	113.34	108.20
2	AB	440	C	C5'-C4'-O4'	6.42	116.81	109.10
2	AB	872	U	O4'-C1'-N1	6.42	113.34	108.20
2	AB	1134	A	O4'-C1'-N9	6.42	113.34	108.20
2	AB	397	U	O4'-C1'-N1	6.42	113.34	108.20
2	AB	2189	U	O4'-C1'-N1	6.42	113.34	108.20
1	AA	64	G	O4'-C1'-N9	6.42	113.34	108.20
2	AB	1174	U	O4'-C1'-N1	6.42	113.34	108.20
2	AB	358	U	O4'-C1'-N1	6.42	113.33	108.20
2	AB	1703	G	C5'-C4'-C3'	-6.42	105.73	116.00
34	BA	641	U	O4'-C4'-C3'	6.42	111.23	106.10
34	BA	771	G	O4'-C1'-N9	6.42	113.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	70	G	O4'-C1'-N9	6.42	113.33	108.20
2	AB	916	G	C8-N9-C4	-6.41	103.83	106.40
2	AB	1114	C	C5'-C4'-O4'	6.41	116.80	109.10
2	AB	1487	U	C5'-C4'-C3'	-6.41	105.74	116.00
34	BA	929	G	O4'-C1'-N9	6.41	113.33	108.20
2	AB	701	G	C5'-C4'-C3'	-6.41	105.74	116.00
2	AB	1952	A	C3'-C2'-C1'	6.41	106.63	101.50
34	BA	1073	U	O4'-C1'-N1	6.41	113.33	108.20
2	AB	1098	A	C5'-C4'-C3'	-6.41	105.75	116.00
2	AB	2091	C	O4'-C1'-N1	6.41	113.33	108.20
2	AB	2146	C	O3'-P-O5'	-6.41	91.83	104.00
2	AB	1258	U	O4'-C1'-N1	6.41	113.33	108.20
2	AB	2683	C	O4'-C1'-N1	6.41	113.33	108.20
34	BA	770	C	C4'-C3'-C2'	-6.41	96.19	102.60
35	BB	65	G	C5'-C4'-C3'	-6.41	105.75	116.00
34	BA	358	U	O4'-C1'-N1	6.40	113.32	108.20
34	BA	933	G	C5'-C4'-O4'	6.40	116.78	109.10
2	AB	1457	U	O4'-C1'-N1	6.40	113.32	108.20
34	BA	1535	C	O5'-C5'-C4'	6.40	123.86	111.70
2	AB	1068	G	O3'-P-O5'	-6.40	91.84	104.00
34	BA	111	G	O4'-C1'-N9	6.40	113.32	108.20
34	BA	70	U	O4'-C1'-N1	6.40	113.32	108.20
34	BA	847	G	C8-N9-C4	-6.40	103.84	106.40
2	AB	1694	C	N1-C2-O2	6.39	122.74	118.90
34	BA	220	G	C8-N9-C4	-6.39	103.84	106.40
2	AB	790	U	O4'-C1'-N1	6.39	113.31	108.20
2	AB	873	C	O4'-C1'-N1	6.39	113.31	108.20
34	BA	1098	C	O4'-C1'-N1	6.39	113.31	108.20
2	AB	2779	U	O4'-C1'-N1	6.39	113.31	108.20
2	AB	286	U	O4'-C1'-N1	6.39	113.31	108.20
2	AB	2585	U	O4'-C1'-N1	6.39	113.31	108.20
34	BA	100	G	C5'-C4'-O4'	6.39	116.76	109.10
34	BA	179	A	C5'-C4'-C3'	-6.39	105.78	116.00
2	AB	1180	U	C5'-C4'-O4'	6.38	116.76	109.10
2	AB	1352	U	O4'-C1'-N1	6.38	113.31	108.20
2	AB	1599	U	O4'-C1'-N1	6.38	113.31	108.20
34	BA	218	U	O4'-C1'-N1	6.38	113.31	108.20
2	AB	2193	G	O4'-C1'-N9	6.38	113.31	108.20
35	BE	58	A	C5'-C4'-C3'	-6.38	105.79	116.00
2	AB	557	C	O4'-C1'-N1	6.38	113.30	108.20
2	AB	314	C	O4'-C1'-N1	6.38	113.30	108.20
2	AB	2854	G	C5'-C4'-O4'	6.38	116.75	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1293	C	O4'-C1'-N1	6.38	113.30	108.20
2	AB	1183	U	C5'-C4'-C3'	-6.38	105.80	116.00
2	AB	248	G	O4'-C1'-N9	6.37	113.30	108.20
2	AB	2016	U	O3'-P-O5'	-6.37	91.89	104.00
34	BA	193	C	C5'-C4'-O4'	6.37	116.74	109.10
1	AA	1	U	O4'-C1'-N1	6.36	113.29	108.20
2	AB	462	C	O4'-C1'-N1	6.36	113.29	108.20
37	BD	31	U	C5'-C4'-O4'	6.36	116.74	109.10
37	BD	34	U	O4'-C1'-N1	6.36	113.29	108.20
34	BA	265	G	C8-N9-C4	-6.36	103.86	106.40
2	AB	493	G	O4'-C1'-N9	6.36	113.29	108.20
2	AB	1054	A	O4'-C1'-N9	6.36	113.29	108.20
2	AB	1116	G	O4'-C1'-N9	6.36	113.29	108.20
2	AB	2379	G	O4'-C1'-N9	6.36	113.29	108.20
28	Ab	53	THR	C-N-CA	6.36	135.66	122.30
2	AB	722	A	C5'-C4'-C3'	-6.36	105.83	116.00
2	AB	1266	G	O4'-C1'-N9	6.36	113.29	108.20
2	AB	2408	U	O4'-C1'-N1	6.36	113.28	108.20
2	AB	2425	A	O4'-C1'-C2'	-6.36	99.44	105.80
2	AB	2718	G	C5'-C4'-O4'	6.36	116.73	109.10
2	AB	2508	G	O4'-C1'-N9	6.35	113.28	108.20
2	AB	845	A	O4'-C1'-N9	6.35	113.28	108.20
34	BA	2	A	C5'-C4'-O4'	6.35	116.72	109.10
34	BA	4	U	C5'-C4'-C3'	-6.35	105.83	116.00
34	BA	653	U	O4'-C1'-N1	6.35	113.28	108.20
2	AB	1731	G	C8-N9-C4	-6.35	103.86	106.40
2	AB	125	A	O4'-C1'-C2'	-6.35	99.45	105.80
2	AB	1872	A	C8-N9-C4	-6.35	103.26	105.80
2	AB	2131	U	O4'-C1'-N1	6.35	113.28	108.20
2	AB	310	A	C5'-C4'-C3'	-6.35	105.84	116.00
2	AB	1989	G	C5'-C4'-O4'	6.35	116.72	109.10
2	AB	2319	G	O4'-C1'-N9	6.35	113.28	108.20
34	BA	486	U	O4'-C1'-N1	6.35	113.28	108.20
2	AB	948	C	O4'-C1'-N1	6.34	113.28	108.20
2	AB	2676	C	O4'-C1'-N1	6.34	113.28	108.20
2	AB	1338	G	O4'-C1'-N9	6.34	113.27	108.20
2	AB	417	C	O4'-C1'-N1	6.34	113.27	108.20
34	BA	1453	G	N3-C4-C5	-6.34	125.43	128.60
2	AB	813	U	O4'-C1'-N1	6.34	113.27	108.20
34	BA	793	U	C1'-O4'-C4'	-6.34	104.83	109.90
34	BA	1308	U	O4'-C1'-N1	6.34	113.27	108.20
34	BA	701	U	C1'-O4'-C4'	-6.34	104.83	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	413	C	O4'-C1'-N1	6.33	113.27	108.20
2	AB	1702	G	O4'-C1'-N9	6.33	113.27	108.20
2	AB	798	G	O4'-C1'-N9	6.33	113.27	108.20
34	BA	228	A	C5'-C4'-C3'	-6.33	105.87	116.00
34	BA	1243	C	O4'-C1'-N1	6.33	113.26	108.20
2	AB	1123	C	C5'-C4'-O4'	6.33	116.69	109.10
2	AB	1746	A	O3'-P-O5'	-6.33	91.98	104.00
34	BA	1487	G	O4'-C1'-N9	6.33	113.26	108.20
1	AA	67	G	C5'-C4'-O4'	6.32	116.69	109.10
2	AB	2521	C	O4'-C1'-N1	6.32	113.26	108.20
34	BA	1268	G	C5'-C4'-O4'	6.32	116.69	109.10
2	AB	2554	U	O4'-C1'-N1	6.32	113.26	108.20
34	BA	812	G	O3'-P-O5'	-6.32	91.99	104.00
2	AB	267	C	O4'-C1'-N1	6.32	113.25	108.20
2	AB	2629	U	O4'-C1'-N1	6.32	113.25	108.20
2	AB	1734	G	O4'-C1'-N9	6.32	113.25	108.20
34	BA	636	U	C4'-C3'-C2'	-6.32	96.28	102.60
2	AB	1722	A	C5'-C4'-C3'	-6.31	105.90	116.00
34	BA	68	G	N9-C1'-C2'	-6.31	105.06	112.00
34	BA	939	G	O4'-C1'-N9	6.31	113.25	108.20
2	AB	2227	A	O4'-C1'-N9	6.31	113.25	108.20
34	BA	843	U	C5'-C4'-C3'	-6.31	105.90	116.00
2	AB	1504	A	O4'-C1'-N9	6.31	113.25	108.20
34	BA	259	G	O4'-C1'-N9	6.31	113.25	108.20
34	BA	884	U	O4'-C1'-N1	6.31	113.25	108.20
2	AB	1103	A	O4'-C1'-N9	6.31	113.25	108.20
2	AB	1811	G	O4'-C1'-N9	6.31	113.25	108.20
34	BA	211	G	C2-N3-C4	6.31	115.05	111.90
34	BA	1477	U	C5'-C4'-O4'	6.31	116.67	109.10
2	AB	895	U	P-O3'-C3'	6.30	127.27	119.70
35	BE	49	C	O4'-C1'-N1	6.30	113.24	108.20
35	BB	15	G	C8-N9-C4	-6.30	103.88	106.40
2	AB	1535	A	O3'-P-O5'	-6.30	92.03	104.00
2	AB	2318	G	O4'-C1'-N9	6.30	113.24	108.20
2	AB	22	C	O4'-C1'-N1	6.30	113.24	108.20
2	AB	2179	C	O4'-C1'-N1	6.30	113.24	108.20
2	AB	2040	G	C5'-C4'-C3'	-6.29	105.93	116.00
2	AB	1183	U	C3'-C2'-C1'	6.29	106.53	101.50
2	AB	1656	C	O4'-C1'-N1	6.29	113.23	108.20
2	AB	2199	A	C5'-C4'-O4'	6.29	116.65	109.10
2	AB	2675	A	O4'-C1'-N9	6.29	113.23	108.20
2	AB	1695	G	N3-C4-C5	-6.29	125.45	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2072	C	O4'-C1'-N1	6.29	113.23	108.20
1	AA	31	C	C5'-C4'-O4'	6.29	116.65	109.10
2	AB	570	G	O4'-C1'-N9	6.29	113.23	108.20
2	AB	995	C	O4'-C1'-N1	6.29	113.23	108.20
2	AB	1806	C	O4'-C1'-N1	6.29	113.23	108.20
2	AB	1763	G	C5'-C4'-C3'	-6.29	105.94	116.00
34	BA	217	C	C5'-C4'-C3'	-6.29	105.94	116.00
34	BA	233	C	O4'-C1'-N1	6.29	113.23	108.20
34	BA	286	C	O4'-C1'-N1	6.29	113.23	108.20
34	BA	620	C	O4'-C1'-N1	6.29	113.23	108.20
34	BA	779	C	O4'-C1'-N1	6.29	113.23	108.20
2	AB	1528	A	O4'-C1'-N9	6.28	113.23	108.20
2	AB	2567	G	N3-C4-C5	-6.28	125.46	128.60
2	AB	647	G	O4'-C1'-N9	6.28	113.22	108.20
2	AB	2568	U	O4'-C1'-N1	6.28	113.22	108.20
2	AB	490	C	C5'-C4'-O4'	6.28	116.64	109.10
1	AA	4	C	O4'-C1'-N1	6.28	113.22	108.20
2	AB	1180	U	O4'-C1'-N1	6.28	113.22	108.20
2	AB	2506	U	O3'-P-O5'	-6.28	92.07	104.00
34	BA	346	G	N3-C4-C5	-6.28	125.46	128.60
2	AB	586	A	O4'-C1'-N9	6.27	113.22	108.20
2	AB	989	G	O4'-C1'-N9	6.27	113.22	108.20
2	AB	47	C	O4'-C1'-N1	6.27	113.22	108.20
2	AB	2214	C	O4'-C1'-N1	6.27	113.22	108.20
34	BA	910	C	O4'-C1'-N1	6.27	113.22	108.20
2	AB	1501	G	O4'-C1'-N9	6.27	113.22	108.20
2	AB	2124	G	C5'-C4'-C3'	-6.27	105.97	116.00
34	BA	854	U	O4'-C1'-N1	6.27	113.22	108.20
34	BA	1353	G	C5'-C4'-O4'	6.27	116.62	109.10
2	AB	275	C	O4'-C1'-N1	6.27	113.21	108.20
34	BA	456	A	O4'-C1'-N9	6.27	113.21	108.20
34	BA	823	C	O4'-C1'-N1	6.27	113.21	108.20
2	AB	2599	G	O4'-C1'-N9	6.26	113.21	108.20
2	AB	1249	U	O4'-C1'-N1	6.26	113.21	108.20
2	AB	1606	C	N1-C2-O2	6.26	122.66	118.90
2	AB	2740	A	C5'-C4'-O4'	6.26	116.61	109.10
36	BC	87	TYR	CB-CG-CD1	-6.26	117.24	121.00
2	AB	2134	A	O4'-C1'-N9	6.26	113.21	108.20
34	BA	801	U	O4'-C1'-N1	6.26	113.21	108.20
2	AB	151	C	O4'-C1'-N1	6.26	113.21	108.20
2	AB	1558	C	O4'-C1'-N1	6.26	113.21	108.20
2	AB	1725	U	C5'-C4'-C3'	-6.26	105.99	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2194	U	O4'-C1'-N1	6.26	113.20	108.20
34	BA	462	G	O4'-C1'-N9	6.26	113.20	108.20
2	AB	364	C	O4'-C1'-N1	6.25	113.20	108.20
34	BA	215	C	O4'-C1'-N1	6.25	113.20	108.20
34	BA	896	C	O4'-C1'-N1	6.25	113.20	108.20
34	BA	1429	A	O4'-C1'-N9	6.25	113.20	108.20
2	AB	2485	G	C3'-C2'-C1'	-6.25	96.50	101.50
2	AB	687	C	O4'-C1'-N1	6.25	113.20	108.20
34	BA	154	U	C5'-C4'-O4'	6.25	116.60	109.10
34	BA	1103	C	C5'-C4'-C3'	-6.25	106.00	116.00
2	AB	184	C	O4'-C1'-N1	6.25	113.20	108.20
2	AB	2185	U	O4'-C1'-N1	6.25	113.20	108.20
2	AB	2291	U	O4'-C1'-N1	6.25	113.20	108.20
2	AB	2796	U	O4'-C1'-N1	6.25	113.20	108.20
2	AB	911	A	O4'-C1'-N9	6.25	113.20	108.20
37	BD	30	U	O4'-C1'-N1	6.25	113.20	108.20
2	AB	2387	U	O4'-C1'-N1	6.24	113.19	108.20
34	BA	931	C	O4'-C1'-N1	6.24	113.19	108.20
2	AB	416	U	O4'-C1'-N1	6.24	113.19	108.20
2	AB	1303	G	C5'-C4'-C3'	-6.24	106.02	116.00
2	AB	2221	G	O4'-C1'-N9	6.24	113.19	108.20
2	AB	460	A	O4'-C1'-N9	6.24	113.19	108.20
2	AB	527	C	O4'-C1'-N1	6.24	113.19	108.20
2	AB	1142	A	P-O3'-C3'	6.24	127.19	119.70
2	AB	1688	U	C5'-C4'-O4'	6.24	116.59	109.10
34	BA	1143	G	C8-N9-C4	-6.24	103.91	106.40
2	AB	578	G	O4'-C1'-N9	6.24	113.19	108.20
2	AB	2012	G	C8-N9-C4	-6.24	103.91	106.40
2	AB	2869	G	O4'-C1'-N9	6.24	113.19	108.20
34	BA	426	U	O4'-C1'-N1	6.24	113.19	108.20
2	AB	1940	U	N1-C1'-C2'	6.23	122.10	114.00
34	BA	1052	U	O4'-C1'-N1	6.23	113.19	108.20
2	AB	131	A	O4'-C1'-N9	6.23	113.18	108.20
2	AB	2067	G	O4'-C1'-N9	6.23	113.18	108.20
34	BA	355	C	O4'-C1'-N1	6.22	113.18	108.20
34	BA	838	G	C8-N9-C4	-6.22	103.91	106.40
2	AB	425	G	O4'-C1'-N9	6.22	113.18	108.20
2	AB	1154	G	C8-N9-C4	-6.22	103.91	106.40
34	BA	406	G	N3-C4-C5	-6.22	125.49	128.60
2	AB	173	A	O4'-C1'-N9	6.22	113.17	108.20
34	BA	897	C	O4'-C1'-N1	6.22	113.17	108.20
2	AB	3	U	O4'-C1'-N1	6.22	113.17	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	172	A	O4'-C1'-N9	6.21	113.17	108.20
2	AB	2442	C	O4'-C1'-N1	6.21	113.17	108.20
2	AB	101	A	O4'-C1'-N9	6.21	113.17	108.20
2	AB	1481	U	O4'-C1'-N1	6.21	113.17	108.20
1	AA	84	G	O4'-C1'-N9	6.21	113.17	108.20
2	AB	103	A	C5'-C4'-O4'	6.21	116.55	109.10
34	BA	847	G	N3-C4-C5	-6.21	125.50	128.60
2	AB	205	G	O4'-C1'-N9	6.21	113.17	108.20
2	AB	1368	G	O4'-C1'-N9	6.21	113.17	108.20
2	AB	1600	C	O4'-C1'-N1	6.21	113.17	108.20
2	AB	2461	A	O4'-C1'-N9	6.21	113.17	108.20
2	AB	369	U	O4'-C1'-N1	6.21	113.17	108.20
2	AB	2769	U	C5'-C4'-O4'	6.21	116.55	109.10
34	BA	998	C	C5'-C4'-C3'	-6.21	106.07	116.00
2	AB	893	C	O4'-C1'-N1	6.20	113.16	108.20
34	BA	1203	C	C5'-C4'-O4'	6.20	116.54	109.10
2	AB	334	C	O4'-C1'-N1	6.20	113.16	108.20
34	BA	1434	A	O4'-C1'-N9	6.20	113.16	108.20
34	BA	1138	G	P-O3'-C3'	6.20	127.14	119.70
34	BA	269	C	O4'-C1'-N1	6.19	113.16	108.20
34	BA	1310	G	O4'-C1'-N9	6.19	113.15	108.20
2	AB	989	G	C1'-O4'-C4'	-6.19	104.95	109.90
2	AB	947	A	O4'-C1'-N9	6.19	113.15	108.20
2	AB	2513	A	C5'-C4'-O4'	6.19	116.52	109.10
34	BA	1446	A	O4'-C1'-N9	6.19	113.15	108.20
35	BB	28	G	N3-C4-C5	-6.19	125.51	128.60
2	AB	988	A	O4'-C1'-N9	6.18	113.15	108.20
2	AB	1573	G	C5'-C4'-O4'	6.18	116.52	109.10
2	AB	122	G	O4'-C1'-N9	6.18	113.15	108.20
2	AB	1467	U	O4'-C1'-N1	6.18	113.15	108.20
2	AB	2746	U	O4'-C1'-N1	6.18	113.15	108.20
35	BB	41	C	O4'-C1'-N1	6.18	113.14	108.20
2	AB	2493	U	O4'-C1'-N1	6.18	113.14	108.20
2	AB	2460	U	O4'-C1'-N1	6.18	113.14	108.20
34	BA	1173	U	O4'-C1'-N1	6.18	113.14	108.20
2	AB	2528	U	O4'-C1'-N1	6.18	113.14	108.20
34	BA	400	C	O4'-C1'-N1	6.18	113.14	108.20
34	BA	410	G	O4'-C1'-N9	6.18	113.14	108.20
2	AB	1936	A	O4'-C1'-N9	6.17	113.14	108.20
2	AB	2112	G	O4'-C1'-N9	6.17	113.14	108.20
2	AB	2753	A	C8-N9-C4	-6.17	103.33	105.80
34	BA	352	C	O4'-C1'-N1	6.17	113.14	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1790	C	O4'-C1'-N1	6.17	113.14	108.20
2	AB	2028	U	C5'-C4'-O4'	6.17	116.51	109.10
2	AB	2829	A	O4'-C1'-N9	6.17	113.14	108.20
2	AB	393	C	O4'-C1'-N1	6.17	113.14	108.20
2	AB	649	G	O4'-C1'-N9	6.17	113.13	108.20
2	AB	1214	A	O4'-C1'-N9	6.17	113.13	108.20
34	BA	644	U	O4'-C1'-N1	6.17	113.13	108.20
2	AB	10	A	C5'-C4'-C3'	-6.16	106.14	116.00
34	BA	1401	G	C8-N9-C4	-6.16	103.94	106.40
34	BA	1002	G	O4'-C1'-N9	6.16	113.13	108.20
34	BA	1089	G	O4'-C1'-N9	6.16	113.13	108.20
34	BA	1196	A	O4'-C1'-N9	6.16	113.13	108.20
2	AB	1390	U	O4'-C1'-N1	6.16	113.12	108.20
2	AB	1407	G	C5'-C4'-O4'	6.16	116.48	109.10
2	AB	650	C	O4'-C1'-N1	6.15	113.12	108.20
2	AB	1871	A	O4'-C1'-N9	6.15	113.12	108.20
2	AB	2214	C	C5'-C4'-O4'	6.15	116.48	109.10
2	AB	2366	A	O4'-C1'-N9	6.15	113.12	108.20
2	AB	2156	G	O4'-C1'-N9	6.15	113.12	108.20
2	AB	1810	A	C5'-C4'-C3'	-6.15	106.16	116.00
2	AB	1890	A	C8-N9-C4	-6.15	103.34	105.80
35	BB	12	U	O4'-C1'-N1	6.15	113.12	108.20
34	BA	934	C	C3'-C2'-C1'	6.14	106.42	101.50
2	AB	731	C	O4'-C1'-N1	6.14	113.11	108.20
2	AB	1119	U	O4'-C1'-N1	6.14	113.11	108.20
2	AB	1367	A	O4'-C1'-N9	6.14	113.11	108.20
2	AB	1082	U	O4'-C1'-N1	6.14	113.11	108.20
34	BA	730	G	C5'-C4'-C3'	-6.14	106.17	116.00
34	BA	1198	G	O4'-C1'-N9	6.14	113.11	108.20
2	AB	444	C	O4'-C1'-N1	6.14	113.11	108.20
2	AB	2567	G	C8-N9-C4	-6.14	103.94	106.40
2	AB	2880	C	N1-C2-O2	6.14	122.58	118.90
34	BA	883	C	O4'-C1'-N1	6.14	113.11	108.20
34	BA	1304	G	C5'-C4'-O4'	6.14	116.47	109.10
2	AB	1483	G	C5'-C4'-C3'	-6.14	106.18	116.00
2	AB	2253	G	O4'-C1'-N9	6.14	113.11	108.20
2	AB	1132	U	O4'-C1'-N1	6.13	113.11	108.20
2	AB	1560	G	C5'-C4'-C3'	-6.13	106.18	116.00
34	BA	1181	G	C5'-C4'-C3'	-6.13	106.18	116.00
2	AB	796	C	O4'-C1'-N1	6.13	113.11	108.20
2	AB	1199	U	O4'-C1'-N1	6.13	113.11	108.20
2	AB	2494	G	C5'-C4'-O4'	6.13	116.46	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2658	C	C5'-C4'-O4'	6.13	116.46	109.10
34	BA	1124	G	O4'-C1'-N9	6.13	113.11	108.20
2	AB	894	U	O4'-C1'-N1	6.13	113.10	108.20
34	BA	1188	A	O4'-C1'-N9	6.13	113.10	108.20
1	AA	95	U	C5'-C4'-C3'	-6.13	106.20	116.00
2	AB	2597	G	C5'-C4'-O4'	6.13	116.45	109.10
2	AB	1530	G	C8-N9-C4	-6.12	103.95	106.40
34	BA	68	G	O4'-C1'-N9	6.12	113.10	108.20
2	AB	210	C	O4'-C1'-N1	6.12	113.10	108.20
2	AB	505	A	O4'-C1'-N9	6.12	113.10	108.20
2	AB	867	C	O4'-C1'-N1	6.12	113.10	108.20
2	AB	1752	C	O4'-C1'-N1	6.12	113.10	108.20
2	AB	2635	A	O4'-C1'-N9	6.12	113.10	108.20
2	AB	2664	G	O4'-C1'-N9	6.12	113.10	108.20
34	BA	1115	U	C5'-C4'-O4'	6.12	116.44	109.10
2	AB	1792	G	C5'-C4'-O4'	6.12	116.44	109.10
2	AB	99	U	O4'-C1'-N1	6.12	113.09	108.20
2	AB	497	A	O4'-C1'-N9	6.12	113.09	108.20
2	AB	525	U	O4'-C1'-N1	6.12	113.09	108.20
34	BA	714	G	O4'-C1'-N9	6.12	113.09	108.20
2	AB	1338	G	C5'-C4'-O4'	6.12	116.44	109.10
2	AB	1446	C	O4'-C1'-N1	6.12	113.09	108.20
2	AB	2233	U	O4'-C1'-N1	6.12	113.09	108.20
2	AB	1313	U	C5'-C4'-O4'	6.11	116.44	109.10
2	AB	1925	C	O4'-C1'-N1	6.11	113.09	108.20
34	BA	249	U	O4'-C1'-N1	6.11	113.09	108.20
34	BA	108	G	N3-C4-C5	-6.11	125.54	128.60
34	BA	749	A	C5'-C4'-O4'	6.11	116.44	109.10
2	AB	289	G	O4'-C1'-N9	6.11	113.09	108.20
2	AB	1415	U	C2'-C3'-O3'	6.11	123.47	113.70
2	AB	1215	G	O4'-C1'-N9	6.11	113.09	108.20
2	AB	2860	A	C5'-C4'-C3'	-6.11	106.23	116.00
34	BA	503	C	C5'-C4'-O4'	6.11	116.43	109.10
34	BA	915	A	O4'-C1'-N9	6.11	113.09	108.20
34	BA	1276	G	C5'-C4'-O4'	6.11	116.43	109.10
2	AB	912	C	C5'-C4'-O4'	6.11	116.43	109.10
2	AB	1533	C	O4'-C1'-N1	6.10	113.08	108.20
2	AB	2059	A	O4'-C1'-N9	6.10	113.08	108.20
2	AB	2664	G	N9-C4-C5	6.10	107.84	105.40
34	BA	19	A	O4'-C1'-N9	6.10	113.08	108.20
35	BE	15	G	O4'-C1'-N9	6.10	113.08	108.20
2	AB	347	A	C5'-C4'-O4'	6.10	116.42	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1479	G	O4'-C1'-N9	6.10	113.08	108.20
34	BA	211	G	C8-N9-C4	-6.10	103.96	106.40
2	AB	607	U	O4'-C1'-N1	6.10	113.08	108.20
2	AB	1554	U	O4'-C1'-N1	6.10	113.08	108.20
2	AB	2255	G	O4'-C1'-N9	6.10	113.08	108.20
2	AB	2311	A	O4'-C1'-N9	6.10	113.08	108.20
1	AA	14	U	C5'-C4'-C3'	-6.09	106.25	116.00
2	AB	2673	G	O4'-C1'-N9	6.09	113.08	108.20
35	BE	61	C	O4'-C1'-N1	6.09	113.08	108.20
2	AB	207	A	O4'-C1'-N9	6.09	113.07	108.20
2	AB	2889	C	O4'-C1'-N1	6.09	113.07	108.20
2	AB	1525	A	O4'-C1'-N9	6.09	113.07	108.20
2	AB	2511	U	O4'-C1'-N1	6.09	113.07	108.20
2	AB	2810	A	C5'-C4'-C3'	-6.09	106.25	116.00
34	BA	254	G	O4'-C1'-N9	6.09	113.07	108.20
1	AA	79	G	C8-N9-C4	-6.09	103.96	106.40
2	AB	237	C	O4'-C1'-N1	6.09	113.07	108.20
2	AB	340	A	O4'-C1'-N9	6.09	113.07	108.20
1	AA	36	C	C5'-C4'-C3'	-6.09	106.26	116.00
2	AB	1280	G	O4'-C1'-N9	6.09	113.07	108.20
2	AB	2031	A	O4'-C4'-C3'	6.09	110.97	106.10
34	BA	57	G	N3-C4-C5	-6.09	125.56	128.60
34	BA	1264	U	C4'-C3'-C2'	-6.09	96.51	102.60
2	AB	2599	G	C4'-C3'-C2'	-6.08	96.52	102.60
2	AB	488	G	C5'-C4'-O4'	6.08	116.40	109.10
2	AB	515	A	O4'-C1'-N9	6.08	113.06	108.20
2	AB	685	A	C8-N9-C4	-6.08	103.37	105.80
2	AB	1375	U	O4'-C1'-N1	6.08	113.06	108.20
2	AB	657	U	C3'-C2'-C1'	6.08	106.36	101.50
2	AB	1445	G	C8-N9-C4	-6.08	103.97	106.40
34	BA	101	A	O4'-C1'-N9	6.08	113.06	108.20
34	BA	1135	U	O4'-C1'-N1	6.08	113.06	108.20
1	AA	77	U	C2'-C3'-O3'	6.08	123.42	113.70
2	AB	2060	A	O4'-C1'-C2'	-6.08	99.72	105.80
34	BA	652	U	O4'-C1'-N1	6.08	113.06	108.20
34	BA	124	C	O4'-C1'-N1	6.08	113.06	108.20
34	BA	251	G	C8-N9-C4	-6.08	103.97	106.40
34	BA	604	G	C3'-C2'-C1'	-6.08	96.64	101.50
34	BA	1424	U	O4'-C1'-N1	6.08	113.06	108.20
2	AB	235	U	O4'-C1'-N1	6.07	113.06	108.20
2	AB	884	U	O4'-C1'-N1	6.07	113.06	108.20
2	AB	1773	A	C5'-C4'-O4'	6.07	116.39	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	407	U	O4'-C1'-N1	6.07	113.06	108.20
2	AB	839	U	O3'-P-O5'	-6.07	92.47	104.00
34	BA	1494	G	C5'-C4'-O4'	6.07	116.39	109.10
2	AB	291	G	O3'-P-O5'	-6.07	92.47	104.00
2	AB	560	C	O4'-C1'-N1	6.07	113.05	108.20
2	AB	907	G	C5'-C4'-O4'	6.07	116.38	109.10
2	AB	1216	G	C5'-C4'-C3'	-6.07	106.29	116.00
2	AB	2118	U	O4'-C1'-N1	6.07	113.05	108.20
34	BA	871	U	O4'-C1'-N1	6.07	113.05	108.20
2	AB	966	G	O4'-C1'-N9	6.06	113.05	108.20
2	AB	461	C	O4'-C1'-N1	6.06	113.05	108.20
2	AB	531	C	C1'-O4'-C4'	-6.06	105.05	109.90
2	AB	1076	C	O4'-C1'-N1	6.06	113.05	108.20
2	AB	2238	G	C5'-C4'-O4'	-6.06	101.83	109.10
35	BB	63	G	O4'-C1'-N9	6.06	113.05	108.20
2	AB	1109	C	O4'-C4'-C3'	6.06	110.94	106.10
2	AB	2087	G	C8-N9-C4	-6.06	103.98	106.40
2	AB	789	A	C5'-C4'-C3'	-6.05	106.32	116.00
34	BA	9	G	N3-C4-C5	-6.05	125.57	128.60
34	BA	760	G	O4'-C1'-N9	6.05	113.04	108.20
34	BA	1429	A	N9-C1'-C2'	-6.05	105.34	112.00
2	AB	793	A	O4'-C1'-N9	6.05	113.04	108.20
34	BA	398	U	O4'-C1'-N1	6.05	113.04	108.20
34	BA	1383	C	O4'-C1'-N1	6.05	113.04	108.20
34	BA	882	C	O4'-C1'-N1	6.05	113.04	108.20
2	AB	688	U	O4'-C1'-N1	6.05	113.04	108.20
2	AB	878	A	C8-N9-C4	-6.05	103.38	105.80
2	AB	913	U	C5'-C4'-C3'	-6.05	106.32	116.00
2	AB	927	A	O4'-C1'-N9	6.05	113.04	108.20
2	AB	2615	U	O4'-C1'-N1	6.05	113.04	108.20
34	BA	986	U	O4'-C1'-N1	6.05	113.04	108.20
2	AB	759	G	N3-C4-C5	-6.04	125.58	128.60
2	AB	760	G	O4'-C1'-N9	6.04	113.03	108.20
1	AA	5	U	O4'-C1'-N1	6.04	113.03	108.20
2	AB	1999	C	C5'-C4'-O4'	6.04	116.35	109.10
34	BA	74	A	O4'-C1'-N9	6.04	113.03	108.20
2	AB	976	G	C8-N9-C4	-6.04	103.98	106.40
2	AB	1550	C	C3'-C2'-C1'	6.04	106.33	101.50
2	AB	2774	C	O4'-C1'-N1	6.04	113.03	108.20
2	AB	190	A	C5'-C4'-C3'	-6.04	106.34	116.00
2	AB	270	A	O4'-C1'-N9	6.04	113.03	108.20
2	AB	1404	C	C5'-C4'-O4'	6.04	116.34	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1567	G	O4'-C1'-N9	6.04	113.03	108.20
2	AB	2559	C	C1'-O4'-C4'	-6.04	105.07	109.90
7	AG	132	ARG	NE-CZ-NH1	-6.04	117.28	120.30
2	AB	2724	U	O4'-C1'-N1	6.03	113.03	108.20
34	BA	588	G	O4'-C1'-N9	6.03	113.03	108.20
2	AB	2870	C	C3'-C2'-C1'	-6.03	96.68	101.50
34	BA	899	C	C4'-C3'-C2'	6.03	108.63	102.60
1	AA	16	G	C8-N9-C4	-6.03	103.99	106.40
2	AB	1645	G	C8-N9-C4	-6.03	103.99	106.40
34	BA	1057	G	O4'-C1'-N9	6.03	113.02	108.20
2	AB	1505	A	O4'-C1'-N9	6.03	113.02	108.20
2	AB	2744	G	C5'-C4'-O4'	6.03	116.33	109.10
34	BA	81	A	O4'-C1'-N9	6.03	113.02	108.20
34	BA	436	C	O4'-C1'-N1	6.03	113.02	108.20
34	BA	971	G	O4'-C1'-N9	6.03	113.02	108.20
2	AB	667	U	O4'-C1'-N1	6.02	113.02	108.20
2	AB	1055	G	C8-N9-C4	-6.02	103.99	106.40
2	AB	2328	A	O3'-P-O5'	-6.02	92.55	104.00
34	BA	165	G	C5'-C4'-C3'	-6.02	106.36	116.00
34	BA	622	A	C8-N9-C4	-6.02	103.39	105.80
2	AB	1456	G	O4'-C1'-N9	6.02	113.02	108.20
2	AB	1604	C	C5'-C4'-O4'	6.02	116.33	109.10
2	AB	1580	A	O4'-C1'-N9	6.02	113.02	108.20
2	AB	2767	C	O4'-C1'-N1	6.02	113.01	108.20
2	AB	377	G	C5'-C4'-C3'	-6.02	106.37	116.00
34	BA	670	G	N9-C1'-C2'	-6.02	105.38	112.00
2	AB	251	A	C8-N9-C4	-6.01	103.39	105.80
2	AB	916	G	O4'-C1'-N9	6.01	113.01	108.20
34	BA	987	G	C8-N9-C4	-6.01	103.99	106.40
34	BA	1137	C	O4'-C1'-N1	6.01	113.01	108.20
2	AB	839	U	O4'-C1'-N1	6.01	113.01	108.20
2	AB	1138	G	O4'-C1'-N9	6.01	113.01	108.20
34	BA	1395	C	C5'-C4'-O4'	6.01	116.31	109.10
2	AB	2190	G	C5'-C4'-O4'	6.01	116.31	109.10
2	AB	2192	U	C5'-C4'-O4'	6.01	116.31	109.10
34	BA	261	U	C5'-C4'-O4'	6.01	116.31	109.10
34	BA	764	C	C5'-C4'-O4'	6.01	116.31	109.10
34	BA	876	C	O4'-C1'-N1	6.01	113.01	108.20
2	AB	1107	G	O4'-C1'-N9	6.00	113.00	108.20
2	AB	1954	G	O4'-C1'-N9	6.00	113.00	108.20
35	BE	10	G	C8-N9-C4	-6.00	104.00	106.40
34	BA	941	G	C5'-C4'-C3'	-6.00	106.40	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1441	G	O4'-C1'-N9	6.00	113.00	108.20
2	AB	1451	C	C2'-C3'-O3'	6.00	123.30	113.70
2	AB	2338	C	O4'-C1'-N1	6.00	113.00	108.20
2	AB	1448	G	C5'-C4'-O4'	6.00	116.30	109.10
2	AB	2398	U	C5'-C4'-O4'	6.00	116.30	109.10
2	AB	2704	C	C5'-C4'-O4'	6.00	116.30	109.10
34	BA	13	U	O4'-C1'-N1	6.00	113.00	108.20
34	BA	846	G	C2-N3-C4	6.00	114.90	111.90
34	BA	1128	C	C5'-C4'-O4'	6.00	116.30	109.10
34	BA	1322	C	N1-C2-O2	6.00	122.50	118.90
34	BA	48	C	O4'-C1'-N1	6.00	113.00	108.20
2	AB	344	A	C3'-C2'-C1'	-5.99	96.70	101.50
2	AB	490	C	C1'-O4'-C4'	-5.99	105.11	109.90
2	AB	1343	G	N3-C4-C5	-5.99	125.60	128.60
2	AB	2008	C	O4'-C1'-N1	5.99	113.00	108.20
2	AB	2411	A	C5'-C4'-O4'	5.99	116.29	109.10
34	BA	1288	A	C8-N9-C4	-5.99	103.40	105.80
34	BA	352	C	N1-C2-O2	5.99	122.50	118.90
34	BA	1490	U	O4'-C1'-N1	5.99	112.99	108.20
2	AB	181	A	C5'-C4'-O4'	5.99	116.29	109.10
2	AB	1033	U	C5'-C4'-O4'	5.99	116.29	109.10
34	BA	415	A	C5'-C4'-O4'	5.99	116.29	109.10
34	BA	438	U	O4'-C1'-N1	5.99	112.99	108.20
34	BA	1156	G	O4'-C1'-N9	5.99	112.99	108.20
34	BA	44	A	O4'-C1'-N9	5.99	112.99	108.20
2	AB	1359	A	O4'-C1'-N9	5.98	112.99	108.20
34	BA	1227	A	O4'-C1'-N9	5.98	112.98	108.20
35	BE	38	A	C5'-C4'-O4'	5.98	116.28	109.10
2	AB	1072	C	O4'-C1'-N1	5.98	112.98	108.20
2	AB	2110	G	O4'-C4'-C3'	5.98	110.88	106.10
2	AB	558	U	O4'-C1'-N1	5.98	112.98	108.20
2	AB	1278	C	O4'-C1'-N1	5.98	112.98	108.20
2	AB	2302	U	C5'-C4'-O4'	5.98	116.27	109.10
34	BA	758	C	N1-C2-O2	5.98	122.49	118.90
34	BA	1482	G	O4'-C1'-N9	5.98	112.98	108.20
35	BE	18	G	C4'-C3'-C2'	-5.98	96.62	102.60
55	BW	77	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	AB	532	A	C1'-O4'-C4'	-5.98	105.12	109.90
2	AB	2150	C	O4'-C1'-N1	5.98	112.98	108.20
2	AB	412	A	C5'-C4'-C3'	-5.97	106.44	116.00
2	AB	1029	A	O4'-C1'-N9	5.97	112.98	108.20
2	AB	2787	C	O4'-C1'-N1	5.97	112.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BE	17	C	N1-C2-O2	5.97	122.48	118.90
2	AB	1840	G	C8-N9-C4	-5.97	104.01	106.40
34	BA	1380	U	O4'-C1'-N1	5.97	112.98	108.20
2	AB	238	C	C5'-C4'-O4'	5.97	116.27	109.10
2	AB	407	G	C8-N9-C4	-5.97	104.01	106.40
2	AB	949	G	C8-N9-C4	-5.97	104.01	106.40
34	BA	1027	C	C5'-C4'-O4'	5.97	116.27	109.10
34	BA	538	G	O4'-C1'-N9	5.97	112.98	108.20
34	BA	948	C	O4'-C1'-N1	5.97	112.97	108.20
2	AB	542	C	C5'-C4'-O4'	5.97	116.26	109.10
2	AB	239	C	O4'-C1'-N1	5.97	112.97	108.20
2	AB	673	C	C5'-C4'-O4'	5.97	116.26	109.10
2	AB	1609	A	O4'-C1'-N9	5.97	112.97	108.20
34	BA	9	G	C8-N9-C4	-5.97	104.01	106.40
34	BA	601	G	C5'-C4'-O4'	5.97	116.26	109.10
2	AB	1475	G	O4'-C1'-N9	5.96	112.97	108.20
2	AB	1748	C	O4'-C1'-N1	5.96	112.97	108.20
34	BA	437	U	O4'-C1'-N1	5.96	112.97	108.20
34	BA	725	G	O4'-C1'-N9	5.96	112.97	108.20
2	AB	767	U	C5'-C4'-O4'	5.96	116.26	109.10
2	AB	2252	G	O4'-C1'-N9	5.96	112.97	108.20
34	BA	108	G	O4'-C1'-N9	5.96	112.97	108.20
2	AB	748	G	C1'-O4'-C4'	-5.96	105.13	109.90
2	AB	326	G	O4'-C1'-N9	5.96	112.97	108.20
2	AB	2059	A	C8-N9-C4	-5.96	103.42	105.80
2	AB	2497	A	O4'-C1'-N9	5.96	112.97	108.20
2	AB	943	A	C5'-C4'-O4'	5.95	116.25	109.10
2	AB	1933	G	C5'-C4'-C3'	-5.95	106.47	116.00
34	BA	1106	G	C8-N9-C4	-5.95	104.02	106.40
34	BA	1120	C	C5'-C4'-O4'	5.95	116.24	109.10
2	AB	1855	U	O4'-C1'-N1	5.95	112.96	108.20
34	BA	639	G	O4'-C1'-N9	5.95	112.96	108.20
2	AB	1363	C	O4'-C1'-N1	5.95	112.96	108.20
2	AB	1996	C	O4'-C1'-N1	5.95	112.96	108.20
34	BA	204	G	C8-N9-C4	-5.95	104.02	106.40
2	AB	121	G	C8-N9-C4	-5.95	104.02	106.40
35	BE	65	G	O4'-C1'-N9	5.95	112.96	108.20
2	AB	1822	C	O4'-C1'-N1	5.95	112.96	108.20
34	BA	1359	C	C5'-C4'-C3'	-5.95	106.49	116.00
35	BE	30	G	O4'-C1'-N9	5.95	112.96	108.20
34	BA	1417	G	C5'-C4'-O4'	5.94	116.23	109.10
2	AB	854	C	O4'-C1'-N1	5.94	112.95	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	270	A	C1'-O4'-C4'	-5.94	105.15	109.90
34	BA	398	U	C5'-C4'-C3'	-5.94	106.50	116.00
34	BA	346	G	C3'-C2'-C1'	5.94	106.25	101.50
34	BA	780	A	O4'-C1'-N9	5.94	112.95	108.20
2	AB	2247	A	C5'-C4'-O4'	5.93	116.22	109.10
34	BA	164	G	C5'-C4'-O4'	5.93	116.22	109.10
34	BA	207	C	O4'-C1'-N1	5.93	112.95	108.20
1	AA	34	A	P-O3'-C3'	5.93	126.82	119.70
2	AB	1727	C	O4'-C1'-N1	5.93	112.94	108.20
2	AB	2874	C	O4'-C1'-N1	5.93	112.94	108.20
2	AB	2784	U	C5'-C4'-C3'	-5.93	106.52	116.00
2	AB	2807	U	C4'-C3'-C2'	-5.93	96.67	102.60
34	BA	272	C	O4'-C1'-N1	5.93	112.94	108.20
2	AB	2716	C	O4'-C1'-N1	5.92	112.94	108.20
34	BA	154	U	O4'-C1'-N1	5.92	112.94	108.20
2	AB	2537	U	C5'-C4'-O4'	5.92	116.21	109.10
2	AB	2377	A	O4'-C1'-N9	5.92	112.94	108.20
2	AB	2514	U	O4'-C1'-N1	5.92	112.94	108.20
35	BB	7	A	O4'-C1'-N9	5.92	112.94	108.20
2	AB	1788	C	C5'-C4'-O4'	5.92	116.20	109.10
34	BA	1213	A	P-O3'-C3'	5.92	126.80	119.70
2	AB	890	C	C5'-C4'-O4'	5.92	116.20	109.10
2	AB	2274	A	C5'-C4'-C3'	-5.92	106.53	116.00
2	AB	2625	G	C5'-C4'-O4'	5.92	116.20	109.10
2	AB	165	A	O4'-C1'-N9	5.92	112.93	108.20
2	AB	997	G	N3-C4-C5	-5.92	125.64	128.60
2	AB	2050	C	O4'-C1'-N1	5.92	112.93	108.20
2	AB	2254	C	C5'-C4'-O4'	5.92	116.20	109.10
2	AB	2500	U	P-O3'-C3'	5.92	126.80	119.70
2	AB	2601	C	C3'-C2'-C1'	5.92	106.23	101.50
2	AB	97	C	O4'-C1'-N1	5.91	112.93	108.20
2	AB	998	C	O4'-C1'-N1	5.91	112.93	108.20
34	BA	501	C	C4'-C3'-C2'	-5.91	96.69	102.60
34	BA	945	G	C5'-C4'-O4'	5.91	116.19	109.10
34	BA	1341	U	O4'-C1'-N1	5.91	112.93	108.20
2	AB	759	G	C8-N9-C4	-5.91	104.04	106.40
2	AB	1078	U	O4'-C1'-N1	5.91	112.93	108.20
2	AB	1623	G	O4'-C1'-N9	5.91	112.93	108.20
2	AB	743	A	C5'-C4'-O4'	5.91	116.19	109.10
2	AB	2074	U	O4'-C1'-N1	5.91	112.92	108.20
2	AB	2222	C	O4'-C1'-N1	5.91	112.92	108.20
34	BA	856	C	O4'-C1'-N1	5.91	112.92	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	656	G	N3-C4-C5	-5.90	125.65	128.60
34	BA	718	A	C5'-C4'-O4'	5.90	116.19	109.10
2	AB	549	G	C2-N3-C4	5.90	114.85	111.90
2	AB	779	U	O4'-C1'-N1	5.90	112.92	108.20
2	AB	1994	C	O4'-C1'-N1	5.90	112.92	108.20
2	AB	2262	U	C5'-C4'-C3'	-5.90	106.56	116.00
2	AB	2318	G	C8-N9-C4	-5.90	104.04	106.40
34	BA	732	C	O4'-C1'-N1	5.90	112.92	108.20
2	AB	1416	G	N9-C4-C5	5.90	107.76	105.40
2	AB	1492	G	O4'-C1'-N9	5.90	112.92	108.20
2	AB	1511	G	C5'-C4'-C3'	-5.90	106.56	116.00
2	AB	274	C	C5'-C4'-O4'	5.90	116.18	109.10
2	AB	1564	C	O4'-C1'-N1	5.90	112.92	108.20
34	BA	177	G	O4'-C1'-N9	5.90	112.92	108.20
35	BE	72	C	O4'-C1'-N1	5.90	112.92	108.20
2	AB	896	A	O3'-P-O5'	-5.90	92.80	104.00
2	AB	1648	U	C5'-C4'-O4'	5.89	116.17	109.10
2	AB	1610	A	O4'-C1'-N9	5.89	112.91	108.20
2	AB	1869	G	O4'-C1'-N9	5.89	112.91	108.20
34	BA	583	A	O4'-C1'-N9	5.89	112.91	108.20
34	BA	1150	A	C5'-C4'-O4'	5.89	116.17	109.10
2	AB	2622	U	C5'-C4'-O4'	5.89	116.17	109.10
34	BA	608	A	C5'-C4'-O4'	5.89	116.17	109.10
2	AB	243	U	O4'-C1'-N1	5.89	112.91	108.20
2	AB	540	C	O4'-C1'-N1	5.89	112.91	108.20
2	AB	1331	G	C5'-C4'-C3'	-5.89	106.58	116.00
2	AB	1331	G	N3-C4-C5	-5.89	125.66	128.60
2	AB	1865	U	P-O3'-C3'	5.89	126.77	119.70
34	BA	327	A	C5'-C4'-C3'	-5.89	106.58	116.00
2	AB	549	G	C5'-C4'-C3'	-5.89	106.58	116.00
2	AB	1036	G	O4'-C1'-N9	5.89	112.91	108.20
2	AB	2550	G	C5'-C4'-C3'	-5.89	106.58	116.00
2	AB	2788	C	C5'-C4'-O4'	5.89	116.16	109.10
2	AB	1690	A	O4'-C1'-N9	5.88	112.91	108.20
2	AB	2768	U	O4'-C1'-N1	5.88	112.91	108.20
34	BA	380	G	O4'-C1'-N9	5.88	112.91	108.20
2	AB	1462	C	O4'-C1'-N1	5.88	112.90	108.20
2	AB	714	U	O4'-C1'-N1	5.88	112.90	108.20
2	AB	1717	A	O4'-C1'-N9	5.88	112.90	108.20
2	AB	2814	A	O4'-C1'-N9	5.88	112.90	108.20
2	AB	2405	G	O4'-C1'-N9	5.88	112.90	108.20
34	BA	1489	G	O4'-C1'-N9	5.88	112.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	253	C	O4'-C1'-N1	5.87	112.90	108.20
34	BA	893	C	O4'-C1'-N1	5.87	112.90	108.20
2	AB	810	U	O4'-C1'-N1	5.87	112.90	108.20
1	AA	50	A	C5'-C4'-C3'	-5.87	106.61	116.00
2	AB	2417	C	O4'-C1'-N1	5.87	112.90	108.20
2	AB	481	G	C8-N9-C4	-5.87	104.05	106.40
34	BA	847	G	O4'-C1'-N9	5.87	112.89	108.20
34	BA	858	G	C8-N9-C4	-5.87	104.05	106.40
2	AB	1643	G	O4'-C1'-N9	5.87	112.89	108.20
2	AB	2639	A	O4'-C1'-N9	5.87	112.89	108.20
34	BA	891	U	O4'-C1'-N1	5.87	112.89	108.20
34	BA	1262	C	O4'-C1'-N1	5.87	112.89	108.20
34	BA	865	A	C3'-C2'-C1'	5.86	106.19	101.50
34	BA	1376	U	O4'-C1'-N1	5.86	112.89	108.20
35	BE	34	G	O4'-C1'-N9	5.86	112.89	108.20
2	AB	2199	A	C5'-C4'-C3'	-5.86	106.62	116.00
2	AB	2328	A	C5'-C4'-C3'	-5.86	106.62	116.00
34	BA	366	A	C4'-C3'-C2'	-5.86	96.74	102.60
34	BA	1366	C	O4'-C1'-N1	5.86	112.89	108.20
2	AB	136	G	C3'-C2'-C1'	-5.86	96.81	101.50
2	AB	1136	G	N3-C4-C5	-5.86	125.67	128.60
34	BA	23	C	O4'-C1'-N1	5.86	112.89	108.20
34	BA	874	G	N3-C4-C5	-5.86	125.67	128.60
2	AB	2862	G	O4'-C1'-N9	5.86	112.89	108.20
34	BA	760	G	N1-C6-O6	-5.86	116.39	119.90
2	AB	1447	C	O4'-C1'-N1	5.85	112.88	108.20
34	BA	1158	C	C3'-C2'-C1'	5.85	106.18	101.50
34	BA	1362	A	C8-N9-C4	-5.85	103.46	105.80
2	AB	1091	G	O4'-C1'-N9	5.85	112.88	108.20
2	AB	2578	G	C5'-C4'-O4'	5.85	116.12	109.10
34	BA	1206	G	C8-N9-C4	-5.85	104.06	106.40
34	BA	1291	U	C5'-C4'-O4'	5.85	116.12	109.10
2	AB	833	A	O4'-C1'-N9	5.85	112.88	108.20
2	AB	2380	C	C5'-C4'-O4'	5.85	116.12	109.10
2	AB	2458	G	O4'-C1'-N9	5.85	112.88	108.20
2	AB	2653	U	O4'-C1'-N1	5.85	112.88	108.20
2	AB	1266	G	C3'-C2'-C1'	-5.84	96.83	101.50
2	AB	1472	C	O4'-C1'-N1	5.84	112.87	108.20
2	AB	1166	G	C5'-C4'-C3'	-5.84	106.66	116.00
2	AB	581	C	O4'-C1'-N1	5.84	112.87	108.20
2	AB	2295	C	O4'-C1'-N1	5.84	112.87	108.20
2	AB	2741	A	C4'-C3'-C2'	-5.84	96.76	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	623	C	C5'-C4'-O4'	5.84	116.11	109.10
34	BA	688	G	C8-N9-C4	-5.84	104.06	106.40
34	BA	1111	A	C5'-C4'-C3'	-5.84	106.66	116.00
2	AB	622	G	O4'-C1'-N9	5.83	112.87	108.20
2	AB	818	G	C8-N9-C4	-5.83	104.07	106.40
2	AB	1930	G	O4'-C4'-C3'	5.83	110.77	106.10
2	AB	2298	A	C5'-C4'-O4'	5.83	116.10	109.10
34	BA	544	G	O4'-C1'-N9	5.83	112.87	108.20
2	AB	90	U	C5'-C4'-C3'	-5.83	106.67	116.00
2	AB	490	C	C5'-C4'-C3'	-5.83	106.67	116.00
34	BA	993	G	N3-C4-C5	-5.83	125.68	128.60
2	AB	1902	C	C5'-C4'-C3'	-5.83	106.67	116.00
34	BA	3	A	P-O3'-C3'	5.83	126.70	119.70
34	BA	466	A	C5'-C4'-C3'	-5.83	106.67	116.00
34	BA	869	G	C8-N9-C4	-5.83	104.07	106.40
2	AB	1404	C	O4'-C1'-N1	5.83	112.86	108.20
2	AB	942	G	O4'-C1'-N9	5.83	112.86	108.20
34	BA	347	G	O4'-C1'-N9	5.83	112.86	108.20
2	AB	396	G	N3-C4-C5	-5.83	125.69	128.60
2	AB	2611	C	C3'-C2'-C1'	5.83	106.16	101.50
34	BA	457	G	O4'-C1'-N9	5.83	112.86	108.20
2	AB	1271	G	N9-C1'-C2'	-5.82	105.59	112.00
2	AB	1411	U	O4'-C1'-N1	5.82	112.86	108.20
34	BA	1049	U	O4'-C1'-N1	5.82	112.86	108.20
2	AB	2563	U	C5'-C4'-O4'	5.82	116.09	109.10
34	BA	1313	U	O4'-C1'-N1	5.82	112.86	108.20
34	BA	205	A	C8-N9-C4	-5.82	103.47	105.80
34	BA	624	C	O4'-C1'-N1	5.82	112.86	108.20
34	BA	1300	G	P-O3'-C3'	5.82	126.68	119.70
34	BA	768	A	O4'-C1'-N9	5.82	112.86	108.20
2	AB	1242	U	N1-C2-N3	5.82	118.39	114.90
2	AB	701	G	N9-C1'-C2'	-5.82	105.60	112.00
2	AB	820	A	C5'-C4'-O4'	5.82	116.08	109.10
2	AB	821	A	O4'-C1'-N9	5.82	112.85	108.20
34	BA	98	A	O4'-C1'-N9	5.82	112.85	108.20
34	BA	474	G	O4'-C1'-N9	5.82	112.85	108.20
34	BA	660	C	O4'-C1'-N1	5.82	112.85	108.20
34	BA	709	U	O4'-C1'-N1	5.82	112.85	108.20
34	BA	1329	A	O4'-C1'-N9	5.82	112.85	108.20
2	AB	1161	C	O4'-C1'-N1	5.81	112.85	108.20
2	AB	2537	U	O4'-C1'-N1	5.81	112.85	108.20
34	BA	1178	G	C8-N9-C4	-5.81	104.08	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	229	U	O4'-C1'-N1	5.81	112.85	108.20
2	AB	33	C	O4'-C1'-N1	5.81	112.85	108.20
2	AB	1149	G	O4'-C1'-N9	5.81	112.84	108.20
2	AB	283	G	C5'-C4'-C3'	-5.81	106.71	116.00
2	AB	2783	U	O4'-C1'-N1	5.81	112.84	108.20
35	BE	4	C	O4'-C1'-N1	5.81	112.84	108.20
2	AB	718	A	C5'-C4'-O4'	5.80	116.06	109.10
2	AB	1866	A	C8-N9-C4	-5.80	103.48	105.80
2	AB	1879	C	O4'-C1'-N1	5.80	112.84	108.20
2	AB	2540	C	O4'-C1'-N1	5.80	112.84	108.20
2	AB	758	C	O4'-C1'-N1	5.80	112.84	108.20
9	AI	25	TYR	CB-CG-CD2	-5.80	117.52	121.00
34	BA	447	G	C8-N9-C4	-5.80	104.08	106.40
2	AB	37	C	C5'-C4'-O4'	5.80	116.06	109.10
2	AB	119	A	C1'-O4'-C4'	-5.80	105.26	109.90
2	AB	1741	C	C5'-C4'-O4'	5.80	116.06	109.10
37	BD	45	G	O4'-C1'-N9	5.80	112.84	108.20
2	AB	864	G	C5'-C4'-C3'	-5.80	106.72	116.00
2	AB	2203	U	O4'-C1'-N1	5.80	112.84	108.20
2	AB	1513	U	O4'-C1'-N1	5.80	112.84	108.20
34	BA	357	G	C5'-C4'-O4'	5.80	116.06	109.10
34	BA	757	U	O3'-P-O5'	-5.80	92.99	104.00
2	AB	726	G	C8-N9-C1'	5.79	134.53	127.00
34	BA	1035	A	C4'-C3'-C2'	-5.79	96.81	102.60
34	BA	1224	U	O3'-P-O5'	-5.79	92.99	104.00
2	AB	91	A	C4'-C3'-C2'	-5.79	96.81	102.60
2	AB	2494	G	O4'-C1'-N9	5.79	112.83	108.20
2	AB	2553	G	C5'-C4'-C3'	-5.79	106.73	116.00
34	BA	868	C	O4'-C1'-N1	5.79	112.83	108.20
34	BA	1116	U	O4'-C1'-N1	5.79	112.83	108.20
35	BE	28	G	O4'-C1'-N9	5.79	112.83	108.20
2	AB	863	A	C8-N9-C4	-5.79	103.48	105.80
2	AB	1964	G	C8-N9-C1'	5.79	134.53	127.00
2	AB	2704	C	C5'-C4'-C3'	-5.79	106.74	116.00
34	BA	1461	G	C5'-C4'-O4'	5.79	116.05	109.10
2	AB	857	G	N9-C4-C5	5.79	107.72	105.40
2	AB	1974	C	O4'-C1'-N1	5.79	112.83	108.20
2	AB	2783	U	C5'-C4'-C3'	-5.79	106.74	116.00
34	BA	590	U	O4'-C1'-N1	5.79	112.83	108.20
34	BA	744	C	O4'-C1'-N1	5.79	112.83	108.20
34	BA	1342	C	O4'-C1'-N1	5.79	112.83	108.20
2	AB	1185	G	N3-C4-C5	-5.79	125.71	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1044	A	C5'-C4'-C3'	-5.79	106.74	116.00
2	AB	2875	C	O4'-C1'-N1	5.78	112.83	108.20
34	BA	762	U	O4'-C1'-N1	5.78	112.83	108.20
2	AB	2480	C	O4'-C1'-N1	5.78	112.83	108.20
2	AB	293	U	O4'-C1'-N1	5.78	112.83	108.20
2	AB	465	G	C5'-C4'-O4'	5.78	116.04	109.10
34	BA	1144	G	C8-N9-C4	-5.78	104.09	106.40
2	AB	10	A	O4'-C1'-N9	5.78	112.82	108.20
2	AB	657	U	O4'-C1'-N1	5.78	112.82	108.20
2	AB	2796	U	C5'-C4'-O4'	5.78	116.03	109.10
34	BA	920	U	O4'-C1'-N1	5.78	112.82	108.20
2	AB	340	A	C5'-C4'-C3'	-5.78	106.76	116.00
2	AB	1033	U	C5'-C4'-C3'	-5.78	106.76	116.00
2	AB	1175	A	C5'-C4'-C3'	-5.78	106.76	116.00
2	AB	1707	G	C8-N9-C4	-5.78	104.09	106.40
2	AB	2855	C	C5'-C4'-C3'	-5.78	106.76	116.00
2	AB	310	A	C5'-C4'-O4'	5.77	116.03	109.10
2	AB	770	G	O4'-C1'-N9	5.77	112.82	108.20
2	AB	1758	U	P-O3'-C3'	5.77	126.63	119.70
2	AB	2118	U	C3'-C2'-C1'	5.77	106.12	101.50
2	AB	2186	G	N3-C4-C5	-5.77	125.71	128.60
2	AB	2863	C	C5'-C4'-O4'	5.77	116.03	109.10
34	BA	950	U	O4'-C1'-N1	5.77	112.82	108.20
34	BA	1447	A	O4'-C1'-N9	5.77	112.82	108.20
2	AB	858	G	O4'-C1'-N9	5.77	112.82	108.20
2	AB	2352	A	C5'-C4'-O4'	5.77	116.03	109.10
34	BA	129	A	O4'-C1'-N9	5.77	112.82	108.20
2	AB	174	U	O4'-C1'-N1	5.77	112.81	108.20
2	AB	1208	C	O4'-C1'-N1	5.77	112.82	108.20
2	AB	1451	C	P-O3'-C3'	5.77	126.62	119.70
1	AA	29	A	O4'-C1'-N9	5.77	112.81	108.20
2	AB	2260	C	O4'-C1'-N1	5.77	112.81	108.20
2	AB	2462	C	O4'-C1'-N1	5.77	112.81	108.20
2	AB	1041	G	C5'-C4'-C3'	-5.77	106.78	116.00
2	AB	1885	A	C5'-C4'-O4'	5.77	116.02	109.10
34	BA	576	C	N1-C2-O2	5.77	122.36	118.90
1	AA	32	U	C3'-C2'-C1'	-5.76	96.89	101.50
2	AB	1648	U	C1'-O4'-C4'	-5.76	105.29	109.90
34	BA	18	C	O4'-C1'-N1	5.76	112.81	108.20
1	AA	54	G	C8-N9-C4	-5.76	104.10	106.40
2	AB	21	A	C5'-C4'-O4'	5.76	116.01	109.10
2	AB	1019	U	C5'-C4'-C3'	-5.76	106.79	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1861	G	C4'-C3'-C2'	-5.76	96.84	102.60
34	BA	271	C	O4'-C1'-N1	5.76	112.81	108.20
34	BA	392	C	O4'-C1'-N1	5.76	112.81	108.20
2	AB	1088	A	C1'-O4'-C4'	-5.76	105.29	109.90
34	BA	1514	G	O4'-C1'-N9	5.76	112.81	108.20
35	BB	18	G	C8-N9-C4	-5.76	104.10	106.40
1	AA	16	G	N3-C4-C5	-5.75	125.72	128.60
2	AB	2112	G	N3-C4-C5	-5.75	125.72	128.60
34	BA	935	A	O4'-C1'-N9	5.75	112.80	108.20
2	AB	937	C	O4'-C1'-N1	5.75	112.80	108.20
2	AB	1928	A	C8-N9-C4	-5.75	103.50	105.80
2	AB	2543	G	C8-N9-C4	-5.75	104.10	106.40
2	AB	2667	C	C5'-C4'-C3'	-5.75	106.80	116.00
2	AB	2801	G	C5'-C4'-C3'	-5.75	106.80	116.00
34	BA	484	G	C3'-C2'-C1'	-5.75	96.90	101.50
34	BA	911	U	O4'-C1'-N1	5.75	112.80	108.20
34	BA	1018	G	O4'-C1'-N9	5.75	112.80	108.20
2	AB	712	G	O4'-C1'-N9	5.75	112.80	108.20
2	AB	1395	A	O4'-C4'-C3'	5.75	110.70	106.10
2	AB	2348	U	O4'-C1'-N1	5.75	112.80	108.20
34	BA	1162	C	O4'-C1'-N1	5.75	112.80	108.20
2	AB	1652	A	C5'-C4'-C3'	-5.75	106.81	116.00
2	AB	2625	G	N3-C4-C5	-5.75	125.73	128.60
34	BA	322	C	O4'-C1'-N1	5.75	112.80	108.20
34	BA	429	U	C5'-C4'-C3'	-5.75	106.80	116.00
34	BA	814	A	C5'-C4'-C3'	-5.75	106.80	116.00
2	AB	1511	G	C5'-C4'-O4'	5.75	115.99	109.10
2	AB	1765	U	O4'-C1'-N1	5.75	112.80	108.20
34	BA	1534	A	C3'-C2'-C1'	5.75	106.10	101.50
2	AB	1033	U	C1'-O4'-C4'	-5.74	105.31	109.90
2	AB	545	U	O4'-C4'-C3'	5.74	110.69	106.10
2	AB	1210	G	P-O3'-C3'	5.74	126.59	119.70
35	BE	63	G	O4'-C1'-N9	5.74	112.79	108.20
2	AB	2452	C	O4'-C1'-N1	5.74	112.79	108.20
2	AB	2692	G	C5'-C4'-O4'	5.74	115.99	109.10
34	BA	505	G	N3-C4-C5	-5.74	125.73	128.60
34	BA	1034	G	C5'-C4'-O4'	5.74	115.99	109.10
2	AB	2399	G	O4'-C1'-N9	5.74	112.79	108.20
2	AB	1627	G	C5'-C4'-O4'	5.74	115.98	109.10
34	BA	236	A	O4'-C1'-N9	5.74	112.79	108.20
34	BA	921	U	O4'-C1'-N1	5.74	112.79	108.20
2	AB	2053	G	O4'-C1'-N9	5.73	112.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2491	U	O4'-C1'-N1	5.73	112.79	108.20
34	BA	678	U	C5'-C4'-O4'	5.73	115.98	109.10
35	BB	17	C	P-O3'-C3'	5.73	126.58	119.70
2	AB	2588	G	N3-C4-C5	-5.73	125.73	128.60
34	BA	329	A	C5'-C4'-C3'	-5.73	106.83	116.00
34	BA	1303	C	O4'-C1'-N1	5.73	112.78	108.20
2	AB	1507	C	O4'-C1'-N1	5.73	112.78	108.20
34	BA	1046	A	C5'-C4'-O4'	5.73	115.98	109.10
1	AA	39	A	O4'-C1'-N9	5.73	112.78	108.20
2	AB	1757	A	P-O3'-C3'	5.73	126.58	119.70
2	AB	2440	C	O4'-C1'-N1	5.73	112.78	108.20
2	AB	1024	G	O4'-C1'-N9	5.73	112.78	108.20
34	BA	156	C	C5'-C4'-C3'	-5.73	106.84	116.00
34	BA	684	U	O4'-C1'-N1	5.73	112.78	108.20
2	AB	368	A	C5'-C4'-C3'	-5.73	106.84	116.00
34	BA	46	G	O4'-C1'-N9	5.73	112.78	108.20
2	AB	1104	C	O4'-C1'-N1	5.72	112.78	108.20
2	AB	1909	C	C4'-C3'-C2'	-5.72	96.88	102.60
34	BA	367	U	C3'-C2'-C1'	5.72	106.08	101.50
1	AA	100	G	C8-N9-C4	-5.72	104.11	106.40
2	AB	1160	G	O4'-C1'-N9	5.72	112.78	108.20
2	AB	1581	G	N9-C4-C5	5.72	107.69	105.40
34	BA	668	G	C5'-C4'-O4'	5.72	115.96	109.10
34	BA	1155	A	C5'-C4'-C3'	-5.72	106.85	116.00
2	AB	820	A	O4'-C1'-N9	5.72	112.78	108.20
2	AB	2196	C	C5'-C4'-O4'	5.72	115.96	109.10
2	AB	52	A	C5'-C4'-C3'	-5.72	106.85	116.00
2	AB	277	G	C2'-C3'-O3'	5.72	122.85	113.70
2	AB	1187	G	C5'-C4'-O4'	5.72	115.96	109.10
2	AB	1510	G	O4'-C1'-N9	5.72	112.77	108.20
2	AB	1645	G	C5'-C4'-C3'	-5.72	106.86	116.00
2	AB	2104	C	O4'-C1'-N1	5.72	112.77	108.20
2	AB	2610	C	C3'-C2'-C1'	-5.71	96.93	101.50
34	BA	281	G	C5'-C4'-O4'	5.71	115.96	109.10
34	BA	751	U	O4'-C1'-N1	5.71	112.77	108.20
34	BA	1535	C	C5'-C4'-C3'	5.71	125.14	116.00
2	AB	295	G	N9-C1'-C2'	-5.71	105.72	112.00
34	BA	410	G	C5'-C4'-C3'	-5.71	106.86	116.00
2	AB	922	C	O4'-C1'-N1	5.71	112.77	108.20
2	AB	2739	U	C4'-C3'-C2'	-5.71	96.89	102.60
2	AB	811	U	C5'-C4'-C3'	-5.71	106.87	116.00
2	AB	1781	U	O4'-C1'-N1	5.71	112.77	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	30	U	C3'-C2'-C1'	5.71	106.07	101.50
34	BA	140	U	O4'-C1'-N1	5.71	112.76	108.20
2	AB	1408	G	O3'-P-O5'	-5.70	93.17	104.00
2	AB	1454	C	N1-C2-O2	5.70	122.32	118.90
35	BB	43	C	O4'-C1'-N1	5.70	112.76	108.20
2	AB	147	C	O4'-C1'-N1	5.70	112.76	108.20
2	AB	1309	G	C8-N9-C4	-5.70	104.12	106.40
2	AB	1501	G	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	2191	A	O4'-C1'-N9	5.70	112.76	108.20
2	AB	2365	G	C5'-C4'-O4'	5.70	115.94	109.10
34	BA	261	U	C5'-C4'-C3'	-5.70	106.88	116.00
34	BA	494	G	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	480	A	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	1840	G	N7-C8-N9	5.70	115.95	113.10
2	AB	2078	C	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	2303	G	C5'-C4'-C3'	-5.70	106.88	116.00
34	BA	111	G	C8-N9-C4	-5.70	104.12	106.40
35	BE	35	A	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	59	U	O4'-C1'-N1	5.70	112.76	108.20
2	AB	566	U	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	1592	C	O4'-C1'-N1	5.70	112.76	108.20
34	BA	787	A	O4'-C1'-N9	5.70	112.76	108.20
2	AB	1560	G	C8-N9-C4	-5.70	104.12	106.40
2	AB	1751	U	O4'-C1'-N1	5.70	112.76	108.20
2	AB	1994	C	C4'-C3'-C2'	-5.70	96.90	102.60
2	AB	2023	C	O4'-C1'-N1	5.69	112.75	108.20
2	AB	141	G	O4'-C1'-N9	5.69	112.75	108.20
2	AB	170	U	O4'-C1'-N1	5.69	112.75	108.20
2	AB	1007	C	C5'-C4'-O4'	5.69	115.93	109.10
2	AB	1543	G	C5'-C4'-O4'	5.69	115.93	109.10
34	BA	1390	U	O4'-C1'-N1	5.69	112.75	108.20
2	AB	1283	G	C8-N9-C4	-5.69	104.12	106.40
34	BA	1201	A	C5'-C4'-O4'	5.69	115.93	109.10
2	AB	317	G	O4'-C1'-N9	5.69	112.75	108.20
2	AB	1420	A	O4'-C1'-N9	5.69	112.75	108.20
2	AB	1325	U	O4'-C1'-N1	5.69	112.75	108.20
34	BA	1035	A	O4'-C1'-N9	5.69	112.75	108.20
2	AB	871	U	C5'-C4'-O4'	5.68	115.92	109.10
2	AB	1416	G	C8-N9-C1'	5.68	134.39	127.00
34	BA	289	G	O4'-C1'-N9	5.68	112.75	108.20
2	AB	549	G	C8-N9-C4	-5.68	104.13	106.40
2	AB	1535	A	N9-C1'-C2'	-5.68	105.75	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1603	A	C5'-C4'-O4'	5.68	115.92	109.10
2	AB	1978	A	O4'-C1'-N9	5.68	112.75	108.20
2	AB	2205	A	O4'-C1'-N9	5.68	112.75	108.20
34	BA	394	G	N9-C4-C5	5.68	107.67	105.40
2	AB	311	A	C3'-C2'-C1'	5.68	106.04	101.50
2	AB	510	C	C5'-C4'-C3'	-5.68	106.91	116.00
2	AB	1203	U	N3-C2-O2	-5.68	118.23	122.20
34	BA	1333	A	C8-N9-C4	-5.68	103.53	105.80
2	AB	1154	G	N7-C8-N9	5.67	115.94	113.10
2	AB	2485	G	N3-C4-C5	-5.67	125.76	128.60
2	AB	2744	G	C1'-O4'-C4'	-5.67	105.36	109.90
34	BA	512	U	C1'-O4'-C4'	-5.67	105.36	109.90
2	AB	783	A	O4'-C1'-N9	5.67	112.74	108.20
2	AB	2076	U	O4'-C1'-N1	5.67	112.74	108.20
2	AB	2705	A	C5'-C4'-C3'	-5.67	106.93	116.00
34	BA	523	A	O4'-C1'-N9	5.67	112.74	108.20
34	BA	822	U	C5'-C4'-O4'	5.67	115.91	109.10
2	AB	738	G	O4'-C1'-N9	5.67	112.74	108.20
2	AB	964	C	O4'-C1'-N1	5.67	112.74	108.20
34	BA	618	C	O4'-C1'-N1	5.67	112.74	108.20
2	AB	863	A	O4'-C1'-N9	5.67	112.73	108.20
2	AB	871	U	C5'-C4'-C3'	-5.67	106.93	116.00
2	AB	1865	U	O4'-C1'-N1	5.67	112.73	108.20
2	AB	1934	C	O4'-C1'-N1	5.67	112.73	108.20
34	BA	352	C	C5'-C4'-O4'	5.67	115.90	109.10
34	BA	1489	G	C8-N9-C4	-5.67	104.13	106.40
34	BA	846	G	N3-C4-C5	-5.67	125.77	128.60
34	BA	1292	G	O4'-C1'-N9	5.67	112.73	108.20
2	AB	2057	G	C4'-C3'-C2'	-5.66	96.94	102.60
2	AB	2650	U	O4'-C1'-N1	5.66	112.73	108.20
34	BA	636	U	C5'-C4'-C3'	-5.66	106.94	116.00
34	BA	1374	A	O4'-C1'-N9	5.66	112.73	108.20
35	BE	57	G	P-O3'-C3'	5.66	126.50	119.70
2	AB	440	C	O4'-C1'-N1	5.66	112.73	108.20
2	AB	1238	G	N3-C4-C5	-5.66	125.77	128.60
2	AB	1695	G	C2-N3-C4	5.66	114.73	111.90
34	BA	1505	G	N9-C4-C5	5.66	107.66	105.40
2	AB	116	C	C5'-C4'-C3'	-5.66	106.95	116.00
34	BA	463	U	O4'-C1'-N1	5.66	112.73	108.20
34	BA	763	G	O4'-C1'-N9	5.66	112.73	108.20
34	BA	1347	G	O4'-C1'-N9	5.66	112.73	108.20
2	AB	2814	A	C5'-C4'-C3'	-5.66	106.95	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	106	C	O4'-C1'-N1	5.66	112.73	108.20
34	BA	719	C	O4'-C1'-N1	5.66	112.72	108.20
2	AB	1695	G	C8-N9-C4	-5.65	104.14	106.40
2	AB	2329	U	O4'-C1'-N1	5.65	112.72	108.20
2	AB	1206	G	C5'-C4'-O4'	5.65	115.88	109.10
34	BA	152	A	O4'-C1'-N9	5.65	112.72	108.20
2	AB	1813	G	C8-N9-C4	-5.65	104.14	106.40
2	AB	2771	C	O4'-C1'-N1	5.65	112.72	108.20
34	BA	40	C	O4'-C1'-N1	5.65	112.72	108.20
34	BA	943	U	O4'-C1'-N1	5.65	112.72	108.20
34	BA	1289	A	C8-N9-C4	-5.65	103.54	105.80
34	BA	1408	A	C5'-C4'-C3'	-5.65	106.96	116.00
2	AB	580	U	O4'-C1'-N1	5.65	112.72	108.20
2	AB	451	U	O4'-C1'-N1	5.65	112.72	108.20
2	AB	1973	G	C5'-C4'-O4'	5.65	115.88	109.10
2	AB	2897	U	C5'-C4'-O4'	5.65	115.88	109.10
2	AB	457	A	P-O3'-C3'	5.65	126.47	119.70
34	BA	686	U	O4'-C4'-C3'	5.65	110.62	106.10
2	AB	133	U	O4'-C1'-N1	5.64	112.72	108.20
2	AB	669	G	N3-C4-C5	-5.64	125.78	128.60
2	AB	1597	A	O4'-C1'-N9	5.64	112.72	108.20
2	AB	2845	U	O4'-C1'-N1	5.64	112.72	108.20
2	AB	368	A	C5'-C4'-O4'	5.64	115.87	109.10
2	AB	1094	U	O4'-C1'-N1	5.64	112.71	108.20
2	AB	2123	G	C8-N9-C4	-5.64	104.14	106.40
2	AB	2214	C	C5'-C4'-C3'	-5.64	106.97	116.00
34	BA	999	C	O4'-C1'-N1	5.64	112.71	108.20
37	BD	28	U	O3'-P-O5'	-5.64	93.28	104.00
2	AB	695	G	O4'-C1'-N9	5.64	112.71	108.20
2	AB	2717	C	C5'-C4'-O4'	5.64	115.87	109.10
2	AB	284	U	O4'-C1'-N1	5.64	112.71	108.20
2	AB	763	G	N3-C4-C5	-5.64	125.78	128.60
2	AB	266	G	N3-C4-C5	-5.64	125.78	128.60
2	AB	1885	A	C5'-C4'-C3'	-5.64	106.98	116.00
2	AB	1346	G	O4'-C1'-N9	5.64	112.71	108.20
2	AB	2350	C	O4'-C1'-N1	5.64	112.71	108.20
2	AB	2821	A	C5'-C4'-C3'	-5.64	106.98	116.00
34	BA	708	C	O4'-C1'-N1	5.64	112.71	108.20
34	BA	1309	G	O4'-C1'-N9	5.64	112.71	108.20
1	AA	50	A	C8-N9-C4	-5.63	103.55	105.80
2	AB	2656	U	O4'-C1'-N1	5.63	112.71	108.20
2	AB	278	A	O3'-P-O5'	-5.63	93.30	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1551	A	O4'-C1'-N9	5.63	112.70	108.20
2	AB	541	A	O4'-C1'-N9	5.63	112.70	108.20
2	AB	1627	G	N3-C4-C5	-5.63	125.79	128.60
2	AB	2337	G	C5'-C4'-C3'	-5.63	106.99	116.00
34	BA	821	G	C5'-C4'-O4'	5.63	115.86	109.10
2	AB	356	G	O4'-C1'-N9	5.63	112.70	108.20
2	AB	392	U	C5'-C4'-O4'	5.63	115.85	109.10
2	AB	1590	A	C5'-C4'-C3'	-5.63	107.00	116.00
2	AB	2731	G	C5'-C4'-O4'	5.63	115.85	109.10
34	BA	607	A	O4'-C1'-N9	5.63	112.70	108.20
35	BE	6	G	O3'-P-O5'	-5.63	93.31	104.00
2	AB	242	G	C3'-C2'-C1'	-5.62	97.00	101.50
2	AB	545	U	C4'-C3'-O3'	5.62	124.25	113.00
34	BA	1100	C	C5'-C4'-O4'	5.62	115.85	109.10
34	BA	1385	G	C5'-C4'-O4'	5.62	115.85	109.10
2	AB	2262	U	C5'-C4'-O4'	5.62	115.85	109.10
34	BA	892	A	C5'-C4'-C3'	-5.62	107.00	116.00
2	AB	1988	G	C5'-C4'-O4'	5.62	115.84	109.10
2	AB	2554	U	O3'-P-O5'	-5.62	93.32	104.00
34	BA	183	C	C5'-C4'-C3'	-5.62	107.00	116.00
34	BA	699	C	O4'-C1'-N1	5.62	112.70	108.20
34	BA	774	G	C5'-C4'-O4'	5.62	115.84	109.10
2	AB	2043	C	C5'-C4'-C3'	-5.62	107.01	116.00
2	AB	2431	U	C2'-C3'-O3'	5.62	122.69	113.70
2	AB	2791	G	C5'-C4'-C3'	-5.62	107.01	116.00
34	BA	1178	G	N9-C4-C5	5.62	107.65	105.40
35	BE	13	C	O3'-P-O5'	5.62	114.68	104.00
2	AB	378	C	C5'-C4'-O4'	5.62	115.84	109.10
2	AB	492	A	C8-N9-C4	-5.62	103.55	105.80
34	BA	416	G	O4'-C1'-N9	5.62	112.69	108.20
2	AB	2885	G	C8-N9-C4	-5.62	104.15	106.40
34	BA	166	U	O4'-C1'-N1	5.62	112.69	108.20
2	AB	424	G	C5'-C4'-C3'	-5.61	107.02	116.00
2	AB	2666	C	N1-C1'-C2'	-5.61	105.83	112.00
34	BA	4	U	C5'-C4'-O4'	5.61	115.84	109.10
34	BA	41	G	O4'-C1'-N9	5.61	112.69	108.20
34	BA	226	G	C5'-C4'-O4'	5.61	115.84	109.10
2	AB	2506	U	C4'-C3'-C2'	-5.61	96.99	102.60
34	BA	130	A	O4'-C1'-N9	5.61	112.69	108.20
2	AB	2560	A	O3'-P-O5'	-5.61	93.34	104.00
34	BA	900	A	C3'-C2'-C1'	5.61	105.99	101.50
1	AA	32	U	N1-C2-N3	5.61	118.27	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	428	A	O4'-C1'-N9	5.61	112.69	108.20
2	AB	2256	G	C8-N9-C4	-5.61	104.16	106.40
2	AB	2853	C	O4'-C1'-N1	5.61	112.69	108.20
34	BA	421	U	O4'-C1'-N1	5.61	112.69	108.20
2	AB	498	G	O4'-C1'-N9	5.61	112.69	108.20
2	AB	674	G	O4'-C1'-N9	5.61	112.68	108.20
2	AB	2648	G	C8-N9-C4	-5.61	104.16	106.40
34	BA	347	G	N3-C4-C5	-5.61	125.80	128.60
34	BA	453	G	N7-C8-N9	5.61	115.90	113.10
34	BA	471	U	O4'-C1'-N1	5.61	112.69	108.20
34	BA	955	U	N1-C1'-C2'	-5.61	105.83	112.00
34	BA	1148	U	O4'-C1'-N1	5.61	112.68	108.20
2	AB	2788	C	O4'-C1'-N1	5.60	112.68	108.20
2	AB	976	G	C5'-C4'-O4'	5.60	115.82	109.10
2	AB	1454	C	O4'-C1'-N1	5.60	112.68	108.20
34	BA	347	G	N9-C1'-C2'	-5.60	105.84	112.00
34	BA	394	G	C5'-C4'-O4'	5.60	115.82	109.10
2	AB	714	U	C5'-C4'-C3'	-5.60	107.04	116.00
2	AB	921	C	C5'-C4'-C3'	-5.60	107.04	116.00
2	AB	1256	G	N3-C4-C5	-5.60	125.80	128.60
2	AB	1511	G	O4'-C1'-N9	5.60	112.68	108.20
2	AB	2040	G	N3-C4-C5	-5.60	125.80	128.60
34	BA	810	C	O4'-C1'-N1	5.60	112.68	108.20
2	AB	439	A	O4'-C1'-N9	5.60	112.68	108.20
34	BA	991	U	O4'-C4'-C3'	5.60	110.58	106.10
2	AB	564	C	O4'-C1'-N1	5.59	112.68	108.20
2	AB	1243	C	O4'-C1'-N1	5.59	112.68	108.20
2	AB	2626	C	O4'-C1'-N1	5.59	112.68	108.20
34	BA	769	G	C5'-C4'-O4'	5.59	115.81	109.10
2	AB	1195	G	N9-C1'-C2'	-5.59	105.85	112.00
2	AB	2272	U	O4'-C1'-N1	5.59	112.67	108.20
34	BA	1201	A	C3'-C2'-C1'	5.59	105.97	101.50
34	BA	585	G	N3-C4-C5	-5.59	125.81	128.60
34	BA	1415	G	O4'-C1'-N9	5.59	112.67	108.20
34	BA	1418	A	O4'-C1'-N9	5.59	112.67	108.20
2	AB	18	U	O4'-C1'-N1	5.59	112.67	108.20
2	AB	141	G	C5'-C4'-O4'	5.59	115.81	109.10
2	AB	969	G	O4'-C1'-N9	5.59	112.67	108.20
2	AB	2317	A	O4'-C1'-N9	5.59	112.67	108.20
2	AB	966	G	C8-N9-C4	-5.59	104.17	106.40
34	BA	1152	A	C3'-C2'-C1'	5.59	105.97	101.50
34	BA	1223	C	O4'-C4'-C3'	5.59	110.57	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	332	A	O4'-C1'-C2'	-5.58	100.22	105.80
2	AB	1986	C	C5'-C4'-C3'	-5.58	107.07	116.00
34	BA	280	C	O4'-C1'-N1	5.58	112.67	108.20
35	BB	28	G	C8-N9-C4	-5.58	104.17	106.40
2	AB	1483	G	C8-N9-C4	-5.58	104.17	106.40
2	AB	1645	G	C3'-C2'-C1'	5.58	105.97	101.50
2	AB	2283	C	O4'-C1'-N1	5.58	112.67	108.20
34	BA	1017	U	C5'-C4'-O4'	5.58	115.80	109.10
34	BA	1200	C	N1-C2-O2	5.58	122.25	118.90
2	AB	11	C	O4'-C1'-C2'	-5.58	100.22	105.80
2	AB	1119	U	C5'-C4'-O4'	5.58	115.80	109.10
2	AB	1624	U	O4'-C1'-N1	5.58	112.66	108.20
34	BA	1440	U	O4'-C1'-N1	5.58	112.66	108.20
2	AB	895	U	O3'-P-O5'	-5.58	93.40	104.00
2	AB	2871	U	O4'-C1'-N1	5.58	112.66	108.20
34	BA	855	U	C5'-C4'-O4'	5.58	115.80	109.10
34	BA	1223	C	C3'-C2'-C1'	5.58	105.96	101.50
34	BA	1277	C	O4'-C1'-N1	5.58	112.66	108.20
2	AB	1069	A	O4'-C4'-C3'	5.58	110.56	106.10
2	AB	2073	C	C5'-C4'-O4'	5.58	115.79	109.10
2	AB	2175	C	C4'-C3'-C2'	5.58	108.17	102.60
2	AB	2756	U	P-O3'-C3'	5.58	126.39	119.70
34	BA	147	G	N3-C4-C5	-5.58	125.81	128.60
1	AA	103	U	O4'-C1'-N1	5.57	112.66	108.20
2	AB	964	C	C5'-C4'-O4'	5.57	115.79	109.10
2	AB	997	G	O4'-C1'-N9	5.57	112.66	108.20
2	AB	1725	U	C5'-C4'-O4'	5.57	115.79	109.10
34	BA	980	C	N1-C2-O2	5.57	122.25	118.90
35	BB	36	A	C5'-C4'-O4'	5.57	115.79	109.10
34	BA	1435	G	C8-N9-C4	-5.57	104.17	106.40
2	AB	1038	G	N3-C4-C5	-5.57	125.81	128.60
2	AB	2477	U	O4'-C4'-C3'	5.57	110.56	106.10
34	BA	56	U	O4'-C1'-N1	5.57	112.66	108.20
34	BA	327	A	O4'-C1'-N9	5.57	112.66	108.20
34	BA	1109	C	C5'-C4'-C3'	-5.57	107.09	116.00
2	AB	325	G	N9-C1'-C2'	-5.57	105.87	112.00
2	AB	2738	A	O4'-C1'-N9	5.57	112.66	108.20
34	BA	651	C	C1'-O4'-C4'	-5.57	105.44	109.90
2	AB	481	G	N3-C4-C5	-5.57	125.82	128.60
2	AB	1652	A	C5'-C4'-O4'	5.57	115.78	109.10
2	AB	2268	A	N9-C1'-C2'	-5.57	105.88	112.00
34	BA	1161	C	O4'-C1'-N1	5.57	112.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1145	C	C5'-C4'-O4'	5.57	115.78	109.10
2	AB	2276	G	C5'-C4'-O4'	5.57	115.78	109.10
34	BA	1337	G	P-O3'-C3'	5.57	126.38	119.70
2	AB	617	G	O4'-C1'-N9	5.56	112.65	108.20
2	AB	1640	A	O4'-C1'-N9	5.56	112.65	108.20
34	BA	1264	U	O4'-C1'-N1	5.56	112.65	108.20
2	AB	681	G	C5'-C4'-O4'	5.56	115.78	109.10
2	AB	1699	G	C5'-C4'-C3'	-5.56	107.10	116.00
2	AB	2133	G	C8-N9-C4	-5.56	104.17	106.40
2	AB	2815	C	C5'-C4'-O4'	5.56	115.78	109.10
34	BA	70	U	N3-C2-O2	-5.56	118.31	122.20
2	AB	767	U	C5'-C4'-C3'	-5.56	107.10	116.00
2	AB	1685	C	O4'-C1'-N1	5.56	112.65	108.20
2	AB	2187	U	C5'-C4'-O4'	5.56	115.77	109.10
2	AB	725	G	P-O3'-C3'	5.56	126.37	119.70
2	AB	862	G	C8-N9-C4	-5.56	104.18	106.40
34	BA	1485	U	O4'-C1'-N1	5.56	112.65	108.20
2	AB	521	U	C5'-C4'-O4'	5.56	115.77	109.10
2	AB	2170	A	O4'-C1'-N9	5.56	112.65	108.20
34	BA	531	U	O4'-C1'-C2'	-5.56	100.24	105.80
2	AB	2161	C	N1-C2-O2	5.55	122.23	118.90
2	AB	182	A	O4'-C1'-N9	5.55	112.64	108.20
2	AB	718	A	C5'-C4'-C3'	-5.55	107.12	116.00
2	AB	1726	C	C5'-C4'-C3'	-5.55	107.12	116.00
2	AB	1933	G	C4'-C3'-C2'	-5.55	97.05	102.60
34	BA	970	C	O4'-C1'-N1	5.55	112.64	108.20
2	AB	427	U	C5'-C4'-O4'	5.55	115.76	109.10
2	AB	2192	U	O4'-C1'-N1	5.55	112.64	108.20
2	AB	2862	G	C5'-C4'-O4'	5.55	115.76	109.10
34	BA	1102	A	C5'-C4'-O4'	5.55	115.76	109.10
34	BA	1118	U	O4'-C1'-N1	5.55	112.64	108.20
1	AA	2	G	N3-C4-C5	-5.55	125.83	128.60
2	AB	817	C	C5'-C4'-O4'	5.55	115.76	109.10
2	AB	1437	C	O4'-C1'-N1	5.55	112.64	108.20
2	AB	2534	A	C5'-C4'-O4'	5.55	115.76	109.10
34	BA	123	U	C5'-C4'-C3'	-5.55	107.13	116.00
2	AB	282	A	O4'-C1'-N9	5.54	112.64	108.20
2	AB	1555	G	C8-N9-C4	-5.54	104.18	106.40
2	AB	1921	G	O4'-C1'-N9	5.54	112.64	108.20
2	AB	2492	U	O4'-C1'-N1	5.54	112.63	108.20
34	BA	61	G	C8-N9-C4	-5.54	104.18	106.40
34	BA	194	C	C5'-C4'-O4'	5.54	115.75	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1108	G	O4'-C1'-N9	5.54	112.64	108.20
2	AB	1454	C	N3-C2-O2	-5.54	118.02	121.90
2	AB	2278	A	O4'-C1'-N9	5.54	112.63	108.20
2	AB	2673	G	C3'-C2'-C1'	-5.54	97.07	101.50
34	BA	1144	G	C5'-C4'-O4'	5.54	115.75	109.10
34	BA	1333	A	C5'-C4'-O4'	5.54	115.75	109.10
2	AB	900	A	C8-N9-C4	-5.54	103.58	105.80
2	AB	1566	A	C5'-C4'-O4'	5.54	115.75	109.10
34	BA	906	A	O4'-C1'-N9	5.54	112.63	108.20
34	BA	1021	A	N9-C1'-C2'	-5.54	105.91	112.00
34	BA	1456	A	O3'-P-O5'	-5.54	93.48	104.00
2	AB	1573	G	C5'-C4'-C3'	-5.54	107.14	116.00
2	AB	1947	C	O4'-C1'-N1	5.54	112.63	108.20
34	BA	637	C	O4'-C1'-N1	5.54	112.63	108.20
1	AA	114	C	O4'-C1'-N1	5.54	112.63	108.20
2	AB	1201	U	O4'-C1'-N1	5.54	112.63	108.20
34	BA	1267	C	O4'-C1'-N1	5.54	112.63	108.20
2	AB	274	C	O4'-C1'-N1	5.53	112.63	108.20
2	AB	1746	A	O4'-C1'-N9	5.53	112.63	108.20
2	AB	2249	U	O4'-C4'-C3'	5.53	110.53	106.10
2	AB	2365	G	C8-N9-C4	-5.53	104.19	106.40
34	BA	480	U	C5'-C4'-C3'	-5.53	107.15	116.00
34	BA	1199	U	O4'-C1'-N1	5.53	112.63	108.20
2	AB	1140	C	O4'-C1'-N1	5.53	112.63	108.20
2	AB	2864	G	C5'-C4'-O4'	5.53	115.74	109.10
34	BA	339	C	O4'-C1'-N1	5.53	112.63	108.20
34	BA	556	C	O4'-C1'-N1	5.53	112.62	108.20
34	BA	601	G	N9-C1'-C2'	-5.53	105.92	112.00
34	BA	844	G	C8-N9-C4	-5.53	104.19	106.40
1	AA	107	G	O4'-C1'-N9	5.53	112.62	108.20
2	AB	1997	C	O4'-C1'-N1	5.53	112.62	108.20
34	BA	200	G	C5'-C4'-C3'	-5.53	107.15	116.00
34	BA	1297	G	O4'-C1'-N9	5.53	112.62	108.20
34	BA	1510	C	C5'-C4'-O4'	5.53	115.74	109.10
37	BD	39	U	O4'-C1'-N1	5.53	112.62	108.20
2	AB	1433	A	O4'-C1'-N9	5.53	112.62	108.20
2	AB	660	C	C5'-C4'-C3'	-5.53	107.16	116.00
2	AB	1685	C	C5'-C4'-O4'	5.53	115.73	109.10
2	AB	2047	C	O4'-C1'-N1	5.53	112.62	108.20
34	BA	1096	C	N1-C2-O2	5.53	122.22	118.90
2	AB	1645	G	O4'-C4'-C3'	5.53	110.52	106.10
2	AB	1740	G	C8-N9-C4	-5.53	104.19	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	14	A	O4'-C1'-N9	5.53	112.62	108.20
34	BA	473	U	O4'-C1'-N1	5.52	112.62	108.20
34	BA	1115	U	O4'-C1'-N1	5.52	112.62	108.20
57	BY	1	PRO	CA-N-CD	-5.52	103.77	111.50
2	AB	1222	U	O4'-C1'-N1	5.52	112.62	108.20
2	AB	2114	A	O4'-C1'-N9	5.52	112.62	108.20
34	BA	521	G	N3-C4-C5	-5.52	125.84	128.60
34	BA	529	G	O4'-C1'-N9	5.52	112.62	108.20
34	BA	1150	A	C5'-C4'-C3'	-5.52	107.16	116.00
2	AB	2786	U	O4'-C1'-N1	5.52	112.62	108.20
2	AB	1804	C	O4'-C1'-N1	5.52	112.62	108.20
1	AA	20	G	C8-N9-C4	-5.52	104.19	106.40
2	AB	469	G	C8-N9-C4	-5.52	104.19	106.40
2	AB	1022	G	O4'-C1'-N9	5.52	112.61	108.20
2	AB	2506	U	O4'-C1'-N1	5.52	112.61	108.20
34	BA	414	A	O4'-C1'-N9	5.52	112.61	108.20
34	BA	643	C	O4'-C1'-N1	5.52	112.61	108.20
34	BA	1502	A	C5'-C4'-C3'	-5.52	107.17	116.00
2	AB	2664	G	N7-C8-N9	5.51	115.86	113.10
34	BA	1284	C	O4'-C1'-N1	5.51	112.61	108.20
2	AB	1092	C	O4'-C1'-N1	5.51	112.61	108.20
2	AB	1890	A	O4'-C1'-N9	5.51	112.61	108.20
2	AB	1796	U	O4'-C1'-N1	5.51	112.61	108.20
2	AB	2627	G	C8-N9-C4	-5.51	104.19	106.40
2	AB	2557	G	O4'-C1'-N9	5.51	112.61	108.20
34	BA	1040	U	C5'-C4'-O4'	5.51	115.71	109.10
34	BA	1074	G	C5'-C4'-O4'	5.51	115.71	109.10
1	AA	105	G	O4'-C1'-N9	5.51	112.61	108.20
2	AB	335	C	O4'-C1'-N1	5.51	112.61	108.20
2	AB	665	U	O4'-C1'-N1	5.51	112.61	108.20
2	AB	1114	C	C5'-C4'-C3'	-5.51	107.19	116.00
2	AB	2087	G	N3-C4-C5	-5.51	125.85	128.60
2	AB	829	A	O4'-C1'-N9	5.51	112.61	108.20
34	BA	357	G	O4'-C1'-N9	5.51	112.61	108.20
34	BA	1289	A	O4'-C1'-N9	5.51	112.61	108.20
34	BA	1386	G	O4'-C1'-N9	5.51	112.61	108.20
2	AB	371	A	O4'-C1'-N9	5.50	112.60	108.20
2	AB	2282	G	O4'-C1'-N9	5.50	112.60	108.20
2	AB	2419	U	O4'-C1'-N1	5.50	112.60	108.20
2	AB	2896	C	C1'-O4'-C4'	-5.50	105.50	109.90
34	BA	1047	G	C8-N9-C4	-5.50	104.20	106.40
1	AA	50	A	C5'-C4'-O4'	5.50	115.70	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	924	G	C3'-C2'-C1'	-5.50	97.10	101.50
2	AB	2299	U	C5'-C4'-C3'	-5.50	107.20	116.00
34	BA	728	A	C5'-C4'-O4'	5.50	115.70	109.10
2	AB	308	G	C3'-C2'-C1'	5.50	105.90	101.50
34	BA	80	A	O4'-C1'-N9	5.50	112.60	108.20
34	BA	139	A	C5'-C4'-C3'	-5.50	107.20	116.00
34	BA	806	C	C5'-C4'-O4'	5.50	115.70	109.10
34	BA	1469	C	C5'-C4'-O4'	5.50	115.70	109.10
2	AB	270	A	C3'-C2'-C1'	-5.50	97.10	101.50
2	AB	356	G	C8-N9-C4	-5.50	104.20	106.40
2	AB	2049	G	O4'-C1'-N9	5.50	112.60	108.20
34	BA	995	C	O4'-C1'-N1	5.50	112.60	108.20
34	BA	1340	A	O4'-C1'-N9	5.50	112.60	108.20
2	AB	740	C	C5'-C4'-O4'	5.49	115.69	109.10
2	AB	2068	U	O4'-C1'-N1	5.49	112.59	108.20
2	AB	1211	C	O4'-C1'-N1	5.49	112.59	108.20
34	BA	164	G	C5'-C4'-C3'	-5.49	107.21	116.00
34	BA	972	C	N1-C1'-C2'	-5.49	105.96	112.00
2	AB	2611	C	C5'-C4'-C3'	-5.49	107.21	116.00
37	BD	35	U	O4'-C1'-N1	5.49	112.59	108.20
1	AA	84	G	N9-C1'-C2'	-5.49	105.96	112.00
2	AB	305	C	C5'-C4'-O4'	5.49	115.69	109.10
2	AB	843	G	N3-C4-C5	-5.49	125.86	128.60
2	AB	2459	A	C8-N9-C4	-5.49	103.60	105.80
2	AB	2647	U	O4'-C1'-N1	5.49	112.59	108.20
34	BA	215	C	C5'-C4'-C3'	-5.49	107.22	116.00
2	AB	278	A	C5'-C4'-O4'	5.49	115.69	109.10
2	AB	1035	U	C5'-C4'-O4'	5.49	115.69	109.10
2	AB	2802	G	N9-C1'-C2'	-5.49	105.96	112.00
2	AB	903	C	C5'-C4'-O4'	5.49	115.68	109.10
2	AB	1084	A	C1'-O4'-C4'	-5.49	105.51	109.90
2	AB	1740	G	O4'-C1'-N9	5.48	112.59	108.20
2	AB	1984	G	O4'-C1'-N9	5.48	112.59	108.20
34	BA	355	C	N3-C2-O2	-5.48	118.06	121.90
2	AB	2408	U	C5'-C4'-O4'	5.48	115.68	109.10
34	BA	740	U	O4'-C1'-N1	5.48	112.58	108.20
34	BA	1022	A	O4'-C1'-N9	5.48	112.58	108.20
2	AB	1574	C	O4'-C1'-N1	5.48	112.58	108.20
2	AB	2472	G	C8-N9-C4	-5.48	104.21	106.40
2	AB	1822	C	C2-N3-C4	5.48	122.64	119.90
2	AB	2588	G	C8-N9-C4	-5.48	104.21	106.40
34	BA	326	G	C8-N9-C4	-5.48	104.21	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1377	A	C4'-C3'-C2'	-5.48	97.12	102.60
2	AB	2878	U	O4'-C1'-N1	5.48	112.58	108.20
2	AB	974	G	N3-C4-C5	-5.47	125.86	128.60
2	AB	1184	U	C5'-C4'-C3'	-5.47	107.24	116.00
2	AB	2606	C	O4'-C1'-N1	5.47	112.58	108.20
1	AA	75	G	C8-N9-C4	-5.47	104.21	106.40
2	AB	635	C	O4'-C1'-N1	5.47	112.58	108.20
2	AB	1852	U	P-O3'-C3'	5.47	126.27	119.70
2	AB	2447	G	P-O3'-C3'	5.47	126.27	119.70
34	BA	1244	G	O4'-C1'-N9	5.47	112.58	108.20
2	AB	1483	G	C5'-C4'-O4'	5.47	115.66	109.10
34	BA	587	G	C5'-C4'-C3'	-5.47	107.25	116.00
34	BA	1228	C	O4'-C4'-C3'	5.47	110.47	106.10
34	BA	1021	A	C4'-C3'-C2'	-5.47	97.13	102.60
2	AB	374	A	C5'-C4'-O4'	5.46	115.66	109.10
2	AB	2400	G	O4'-C1'-N9	5.46	112.57	108.20
34	BA	32	A	O4'-C1'-N9	5.46	112.57	108.20
34	BA	346	G	C2-N3-C4	5.46	114.63	111.90
2	AB	2685	G	O4'-C1'-N9	5.46	112.57	108.20
34	BA	545	C	O4'-C1'-N1	5.46	112.57	108.20
2	AB	1724	G	N3-C4-C5	-5.46	125.87	128.60
2	AB	2308	G	C8-N9-C4	-5.46	104.22	106.40
2	AB	119	A	C5'-C4'-C3'	-5.46	107.26	116.00
2	AB	1355	G	O4'-C1'-N9	5.46	112.57	108.20
34	BA	12	U	O4'-C1'-N1	5.46	112.57	108.20
2	AB	398	C	O4'-C1'-N1	5.46	112.57	108.20
2	AB	671	C	C4'-C3'-C2'	-5.46	97.14	102.60
2	AB	984	A	N9-C1'-C2'	5.46	121.09	114.00
18	AR	23	TYR	CB-CG-CD1	-5.46	117.72	121.00
2	AB	2354	C	O4'-C1'-N1	5.46	112.57	108.20
2	AB	479	A	P-O3'-C3'	5.46	126.25	119.70
2	AB	554	U	C5'-C4'-C3'	-5.46	107.27	116.00
2	AB	2451	A	O4'-C1'-N9	5.45	112.56	108.20
2	AB	2846	G	C8-N9-C4	-5.45	104.22	106.40
34	BA	964	A	O4'-C1'-N9	5.45	112.56	108.20
1	AA	38	C	O4'-C1'-N1	5.45	112.56	108.20
34	BA	731	G	C5'-C4'-O4'	5.45	115.64	109.10
2	AB	623	C	O4'-C1'-N1	5.45	112.56	108.20
2	AB	656	G	C8-N9-C4	-5.45	104.22	106.40
2	AB	925	A	O4'-C1'-N9	5.45	112.56	108.20
2	AB	1561	C	O4'-C1'-N1	5.45	112.56	108.20
34	BA	107	G	C5'-C4'-O4'	5.45	115.64	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	527	C	N1-C2-O2	5.45	122.17	118.90
2	AB	1002	G	C8-N9-C4	-5.45	104.22	106.40
35	BB	53	G	O4'-C1'-N9	5.45	112.56	108.20
1	AA	32	U	N3-C2-O2	-5.45	118.39	122.20
2	AB	345	A	P-O3'-C3'	5.44	126.23	119.70
2	AB	2640	G	C5'-C4'-O4'	5.44	115.63	109.10
2	AB	1723	G	C8-N9-C4	-5.44	104.22	106.40
3	AC	228	GLY	C-N-CA	5.44	135.31	121.70
34	BA	790	A	C5'-C4'-O4'	5.44	115.63	109.10
34	BA	1272	G	O4'-C1'-N9	5.44	112.55	108.20
2	AB	40	U	O4'-C1'-N1	5.44	112.55	108.20
2	AB	549	G	N3-C4-C5	-5.44	125.88	128.60
2	AB	1360	G	N9-C4-C5	5.44	107.58	105.40
34	BA	292	G	C4'-C3'-C2'	-5.44	97.16	102.60
2	AB	6	A	C5'-C4'-O4'	5.44	115.63	109.10
2	AB	2439	A	C5'-C4'-C3'	-5.44	107.30	116.00
2	AB	832	U	C5'-C4'-C3'	-5.44	107.30	116.00
2	AB	917	A	O4'-C1'-N9	5.44	112.55	108.20
2	AB	1410	G	N3-C4-C5	-5.44	125.88	128.60
2	AB	2401	U	O4'-C1'-N1	5.44	112.55	108.20
37	BD	37	U	O4'-C1'-N1	5.44	112.55	108.20
1	AA	14	U	C1'-O4'-C4'	-5.44	105.55	109.90
2	AB	545	U	O4'-C1'-N1	5.43	112.55	108.20
2	AB	690	G	C8-N9-C4	-5.43	104.23	106.40
2	AB	768	G	C5'-C4'-O4'	5.43	115.62	109.10
2	AB	1507	C	C4'-C3'-C2'	-5.43	97.17	102.60
2	AB	1847	A	C1'-O4'-C4'	-5.43	105.55	109.90
2	AB	2488	G	N3-C4-C5	-5.43	125.88	128.60
34	BA	347	G	C8-N9-C4	-5.43	104.23	106.40
34	BA	636	U	C5'-C4'-O4'	5.43	115.62	109.10
2	AB	2363	G	C8-N9-C4	-5.43	104.23	106.40
34	BA	9	G	O4'-C1'-N9	5.43	112.55	108.20
34	BA	1086	U	C5'-C4'-O4'	5.43	115.62	109.10
2	AB	217	A	C5'-C4'-C3'	-5.43	107.31	116.00
1	AA	43	C	O4'-C1'-N1	5.43	112.54	108.20
2	AB	15	G	N7-C8-N9	5.43	115.81	113.10
2	AB	421	C	O4'-C1'-N1	5.43	112.54	108.20
2	AB	547	A	O4'-C1'-N9	5.43	112.54	108.20
2	AB	1893	C	O4'-C1'-N1	5.43	112.54	108.20
2	AB	2136	G	C5'-C4'-O4'	5.43	115.62	109.10
2	AB	2711	A	O4'-C1'-N9	5.43	112.54	108.20
34	BA	1184	G	C5'-C4'-O4'	5.43	115.62	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2162	G	C5'-C4'-C3'	-5.43	107.31	116.00
34	BA	139	A	C4'-C3'-C2'	-5.43	97.17	102.60
34	BA	1319	A	O4'-C1'-N9	5.43	112.54	108.20
2	AB	242	G	C5'-C4'-C3'	-5.43	107.32	116.00
2	AB	2705	A	C4'-C3'-C2'	-5.43	97.17	102.60
34	BA	1061	G	N7-C8-N9	5.43	115.81	113.10
34	BA	1213	A	C2'-C3'-O3'	5.43	122.38	113.70
2	AB	623	C	C5'-C4'-C3'	-5.42	107.32	116.00
2	AB	2020	A	C1'-O4'-C4'	-5.42	105.56	109.90
2	AB	2571	U	P-O3'-C3'	5.42	126.21	119.70
34	BA	168	G	C5'-C4'-O4'	5.42	115.61	109.10
2	AB	240	C	O4'-C1'-N1	5.42	112.54	108.20
2	AB	253	C	C5'-C4'-O4'	5.42	115.61	109.10
2	AB	764	A	O4'-C1'-N9	5.42	112.54	108.20
2	AB	767	U	O4'-C1'-N1	5.42	112.54	108.20
34	BA	403	C	C5'-C4'-O4'	5.42	115.61	109.10
34	BA	1280	A	C5'-C4'-C3'	-5.42	107.33	116.00
2	AB	119	A	O4'-C1'-N9	5.42	112.54	108.20
2	AB	1410	G	C8-N9-C4	-5.42	104.23	106.40
2	AB	2562	U	O4'-C1'-N1	5.42	112.54	108.20
34	BA	85	U	C1'-O4'-C4'	-5.42	105.56	109.90
2	AB	1603	A	C5'-C4'-C3'	-5.42	107.33	116.00
34	BA	439	U	N1-C2-N3	5.42	118.15	114.90
34	BA	909	A	O3'-P-O5'	5.42	114.29	104.00
1	AA	75	G	O4'-C1'-N9	5.42	112.53	108.20
2	AB	531	C	O4'-C4'-C3'	5.42	110.43	106.10
2	AB	987	C	O4'-C1'-N1	5.42	112.53	108.20
2	AB	2263	C	O4'-C1'-N1	5.42	112.53	108.20
34	BA	234	C	O4'-C1'-N1	5.42	112.53	108.20
34	BA	1230	C	O4'-C1'-N1	5.42	112.53	108.20
2	AB	769	U	C5'-C4'-O4'	5.42	115.60	109.10
2	AB	1952	A	O4'-C4'-C3'	5.41	110.43	106.10
2	AB	2186	G	O4'-C1'-N9	5.41	112.53	108.20
2	AB	2806	C	O4'-C1'-N1	5.41	112.53	108.20
34	BA	715	A	O4'-C1'-N9	5.41	112.53	108.20
2	AB	536	G	O4'-C1'-N9	5.41	112.53	108.20
2	AB	763	G	C8-N9-C4	-5.41	104.23	106.40
34	BA	336	A	O4'-C1'-N9	5.41	112.53	108.20
1	AA	107	G	N7-C8-N9	5.41	115.81	113.10
2	AB	735	A	O4'-C1'-N9	5.41	112.53	108.20
2	AB	824	U	C5'-C4'-O4'	5.41	115.59	109.10
2	AB	1495	A	O4'-C1'-N9	5.41	112.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	491	G	C8-N9-C4	-5.41	104.24	106.40
2	AB	554	U	C5'-C4'-O4'	5.41	115.59	109.10
2	AB	787	C	O4'-C1'-N1	5.41	112.53	108.20
2	AB	1139	G	O4'-C1'-N9	5.41	112.53	108.20
2	AB	2174	C	O4'-C1'-N1	5.41	112.53	108.20
34	BA	136	C	O4'-C1'-N1	5.41	112.53	108.20
34	BA	861	G	N3-C4-C5	-5.41	125.90	128.60
34	BA	1008	U	C5'-C4'-O4'	5.41	115.59	109.10
34	BA	1256	A	O4'-C1'-N9	5.41	112.53	108.20
34	BA	277	C	N1-C1'-C2'	-5.41	106.05	112.00
2	AB	842	U	C5'-C4'-C3'	-5.41	107.35	116.00
2	AB	1566	A	C5'-C4'-C3'	-5.41	107.35	116.00
2	AB	742	A	O4'-C1'-N9	5.40	112.52	108.20
2	AB	2735	G	C5'-C4'-O4'	5.40	115.58	109.10
34	BA	175	C	C5'-C4'-O4'	5.40	115.58	109.10
34	BA	1242	G	C8-N9-C4	-5.40	104.24	106.40
2	AB	545	U	O3'-P-O5'	-5.40	93.74	104.00
2	AB	1332	G	N3-C4-C5	-5.40	125.90	128.60
2	AB	2398	U	C5'-C4'-C3'	-5.40	107.36	116.00
34	BA	356	A	O4'-C1'-N9	5.40	112.52	108.20
34	BA	793	U	O3'-P-O5'	-5.40	93.74	104.00
34	BA	1090	U	N1-C1'-C2'	-5.40	106.06	112.00
2	AB	383	C	N1-C2-O2	5.40	122.14	118.90
2	AB	996	A	C5'-C4'-O4'	5.40	115.58	109.10
2	AB	2309	A	O4'-C1'-N9	5.40	112.52	108.20
34	BA	705	G	C8-N9-C4	-5.40	104.24	106.40
34	BA	913	A	P-O3'-C3'	5.40	126.18	119.70
2	AB	1292	G	O3'-P-O5'	-5.40	93.74	104.00
34	BA	1138	G	N3-C4-C5	-5.40	125.90	128.60
1	AA	13	G	C4'-C3'-O3'	5.40	123.80	113.00
2	AB	1164	C	O4'-C1'-N1	5.40	112.52	108.20
2	AB	389	G	C8-N9-C4	-5.40	104.24	106.40
2	AB	1118	C	C5'-C4'-C3'	-5.40	107.37	116.00
2	AB	2234	G	C8-N9-C4	-5.40	104.24	106.40
2	AB	2299	U	C5'-C4'-O4'	5.40	115.58	109.10
34	BA	253	A	O3'-P-O5'	-5.40	93.75	104.00
2	AB	1710	G	C5'-C4'-C3'	-5.39	107.37	116.00
2	AB	2677	G	O4'-C1'-N9	5.39	112.52	108.20
2	AB	2902	C	O4'-C1'-N1	5.39	112.52	108.20
34	BA	310	G	N3-C4-C5	-5.39	125.90	128.60
2	AB	1799	G	O4'-C1'-N9	5.39	112.52	108.20
2	AB	1822	C	N1-C2-O2	5.39	122.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2471	A	O4'-C1'-N9	5.39	112.51	108.20
34	BA	1061	G	N3-C4-C5	-5.39	125.90	128.60
2	AB	72	U	O4'-C4'-C3'	5.39	110.41	106.10
2	AB	121	G	N3-C4-C5	-5.39	125.91	128.60
2	AB	123	G	C5'-C4'-O4'	5.39	115.57	109.10
2	AB	654	A	P-O3'-C3'	5.39	126.17	119.70
2	AB	2006	C	C5'-C4'-O4'	5.39	115.56	109.10
34	BA	843	U	C3'-C2'-C1'	5.39	105.81	101.50
1	AA	51	G	C8-N9-C4	-5.39	104.25	106.40
2	AB	589	U	O4'-C1'-N1	5.39	112.51	108.20
2	AB	942	G	C8-N9-C4	-5.39	104.25	106.40
34	BA	415	A	N9-C1'-C2'	-5.39	106.08	112.00
2	AB	216	A	N9-C1'-C2'	-5.38	106.08	112.00
2	AB	2842	G	O4'-C1'-N9	5.38	112.51	108.20
34	BA	917	G	N3-C4-C5	-5.38	125.91	128.60
34	BA	1395	C	C5'-C4'-C3'	-5.38	107.38	116.00
2	AB	1403	A	O4'-C1'-N9	5.38	112.51	108.20
34	BA	188	C	O3'-P-O5'	-5.38	93.77	104.00
34	BA	240	G	O4'-C1'-N9	5.38	112.51	108.20
34	BA	378	G	O4'-C1'-N9	5.38	112.51	108.20
2	AB	1444	G	C8-N9-C4	-5.38	104.25	106.40
2	AB	1666	G	O4'-C1'-N9	5.38	112.51	108.20
2	AB	2614	A	O4'-C1'-N9	5.38	112.50	108.20
34	BA	542	G	O4'-C1'-N9	5.38	112.51	108.20
35	BB	72	C	O4'-C1'-N1	5.38	112.50	108.20
2	AB	426	C	O4'-C1'-N1	5.38	112.50	108.20
2	AB	2328	A	C5'-C4'-O4'	5.38	115.55	109.10
2	AB	2890	G	C8-N9-C4	-5.38	104.25	106.40
37	BD	26	U	N3-C2-O2	-5.38	118.44	122.20
34	BA	688	G	N3-C4-C5	-5.38	125.91	128.60
2	AB	337	C	O4'-C1'-N1	5.38	112.50	108.20
2	AB	1214	A	C5'-C4'-C3'	-5.38	107.40	116.00
2	AB	1566	A	C3'-C2'-C1'	5.38	105.80	101.50
2	AB	1812	U	O4'-C1'-N1	5.38	112.50	108.20
34	BA	1001	C	C5'-C4'-C3'	-5.38	107.40	116.00
34	BA	1107	C	O4'-C1'-N1	5.38	112.50	108.20
2	AB	54	G	C8-N9-C4	-5.37	104.25	106.40
2	AB	2083	G	C8-N9-C4	-5.37	104.25	106.40
2	AB	2619	C	C5'-C4'-O4'	5.37	115.55	109.10
34	BA	75	G	O4'-C1'-N9	5.37	112.50	108.20
34	BA	470	C	O4'-C1'-N1	5.37	112.50	108.20
34	BA	1512	U	O4'-C1'-N1	5.37	112.50	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1171	G	O4'-C1'-N9	5.37	112.50	108.20
2	AB	1767	G	N3-C4-C5	-5.37	125.92	128.60
2	AB	2202	U	C5'-C4'-O4'	5.37	115.55	109.10
34	BA	422	C	O4'-C1'-N1	5.37	112.50	108.20
34	BA	1076	U	C2'-C3'-O3'	5.37	122.29	113.70
34	BA	235	C	C5'-C4'-O4'	5.37	115.54	109.10
2	AB	98	G	C8-N9-C4	-5.37	104.25	106.40
34	BA	749	A	C3'-C2'-C1'	-5.37	97.20	101.50
34	BA	777	A	C5'-C4'-C3'	-5.37	107.41	116.00
34	BA	743	A	C5'-C4'-O4'	5.37	115.54	109.10
2	AB	79	C	O4'-C1'-N1	5.37	112.49	108.20
2	AB	329	G	C8-N9-C4	-5.37	104.25	106.40
2	AB	687	C	N1-C2-O2	5.37	122.12	118.90
2	AB	1868	C	C5'-C4'-C3'	-5.37	107.42	116.00
2	AB	2123	G	N9-C4-C5	5.37	107.55	105.40
2	AB	494	G	N9-C1'-C2'	-5.36	106.10	112.00
2	AB	686	U	C5'-C4'-O4'	5.36	115.54	109.10
2	AB	1454	C	C6-N1-C2	-5.36	118.16	120.30
2	AB	2135	A	C3'-C2'-C1'	5.36	105.79	101.50
2	AB	2792	A	P-O5'-C5'	5.36	129.48	120.90
34	BA	72	A	C5'-C4'-C3'	-5.36	107.42	116.00
34	BA	318	G	C3'-C2'-C1'	-5.36	97.21	101.50
2	AB	1718	G	C5'-C4'-O4'	5.36	115.53	109.10
2	AB	401	A	C5'-C4'-C3'	-5.36	107.42	116.00
2	AB	807	U	C4'-C3'-C2'	-5.36	97.24	102.60
2	AB	866	A	C5'-C4'-O4'	5.36	115.53	109.10
2	AB	1138	G	N3-C4-C5	-5.36	125.92	128.60
2	AB	2631	G	C5'-C4'-O4'	5.36	115.53	109.10
34	BA	1038	C	O4'-C1'-N1	5.36	112.49	108.20
35	BE	52	G	O4'-C1'-N9	5.36	112.49	108.20
2	AB	181	A	C3'-C2'-C1'	-5.36	97.21	101.50
2	AB	2800	A	C5'-C4'-C3'	-5.36	107.43	116.00
2	AB	857	G	C8-N9-C1'	5.36	133.96	127.00
2	AB	981	A	C5'-C4'-O4'	5.36	115.53	109.10
2	AB	1474	U	O4'-C1'-N1	5.36	112.48	108.20
2	AB	2186	G	C8-N9-C4	-5.36	104.26	106.40
2	AB	2258	C	P-O3'-C3'	5.35	126.12	119.70
35	BB	69	G	O4'-C1'-N9	5.35	112.48	108.20
2	AB	843	G	C8-N9-C4	-5.35	104.26	106.40
34	BA	1255	G	N9-C4-C5	5.35	107.54	105.40
34	BA	1533	C	O4'-C1'-N1	5.35	112.48	108.20
2	AB	712	G	C8-N9-C4	-5.35	104.26	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1540	G	N3-C4-C5	-5.35	125.93	128.60
2	AB	1737	G	C5'-C4'-C3'	-5.35	107.44	116.00
34	BA	633	G	O4'-C1'-N9	5.35	112.48	108.20
2	AB	841	G	C1'-O4'-C4'	-5.35	105.62	109.90
2	AB	1538	G	O4'-C1'-N9	5.35	112.48	108.20
34	BA	251	G	O4'-C1'-N9	5.35	112.48	108.20
34	BA	1344	C	O4'-C1'-N1	5.35	112.48	108.20
2	AB	545	U	C3'-C2'-C1'	5.35	105.78	101.50
2	AB	2039	U	C5'-C4'-C3'	-5.34	107.45	116.00
2	AB	2345	G	N3-C4-C5	-5.34	125.93	128.60
34	BA	435	A	O4'-C1'-N9	5.34	112.48	108.20
35	BE	6	G	P-O3'-C3'	5.34	126.11	119.70
2	AB	2219	U	O4'-C1'-N1	5.34	112.47	108.20
2	AB	2344	U	O4'-C1'-N1	5.34	112.47	108.20
2	AB	757	G	O4'-C1'-N9	5.34	112.47	108.20
2	AB	1186	G	C8-N9-C4	-5.34	104.26	106.40
34	BA	756	C	O4'-C1'-N1	5.34	112.47	108.20
34	BA	996	A	C5'-C4'-O4'	5.34	115.51	109.10
2	AB	2036	C	N1-C2-O2	5.34	122.10	118.90
2	AB	2639	A	C5'-C4'-C3'	-5.34	107.46	116.00
35	BE	12	U	O4'-C1'-N1	5.34	112.47	108.20
35	BE	19	G	N3-C4-C5	-5.34	125.93	128.60
34	BA	115	G	O4'-C1'-N9	5.33	112.47	108.20
34	BA	1013	G	O4'-C1'-N9	5.33	112.47	108.20
2	AB	1446	C	C5'-C4'-O4'	5.33	115.50	109.10
2	AB	2680	U	O4'-C1'-N1	5.33	112.47	108.20
34	BA	79	G	O4'-C1'-N9	5.33	112.47	108.20
35	BB	66	U	C5'-C4'-O4'	5.33	115.50	109.10
35	BE	61	C	C5'-C4'-C3'	-5.33	107.47	116.00
2	AB	323	C	C5'-C4'-C3'	-5.33	107.47	116.00
2	AB	2666	C	N1-C2-O2	5.33	122.10	118.90
34	BA	909	A	C8-N9-C4	-5.33	103.67	105.80
35	BE	18	G	P-O3'-C3'	5.33	126.10	119.70
2	AB	2550	G	C5'-C4'-O4'	5.33	115.50	109.10
34	BA	1373	G	C5'-C4'-O4'	5.33	115.50	109.10
2	AB	1117	C	O4'-C1'-N1	5.33	112.46	108.20
2	AB	1451	C	C5'-C4'-O4'	5.33	115.49	109.10
2	AB	1680	U	C5'-C4'-O4'	5.33	115.49	109.10
2	AB	1776	G	C5'-C4'-O4'	5.33	115.50	109.10
2	AB	2357	G	C5'-C4'-O4'	5.33	115.50	109.10
2	AB	2399	G	C8-N9-C4	-5.33	104.27	106.40
34	BA	981	U	C5'-C4'-C3'	-5.33	107.47	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BD	44	U	O4'-C1'-N1	5.33	112.46	108.20
1	AA	13	G	N3-C4-C5	-5.33	125.94	128.60
2	AB	1451	C	N1-C2-O2	5.33	122.10	118.90
2	AB	1732	C	O4'-C4'-C3'	5.33	110.36	106.10
2	AB	171	U	O4'-C1'-N1	5.33	112.46	108.20
2	AB	227	A	O4'-C1'-N9	5.33	112.46	108.20
2	AB	968	C	O4'-C1'-N1	5.33	112.46	108.20
2	AB	1455	G	C5'-C4'-O4'	5.33	115.49	109.10
2	AB	1873	G	N3-C4-C5	-5.33	125.94	128.60
2	AB	1159	U	C5'-C4'-O4'	5.32	115.49	109.10
2	AB	2587	A	O4'-C1'-N9	5.32	112.46	108.20
34	BA	602	A	O4'-C1'-N9	5.32	112.46	108.20
35	BE	75	C	O4'-C1'-N1	5.32	112.46	108.20
2	AB	1385	A	C4'-C3'-C2'	-5.32	97.28	102.60
34	BA	1386	G	C8-N9-C4	-5.32	104.27	106.40
2	AB	1236	G	O4'-C1'-N9	5.32	112.46	108.20
2	AB	2261	C	O4'-C1'-N1	5.32	112.46	108.20
2	AB	424	G	N3-C4-C5	-5.32	125.94	128.60
2	AB	514	A	C5'-C4'-O4'	5.32	115.48	109.10
2	AB	2019	A	O4'-C1'-N9	5.32	112.45	108.20
2	AB	875	G	N3-C4-C5	-5.32	125.94	128.60
34	BA	351	G	O4'-C1'-N9	5.32	112.45	108.20
1	AA	3	C	C5'-C4'-O4'	5.32	115.48	109.10
2	AB	1107	G	N3-C4-C5	-5.32	125.94	128.60
34	BA	1310	G	C5'-C4'-O4'	5.32	115.48	109.10
2	AB	1241	A	O4'-C1'-N9	5.31	112.45	108.20
2	AB	2731	G	C8-N9-C4	-5.31	104.27	106.40
34	BA	520	A	C8-N9-C4	-5.31	103.67	105.80
2	AB	1718	G	C8-N9-C4	-5.31	104.28	106.40
2	AB	2301	C	O4'-C1'-N1	5.31	112.45	108.20
35	BE	28	G	N3-C4-C5	-5.31	125.94	128.60
2	AB	1490	A	C8-N9-C4	-5.31	103.68	105.80
2	AB	1552	A	C1'-O4'-C4'	-5.31	105.65	109.90
2	AB	468	G	C8-N9-C4	-5.31	104.28	106.40
34	BA	1058	G	O4'-C1'-N9	5.31	112.45	108.20
2	AB	15	G	N3-C4-C5	-5.31	125.95	128.60
2	AB	2488	G	C8-N9-C4	-5.31	104.28	106.40
34	BA	86	G	C3'-C2'-C1'	5.31	105.75	101.50
34	BA	765	G	C8-N9-C4	-5.31	104.28	106.40
34	BA	933	G	C5'-C4'-C3'	-5.31	107.51	116.00
34	BA	1053	G	P-O3'-C3'	5.31	126.07	119.70
34	BA	1279	G	O5'-C5'-C4'	-5.31	101.61	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	618	G	C8-N9-C4	-5.31	104.28	106.40
2	AB	1817	G	C8-N9-C4	-5.31	104.28	106.40
2	AB	53	A	O4'-C1'-N9	5.30	112.44	108.20
2	AB	678	C	O4'-C1'-N1	5.30	112.44	108.20
2	AB	1588	G	C3'-C2'-C1'	-5.30	97.26	101.50
2	AB	1850	G	O4'-C1'-N9	5.30	112.44	108.20
2	AB	1995	U	O4'-C1'-N1	5.30	112.44	108.20
34	BA	257	G	C5'-C4'-O4'	5.30	115.47	109.10
34	BA	789	U	C5'-C4'-O4'	5.30	115.47	109.10
2	AB	17	G	C8-N9-C4	-5.30	104.28	106.40
2	AB	1726	C	O4'-C1'-N1	5.30	112.44	108.20
2	AB	2190	G	C5'-C4'-C3'	-5.30	107.52	116.00
34	BA	331	G	O4'-C1'-N9	5.30	112.44	108.20
2	AB	1263	U	O4'-C1'-N1	5.30	112.44	108.20
34	BA	376	G	O4'-C1'-N9	5.30	112.44	108.20
34	BA	815	A	C4'-C3'-C2'	-5.30	97.30	102.60
2	AB	1165	A	C5'-C4'-O4'	5.30	115.46	109.10
2	AB	2238	G	N3-C4-C5	-5.30	125.95	128.60
2	AB	2692	G	N3-C4-C5	-5.30	125.95	128.60
2	AB	532	A	O4'-C4'-C3'	5.30	110.34	106.10
2	AB	301	G	N9-C4-C5	5.30	107.52	105.40
2	AB	347	A	C8-N9-C4	-5.30	103.68	105.80
34	BA	938	A	C5'-C4'-O4'	5.30	115.46	109.10
34	BA	1033	G	N3-C4-C5	-5.30	125.95	128.60
2	AB	2248	C	O4'-C1'-N1	5.29	112.44	108.20
34	BA	1257	A	O4'-C4'-C3'	5.29	110.34	106.10
2	AB	1869	G	N9-C4-C5	5.29	107.52	105.40
2	AB	1972	G	O4'-C1'-N9	5.29	112.44	108.20
35	BE	73	A	O4'-C1'-N9	5.29	112.44	108.20
2	AB	1502	A	O4'-C1'-N9	5.29	112.43	108.20
2	AB	1569	A	C5'-C4'-O4'	5.29	115.45	109.10
2	AB	2448	A	C1'-O4'-C4'	-5.29	105.67	109.90
2	AB	2483	C	O4'-C1'-N1	5.29	112.43	108.20
2	AB	2881	U	C2-N3-C4	-5.29	123.83	127.00
34	BA	367	U	O4'-C4'-C3'	5.29	110.33	106.10
34	BA	426	U	O3'-P-O5'	-5.29	93.94	104.00
2	AB	2296	U	O4'-C4'-C3'	5.29	110.33	106.10
34	BA	1520	C	O4'-C1'-N1	5.29	112.43	108.20
35	BB	26	A	O4'-C1'-N9	5.29	112.43	108.20
2	AB	2049	G	C4'-C3'-C2'	-5.29	97.31	102.60
2	AB	2429	G	P-O3'-C3'	5.29	126.05	119.70
34	BA	112	G	C1'-O4'-C4'	-5.29	105.67	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1144	G	N3-C4-C5	-5.29	125.96	128.60
34	BA	227	G	O4'-C1'-N9	5.29	112.43	108.20
1	AA	15	A	O3'-P-O5'	-5.28	93.96	104.00
1	AA	72	G	C8-N9-C4	-5.28	104.29	106.40
2	AB	21	A	C5'-C4'-C3'	-5.28	107.55	116.00
2	AB	1165	A	N9-C1'-C2'	-5.28	106.19	112.00
2	AB	1975	G	N9-C1'-C2'	-5.28	106.19	112.00
2	AB	2394	C	C4'-C3'-C2'	-5.28	97.32	102.60
2	AB	2553	G	C4'-C3'-C2'	-5.28	97.32	102.60
34	BA	1279	G	C1'-O4'-C4'	-5.28	105.67	109.90
2	AB	729	G	N3-C4-C5	-5.28	125.96	128.60
2	AB	1559	U	O4'-C1'-N1	5.28	112.42	108.20
34	BA	38	G	C8-N9-C4	-5.28	104.29	106.40
34	BA	276	G	C5'-C4'-O4'	5.28	115.44	109.10
35	BE	34	G	C5'-C4'-C3'	-5.28	107.55	116.00
2	AB	447	A	C8-N9-C4	-5.28	103.69	105.80
34	BA	214	C	N3-C2-O2	-5.28	118.20	121.90
34	BA	439	U	O4'-C1'-N1	5.28	112.42	108.20
34	BA	689	C	O4'-C1'-N1	5.28	112.42	108.20
34	BA	793	U	C5'-C4'-O4'	5.28	115.43	109.10
2	AB	458	G	C3'-C2'-C1'	-5.28	97.28	101.50
2	AB	533	G	N3-C4-C5	-5.28	125.96	128.60
2	AB	671	C	O4'-C1'-N1	5.28	112.42	108.20
2	AB	1786	A	C1'-O4'-C4'	-5.28	105.68	109.90
2	AB	2302	U	O4'-C1'-N1	5.28	112.42	108.20
35	BE	66	U	N1-C2-N3	5.28	118.06	114.90
2	AB	910	A	O4'-C1'-N9	5.27	112.42	108.20
34	BA	1225	A	O5'-C5'-C4'	-5.27	101.68	111.70
2	AB	690	G	N3-C4-C5	-5.27	125.96	128.60
2	AB	1042	G	C5'-C4'-O4'	5.27	115.43	109.10
2	AB	1138	G	C8-N9-C4	-5.27	104.29	106.40
2	AB	1538	G	N3-C4-C5	-5.27	125.96	128.60
2	AB	2625	G	C8-N9-C4	-5.27	104.29	106.40
34	BA	39	G	C4'-C3'-C2'	-5.27	97.33	102.60
34	BA	42	G	C5'-C4'-C3'	-5.27	107.56	116.00
34	BA	100	G	O4'-C1'-N9	5.27	112.42	108.20
2	AB	1838	C	N1-C2-O2	5.27	122.06	118.90
2	AB	2665	A	O4'-C1'-N9	5.27	112.42	108.20
2	AB	333	G	C8-N9-C4	-5.27	104.29	106.40
2	AB	485	C	C5'-C4'-C3'	-5.27	107.57	116.00
2	AB	1024	G	C8-N9-C4	-5.27	104.29	106.40
2	AB	1291	C	C5'-C4'-C3'	-5.27	107.57	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1900	A	O4'-C1'-N9	5.27	112.42	108.20
2	AB	1992	G	O4'-C1'-N9	5.27	112.42	108.20
34	BA	408	A	C8-N9-C4	-5.27	103.69	105.80
34	BA	686	U	C4'-C3'-C2'	-5.27	97.33	102.60
34	BA	1042	A	O4'-C1'-N9	5.27	112.42	108.20
2	AB	1895	C	C5'-C4'-O4'	5.27	115.42	109.10
34	BA	651	C	C5'-C4'-C3'	-5.27	107.57	116.00
34	BA	842	U	C5'-C4'-C3'	-5.27	107.57	116.00
34	BA	1072	G	C8-N9-C4	-5.27	104.29	106.40
34	BA	1397	C	C5'-C4'-C3'	-5.27	107.57	116.00
2	AB	346	A	C5'-C4'-O4'	5.26	115.42	109.10
34	BA	300	A	O4'-C1'-N9	5.26	112.41	108.20
34	BA	511	C	O3'-P-O5'	-5.26	94.00	104.00
2	AB	2706	A	O4'-C1'-N9	5.26	112.41	108.20
34	BA	738	C	O4'-C1'-N1	5.26	112.41	108.20
34	BA	1312	G	N3-C4-C5	-5.26	125.97	128.60
2	AB	1345	C	C5'-C4'-C3'	-5.26	107.58	116.00
2	AB	1989	G	C5'-C4'-C3'	-5.26	107.58	116.00
2	AB	2241	A	O4'-C1'-N9	5.26	112.41	108.20
34	BA	193	C	O4'-C1'-N1	5.26	112.41	108.20
34	BA	1041	G	C5'-C4'-O4'	5.26	115.41	109.10
34	BA	1233	G	C5'-C4'-O4'	5.26	115.41	109.10
2	AB	1042	G	C5'-C4'-C3'	-5.26	107.58	116.00
2	AB	1307	A	O4'-C1'-N9	5.26	112.41	108.20
2	AB	2212	A	N9-C1'-C2'	-5.26	106.22	112.00
2	AB	2285	C	C5'-C4'-O4'	5.26	115.41	109.10
34	BA	525	C	C5'-C4'-O4'	5.26	115.41	109.10
34	BA	579	A	O4'-C1'-N9	5.26	112.41	108.20
35	BE	28	G	C8-N9-C4	-5.26	104.30	106.40
2	AB	4	U	C5'-C4'-O4'	5.26	115.41	109.10
2	AB	916	G	N3-C4-C5	-5.26	125.97	128.60
34	BA	14	U	O4'-C1'-N1	5.26	112.41	108.20
34	BA	1040	U	C5'-C4'-C3'	-5.26	107.59	116.00
2	AB	187	G	N3-C4-C5	-5.25	125.97	128.60
2	AB	1186	G	C5'-C4'-O4'	5.25	115.41	109.10
2	AB	474	G	O4'-C1'-N9	5.25	112.40	108.20
2	AB	1738	G	N9-C4-C5	5.25	107.50	105.40
34	BA	70	U	N1-C2-N3	5.25	118.05	114.90
34	BA	268	U	C5'-C4'-C3'	-5.25	107.60	116.00
34	BA	1043	G	C8-N9-C4	-5.25	104.30	106.40
34	BA	1426	G	C8-N9-C4	-5.25	104.30	106.40
35	BB	18	G	N3-C4-C5	-5.25	125.97	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1201	U	C5'-C4'-O4'	5.25	115.40	109.10
2	AB	2637	U	N1-C2-N3	5.25	118.05	114.90
34	BA	162	A	C8-N9-C4	-5.25	103.70	105.80
34	BA	794	A	C5'-C4'-O4'	5.25	115.40	109.10
2	AB	550	C	P-O5'-C5'	5.25	129.30	120.90
2	AB	1508	A	C3'-C2'-C1'	5.25	105.70	101.50
2	AB	2380	C	C4'-C3'-C2'	-5.25	97.35	102.60
2	AB	2462	C	N3-C2-O2	-5.25	118.23	121.90
2	AB	2648	G	C5'-C4'-O4'	5.25	115.40	109.10
34	BA	660	C	C4'-C3'-C2'	-5.25	97.35	102.60
34	BA	1016	A	C5'-C4'-O4'	5.25	115.40	109.10
34	BA	1138	G	O4'-C1'-N9	5.25	112.40	108.20
35	BB	18	G	C3'-C2'-C1'	5.25	105.70	101.50
35	BB	22	G	N3-C4-C5	-5.25	125.98	128.60
2	AB	305	C	O4'-C1'-N1	5.25	112.40	108.20
2	AB	1040	A	O4'-C1'-N9	5.25	112.40	108.20
2	AB	2728	U	O4'-C1'-N1	5.25	112.40	108.20
2	AB	2808	G	P-O3'-C3'	5.25	126.00	119.70
34	BA	172	A	C8-N9-C4	-5.25	103.70	105.80
2	AB	2028	U	C3'-C2'-C1'	-5.25	97.30	101.50
2	AB	2822	G	C5'-C4'-O4'	5.25	115.39	109.10
2	AB	616	A	C5'-C4'-O4'	5.24	115.39	109.10
2	AB	1241	A	C8-N9-C4	-5.24	103.70	105.80
2	AB	2485	G	C8-N9-C4	-5.24	104.30	106.40
2	AB	2512	C	O4'-C1'-N1	5.24	112.39	108.20
2	AB	2777	G	N3-C4-C5	-5.24	125.98	128.60
2	AB	1243	C	C5'-C4'-C3'	-5.24	107.61	116.00
2	AB	2029	G	C5'-C4'-O4'	5.24	115.39	109.10
1	AA	18	G	C5'-C4'-O4'	5.24	115.39	109.10
34	BA	310	G	N7-C8-N9	5.24	115.72	113.10
2	AB	523	C	C5'-C4'-O4'	5.24	115.39	109.10
2	AB	712	G	N3-C4-C5	-5.24	125.98	128.60
2	AB	722	A	O4'-C1'-N9	5.24	112.39	108.20
2	AB	1330	C	C5'-C4'-O4'	5.24	115.39	109.10
2	AB	1530	G	C5'-C4'-O4'	5.24	115.39	109.10
34	BA	858	G	C5'-C4'-O4'	5.24	115.39	109.10
34	BA	1203	C	O4'-C1'-N1	5.24	112.39	108.20
2	AB	852	U	N1-C2-N3	5.24	118.04	114.90
1	AA	51	G	O4'-C1'-N9	5.23	112.39	108.20
2	AB	2133	G	O4'-C1'-C2'	-5.23	100.57	105.80
34	BA	1233	G	N3-C4-C5	-5.23	125.98	128.60
1	AA	75	G	O5'-C5'-C4'	-5.23	101.76	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	76	G	O4'-C1'-N9	5.23	112.38	108.20
2	AB	2119	A	C3'-C2'-C1'	5.23	105.69	101.50
34	BA	77	A	O4'-C1'-N9	5.23	112.39	108.20
34	BA	1501	C	C3'-C2'-C1'	5.23	105.68	101.50
2	AB	2685	G	C5'-C4'-O4'	5.23	115.38	109.10
2	AB	756	A	C3'-C2'-C1'	-5.23	97.32	101.50
2	AB	1941	C	C3'-C2'-C1'	5.23	105.68	101.50
2	AB	2051	A	C5'-C4'-C3'	-5.23	107.64	116.00
2	AB	2104	C	C5'-C4'-C3'	-5.23	107.64	116.00
2	AB	2749	A	O4'-C1'-N9	5.23	112.38	108.20
1	AA	11	C	N1-C2-O2	5.23	122.04	118.90
2	AB	167	A	C8-N9-C4	-5.23	103.71	105.80
2	AB	344	A	O4'-C1'-N9	5.23	112.38	108.20
2	AB	69	C	C5'-C4'-O4'	5.22	115.37	109.10
2	AB	724	U	O4'-C1'-N1	5.22	112.38	108.20
2	AB	1104	C	C2-N3-C4	5.22	122.51	119.90
34	BA	1347	G	C3'-C2'-C1'	-5.22	97.32	101.50
2	AB	1017	G	O4'-C1'-N9	5.22	112.38	108.20
2	AB	1395	A	C5'-C4'-C3'	-5.22	107.64	116.00
2	AB	1782	U	O4'-C1'-N1	5.22	112.38	108.20
34	BA	122	G	N3-C4-C5	-5.22	125.99	128.60
34	BA	625	U	O4'-C1'-N1	5.22	112.38	108.20
34	BA	749	A	C5'-C4'-C3'	-5.22	107.64	116.00
35	BB	19	G	O4'-C1'-N9	5.22	112.38	108.20
34	BA	295	C	O4'-C1'-N1	5.22	112.38	108.20
34	BA	1032	G	N3-C4-C5	-5.22	125.99	128.60
2	AB	1816	C	C1'-O4'-C4'	-5.22	105.72	109.90
2	AB	2791	G	C1'-O4'-C4'	-5.22	105.72	109.90
34	BA	817	C	O4'-C4'-C3'	5.22	110.28	106.10
2	AB	1498	C	O4'-C1'-N1	5.22	112.37	108.20
34	BA	1176	A	C8-N9-C4	-5.22	103.71	105.80
2	AB	555	G	N3-C4-C5	-5.22	125.99	128.60
2	AB	1850	G	C8-N9-C4	-5.22	104.31	106.40
2	AB	2190	G	O4'-C1'-N9	5.22	112.37	108.20
34	BA	729	A	O4'-C1'-N9	5.22	112.37	108.20
34	BA	989	U	O4'-C1'-N1	5.22	112.37	108.20
1	AA	110	C	O4'-C1'-N1	5.21	112.37	108.20
2	AB	205	G	C8-N9-C4	-5.21	104.31	106.40
2	AB	1048	A	C8-N9-C4	-5.21	103.71	105.80
34	BA	911	U	C5'-C4'-C3'	-5.21	107.66	116.00
1	AA	107	G	N3-C4-C5	-5.21	125.99	128.60
2	AB	979	A	C5'-C4'-C3'	-5.21	107.66	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	378	C	C5'-C4'-C3'	-5.21	107.66	116.00
2	AB	533	G	O4'-C4'-C3'	5.21	110.27	106.10
2	AB	711	G	C8-N9-C4	-5.21	104.32	106.40
2	AB	766	U	C5'-C4'-O4'	5.21	115.35	109.10
2	AB	1537	G	N3-C4-C5	-5.21	126.00	128.60
2	AB	1875	G	O3'-P-O5'	-5.21	94.10	104.00
34	BA	477	C	O4'-C4'-C3'	5.21	110.27	106.10
34	BA	851	G	C3'-C2'-C1'	-5.21	97.33	101.50
34	BA	1295	U	O4'-C1'-N1	5.21	112.37	108.20
1	AA	72	G	C5'-C4'-O4'	5.21	115.35	109.10
2	AB	509	C	O4'-C4'-C3'	5.21	110.27	106.10
2	AB	1411	U	C5'-C4'-C3'	-5.21	107.66	116.00
2	AB	1491	G	N3-C4-C5	-5.21	126.00	128.60
2	AB	2401	U	C5'-C4'-C3'	-5.21	107.66	116.00
34	BA	1047	G	C5'-C4'-O4'	5.21	115.35	109.10
2	AB	407	G	N3-C4-C5	-5.21	126.00	128.60
2	AB	483	A	O4'-C1'-N9	5.21	112.37	108.20
2	AB	509	C	O4'-C1'-N1	5.21	112.37	108.20
2	AB	1358	G	C8-N9-C4	-5.21	104.32	106.40
2	AB	2094	A	O4'-C1'-N9	5.21	112.37	108.20
2	AB	2618	G	C5'-C4'-O4'	5.21	115.35	109.10
34	BA	781	A	C5'-C4'-O4'	5.21	115.35	109.10
34	BA	1006	G	C8-N9-C4	-5.21	104.32	106.40
35	BE	2	C	C5'-C4'-O4'	5.21	115.35	109.10
34	BA	1446	A	C5'-C4'-C3'	-5.21	107.67	116.00
2	AB	646	U	C4'-C3'-C2'	-5.21	97.39	102.60
2	AB	824	U	C5'-C4'-C3'	-5.20	107.67	116.00
2	AB	844	A	O4'-C1'-N9	5.20	112.36	108.20
2	AB	983	A	O4'-C4'-C3'	5.20	110.26	106.10
2	AB	1197	G	C5'-C4'-O4'	5.20	115.34	109.10
2	AB	1594	U	O4'-C1'-N1	5.20	112.36	108.20
2	AB	2256	G	O4'-C1'-N9	5.20	112.36	108.20
34	BA	232	G	C5'-C4'-O4'	5.20	115.34	109.10
34	BA	1091	U	C5'-C4'-C3'	-5.20	107.67	116.00
34	BA	1314	C	N1-C2-O2	5.20	122.02	118.90
2	AB	1385	A	C1'-O4'-C4'	-5.20	105.74	109.90
2	AB	604	G	N9-C1'-C2'	-5.20	106.28	112.00
2	AB	1538	G	C8-N9-C4	-5.20	104.32	106.40
2	AB	1569	A	C5'-C4'-C3'	-5.20	107.68	116.00
2	AB	1757	A	O4'-C4'-C3'	5.20	110.26	106.10
2	AB	2168	G	C8-N9-C4	-5.20	104.32	106.40
34	BA	987	G	N3-C4-C5	-5.20	126.00	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1641	A	C5'-C4'-O4'	5.20	115.34	109.10
2	AB	2407	A	C4'-C3'-C2'	-5.20	97.40	102.60
2	AB	240	C	N1-C2-O2	5.20	122.02	118.90
34	BA	447	G	N3-C4-C5	-5.20	126.00	128.60
2	AB	316	C	N1-C1'-C2'	-5.20	106.28	112.00
2	AB	651	G	C5'-C4'-C3'	5.20	124.31	116.00
34	BA	1481	U	C5'-C4'-O4'	5.20	115.33	109.10
2	AB	305	C	C4'-C3'-C2'	-5.19	97.41	102.60
34	BA	252	U	O4'-C1'-N1	5.19	112.36	108.20
2	AB	684	G	O4'-C1'-N9	5.19	112.35	108.20
2	AB	811	U	O4'-C1'-C2'	-5.19	100.61	105.80
2	AB	1360	G	O4'-C1'-N9	5.19	112.35	108.20
2	AB	705	A	C8-N9-C4	-5.19	103.72	105.80
2	AB	1579	A	C5'-C4'-O4'	5.19	115.33	109.10
34	BA	140	U	C5'-C4'-O4'	5.19	115.33	109.10
2	AB	1848	A	C5'-C4'-O4'	5.19	115.33	109.10
34	BA	563	A	C1'-O4'-C4'	-5.19	105.75	109.90
2	AB	555	G	C2-N3-C4	5.19	114.49	111.90
2	AB	1537	G	C8-N9-C4	-5.19	104.33	106.40
2	AB	1855	U	C5'-C4'-O4'	5.19	115.32	109.10
2	AB	2344	U	P-O3'-C3'	5.19	125.92	119.70
34	BA	1399	C	O4'-C1'-N1	5.19	112.35	108.20
2	AB	2300	C	C5'-C4'-O4'	5.19	115.32	109.10
1	AA	62	C	O4'-C1'-N1	5.18	112.35	108.20
2	AB	978	G	C3'-C2'-C1'	-5.18	97.35	101.50
2	AB	2653	U	C5'-C4'-O4'	5.18	115.32	109.10
2	AB	2799	A	O4'-C1'-C2'	-5.18	100.62	105.80
2	AB	992	C	O4'-C1'-N1	5.18	112.35	108.20
34	BA	668	G	C5'-C4'-C3'	-5.18	107.71	116.00
2	AB	1209	U	C2-N1-C1'	5.18	123.92	117.70
2	AB	1396	U	C5'-C4'-C3'	-5.18	107.71	116.00
2	AB	1583	A	C4'-C3'-O3'	5.18	123.36	113.00
2	AB	1731	G	N9-C4-C5	5.18	107.47	105.40
2	AB	2801	G	C5'-C4'-O4'	5.18	115.31	109.10
34	BA	601	G	C5'-C4'-C3'	-5.18	107.71	116.00
34	BA	1149	C	C5'-C4'-O4'	5.18	115.31	109.10
2	AB	2158	A	P-O3'-C3'	5.18	125.91	119.70
2	AB	14	A	C5'-C4'-O4'	5.18	115.31	109.10
2	AB	957	C	O3'-P-O5'	-5.18	94.17	104.00
2	AB	1082	U	C5'-C4'-O4'	5.18	115.31	109.10
2	AB	1845	G	C8-N9-C4	-5.18	104.33	106.40
2	AB	2276	G	N9-C1'-C2'	-5.18	106.31	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	177	G	O4'-C1'-N9	5.17	112.34	108.20
2	AB	1331	G	C5'-C4'-O4'	5.17	115.31	109.10
2	AB	1902	C	C5'-C4'-O4'	5.17	115.31	109.10
2	AB	2228	G	C8-N9-C4	-5.17	104.33	106.40
34	BA	1279	G	N3-C4-C5	-5.17	126.01	128.60
1	AA	38	C	N1-C1'-C2'	-5.17	106.31	112.00
2	AB	2055	C	O4'-C1'-N1	5.17	112.34	108.20
34	BA	340	U	C5'-C4'-O4'	5.17	115.31	109.10
34	BA	662	U	O4'-C1'-N1	5.17	112.34	108.20
1	AA	45	A	C5'-C4'-C3'	-5.17	107.72	116.00
2	AB	855	G	C5'-C4'-C3'	-5.17	107.73	116.00
2	AB	1927	A	O4'-C1'-N9	5.17	112.34	108.20
34	BA	370	C	O4'-C1'-N1	5.17	112.34	108.20
34	BA	597	G	N3-C4-C5	-5.17	126.01	128.60
34	BA	726	C	O4'-C1'-N1	5.17	112.34	108.20
35	BE	3	C	C5'-C4'-O4'	5.17	115.31	109.10
2	AB	592	A	O4'-C1'-N9	5.17	112.34	108.20
2	AB	793	A	C8-N9-C4	-5.17	103.73	105.80
34	BA	1315	U	O4'-C1'-N1	5.17	112.34	108.20
2	AB	573	U	C5'-C4'-C3'	-5.17	107.73	116.00
2	AB	979	A	O4'-C1'-N9	5.17	112.33	108.20
2	AB	1521	G	O4'-C1'-N9	5.17	112.33	108.20
2	AB	2164	C	N1-C2-O2	5.17	122.00	118.90
2	AB	2533	U	N1-C1'-C2'	-5.17	106.31	112.00
2	AB	732	C	O4'-C1'-N1	5.17	112.33	108.20
2	AB	1372	U	C5'-C4'-O4'	5.17	115.30	109.10
34	BA	335	C	C5'-C4'-O4'	5.17	115.30	109.10
34	BA	1120	C	O3'-P-O5'	-5.17	94.18	104.00
37	BD	29	G	O4'-C4'-C3'	5.17	110.23	106.10
34	BA	1360	A	O4'-C1'-N9	5.17	112.33	108.20
2	AB	2393	U	O4'-C1'-N1	5.16	112.33	108.20
34	BA	1204	A	C5'-C4'-O4'	5.16	115.30	109.10
35	BB	45	U	O4'-C1'-N1	5.16	112.33	108.20
2	AB	179	C	C5'-C4'-O4'	5.16	115.30	109.10
2	AB	277	G	N9-C1'-C2'	5.16	120.71	114.00
2	AB	489	G	N9-C1'-C2'	-5.16	106.32	112.00
2	AB	597	G	O4'-C1'-N9	5.16	112.33	108.20
2	AB	2111	U	P-O3'-C3'	5.16	125.89	119.70
2	AB	1525	A	C5'-C4'-O4'	5.16	115.29	109.10
34	BA	245	U	C1'-O4'-C4'	-5.16	105.77	109.90
34	BA	441	A	O4'-C1'-N9	5.16	112.33	108.20
2	AB	716	A	C1'-O4'-C4'	-5.16	105.77	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1219	U	O4'-C1'-N1	5.16	112.33	108.20
2	AB	1408	G	C3'-C2'-C1'	-5.16	97.37	101.50
2	AB	1461	C	C1'-O4'-C4'	-5.16	105.77	109.90
2	AB	1591	A	C5'-C4'-C3'	-5.16	107.75	116.00
2	AB	1722	A	C8-N9-C4	-5.16	103.74	105.80
2	AB	2234	G	N7-C8-N9	5.16	115.68	113.10
2	AB	2324	U	O4'-C4'-C3'	5.16	110.23	106.10
34	BA	932	C	O4'-C1'-N1	5.16	112.33	108.20
1	AA	77	U	C3'-C2'-C1'	-5.16	97.38	101.50
2	AB	1646	C	O4'-C1'-N1	5.16	112.33	108.20
2	AB	1800	C	C6-N1-C2	-5.16	118.24	120.30
34	BA	1057	G	N3-C4-C5	-5.16	126.02	128.60
2	AB	573	U	C4'-C3'-C2'	-5.15	97.45	102.60
2	AB	1888	G	C8-N9-C4	-5.15	104.34	106.40
34	BA	916	U	O4'-C1'-N1	5.15	112.32	108.20
34	BA	1094	G	C8-N9-C4	-5.15	104.34	106.40
2	AB	367	G	C5'-C4'-C3'	-5.15	107.76	116.00
2	AB	1786	A	C5'-C4'-C3'	-5.15	107.76	116.00
2	AB	2517	C	N1-C2-O2	5.15	121.99	118.90
2	AB	2870	C	C5'-C4'-O4'	5.15	115.28	109.10
34	BA	434	U	C5'-C4'-O4'	5.15	115.28	109.10
34	BA	688	G	O4'-C1'-N9	5.15	112.32	108.20
34	BA	812	G	N3-C4-C5	-5.15	126.02	128.60
34	BA	1217	C	O4'-C1'-N1	5.15	112.32	108.20
2	AB	214	G	C8-N9-C4	-5.15	104.34	106.40
2	AB	302	C	C4'-C3'-C2'	-5.15	97.45	102.60
2	AB	2476	A	C2'-C3'-O3'	5.15	121.94	113.70
34	BA	50	A	O4'-C1'-N9	5.15	112.32	108.20
34	BA	430	A	C5'-C4'-O4'	5.15	115.28	109.10
2	AB	1324	G	O4'-C1'-N9	5.15	112.32	108.20
34	BA	212	G	N3-C4-C5	-5.15	126.03	128.60
34	BA	886	G	N9-C1'-C2'	-5.15	106.34	112.00
34	BA	998	C	O4'-C1'-N1	5.15	112.32	108.20
34	BA	1291	U	O4'-C1'-N1	5.15	112.32	108.20
2	AB	890	C	O4'-C1'-N1	5.15	112.32	108.20
34	BA	1081	A	O4'-C1'-N9	5.15	112.32	108.20
35	BE	27	G	O4'-C1'-N9	5.15	112.32	108.20
2	AB	345	A	C5'-C4'-O4'	5.15	115.28	109.10
2	AB	363	G	C5'-C4'-C3'	-5.15	107.77	116.00
2	AB	2378	A	C5'-C4'-O4'	5.15	115.28	109.10
34	BA	394	G	C8-N9-C4	-5.15	104.34	106.40
2	AB	1011	G	N9-C4-C5	5.14	107.46	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2638	G	C5'-C4'-C3'	-5.14	107.77	116.00
34	BA	183	C	O4'-C1'-N1	5.14	112.31	108.20
2	AB	81	G	O4'-C1'-N9	5.14	112.31	108.20
2	AB	1308	A	C5'-C4'-C3'	-5.14	107.77	116.00
2	AB	726	G	C4-N9-C1'	-5.14	119.82	126.50
2	AB	1478	G	C5'-C4'-O4'	5.14	115.27	109.10
2	AB	1776	G	N3-C4-C5	-5.14	126.03	128.60
34	BA	146	G	O4'-C1'-N9	5.14	112.31	108.20
34	BA	332	G	C1'-O4'-C4'	-5.14	105.79	109.90
34	BA	764	C	O4'-C1'-N1	5.14	112.31	108.20
34	BA	1051	C	P-O3'-C3'	5.14	125.87	119.70
43	BK	1	PRO	CA-N-CD	-5.14	104.31	111.50
2	AB	380	G	C5'-C4'-O4'	5.14	115.27	109.10
2	AB	669	G	C2-N3-C4	5.14	114.47	111.90
2	AB	2840	C	O4'-C1'-N1	5.14	112.31	108.20
34	BA	1020	G	C5'-C4'-O4'	5.14	115.27	109.10
2	AB	1379	U	O4'-C1'-N1	5.14	112.31	108.20
2	AB	1830	C	C5'-C4'-O4'	5.14	115.26	109.10
2	AB	1898	U	C5'-C4'-O4'	5.14	115.27	109.10
2	AB	2041	U	O4'-C1'-N1	5.14	112.31	108.20
2	AB	2801	G	N9-C1'-C2'	-5.14	106.35	112.00
34	BA	406	G	C8-N9-C4	-5.14	104.35	106.40
34	BA	885	G	N3-C4-C5	-5.14	126.03	128.60
34	BA	1119	C	O4'-C1'-N1	5.14	112.31	108.20
34	BA	1162	C	C5'-C4'-C3'	-5.14	107.78	116.00
35	BB	2	C	O4'-C1'-N1	5.14	112.31	108.20
2	AB	190	A	O5'-C5'-C4'	5.13	121.45	111.70
2	AB	898	C	C1'-O4'-C4'	-5.13	105.79	109.90
1	AA	49	C	N1-C1'-C2'	-5.13	106.35	112.00
2	AB	2177	C	N1-C2-O2	5.13	121.98	118.90
2	AB	2885	G	C4'-C3'-O3'	5.13	123.27	113.00
1	AA	77	U	C5'-C4'-O4'	5.13	115.26	109.10
2	AB	1034	G	O4'-C1'-N9	5.13	112.31	108.20
2	AB	2477	U	C4'-C3'-C2'	-5.13	97.47	102.60
26	AZ	7	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	AB	1422	G	C3'-C2'-C1'	-5.13	97.40	101.50
2	AB	2543	G	C5'-C4'-O4'	5.13	115.26	109.10
2	AB	167	A	C5'-C4'-O4'	5.13	115.25	109.10
2	AB	389	G	N3-C4-C5	-5.13	126.04	128.60
2	AB	1360	G	C8-N9-C4	-5.13	104.35	106.40
2	AB	2230	G	N3-C4-C5	-5.13	126.04	128.60
2	AB	2540	C	C1'-O4'-C4'	-5.13	105.80	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1361	G	C8-N9-C4	-5.13	104.35	106.40
34	BA	1380	U	C1'-O4'-C4'	-5.13	105.80	109.90
2	AB	1154	G	N3-C4-C5	-5.13	126.04	128.60
2	AB	1203	U	C2-N3-C4	-5.13	123.92	127.00
2	AB	1743	G	C4'-C3'-C2'	-5.13	97.47	102.60
34	BA	540	G	O4'-C1'-N9	5.13	112.30	108.20
34	BA	1084	G	C2'-C3'-O3'	5.13	121.90	113.70
31	Ae	19	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	AA	88	C	O4'-C1'-N1	5.12	112.30	108.20
2	AB	841	G	O4'-C1'-C2'	5.12	112.21	107.60
2	AB	1555	G	N9-C4-C5	5.12	107.45	105.40
2	AB	1560	G	N3-C4-C5	-5.12	126.04	128.60
2	AB	2666	C	C4'-C3'-C2'	-5.12	97.48	102.60
2	AB	2765	A	O4'-C1'-N9	5.12	112.30	108.20
2	AB	1799	G	C8-N9-C4	-5.12	104.35	106.40
2	AB	1989	G	C8-N9-C4	-5.12	104.35	106.40
2	AB	2588	G	O4'-C1'-N9	5.12	112.30	108.20
34	BA	94	G	N3-C4-C5	-5.12	126.04	128.60
2	AB	381	G	O4'-C1'-N9	5.12	112.30	108.20
34	BA	393	A	O4'-C1'-N9	5.12	112.30	108.20
35	BB	18	G	O4'-C1'-N9	5.12	112.30	108.20
2	AB	202	U	O4'-C1'-N1	5.12	112.30	108.20
2	AB	242	G	O4'-C1'-N9	5.12	112.30	108.20
2	AB	1645	G	N3-C4-C5	-5.12	126.04	128.60
2	AB	1776	G	C5'-C4'-C3'	-5.12	107.81	116.00
2	AB	2731	G	C5'-C4'-C3'	-5.12	107.81	116.00
34	BA	502	A	O4'-C1'-N9	5.12	112.30	108.20
34	BA	1159	U	O4'-C1'-N1	5.12	112.30	108.20
2	AB	277	G	O4'-C1'-N9	5.12	112.29	108.20
2	AB	2060	A	O4'-C1'-N9	5.12	112.29	108.20
34	BA	176	C	O4'-C1'-N1	5.12	112.29	108.20
34	BA	884	U	C1'-O4'-C4'	-5.12	105.81	109.90
2	AB	150	U	O4'-C1'-N1	5.12	112.29	108.20
2	AB	483	A	C5'-C4'-O4'	5.12	115.24	109.10
2	AB	1881	C	C5'-C4'-C3'	-5.12	107.81	116.00
2	AB	1938	A	C5'-C4'-O4'	5.12	115.24	109.10
34	BA	549	C	C5'-C4'-O4'	5.12	115.24	109.10
34	BA	1227	A	C8-N9-C4	-5.12	103.75	105.80
2	AB	168	G	C3'-C2'-C1'	-5.11	97.41	101.50
2	AB	663	G	C8-N9-C4	-5.11	104.36	106.40
2	AB	1332	G	O3'-P-O5'	-5.11	94.28	104.00
2	AB	2292	U	O4'-C1'-N1	5.11	112.29	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	522	C	O4'-C1'-N1	5.11	112.29	108.20
34	BA	901	A	C4'-C3'-C2'	-5.11	97.49	102.60
34	BA	1426	G	O4'-C1'-N9	5.11	112.29	108.20
2	AB	231	A	C5'-C4'-C3'	-5.11	107.82	116.00
2	AB	326	G	C8-N9-C4	-5.11	104.36	106.40
2	AB	2898	U	O4'-C1'-N1	5.11	112.29	108.20
2	AB	1230	A	C5'-C4'-C3'	-5.11	107.82	116.00
34	BA	305	G	P-O3'-C3'	5.11	125.83	119.70
34	BA	991	U	O4'-C1'-N1	5.11	112.29	108.20
2	AB	287	G	N3-C4-C5	-5.11	126.05	128.60
2	AB	473	G	C5'-C4'-C3'	-5.11	107.83	116.00
2	AB	511	U	C5'-C4'-C3'	-5.11	107.83	116.00
2	AB	2872	A	C1'-O4'-C4'	-5.11	105.81	109.90
34	BA	1452	C	O4'-C1'-N1	5.11	112.29	108.20
1	AA	43	C	C3'-C2'-C1'	5.11	105.59	101.50
2	AB	1705	A	O4'-C1'-N9	5.11	112.29	108.20
2	AB	2831	G	O3'-P-O5'	-5.11	94.30	104.00
34	BA	758	C	N3-C2-O2	-5.11	118.33	121.90
51	BS	88	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	AA	111	U	C5'-C4'-C3'	-5.11	107.83	116.00
2	AB	663	G	O4'-C1'-N9	5.11	112.28	108.20
2	AB	725	G	C2'-C3'-O3'	5.11	121.87	113.70
2	AB	2530	A	C5'-C4'-O4'	5.11	115.23	109.10
2	AB	2642	G	N3-C4-C5	-5.11	126.05	128.60
34	BA	11	G	C5'-C4'-O4'	5.11	115.23	109.10
34	BA	1256	A	O3'-P-O5'	-5.11	94.30	104.00
35	BB	60	U	O4'-C1'-C2'	-5.11	100.69	105.80
2	AB	90	U	P-O3'-C3'	5.10	125.82	119.70
2	AB	136	G	N9-C1'-C2'	-5.10	106.39	112.00
2	AB	1491	G	C8-N9-C4	-5.10	104.36	106.40
2	AB	2031	A	C3'-C2'-C1'	5.10	105.58	101.50
2	AB	178	G	O4'-C1'-N9	5.10	112.28	108.20
2	AB	1530	G	N3-C4-C5	-5.10	126.05	128.60
2	AB	2162	G	N9-C4-C5	5.10	107.44	105.40
2	AB	2537	U	C5'-C4'-C3'	-5.10	107.83	116.00
2	AB	2825	G	N3-C4-C5	-5.10	126.05	128.60
34	BA	1047	G	N3-C4-C5	-5.10	126.05	128.60
1	AA	34	A	C8-N9-C4	-5.10	103.76	105.80
2	AB	532	A	O4'-C1'-C2'	-5.10	100.70	105.80
2	AB	1345	C	O4'-C1'-N1	5.10	112.28	108.20
34	BA	933	G	C8-N9-C4	-5.10	104.36	106.40
34	BA	194	C	N1-C2-O2	5.10	121.96	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1333	A	O4'-C1'-N9	5.10	112.28	108.20
2	AB	915	C	O4'-C1'-N1	5.10	112.28	108.20
2	AB	1446	C	C5'-C4'-C3'	-5.10	107.84	116.00
2	AB	2749	A	C3'-C2'-C1'	-5.10	97.42	101.50
34	BA	330	C	C5'-C4'-C3'	-5.10	107.84	116.00
34	BA	591	U	C5'-C4'-O4'	5.10	115.22	109.10
34	BA	936	C	C5'-C4'-C3'	-5.10	107.84	116.00
34	BA	874	G	C8-N9-C4	-5.10	104.36	106.40
2	AB	1785	A	C4'-C3'-C2'	-5.09	97.50	102.60
2	AB	1826	G	N3-C4-C5	-5.09	126.05	128.60
2	AB	111	A	O4'-C1'-N9	5.09	112.27	108.20
2	AB	388	G	P-O3'-C3'	5.09	125.81	119.70
2	AB	1586	A	C4'-C3'-C2'	-5.09	97.51	102.60
2	AB	1892	C	O4'-C1'-N1	5.09	112.28	108.20
34	BA	217	C	C5'-C4'-O4'	5.09	115.21	109.10
2	AB	141	G	C1'-O4'-C4'	-5.09	105.83	109.90
2	AB	739	A	O4'-C1'-N9	-5.09	104.13	108.20
2	AB	1854	A	C5'-C4'-C3'	-5.09	107.85	116.00
2	AB	2211	A	O4'-C1'-N9	5.09	112.27	108.20
2	AB	2782	G	C5'-C4'-O4'	5.09	115.21	109.10
2	AB	1848	A	C8-N9-C4	-5.09	103.77	105.80
2	AB	2464	G	N9-C4-C5	5.09	107.44	105.40
34	BA	335	C	O4'-C1'-N1	5.09	112.27	108.20
34	BA	596	A	C5'-C4'-C3'	-5.09	107.86	116.00
2	AB	1559	U	N1-C1'-C2'	5.09	120.61	114.00
2	AB	2490	G	C8-N9-C4	-5.09	104.36	106.40
35	BB	48	C	C5'-C4'-O4'	5.09	115.21	109.10
2	AB	255	A	C5'-C4'-C3'	-5.09	107.86	116.00
2	AB	710	U	O3'-P-O5'	-5.09	94.33	104.00
2	AB	1800	C	C3'-C2'-C1'	5.09	105.57	101.50
4	AD	132	ARG	NE-CZ-NH1	5.09	122.84	120.30
34	BA	318	G	C5'-C4'-O4'	5.09	115.20	109.10
35	BE	23	A	O4'-C1'-N9	5.09	112.27	108.20
1	AA	37	C	C6-N1-C2	-5.08	118.27	120.30
34	BA	1143	G	N3-C4-C5	-5.08	126.06	128.60
2	AB	570	G	C5'-C4'-O4'	5.08	115.20	109.10
2	AB	1234	U	O4'-C1'-N1	5.08	112.27	108.20
2	AB	1313	U	C5'-C4'-C3'	-5.08	107.86	116.00
2	AB	1500	G	C5'-C4'-O4'	5.08	115.20	109.10
34	BA	120	A	C5'-C4'-C3'	-5.08	107.87	116.00
34	BA	929	G	N9-C1'-C2'	-5.08	106.41	112.00
2	AB	425	G	N9-C1'-C2'	-5.08	106.41	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2081	U	O4'-C1'-N1	5.08	112.27	108.20
34	BA	111	G	N3-C4-C5	-5.08	126.06	128.60
34	BA	440	C	O4'-C1'-N1	5.08	112.27	108.20
2	AB	624	C	O4'-C1'-N1	5.08	112.26	108.20
2	AB	1489	C	O4'-C1'-N1	5.08	112.26	108.20
34	BA	760	G	N9-C1'-C2'	-5.08	106.41	112.00
1	AA	20	G	N3-C4-C5	-5.08	126.06	128.60
2	AB	315	G	N9-C4-C5	5.08	107.43	105.40
2	AB	516	C	O4'-C1'-N1	5.08	112.26	108.20
2	AB	530	G	C5'-C4'-C3'	-5.08	107.87	116.00
7	AG	132	ARG	CD-NE-CZ	5.08	130.71	123.60
34	BA	167	A	O4'-C1'-N9	5.08	112.26	108.20
34	BA	340	U	O4'-C1'-N1	5.08	112.26	108.20
34	BA	1270	G	N9-C4-C5	5.08	107.43	105.40
34	BA	1378	C	C4'-C3'-C2'	-5.08	97.52	102.60
2	AB	914	G	C2-N3-C4	5.08	114.44	111.90
2	AB	949	G	N3-C4-C5	-5.08	126.06	128.60
2	AB	1151	A	O4'-C1'-N9	5.08	112.26	108.20
2	AB	619	G	C8-N9-C4	-5.08	104.37	106.40
2	AB	1162	G	N9-C1'-C2'	-5.08	106.42	112.00
2	AB	1345	C	C5'-C4'-O4'	5.08	115.19	109.10
34	BA	42	G	O4'-C1'-N9	5.08	112.26	108.20
34	BA	481	G	C2'-C3'-O3'	5.08	121.82	113.70
34	BA	1001	C	O4'-C1'-N1	5.08	112.26	108.20
34	BA	1164	G	O4'-C1'-N9	5.08	112.26	108.20
34	BA	1359	C	O4'-C4'-C3'	5.08	110.16	106.10
41	BI	145	ASN	C-N-CA	5.08	134.39	121.70
2	AB	21	A	N9-C1'-C2'	-5.07	106.42	112.00
2	AB	407	G	C3'-C2'-C1'	-5.07	97.44	101.50
2	AB	1761	C	C2'-C3'-O3'	5.07	121.82	113.70
2	AB	1882	U	C5'-C4'-C3'	-5.07	107.88	116.00
2	AB	2811	G	N9-C1'-C2'	-5.07	106.42	112.00
34	BA	543	U	C5'-C4'-O4'	5.07	115.19	109.10
2	AB	514	A	O4'-C1'-N9	5.07	112.26	108.20
2	AB	2823	A	C3'-C2'-C1'	5.07	105.56	101.50
14	AN	38	ARG	NE-CZ-NH1	5.07	122.84	120.30
34	BA	599	C	O4'-C1'-N1	5.07	112.26	108.20
34	BA	648	A	C5'-C4'-C3'	-5.07	107.89	116.00
2	AB	1509	A	P-O3'-C3'	5.07	125.78	119.70
34	BA	292	G	C8-N9-C4	-5.07	104.37	106.40
2	AB	2565	A	C8-N9-C4	-5.07	103.77	105.80
2	AB	2692	G	C5'-C4'-C3'	-5.07	107.89	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	454	G	C8-N9-C4	-5.07	104.37	106.40
34	BA	1047	G	C1'-O4'-C4'	-5.07	105.84	109.90
34	BA	1078	U	N3-C2-O2	-5.07	118.65	122.20
34	BA	1228	C	C5'-C4'-O4'	5.07	115.18	109.10
1	AA	54	G	N9-C4-C5	5.07	107.43	105.40
2	AB	1193	G	C5'-C4'-C3'	-5.07	107.89	116.00
2	AB	2093	G	O5'-C5'-C4'	-5.07	102.07	111.70
2	AB	2664	G	N3-C4-C5	-5.07	126.07	128.60
34	BA	441	A	C8-N9-C4	-5.07	103.77	105.80
34	BA	682	G	N9-C1'-C2'	-5.07	106.42	112.00
34	BA	1381	U	O4'-C1'-N1	5.07	112.25	108.20
2	AB	1340	U	O4'-C1'-N1	5.07	112.25	108.20
2	AB	2332	C	O4'-C1'-N1	5.06	112.25	108.20
34	BA	163	C	C4'-C3'-C2'	-5.06	97.54	102.60
34	BA	727	G	C5'-C4'-O4'	5.06	115.18	109.10
2	AB	529	A	C1'-O4'-C4'	-5.06	105.85	109.90
34	BA	1022	A	C8-N9-C4	-5.06	103.78	105.80
34	BA	1056	U	C5'-C4'-O4'	5.06	115.17	109.10
34	BA	1450	U	C3'-C2'-C1'	5.06	105.55	101.50
50	BR	58	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	AA	77	U	O4'-C1'-N1	5.06	112.25	108.20
2	AB	7	G	C5'-C4'-C3'	-5.06	107.90	116.00
2	AB	380	G	N9-C1'-C2'	-5.06	106.43	112.00
34	BA	887	G	N9-C1'-C2'	-5.06	106.43	112.00
55	BW	1	PRO	CA-N-CD	-5.06	104.42	111.50
2	AB	1694	C	O4'-C1'-N1	5.06	112.25	108.20
2	AB	2584	U	O4'-C1'-N1	5.06	112.25	108.20
34	BA	17	U	O4'-C1'-N1	5.06	112.25	108.20
34	BA	30	U	O4'-C4'-C3'	5.06	110.15	106.10
34	BA	620	C	C1'-O4'-C4'	-5.06	105.85	109.90
34	BA	1000	A	C5'-C4'-O4'	5.06	115.17	109.10
2	AB	1189	A	C5'-C4'-O4'	5.06	115.17	109.10
2	AB	2195	U	C5'-C4'-C3'	-5.06	107.91	116.00
2	AB	2423	U	O4'-C1'-N1	5.06	112.25	108.20
34	BA	1436	U	C4'-C3'-C2'	-5.06	97.54	102.60
2	AB	1206	G	C5'-C4'-C3'	-5.06	107.91	116.00
2	AB	1619	G	C8-N9-C4	-5.06	104.38	106.40
2	AB	1971	U	O4'-C1'-N1	5.06	112.25	108.20
34	BA	503	C	N1-C2-O2	5.06	121.93	118.90
1	AA	55	U	O4'-C1'-N1	5.05	112.24	108.20
2	AB	62	U	O4'-C1'-N1	5.05	112.24	108.20
2	AB	69	C	O4'-C1'-N1	5.05	112.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	481	G	C2-N3-C4	5.05	114.43	111.90
2	AB	520	G	C5'-C4'-C3'	-5.05	107.91	116.00
2	AB	533	G	C8-N9-C4	-5.05	104.38	106.40
2	AB	877	A	O3'-P-O5'	-5.05	94.40	104.00
2	AB	2478	A	C3'-C2'-C1'	-5.05	97.46	101.50
2	AB	1778	U	P-O3'-C3'	5.05	125.76	119.70
34	BA	893	C	C5'-C4'-O4'	5.05	115.16	109.10
35	BE	74	C	O4'-C1'-N1	5.05	112.24	108.20
2	AB	1938	A	C5'-C4'-C3'	-5.05	107.92	116.00
2	AB	2035	G	O4'-C1'-N9	5.05	112.24	108.20
2	AB	2617	U	O4'-C1'-N1	5.05	112.24	108.20
34	BA	663	A	C8-N9-C4	-5.05	103.78	105.80
34	BA	846	G	C8-N9-C4	-5.05	104.38	106.40
2	AB	1064	C	O3'-P-O5'	-5.05	94.41	104.00
2	AB	1390	U	C5'-C4'-C3'	-5.05	107.92	116.00
2	AB	1980	G	P-O3'-C3'	5.05	125.76	119.70
2	AB	2516	A	O4'-C1'-N9	5.05	112.24	108.20
34	BA	164	G	N3-C4-C5	-5.05	126.08	128.60
2	AB	103	A	C8-N9-C4	-5.05	103.78	105.80
2	AB	468	G	N3-C4-C5	-5.05	126.08	128.60
2	AB	1099	G	C4'-C3'-C2'	-5.05	97.55	102.60
2	AB	1416	G	C4-C5-N7	-5.05	108.78	110.80
2	AB	1418	G	C5'-C4'-O4'	5.05	115.16	109.10
2	AB	1888	G	N3-C4-C5	-5.05	126.08	128.60
34	BA	907	A	C5'-C4'-O4'	5.05	115.16	109.10
35	BB	73	A	O4'-C1'-N9	5.05	112.24	108.20
2	AB	1187	G	C8-N9-C4	-5.04	104.38	106.40
2	AB	2854	G	C5'-C4'-C3'	-5.04	107.93	116.00
7	AG	19	PHE	CB-CG-CD1	-5.04	117.27	120.80
34	BA	1231	G	C3'-C2'-C1'	-5.04	97.46	101.50
34	BA	1266	G	C3'-C2'-C1'	-5.04	97.46	101.50
2	AB	900	A	O4'-C1'-N9	5.04	112.23	108.20
2	AB	1603	A	C3'-C2'-C1'	-5.04	97.47	101.50
2	AB	1649	G	C1'-O4'-C4'	-5.04	105.86	109.90
2	AB	2186	G	N9-C1'-C2'	-5.04	106.45	112.00
2	AB	2347	C	P-O3'-C3'	5.04	125.75	119.70
34	BA	1527	U	O4'-C1'-N1	5.04	112.23	108.20
35	BE	10	G	N3-C4-C5	-5.04	126.08	128.60
2	AB	1046	A	C4'-C3'-C2'	-5.04	97.56	102.60
2	AB	1289	C	C5'-C4'-O4'	5.04	115.15	109.10
34	BA	445	G	O4'-C1'-N9	5.04	112.23	108.20
34	BA	521	G	C5'-C4'-O4'	5.04	115.15	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1517	G	N3-C4-C5	-5.04	126.08	128.60
2	AB	219	A	O4'-C1'-N9	5.04	112.23	108.20
2	AB	1191	G	N3-C4-C5	-5.04	126.08	128.60
2	AB	1711	A	O4'-C1'-N9	5.04	112.23	108.20
2	AB	776	G	C8-N9-C4	-5.04	104.38	106.40
2	AB	1587	G	C4'-C3'-C2'	-5.04	97.56	102.60
34	BA	481	G	C8-N9-C4	-5.04	104.38	106.40
34	BA	1041	G	O4'-C1'-N9	5.04	112.23	108.20
34	BA	1353	G	C5'-C4'-C3'	-5.04	107.94	116.00
34	BA	95	C	O4'-C1'-N1	5.04	112.23	108.20
2	AB	133	U	C5'-C4'-O4'	5.04	115.14	109.10
2	AB	1731	G	N3-C4-C5	-5.04	126.08	128.60
2	AB	2280	G	O4'-C1'-N9	5.04	112.23	108.20
2	AB	2699	C	C5'-C4'-C3'	-5.04	107.94	116.00
34	BA	171	A	C5'-C4'-O4'	5.04	115.14	109.10
34	BA	1002	G	C5'-C4'-O4'	5.04	115.14	109.10
34	BA	1021	A	C5'-C4'-C3'	-5.04	107.94	116.00
34	BA	1200	C	P-O3'-C3'	5.04	125.74	119.70
2	AB	1619	G	N3-C4-C5	-5.03	126.08	128.60
2	AB	2145	C	N1-C2-O2	5.03	121.92	118.90
2	AB	416	U	C5'-C4'-C3'	-5.03	107.95	116.00
34	BA	407	U	C4'-C3'-C2'	-5.03	97.57	102.60
2	AB	1606	C	N3-C2-O2	-5.03	118.38	121.90
2	AB	2051	A	O4'-C4'-C3'	5.03	110.12	106.10
2	AB	2194	U	C5'-C4'-C3'	-5.03	107.95	116.00
2	AB	2367	G	C3'-C2'-C1'	-5.03	97.48	101.50
37	BD	25	U	O4'-C1'-N1	5.03	112.22	108.20
2	AB	1504	A	C5'-C4'-C3'	-5.03	107.95	116.00
34	BA	1329	A	C4'-C3'-C2'	-5.03	97.57	102.60
2	AB	301	G	P-O3'-C3'	5.03	125.73	119.70
2	AB	390	U	C5'-C4'-O4'	5.03	115.13	109.10
2	AB	1736	U	N1-C2-N3	5.03	117.92	114.90
34	BA	1528	U	C4'-C3'-C2'	-5.03	97.57	102.60
1	AA	32	U	C2-N3-C4	-5.02	123.98	127.00
2	AB	1480	C	O4'-C1'-N1	5.02	112.22	108.20
2	AB	1583	A	P-O3'-C3'	5.02	125.73	119.70
34	BA	214	C	C3'-C2'-C1'	-5.02	97.48	101.50
2	AB	214	G	N3-C4-C5	-5.02	126.09	128.60
2	AB	301	G	C8-N9-C4	-5.02	104.39	106.40
2	AB	1333	G	C5'-C4'-O4'	5.02	115.13	109.10
2	AB	1348	C	C5'-C4'-O4'	5.02	115.13	109.10
34	BA	1511	G	C5'-C4'-C3'	-5.02	107.96	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	69	G	C5'-C4'-C3'	-5.02	107.96	116.00
2	AB	23	G	C8-N9-C4	-5.02	104.39	106.40
2	AB	35	G	C8-N9-C4	-5.02	104.39	106.40
2	AB	1066	U	C5'-C4'-C3'	-5.02	107.97	116.00
2	AB	2000	C	O4'-C1'-N1	5.02	112.22	108.20
2	AB	938	G	O4'-C1'-N9	5.02	112.22	108.20
2	AB	942	G	N3-C4-C5	-5.02	126.09	128.60
2	AB	1191	G	C4'-C3'-C2'	-5.02	97.58	102.60
2	AB	2378	A	C5'-C4'-C3'	-5.02	107.97	116.00
34	BA	1026	G	C8-N9-C4	-5.02	104.39	106.40
2	AB	2117	A	P-O3'-C3'	5.02	125.72	119.70
2	AB	1171	G	C4'-C3'-C2'	-5.02	97.58	102.60
2	AB	1954	G	C3'-C2'-C1'	-5.02	97.49	101.50
34	BA	847	G	C2-N3-C4	5.02	114.41	111.90
34	BA	1403	C	C5'-C4'-C3'	-5.02	107.97	116.00
1	AA	79	G	N3-C4-C5	-5.01	126.09	128.60
2	AB	1734	G	N3-C4-C5	-5.01	126.09	128.60
34	BA	911	U	C1'-O4'-C4'	-5.01	105.89	109.90
34	BA	1219	A	O4'-C1'-N9	5.01	112.21	108.20
35	BE	10	G	C5'-C4'-O4'	5.01	115.12	109.10
2	AB	1799	G	N9-C4-C5	5.01	107.41	105.40
2	AB	2010	G	C5'-C4'-O4'	5.01	115.12	109.10
2	AB	2288	A	O4'-C1'-N9	5.01	112.21	108.20
34	BA	989	U	C5'-C4'-O4'	5.01	115.12	109.10
34	BA	1532	U	O4'-C1'-N1	5.01	112.21	108.20
35	BE	49	C	C5'-C4'-O4'	5.01	115.11	109.10
2	AB	323	C	N1-C2-O2	5.01	121.91	118.90
2	AB	2741	A	C5'-C4'-C3'	-5.01	107.98	116.00
2	AB	860	U	O4'-C1'-N1	5.01	112.21	108.20
2	AB	912	C	O4'-C1'-N1	5.01	112.21	108.20
2	AB	948	C	N1-C2-O2	5.01	121.91	118.90
2	AB	1245	G	C4'-C3'-C2'	-5.01	97.59	102.60
2	AB	1533	C	N1-C2-O2	5.01	121.91	118.90
2	AB	1763	G	O3'-P-O5'	-5.01	94.48	104.00
2	AB	1937	A	O4'-C1'-N9	5.01	112.21	108.20
2	AB	2722	G	C8-N9-C4	-5.01	104.40	106.40
2	AB	1171	G	C8-N9-C4	-5.01	104.40	106.40
2	AB	2297	A	C5'-C4'-O4'	5.01	115.11	109.10
2	AB	420	C	N3-C2-O2	-5.01	118.40	121.90
2	AB	1228	G	O4'-C1'-N9	5.01	112.20	108.20
2	AB	1359	A	N9-C1'-C2'	-5.01	106.49	112.00
2	AB	1501	G	C2-N3-C4	5.01	114.40	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2278	A	C4'-C3'-C2'	-5.01	97.59	102.60
2	AB	2395	C	C5'-C4'-C3'	-5.01	107.99	116.00
2	AB	2770	G	O4'-C1'-N9	5.01	112.20	108.20
34	BA	590	U	C5'-C4'-C3'	-5.01	107.99	116.00
34	BA	1153	G	N9-C1'-C2'	-5.01	106.49	112.00
34	BA	1259	C	C5'-C4'-O4'	5.01	115.11	109.10
2	AB	720	U	C5'-C4'-C3'	-5.00	107.99	116.00
2	AB	1054	A	P-O3'-C3'	5.00	125.71	119.70
2	AB	1266	G	N9-C4-C5	5.00	107.40	105.40
34	BA	350	G	P-O3'-C3'	5.00	125.71	119.70
1	AA	43	C	N1-C2-O2	5.00	121.90	118.90
2	AB	840	C	O4'-C1'-N1	5.00	112.20	108.20
2	AB	2870	C	O4'-C1'-N1	5.00	112.20	108.20
34	BA	761	G	O4'-C1'-N9	5.00	112.20	108.20
34	BA	1475	G	C8-N9-C4	-5.00	104.40	106.40
2	AB	8	C	O4'-C1'-N1	5.00	112.20	108.20
35	BE	2	C	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (1392) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	103	U	Sidechain
1	AA	107	G	Sidechain
1	AA	108	A	Sidechain
1	AA	109	A	Sidechain
1	AA	13	G	Sidechain
1	AA	14	U	Sidechain
1	AA	15	A	Sidechain
1	AA	19	C	Sidechain
1	AA	2	G	Sidechain
1	AA	26	C	Sidechain
1	AA	36	C	Sidechain
1	AA	37	C	Sidechain
1	AA	40	U	Sidechain
1	AA	41	G	Sidechain
1	AA	48	U	Sidechain
1	AA	52	A	Sidechain
1	AA	62	C	Sidechain
1	AA	64	G	Sidechain
1	AA	65	U	Sidechain
1	AA	66	A	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	67	G	Sidechain
1	AA	7	G	Sidechain
1	AA	72	G	Sidechain
1	AA	87	U	Sidechain
1	AA	88	C	Sidechain
1	AA	95	U	Sidechain
1	AA	99	A	Sidechain
2	AB	1000	A	Sidechain
2	AB	1003	G	Sidechain
2	AB	1004	U	Sidechain
2	AB	1005	C	Sidechain
2	AB	1006	C	Sidechain
2	AB	1010	A	Sidechain
2	AB	1011	G	Sidechain
2	AB	1012	U	Sidechain
2	AB	1014	A	Sidechain
2	AB	1017	G	Sidechain
2	AB	1022	G	Sidechain
2	AB	1025	G	Sidechain
2	AB	1026	G	Sidechain
2	AB	1027	A	Sidechain
2	AB	1028	A	Sidechain
2	AB	1029	A	Sidechain
2	AB	103	A	Sidechain
2	AB	104	A	Sidechain
2	AB	1042	G	Sidechain
2	AB	1048	A	Sidechain
2	AB	105	C	Sidechain
2	AB	1052	C	Sidechain
2	AB	1053	C	Sidechain
2	AB	1054	A	Sidechain
2	AB	1057	A	Sidechain
2	AB	1059	G	Sidechain
2	AB	1061	U	Sidechain
2	AB	1063	G	Sidechain
2	AB	1064	C	Sidechain
2	AB	1067	A	Sidechain
2	AB	1069	A	Sidechain
2	AB	1073	A	Sidechain
2	AB	1074	G	Sidechain
2	AB	1075	C	Sidechain
2	AB	1076	C	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	1084	A	Sidechain
2	AB	1087	G	Sidechain
2	AB	1094	U	Sidechain
2	AB	1096	A	Sidechain
2	AB	1097	U	Sidechain
2	AB	1098	A	Sidechain
2	AB	1099	G	Sidechain
2	AB	1111	A	Sidechain
2	AB	1116	G	Sidechain
2	AB	1117	C	Sidechain
2	AB	1118	C	Sidechain
2	AB	112	U	Sidechain
2	AB	1120	G	Sidechain
2	AB	1121	C	Sidechain
2	AB	1123	C	Sidechain
2	AB	1124	G	Sidechain
2	AB	1130	U	Sidechain
2	AB	1131	G	Sidechain
2	AB	1132	U	Sidechain
2	AB	1133	A	Sidechain
2	AB	1135	C	Sidechain
2	AB	1138	G	Sidechain
2	AB	1141	U	Sidechain
2	AB	1143	A	Sidechain
2	AB	1144	A	Sidechain
2	AB	1145	C	Sidechain
2	AB	115	C	Sidechain
2	AB	1153	C	Sidechain
2	AB	1154	G	Sidechain
2	AB	116	C	Sidechain
2	AB	1161	C	Sidechain
2	AB	1174	U	Sidechain
2	AB	1179	G	Sidechain
2	AB	118	A	Sidechain
2	AB	1182	G	Sidechain
2	AB	119	A	Sidechain
2	AB	1198	U	Sidechain
2	AB	1199	U	Sidechain
2	AB	1203	U	Sidechain
2	AB	1204	A	Sidechain
2	AB	1212	G	Sidechain
2	AB	1224	U	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	1226	A	Sidechain
2	AB	1227	G	Sidechain
2	AB	1230	A	Sidechain
2	AB	1234	U	Sidechain
2	AB	1236	G	Sidechain
2	AB	1242	U	Sidechain
2	AB	1246	A	Sidechain
2	AB	1256	G	Sidechain
2	AB	1262	A	Sidechain
2	AB	1263	U	Sidechain
2	AB	1266	G	Sidechain
2	AB	1268	A	Sidechain
2	AB	127	A	Sidechain
2	AB	1271	G	Sidechain
2	AB	1276	A	Sidechain
2	AB	1281	G	Sidechain
2	AB	1282	U	Sidechain
2	AB	1283	G	Sidechain
2	AB	1284	A	Sidechain
2	AB	1287	A	Sidechain
2	AB	1288	G	Sidechain
2	AB	1289	C	Sidechain
2	AB	129	C	Sidechain
2	AB	1293	C	Sidechain
2	AB	1295	C	Sidechain
2	AB	1296	G	Sidechain
2	AB	1299	G	Sidechain
2	AB	1309	G	Sidechain
2	AB	1317	G	Sidechain
2	AB	132	G	Sidechain
2	AB	1321	A	Sidechain
2	AB	1324	G	Sidechain
2	AB	1327	A	Sidechain
2	AB	133	U	Sidechain
2	AB	1330	C	Sidechain
2	AB	1334	G	Sidechain
2	AB	1335	C	Sidechain
2	AB	1345	C	Sidechain
2	AB	1353	A	Sidechain
2	AB	1356	G	Sidechain
2	AB	1359	A	Sidechain
2	AB	1368	G	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	137	U	Sidechain
2	AB	1371	G	Sidechain
2	AB	1376	C	Sidechain
2	AB	1377	G	Sidechain
2	AB	1379	U	Sidechain
2	AB	138	U	Sidechain
2	AB	1381	G	Sidechain
2	AB	1389	G	Sidechain
2	AB	1390	U	Sidechain
2	AB	1392	A	Sidechain
2	AB	1393	A	Sidechain
2	AB	1394	U	Sidechain
2	AB	1396	U	Sidechain
2	AB	1398	C	Sidechain
2	AB	1399	C	Sidechain
2	AB	140	C	Sidechain
2	AB	1400	U	Sidechain
2	AB	141	G	Sidechain
2	AB	1410	G	Sidechain
2	AB	1416	G	Sidechain
2	AB	1417	C	Sidechain
2	AB	1418	G	Sidechain
2	AB	1419	A	Sidechain
2	AB	1424	G	Sidechain
2	AB	1426	G	Sidechain
2	AB	1427	A	Sidechain
2	AB	143	C	Sidechain
2	AB	1436	G	Sidechain
2	AB	1440	U	Sidechain
2	AB	1442	U	Sidechain
2	AB	145	C	Sidechain
2	AB	1453	A	Sidechain
2	AB	1454	C	Sidechain
2	AB	1456	G	Sidechain
2	AB	1458	U	Sidechain
2	AB	1459	G	Sidechain
2	AB	146	A	Sidechain
2	AB	1471	G	Sidechain
2	AB	1473	G	Sidechain
2	AB	1481	U	Sidechain
2	AB	149	A	Sidechain
2	AB	1495	A	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	1501	G	Sidechain
2	AB	1514	G	Sidechain
2	AB	1521	G	Sidechain
2	AB	1527	G	Sidechain
2	AB	1532	A	Sidechain
2	AB	1535	A	Sidechain
2	AB	1537	G	Sidechain
2	AB	1544	A	Sidechain
2	AB	1546	G	Sidechain
2	AB	1548	A	Sidechain
2	AB	1549	A	Sidechain
2	AB	1552	A	Sidechain
2	AB	1553	A	Sidechain
2	AB	1554	U	Sidechain
2	AB	1555	G	Sidechain
2	AB	1564	C	Sidechain
2	AB	1566	A	Sidechain
2	AB	1568	G	Sidechain
2	AB	1577	C	Sidechain
2	AB	1578	U	Sidechain
2	AB	1581	G	Sidechain
2	AB	1588	G	Sidechain
2	AB	1592	C	Sidechain
2	AB	1596	A	Sidechain
2	AB	1603	A	Sidechain
2	AB	1605	C	Sidechain
2	AB	1606	C	Sidechain
2	AB	1607	C	Sidechain
2	AB	1608	A	Sidechain
2	AB	1609	A	Sidechain
2	AB	161	A	Sidechain
2	AB	1620	G	Sidechain
2	AB	1622	G	Sidechain
2	AB	163	C	Sidechain
2	AB	1631	G	Sidechain
2	AB	1632	A	Sidechain
2	AB	164	C	Sidechain
2	AB	1641	A	Sidechain
2	AB	1644	C	Sidechain
2	AB	1646	C	Sidechain
2	AB	1652	A	Sidechain
2	AB	1656	C	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	166	U	Sidechain
2	AB	1664	A	Sidechain
2	AB	1671	U	Sidechain
2	AB	1672	A	Sidechain
2	AB	1675	C	Sidechain
2	AB	1680	U	Sidechain
2	AB	1687	G	Sidechain
2	AB	1689	A	Sidechain
2	AB	169	G	Sidechain
2	AB	1690	A	Sidechain
2	AB	1693	U	Sidechain
2	AB	1695	G	Sidechain
2	AB	17	G	Sidechain
2	AB	1701	A	Sidechain
2	AB	1706	C	Sidechain
2	AB	1710	G	Sidechain
2	AB	1711	A	Sidechain
2	AB	1721	G	Sidechain
2	AB	1722	A	Sidechain
2	AB	1723	G	Sidechain
2	AB	1726	C	Sidechain
2	AB	1733	G	Sidechain
2	AB	1734	G	Sidechain
2	AB	1736	U	Sidechain
2	AB	1738	G	Sidechain
2	AB	1739	A	Sidechain
2	AB	174	U	Sidechain
2	AB	1740	G	Sidechain
2	AB	1742	U	Sidechain
2	AB	1750	G	Sidechain
2	AB	1752	C	Sidechain
2	AB	1755	A	Sidechain
2	AB	1757	A	Sidechain
2	AB	177	G	Sidechain
2	AB	1777	U	Sidechain
2	AB	1780	A	Sidechain
2	AB	1788	C	Sidechain
2	AB	1791	A	Sidechain
2	AB	1797	G	Sidechain
2	AB	1799	G	Sidechain
2	AB	180	G	Sidechain
2	AB	1800	C	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	1801	A	Sidechain
2	AB	1802	A	Sidechain
2	AB	1805	A	Sidechain
2	AB	1806	C	Sidechain
2	AB	1809	A	Sidechain
2	AB	1810	A	Sidechain
2	AB	1818	U	Sidechain
2	AB	1819	A	Sidechain
2	AB	1820	U	Sidechain
2	AB	1822	C	Sidechain
2	AB	1825	U	Sidechain
2	AB	1828	G	Sidechain
2	AB	1831	G	Sidechain
2	AB	1834	U	Sidechain
2	AB	1836	C	Sidechain
2	AB	1837	C	Sidechain
2	AB	1839	G	Sidechain
2	AB	1841	U	Sidechain
2	AB	1846	G	Sidechain
2	AB	1847	A	Sidechain
2	AB	1848	A	Sidechain
2	AB	1850	G	Sidechain
2	AB	1852	U	Sidechain
2	AB	1854	A	Sidechain
2	AB	1857	G	Sidechain
2	AB	1865	U	Sidechain
2	AB	1869	G	Sidechain
2	AB	1870	C	Sidechain
2	AB	1871	A	Sidechain
2	AB	1872	A	Sidechain
2	AB	1878	G	Sidechain
2	AB	188	G	Sidechain
2	AB	1886	U	Sidechain
2	AB	1887	C	Sidechain
2	AB	1888	G	Sidechain
2	AB	189	G	Sidechain
2	AB	1898	U	Sidechain
2	AB	190	A	Sidechain
2	AB	1903	G	Sidechain
2	AB	1906	G	Sidechain
2	AB	1909	C	Sidechain
2	AB	1912	A	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	1918	A	Sidechain
2	AB	192	C	Sidechain
2	AB	1920	C	Sidechain
2	AB	1924	C	Sidechain
2	AB	1925	C	Sidechain
2	AB	1926	U	Sidechain
2	AB	1927	A	Sidechain
2	AB	1928	A	Sidechain
2	AB	1929	G	Sidechain
2	AB	1932	A	Sidechain
2	AB	1938	A	Sidechain
2	AB	194	G	Sidechain
2	AB	1942	C	Sidechain
2	AB	195	A	Sidechain
2	AB	1959	G	Sidechain
2	AB	1961	C	Sidechain
2	AB	1968	G	Sidechain
2	AB	1969	A	Sidechain
2	AB	1970	A	Sidechain
2	AB	1973	G	Sidechain
2	AB	1975	G	Sidechain
2	AB	1976	U	Sidechain
2	AB	1995	U	Sidechain
2	AB	1996	C	Sidechain
2	AB	1997	C	Sidechain
2	AB	20	C	Sidechain
2	AB	2002	G	Sidechain
2	AB	2005	A	Sidechain
2	AB	2017	U	Sidechain
2	AB	2020	A	Sidechain
2	AB	2021	C	Sidechain
2	AB	2025	C	Sidechain
2	AB	2029	G	Sidechain
2	AB	2031	A	Sidechain
2	AB	2032	G	Sidechain
2	AB	2033	A	Sidechain
2	AB	2034	U	Sidechain
2	AB	204	A	Sidechain
2	AB	2040	G	Sidechain
2	AB	2042	A	Sidechain
2	AB	2046	G	Sidechain
2	AB	2048	G	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	2051	A	Sidechain
2	AB	2053	G	Sidechain
2	AB	2055	C	Sidechain
2	AB	2058	A	Sidechain
2	AB	2059	A	Sidechain
2	AB	206	U	Sidechain
2	AB	2064	C	Sidechain
2	AB	2068	U	Sidechain
2	AB	2071	A	Sidechain
2	AB	2072	C	Sidechain
2	AB	2073	C	Sidechain
2	AB	2074	U	Sidechain
2	AB	2075	U	Sidechain
2	AB	2077	A	Sidechain
2	AB	2079	U	Sidechain
2	AB	2092	U	Sidechain
2	AB	2094	A	Sidechain
2	AB	2097	A	Sidechain
2	AB	2107	G	Sidechain
2	AB	2112	G	Sidechain
2	AB	2113	U	Sidechain
2	AB	2115	G	Sidechain
2	AB	2117	A	Sidechain
2	AB	2126	A	Sidechain
2	AB	2127	G	Sidechain
2	AB	2128	G	Sidechain
2	AB	213	A	Sidechain
2	AB	2133	G	Sidechain
2	AB	2134	A	Sidechain
2	AB	215	G	Sidechain
2	AB	2159	G	Sidechain
2	AB	2160	C	Sidechain
2	AB	2168	G	Sidechain
2	AB	2179	C	Sidechain
2	AB	2183	A	Sidechain
2	AB	2185	U	Sidechain
2	AB	2188	U	Sidechain
2	AB	2190	G	Sidechain
2	AB	2193	G	Sidechain
2	AB	2198	A	Sidechain
2	AB	22	C	Sidechain
2	AB	2202	U	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	2204	G	Sidechain
2	AB	2218	G	Sidechain
2	AB	2223	G	Sidechain
2	AB	2226	C	Sidechain
2	AB	2233	U	Sidechain
2	AB	2234	G	Sidechain
2	AB	2238	G	Sidechain
2	AB	2250	G	Sidechain
2	AB	2259	U	Sidechain
2	AB	226	A	Sidechain
2	AB	2261	C	Sidechain
2	AB	2262	U	Sidechain
2	AB	2263	C	Sidechain
2	AB	2268	A	Sidechain
2	AB	2269	G	Sidechain
2	AB	227	A	Sidechain
2	AB	2271	G	Sidechain
2	AB	2273	A	Sidechain
2	AB	2274	A	Sidechain
2	AB	2275	C	Sidechain
2	AB	2277	G	Sidechain
2	AB	2282	G	Sidechain
2	AB	2285	C	Sidechain
2	AB	2287	A	Sidechain
2	AB	2289	G	Sidechain
2	AB	2299	U	Sidechain
2	AB	23	G	Sidechain
2	AB	2301	C	Sidechain
2	AB	2304	G	Sidechain
2	AB	2306	C	Sidechain
2	AB	2307	G	Sidechain
2	AB	2308	G	Sidechain
2	AB	231	A	Sidechain
2	AB	2310	C	Sidechain
2	AB	2317	A	Sidechain
2	AB	2318	G	Sidechain
2	AB	2321	U	Sidechain
2	AB	2323	G	Sidechain
2	AB	2324	U	Sidechain
2	AB	2325	G	Sidechain
2	AB	2328	A	Sidechain
2	AB	2330	G	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	2331	G	Sidechain
2	AB	2333	A	Sidechain
2	AB	2335	A	Sidechain
2	AB	2338	C	Sidechain
2	AB	2342	C	Sidechain
2	AB	2344	U	Sidechain
2	AB	2348	U	Sidechain
2	AB	2357	G	Sidechain
2	AB	2359	C	Sidechain
2	AB	2362	C	Sidechain
2	AB	2365	G	Sidechain
2	AB	2375	G	Sidechain
2	AB	2376	A	Sidechain
2	AB	2380	C	Sidechain
2	AB	2383	G	Sidechain
2	AB	2387	U	Sidechain
2	AB	2389	G	Sidechain
2	AB	2391	G	Sidechain
2	AB	24	G	Sidechain
2	AB	2402	U	Sidechain
2	AB	2407	A	Sidechain
2	AB	241	A	Sidechain
2	AB	2411	A	Sidechain
2	AB	2414	G	Sidechain
2	AB	2416	C	Sidechain
2	AB	2419	U	Sidechain
2	AB	242	G	Sidechain
2	AB	2420	C	Sidechain
2	AB	2424	C	Sidechain
2	AB	2427	C	Sidechain
2	AB	2430	A	Sidechain
2	AB	2434	A	Sidechain
2	AB	2450	A	Sidechain
2	AB	2458	G	Sidechain
2	AB	2460	U	Sidechain
2	AB	2464	G	Sidechain
2	AB	2466	C	Sidechain
2	AB	2471	A	Sidechain
2	AB	2480	C	Sidechain
2	AB	2490	G	Sidechain
2	AB	2492	U	Sidechain
2	AB	2496	C	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	2497	A	Sidechain
2	AB	250	G	Sidechain
2	AB	2500	U	Sidechain
2	AB	2505	G	Sidechain
2	AB	2507	C	Sidechain
2	AB	2510	C	Sidechain
2	AB	2515	C	Sidechain
2	AB	2516	A	Sidechain
2	AB	2519	U	Sidechain
2	AB	252	G	Sidechain
2	AB	2521	C	Sidechain
2	AB	2526	G	Sidechain
2	AB	2529	G	Sidechain
2	AB	2531	A	Sidechain
2	AB	2533	U	Sidechain
2	AB	2536	G	Sidechain
2	AB	2538	C	Sidechain
2	AB	2539	C	Sidechain
2	AB	2547	A	Sidechain
2	AB	2550	G	Sidechain
2	AB	2554	U	Sidechain
2	AB	2563	U	Sidechain
2	AB	2565	A	Sidechain
2	AB	2569	G	Sidechain
2	AB	257	C	Sidechain
2	AB	2573	C	Sidechain
2	AB	2574	G	Sidechain
2	AB	2576	G	Sidechain
2	AB	2579	C	Sidechain
2	AB	2581	G	Sidechain
2	AB	2583	G	Sidechain
2	AB	2587	A	Sidechain
2	AB	2588	G	Sidechain
2	AB	2589	A	Sidechain
2	AB	259	G	Sidechain
2	AB	2592	G	Sidechain
2	AB	2595	G	Sidechain
2	AB	2599	G	Sidechain
2	AB	260	G	Sidechain
2	AB	261	G	Sidechain
2	AB	2611	C	Sidechain
2	AB	2612	C	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	2616	C	Sidechain
2	AB	262	A	Sidechain
2	AB	2621	G	Sidechain
2	AB	2625	G	Sidechain
2	AB	2627	G	Sidechain
2	AB	263	G	Sidechain
2	AB	2637	U	Sidechain
2	AB	2643	G	Sidechain
2	AB	2644	G	Sidechain
2	AB	2645	G	Sidechain
2	AB	265	A	Sidechain
2	AB	2658	C	Sidechain
2	AB	2659	G	Sidechain
2	AB	266	G	Sidechain
2	AB	2660	A	Sidechain
2	AB	2661	G	Sidechain
2	AB	2662	A	Sidechain
2	AB	2663	G	Sidechain
2	AB	2664	G	Sidechain
2	AB	2666	C	Sidechain
2	AB	2671	G	Sidechain
2	AB	2677	G	Sidechain
2	AB	268	C	Sidechain
2	AB	2680	U	Sidechain
2	AB	2683	C	Sidechain
2	AB	2684	U	Sidechain
2	AB	2688	G	Sidechain
2	AB	2693	G	Sidechain
2	AB	2696	U	Sidechain
2	AB	2701	U	Sidechain
2	AB	2706	A	Sidechain
2	AB	271	G	Sidechain
2	AB	2720	U	Sidechain
2	AB	2722	G	Sidechain
2	AB	2727	A	Sidechain
2	AB	2728	U	Sidechain
2	AB	2731	G	Sidechain
2	AB	2732	G	Sidechain
2	AB	2737	G	Sidechain
2	AB	2739	U	Sidechain
2	AB	2740	A	Sidechain
2	AB	275	C	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	2756	U	Sidechain
2	AB	276	U	Sidechain
2	AB	2763	G	Sidechain
2	AB	2764	A	Sidechain
2	AB	2765	A	Sidechain
2	AB	2770	G	Sidechain
2	AB	2783	U	Sidechain
2	AB	2785	C	Sidechain
2	AB	2787	C	Sidechain
2	AB	2791	G	Sidechain
2	AB	2792	A	Sidechain
2	AB	2797	U	Sidechain
2	AB	2799	A	Sidechain
2	AB	2801	G	Sidechain
2	AB	2805	C	Sidechain
2	AB	2807	U	Sidechain
2	AB	2808	G	Sidechain
2	AB	281	C	Sidechain
2	AB	2813	A	Sidechain
2	AB	2815	C	Sidechain
2	AB	2818	U	Sidechain
2	AB	2819	G	Sidechain
2	AB	2824	C	Sidechain
2	AB	283	G	Sidechain
2	AB	2832	U	Sidechain
2	AB	2843	G	Sidechain
2	AB	2849	U	Sidechain
2	AB	2854	G	Sidechain
2	AB	2857	G	Sidechain
2	AB	2859	G	Sidechain
2	AB	2861	U	Sidechain
2	AB	2862	G	Sidechain
2	AB	2864	G	Sidechain
2	AB	2872	A	Sidechain
2	AB	2873	A	Sidechain
2	AB	2881	U	Sidechain
2	AB	2882	A	Sidechain
2	AB	2884	U	Sidechain
2	AB	2890	G	Sidechain
2	AB	2892	G	Sidechain
2	AB	2894	G	Sidechain
2	AB	2895	G	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	29	U	Sidechain
2	AB	291	G	Sidechain
2	AB	293	U	Sidechain
2	AB	294	A	Sidechain
2	AB	299	A	Sidechain
2	AB	300	A	Sidechain
2	AB	303	G	Sidechain
2	AB	306	U	Sidechain
2	AB	307	G	Sidechain
2	AB	308	G	Sidechain
2	AB	310	A	Sidechain
2	AB	311	A	Sidechain
2	AB	313	G	Sidechain
2	AB	315	G	Sidechain
2	AB	319	G	Sidechain
2	AB	32	C	Sidechain
2	AB	321	U	Sidechain
2	AB	329	G	Sidechain
2	AB	33	C	Sidechain
2	AB	339	U	Sidechain
2	AB	34	U	Sidechain
2	AB	340	A	Sidechain
2	AB	341	C	Sidechain
2	AB	342	A	Sidechain
2	AB	345	A	Sidechain
2	AB	346	A	Sidechain
2	AB	347	A	Sidechain
2	AB	356	G	Sidechain
2	AB	360	U	Sidechain
2	AB	362	A	Sidechain
2	AB	363	G	Sidechain
2	AB	364	C	Sidechain
2	AB	365	U	Sidechain
2	AB	367	G	Sidechain
2	AB	368	A	Sidechain
2	AB	369	U	Sidechain
2	AB	378	C	Sidechain
2	AB	382	A	Sidechain
2	AB	391	A	Sidechain
2	AB	392	U	Sidechain
2	AB	394	C	Sidechain
2	AB	395	U	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	401	A	Sidechain
2	AB	405	U	Sidechain
2	AB	407	G	Sidechain
2	AB	411	G	Sidechain
2	AB	412	A	Sidechain
2	AB	421	C	Sidechain
2	AB	422	A	Sidechain
2	AB	424	G	Sidechain
2	AB	429	A	Sidechain
2	AB	430	A	Sidechain
2	AB	432	A	Sidechain
2	AB	442	G	Sidechain
2	AB	445	C	Sidechain
2	AB	446	G	Sidechain
2	AB	448	U	Sidechain
2	AB	449	A	Sidechain
2	AB	45	G	Sidechain
2	AB	452	G	Sidechain
2	AB	456	C	Sidechain
2	AB	458	G	Sidechain
2	AB	460	A	Sidechain
2	AB	463	G	Sidechain
2	AB	464	U	Sidechain
2	AB	465	G	Sidechain
2	AB	467	G	Sidechain
2	AB	47	C	Sidechain
2	AB	470	A	Sidechain
2	AB	473	G	Sidechain
2	AB	476	G	Sidechain
2	AB	478	A	Sidechain
2	AB	480	A	Sidechain
2	AB	481	G	Sidechain
2	AB	484	C	Sidechain
2	AB	487	C	Sidechain
2	AB	489	G	Sidechain
2	AB	492	A	Sidechain
2	AB	493	G	Sidechain
2	AB	494	G	Sidechain
2	AB	498	G	Sidechain
2	AB	499	U	Sidechain
2	AB	501	A	Sidechain
2	AB	507	A	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	511	U	Sidechain
2	AB	512	G	Sidechain
2	AB	517	C	Sidechain
2	AB	518	G	Sidechain
2	AB	520	G	Sidechain
2	AB	522	A	Sidechain
2	AB	526	A	Sidechain
2	AB	527	C	Sidechain
2	AB	535	G	Sidechain
2	AB	536	G	Sidechain
2	AB	539	G	Sidechain
2	AB	546	U	Sidechain
2	AB	547	A	Sidechain
2	AB	551	G	Sidechain
2	AB	553	G	Sidechain
2	AB	554	U	Sidechain
2	AB	555	G	Sidechain
2	AB	572	A	Sidechain
2	AB	582	A	Sidechain
2	AB	585	G	Sidechain
2	AB	586	A	Sidechain
2	AB	588	U	Sidechain
2	AB	590	A	Sidechain
2	AB	591	U	Sidechain
2	AB	594	U	Sidechain
2	AB	595	C	Sidechain
2	AB	60	G	Sidechain
2	AB	604	G	Sidechain
2	AB	608	A	Sidechain
2	AB	611	C	Sidechain
2	AB	612	G	Sidechain
2	AB	613	A	Sidechain
2	AB	614	A	Sidechain
2	AB	62	U	Sidechain
2	AB	630	G	Sidechain
2	AB	631	A	Sidechain
2	AB	632	A	Sidechain
2	AB	635	C	Sidechain
2	AB	642	U	Sidechain
2	AB	644	A	Sidechain
2	AB	647	G	Sidechain
2	AB	65	U	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	655	A	Sidechain
2	AB	666	A	Sidechain
2	AB	674	G	Sidechain
2	AB	676	A	Sidechain
2	AB	678	C	Sidechain
2	AB	68	G	Sidechain
2	AB	692	C	Sidechain
2	AB	693	A	Sidechain
2	AB	696	G	Sidechain
2	AB	697	G	Sidechain
2	AB	7	G	Sidechain
2	AB	700	G	Sidechain
2	AB	701	G	Sidechain
2	AB	704	G	Sidechain
2	AB	71	A	Sidechain
2	AB	714	U	Sidechain
2	AB	716	A	Sidechain
2	AB	717	C	Sidechain
2	AB	72	U	Sidechain
2	AB	721	A	Sidechain
2	AB	726	G	Sidechain
2	AB	727	A	Sidechain
2	AB	730	A	Sidechain
2	AB	738	G	Sidechain
2	AB	739	A	Sidechain
2	AB	74	A	Sidechain
2	AB	744	U	Sidechain
2	AB	750	A	Sidechain
2	AB	751	A	Sidechain
2	AB	753	A	Sidechain
2	AB	757	G	Sidechain
2	AB	758	C	Sidechain
2	AB	765	C	Sidechain
2	AB	766	U	Sidechain
2	AB	767	U	Sidechain
2	AB	77	G	Sidechain
2	AB	775	G	Sidechain
2	AB	778	G	Sidechain
2	AB	780	G	Sidechain
2	AB	788	A	Sidechain
2	AB	789	A	Sidechain
2	AB	791	C	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	794	A	Sidechain
2	AB	798	G	Sidechain
2	AB	801	G	Sidechain
2	AB	809	G	Sidechain
2	AB	81	G	Sidechain
2	AB	810	U	Sidechain
2	AB	814	C	Sidechain
2	AB	816	C	Sidechain
2	AB	818	G	Sidechain
2	AB	83	A	Sidechain
2	AB	834	G	Sidechain
2	AB	836	G	Sidechain
2	AB	839	U	Sidechain
2	AB	841	G	Sidechain
2	AB	843	G	Sidechain
2	AB	844	A	Sidechain
2	AB	845	A	Sidechain
2	AB	847	U	Sidechain
2	AB	848	C	Sidechain
2	AB	852	U	Sidechain
2	AB	856	G	Sidechain
2	AB	857	G	Sidechain
2	AB	858	G	Sidechain
2	AB	859	G	Sidechain
2	AB	864	G	Sidechain
2	AB	866	A	Sidechain
2	AB	867	C	Sidechain
2	AB	868	U	Sidechain
2	AB	870	U	Sidechain
2	AB	871	U	Sidechain
2	AB	872	U	Sidechain
2	AB	88	G	Sidechain
2	AB	882	G	Sidechain
2	AB	886	A	Sidechain
2	AB	887	U	Sidechain
2	AB	888	C	Sidechain
2	AB	892	A	Sidechain
2	AB	894	U	Sidechain
2	AB	895	U	Sidechain
2	AB	896	A	Sidechain
2	AB	898	C	Sidechain
2	AB	901	C	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	910	A	Sidechain
2	AB	911	A	Sidechain
2	AB	912	C	Sidechain
2	AB	913	U	Sidechain
2	AB	918	A	Sidechain
2	AB	92	U	Sidechain
2	AB	924	G	Sidechain
2	AB	925	A	Sidechain
2	AB	930	G	Sidechain
2	AB	932	U	Sidechain
2	AB	933	A	Sidechain
2	AB	936	A	Sidechain
2	AB	945	A	Sidechain
2	AB	947	A	Sidechain
2	AB	949	G	Sidechain
2	AB	95	A	Sidechain
2	AB	960	A	Sidechain
2	AB	961	C	Sidechain
2	AB	962	G	Sidechain
2	AB	965	C	Sidechain
2	AB	966	G	Sidechain
2	AB	976	G	Sidechain
2	AB	978	G	Sidechain
2	AB	979	A	Sidechain
2	AB	98	G	Sidechain
2	AB	980	A	Sidechain
2	AB	983	A	Sidechain
2	AB	99	U	Sidechain
2	AB	990	A	Sidechain
2	AB	993	G	Sidechain
3	AC	43	ASP	Peptide
3	AC	44	VAL	Peptide
5	AE	24	VAL	Mainchain
5	AE	47	ALA	Peptide,Mainchain
6	AF	77	ILE	Peptide
8	AH	107	GLY	Peptide
8	AH	39	ALA	Peptide
9	AI	117	LEU	Peptide
9	AI	31	VAL	Mainchain
11	AK	51	GLY	Peptide
11	AK	75	TYR	Sidechain
15	AO	16	HIS	Sidechain

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Mol	Chain	Res	Type	Group
17	AQ	98	TYR	Sidechain
18	AR	4	LYS	Peptide
28	Ab	54	GLY	Mainchain
30	Ad	48	TYR	Sidechain
31	Ae	45	SER	Peptide
31	Ae	6	GLN	Peptide
34	BA	100	G	Sidechain
34	BA	1003	G	Sidechain
34	BA	1008	U	Sidechain
34	BA	1009	U	Sidechain
34	BA	1010	U	Sidechain
34	BA	1013	G	Sidechain
34	BA	1014	A	Sidechain
34	BA	1016	A	Sidechain
34	BA	1026	G	Sidechain
34	BA	1027	C	Sidechain
34	BA	1032	G	Sidechain
34	BA	104	G	Sidechain
34	BA	1048	G	Sidechain
34	BA	1058	G	Sidechain
34	BA	1061	G	Sidechain
34	BA	1062	U	Sidechain
34	BA	1065	U	Sidechain
34	BA	1068	G	Sidechain
34	BA	1071	C	Sidechain
34	BA	1072	G	Sidechain
34	BA	1074	G	Sidechain
34	BA	1077	G	Sidechain
34	BA	1078	U	Sidechain
34	BA	1079	G	Sidechain
34	BA	1086	U	Sidechain
34	BA	1091	U	Sidechain
34	BA	1092	A	Sidechain
34	BA	1093	A	Sidechain
34	BA	1094	G	Sidechain
34	BA	1095	U	Sidechain
34	BA	1097	C	Sidechain
34	BA	11	G	Sidechain
34	BA	1100	C	Sidechain
34	BA	1101	A	Sidechain
34	BA	1106	G	Sidechain
34	BA	1119	C	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	1120	C	Sidechain
34	BA	1121	U	Sidechain
34	BA	1122	U	Sidechain
34	BA	1123	U	Sidechain
34	BA	1124	G	Sidechain
34	BA	1126	U	Sidechain
34	BA	1127	G	Sidechain
34	BA	113	G	Sidechain
34	BA	1130	A	Sidechain
34	BA	1132	C	Sidechain
34	BA	1134	G	Sidechain
34	BA	1135	U	Sidechain
34	BA	1136	C	Sidechain
34	BA	1140	C	Sidechain
34	BA	1141	C	Sidechain
34	BA	1144	G	Sidechain
34	BA	1148	U	Sidechain
34	BA	1149	C	Sidechain
34	BA	1151	A	Sidechain
34	BA	1153	G	Sidechain
34	BA	1155	A	Sidechain
34	BA	1158	C	Sidechain
34	BA	1159	U	Sidechain
34	BA	116	A	Sidechain
34	BA	1160	G	Sidechain
34	BA	1167	A	Sidechain
34	BA	1169	A	Sidechain
34	BA	1176	A	Sidechain
34	BA	1177	G	Sidechain
34	BA	1179	A	Sidechain
34	BA	1181	G	Sidechain
34	BA	1182	G	Sidechain
34	BA	1183	U	Sidechain
34	BA	1197	A	Sidechain
34	BA	1201	A	Sidechain
34	BA	1202	U	Sidechain
34	BA	1206	G	Sidechain
34	BA	1212	U	Sidechain
34	BA	1213	A	Sidechain
34	BA	1214	C	Sidechain
34	BA	1216	A	Sidechain
34	BA	1222	G	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	1225	A	Sidechain
34	BA	1227	A	Sidechain
34	BA	1232	U	Sidechain
34	BA	1233	G	Sidechain
34	BA	1234	C	Sidechain
34	BA	1235	U	Sidechain
34	BA	1240	U	Sidechain
34	BA	1242	G	Sidechain
34	BA	1249	C	Sidechain
34	BA	1250	A	Sidechain
34	BA	1256	A	Sidechain
34	BA	1258	G	Sidechain
34	BA	1260	G	Sidechain
34	BA	1266	G	Sidechain
34	BA	1267	C	Sidechain
34	BA	1269	A	Sidechain
34	BA	1277	C	Sidechain
34	BA	128	G	Sidechain
34	BA	1285	A	Sidechain
34	BA	1288	A	Sidechain
34	BA	1289	A	Sidechain
34	BA	1298	U	Sidechain
34	BA	1301	U	Sidechain
34	BA	1303	C	Sidechain
34	BA	1305	G	Sidechain
34	BA	1307	U	Sidechain
34	BA	1319	A	Sidechain
34	BA	1322	C	Sidechain
34	BA	1323	G	Sidechain
34	BA	1326	U	Sidechain
34	BA	1333	A	Sidechain
34	BA	1335	U	Sidechain
34	BA	1337	G	Sidechain
34	BA	134	G	Sidechain
34	BA	1340	A	Sidechain
34	BA	1341	U	Sidechain
34	BA	1343	G	Sidechain
34	BA	1345	U	Sidechain
34	BA	1346	A	Sidechain
34	BA	1347	G	Sidechain
34	BA	1354	U	Sidechain
34	BA	1356	G	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	1357	A	Sidechain
34	BA	1358	U	Sidechain
34	BA	1364	U	Sidechain
34	BA	137	U	Sidechain
34	BA	1371	G	Sidechain
34	BA	1373	G	Sidechain
34	BA	1376	U	Sidechain
34	BA	1377	A	Sidechain
34	BA	1378	C	Sidechain
34	BA	1379	G	Sidechain
34	BA	138	G	Sidechain
34	BA	1382	C	Sidechain
34	BA	1383	C	Sidechain
34	BA	1390	U	Sidechain
34	BA	1391	U	Sidechain
34	BA	1392	G	Sidechain
34	BA	1398	A	Sidechain
34	BA	1403	C	Sidechain
34	BA	1411	C	Sidechain
34	BA	1412	C	Sidechain
34	BA	1414	U	Sidechain
34	BA	1416	G	Sidechain
34	BA	1417	G	Sidechain
34	BA	142	G	Sidechain
34	BA	1424	U	Sidechain
34	BA	1425	U	Sidechain
34	BA	1429	A	Sidechain
34	BA	143	A	Sidechain
34	BA	1432	G	Sidechain
34	BA	1433	A	Sidechain
34	BA	1438	G	Sidechain
34	BA	1441	A	Sidechain
34	BA	1444	U	Sidechain
34	BA	1446	A	Sidechain
34	BA	1447	A	Sidechain
34	BA	1450	U	Sidechain
34	BA	1456	A	Sidechain
34	BA	1459	G	Sidechain
34	BA	1464	U	Sidechain
34	BA	1465	A	Sidechain
34	BA	1467	C	Sidechain
34	BA	1469	C	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	1470	U	Sidechain
34	BA	1477	U	Sidechain
34	BA	1478	U	Sidechain
34	BA	1479	C	Sidechain
34	BA	1482	G	Sidechain
34	BA	1483	A	Sidechain
34	BA	149	A	Sidechain
34	BA	1491	G	Sidechain
34	BA	1492	A	Sidechain
34	BA	1499	A	Sidechain
34	BA	15	G	Sidechain
34	BA	150	U	Sidechain
34	BA	1501	C	Sidechain
34	BA	1502	A	Sidechain
34	BA	1503	A	Sidechain
34	BA	1505	G	Sidechain
34	BA	1509	C	Sidechain
34	BA	1512	U	Sidechain
34	BA	1517	G	Sidechain
34	BA	152	A	Sidechain
34	BA	1520	C	Sidechain
34	BA	1521	C	Sidechain
34	BA	1522	U	Sidechain
34	BA	1528	U	Sidechain
34	BA	1529	G	Sidechain
34	BA	153	C	Sidechain
34	BA	1530	G	Sidechain
34	BA	1531	A	Sidechain
34	BA	1536	C	Sidechain
34	BA	1540	U	Sidechain
34	BA	1541	U	Sidechain
34	BA	1542	A	Sidechain
34	BA	159	G	Sidechain
34	BA	16	A	Sidechain
34	BA	163	C	Sidechain
34	BA	167	A	Sidechain
34	BA	173	U	Sidechain
34	BA	182	A	Sidechain
34	BA	183	C	Sidechain
34	BA	184	G	Sidechain
34	BA	187	G	Sidechain
34	BA	188	C	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	189	A	Sidechain
34	BA	190	A	Sidechain
34	BA	193	C	Sidechain
34	BA	194	C	Sidechain
34	BA	195	A	Sidechain
34	BA	196	A	Sidechain
34	BA	197	A	Sidechain
34	BA	202	G	Sidechain
34	BA	203	G	Sidechain
34	BA	205	A	Sidechain
34	BA	206	C	Sidechain
34	BA	211	G	Sidechain
34	BA	215	C	Sidechain
34	BA	22	G	Sidechain
34	BA	222	C	Sidechain
34	BA	223	A	Sidechain
34	BA	224	U	Sidechain
34	BA	229	U	Sidechain
34	BA	235	C	Sidechain
34	BA	236	A	Sidechain
34	BA	237	G	Sidechain
34	BA	239	U	Sidechain
34	BA	246	A	Sidechain
34	BA	25	C	Sidechain
34	BA	252	U	Sidechain
34	BA	254	G	Sidechain
34	BA	257	G	Sidechain
34	BA	265	G	Sidechain
34	BA	269	C	Sidechain
34	BA	27	G	Sidechain
34	BA	274	A	Sidechain
34	BA	285	C	Sidechain
34	BA	29	U	Sidechain
34	BA	290	C	Sidechain
34	BA	298	A	Sidechain
34	BA	299	G	Sidechain
34	BA	3	A	Sidechain
34	BA	305	G	Sidechain
34	BA	306	A	Sidechain
34	BA	307	C	Sidechain
34	BA	31	G	Sidechain
34	BA	313	A	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	315	A	Sidechain
34	BA	320	A	Sidechain
34	BA	323	U	Sidechain
34	BA	325	A	Sidechain
34	BA	329	A	Sidechain
34	BA	33	A	Sidechain
34	BA	330	C	Sidechain
34	BA	332	G	Sidechain
34	BA	333	U	Sidechain
34	BA	334	C	Sidechain
34	BA	34	C	Sidechain
34	BA	340	U	Sidechain
34	BA	346	G	Sidechain
34	BA	347	G	Sidechain
34	BA	348	G	Sidechain
34	BA	349	A	Sidechain
34	BA	350	G	Sidechain
34	BA	354	G	Sidechain
34	BA	356	A	Sidechain
34	BA	362	G	Sidechain
34	BA	363	A	Sidechain
34	BA	365	U	Sidechain
34	BA	368	U	Sidechain
34	BA	370	C	Sidechain
34	BA	380	G	Sidechain
34	BA	383	A	Sidechain
34	BA	387	U	Sidechain
34	BA	388	G	Sidechain
34	BA	39	G	Sidechain
34	BA	391	G	Sidechain
34	BA	394	G	Sidechain
34	BA	396	C	Sidechain
34	BA	399	G	Sidechain
34	BA	4	U	Sidechain
34	BA	408	A	Sidechain
34	BA	413	G	Sidechain
34	BA	414	A	Sidechain
34	BA	415	A	Sidechain
34	BA	417	G	Sidechain
34	BA	427	U	Sidechain
34	BA	428	G	Sidechain
34	BA	43	C	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	430	A	Sidechain
34	BA	442	G	Sidechain
34	BA	446	G	Sidechain
34	BA	447	G	Sidechain
34	BA	448	A	Sidechain
34	BA	452	A	Sidechain
34	BA	456	A	Sidechain
34	BA	459	A	Sidechain
34	BA	464	U	Sidechain
34	BA	465	A	Sidechain
34	BA	466	A	Sidechain
34	BA	467	U	Sidechain
34	BA	469	C	Sidechain
34	BA	470	C	Sidechain
34	BA	471	U	Sidechain
34	BA	476	U	Sidechain
34	BA	477	C	Sidechain
34	BA	479	U	Sidechain
34	BA	480	U	Sidechain
34	BA	481	G	Sidechain
34	BA	483	C	Sidechain
34	BA	486	U	Sidechain
34	BA	487	A	Sidechain
34	BA	489	C	Sidechain
34	BA	491	G	Sidechain
34	BA	493	A	Sidechain
34	BA	496	A	Sidechain
34	BA	5	U	Sidechain
34	BA	50	A	Sidechain
34	BA	508	U	Sidechain
34	BA	510	A	Sidechain
34	BA	511	C	Sidechain
34	BA	517	G	Sidechain
34	BA	519	C	Sidechain
34	BA	520	A	Sidechain
34	BA	523	A	Sidechain
34	BA	525	C	Sidechain
34	BA	532	A	Sidechain
34	BA	533	A	Sidechain
34	BA	542	G	Sidechain
34	BA	546	A	Sidechain
34	BA	556	C	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	565	U	Sidechain
34	BA	568	G	Sidechain
34	BA	576	C	Sidechain
34	BA	577	G	Sidechain
34	BA	589	U	Sidechain
34	BA	594	U	Sidechain
34	BA	596	A	Sidechain
34	BA	597	G	Sidechain
34	BA	608	A	Sidechain
34	BA	609	A	Sidechain
34	BA	61	G	Sidechain
34	BA	613	C	Sidechain
34	BA	614	C	Sidechain
34	BA	618	C	Sidechain
34	BA	62	U	Sidechain
34	BA	636	U	Sidechain
34	BA	64	G	Sidechain
34	BA	641	U	Sidechain
34	BA	642	A	Sidechain
34	BA	646	G	Sidechain
34	BA	654	G	Sidechain
34	BA	66	A	Sidechain
34	BA	660	C	Sidechain
34	BA	661	G	Sidechain
34	BA	670	G	Sidechain
34	BA	671	G	Sidechain
34	BA	673	A	Sidechain
34	BA	682	G	Sidechain
34	BA	686	U	Sidechain
34	BA	687	A	Sidechain
34	BA	688	G	Sidechain
34	BA	69	G	Sidechain
34	BA	692	U	Sidechain
34	BA	693	G	Sidechain
34	BA	694	A	Sidechain
34	BA	697	U	Sidechain
34	BA	7	A	Sidechain
34	BA	701	U	Sidechain
34	BA	702	A	Sidechain
34	BA	704	A	Sidechain
34	BA	705	G	Sidechain
34	BA	71	A	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	713	G	Sidechain
34	BA	714	G	Sidechain
34	BA	719	C	Sidechain
34	BA	721	G	Sidechain
34	BA	723	U	Sidechain
34	BA	728	A	Sidechain
34	BA	73	C	Sidechain
34	BA	737	C	Sidechain
34	BA	738	C	Sidechain
34	BA	739	C	Sidechain
34	BA	745	G	Sidechain
34	BA	748	G	Sidechain
34	BA	749	A	Sidechain
34	BA	751	U	Sidechain
34	BA	752	G	Sidechain
34	BA	754	C	Sidechain
34	BA	757	U	Sidechain
34	BA	758	C	Sidechain
34	BA	76	G	Sidechain
34	BA	762	U	Sidechain
34	BA	765	G	Sidechain
34	BA	771	G	Sidechain
34	BA	773	G	Sidechain
34	BA	775	G	Sidechain
34	BA	776	G	Sidechain
34	BA	786	G	Sidechain
34	BA	789	U	Sidechain
34	BA	790	A	Sidechain
34	BA	792	A	Sidechain
34	BA	794	A	Sidechain
34	BA	797	C	Sidechain
34	BA	8	A	Sidechain
34	BA	804	U	Sidechain
34	BA	817	C	Sidechain
34	BA	82	G	Sidechain
34	BA	820	U	Sidechain
34	BA	823	C	Sidechain
34	BA	828	U	Sidechain
34	BA	833	G	Sidechain
34	BA	838	G	Sidechain
34	BA	84	U	Sidechain
34	BA	840	C	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	841	C	Sidechain
34	BA	842	U	Sidechain
34	BA	843	U	Sidechain
34	BA	847	G	Sidechain
34	BA	849	G	Sidechain
34	BA	85	U	Sidechain
34	BA	851	G	Sidechain
34	BA	854	U	Sidechain
34	BA	861	G	Sidechain
34	BA	864	A	Sidechain
34	BA	866	C	Sidechain
34	BA	869	G	Sidechain
34	BA	870	U	Sidechain
34	BA	873	A	Sidechain
34	BA	874	G	Sidechain
34	BA	876	C	Sidechain
34	BA	877	G	Sidechain
34	BA	88	U	Sidechain
34	BA	880	C	Sidechain
34	BA	884	U	Sidechain
34	BA	888	G	Sidechain
34	BA	89	U	Sidechain
34	BA	899	C	Sidechain
34	BA	900	A	Sidechain
34	BA	901	A	Sidechain
34	BA	902	G	Sidechain
34	BA	908	A	Sidechain
34	BA	91	U	Sidechain
34	BA	919	A	Sidechain
34	BA	92	U	Sidechain
34	BA	920	U	Sidechain
34	BA	923	A	Sidechain
34	BA	928	G	Sidechain
34	BA	933	G	Sidechain
34	BA	934	C	Sidechain
34	BA	935	A	Sidechain
34	BA	937	A	Sidechain
34	BA	938	A	Sidechain
34	BA	94	G	Sidechain
34	BA	940	C	Sidechain
34	BA	946	A	Sidechain
34	BA	948	C	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	951	G	Sidechain
34	BA	955	U	Sidechain
34	BA	958	A	Sidechain
34	BA	959	A	Sidechain
34	BA	960	U	Sidechain
34	BA	972	C	Sidechain
34	BA	975	A	Sidechain
34	BA	977	A	Sidechain
34	BA	978	A	Sidechain
34	BA	980	C	Sidechain
34	BA	983	A	Sidechain
34	BA	984	C	Sidechain
34	BA	99	C	Sidechain
34	BA	991	U	Sidechain
34	BA	992	U	Sidechain
34	BA	994	A	Sidechain
34	BA	995	C	Sidechain
35	BB	15	G	Sidechain
35	BB	40	C	Sidechain
35	BB	48	C	Sidechain
35	BB	50	U	Sidechain
35	BB	51	U	Sidechain
35	BB	56	C	Sidechain
35	BB	58	A	Sidechain
35	BB	59	U	Sidechain
35	BB	60	U	Sidechain
35	BB	68	C	Sidechain
35	BB	7	A	Sidechain
35	BB	74	C	Sidechain
37	BD	24	A	Sidechain
37	BD	25	U	Sidechain
37	BD	37	U	Sidechain
37	BD	47	C	Sidechain
35	BE	15	G	Sidechain
35	BE	18	G	Sidechain
35	BE	19	G	Sidechain
35	BE	21	A	Sidechain
35	BE	22	G	Sidechain
35	BE	24	G	Sidechain
35	BE	34	G	Sidechain
35	BE	44	G	Sidechain
35	BE	56	C	Sidechain

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Mol	Chain	Res	Type	Group
35	BE	57	G	Sidechain
35	BE	59	U	Sidechain
35	BE	6	G	Sidechain
35	BE	63	G	Sidechain
35	BE	65	G	Sidechain
35	BE	68	C	Sidechain
38	BF	21	TYR	Sidechain
39	BG	221	ALA	Peptide
39	BG	223	PRO	Mainchain
40	BH	102	TYR	Sidechain
40	BH	203	TYR	Sidechain
41	BI	146	MET	Peptide,Mainchain
41	BI	154	ALA	Peptide
42	BJ	87	SER	Peptide
43	BK	172	PRO	Mainchain
43	BK	5	VAL	Peptide
45	BM	6	TYR	Sidechain
45	BM	63	TYR	Sidechain
47	BO	81	LEU	Peptide
48	BP	16	ALA	Mainchain
50	BR	60	ARG	Mainchain
54	BV	3	TYR	Sidechain
55	BW	77	ARG	Sidechain
57	BY	17	ARG	Sidechain
57	BY	37	TYR	Sidechain
57	BY	4	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2566	0	1302	0	0
2	AB	62351	0	31387	0	0
3	AC	1733	0	1824	0	0
4	AD	2092	0	2170	0	0
5	AE	1565	0	1616	0	0
6	AF	1552	0	1619	0	0
7	AG	1420	0	1460	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AH	1323	0	1374	0	0
9	AI	1111	0	1148	0	0
10	AJ	1032	0	1088	0	0
11	AK	1129	0	1162	0	0
12	AL	947	0	1023	0	0
13	AM	1053	0	1129	0	0
14	AN	1074	0	1157	0	0
15	AO	1008	0	1045	0	0
16	AP	900	0	935	0	0
17	AQ	917	0	965	0	0
18	AR	947	0	1022	0	0
19	AS	816	0	839	0	0
20	AT	857	0	922	0	0
21	AU	787	0	846	0	0
22	AV	789	0	847	0	0
23	AW	753	0	780	0	0
24	AX	634	0	656	0	0
25	AY	625	0	655	0	0
26	AZ	509	0	543	0	0
27	Aa	449	0	491	0	0
28	Ab	549	0	552	0	0
29	Ac	444	0	461	0	0
30	Ad	441	0	485	0	0
31	Ae	377	0	418	0	0
32	Af	504	0	574	0	0
33	Ag	302	0	343	0	0
34	BA	33089	0	16678	0	0
35	BB	1635	0	849	0	0
35	BE	1635	0	849	0	0
36	BC	3036	0	3052	0	0
37	BD	495	0	249	0	0
38	BF	1872	0	1885	0	0
39	BG	1822	0	1913	0	0
40	BH	1643	0	1710	0	0
41	BI	1225	0	1273	0	0
42	BJ	1101	0	1050	0	0
43	BK	1400	0	1449	0	0
44	BL	979	0	1034	0	0
45	BM	1036	0	1084	0	0
46	BN	825	0	865	0	0
47	BO	965	0	997	0	0
48	BP	955	0	1019	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	BQ	910	0	981	0	0
50	BR	805	0	847	0	0
51	BS	716	0	742	0	0
52	BT	649	0	666	0	0
53	BU	672	0	716	0	0
54	BV	626	0	651	0	0
55	BW	727	0	769	0	0
56	BX	670	0	722	0	0
57	BY	590	0	631	0	0
All	All	153634	0	105519	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

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	
3	AC	232/234 (99%)	204 (88%)	25 (11%)	3 (1%)	12	48
4	AD	270/273 (99%)	239 (88%)	23 (8%)	8 (3%)	4	28
5	AE	207/209 (99%)	186 (90%)	15 (7%)	6 (3%)	4	29
6	AF	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	10	46
7	AG	176/179 (98%)	147 (84%)	27 (15%)	2 (1%)	14	52
8	AH	174/177 (98%)	163 (94%)	8 (5%)	3 (2%)	9	42
9	AI	147/149 (99%)	126 (86%)	16 (11%)	5 (3%)	3	26
10	AJ	139/142 (98%)	123 (88%)	15 (11%)	1 (1%)	22	63
11	AK	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
12	AL	121/123 (98%)	106 (88%)	13 (11%)	2 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AM	142/144 (99%)	125 (88%)	15 (11%)	2 (1%)	11	46
14	AN	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	6	35
15	AO	125/127 (98%)	117 (94%)	7 (6%)	1 (1%)	19	60
16	AP	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	17	57
17	AQ	112/115 (97%)	100 (89%)	10 (9%)	2 (2%)	8	40
18	AR	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	57
19	AS	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	3	23
20	AT	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	17	57
21	AU	98/100 (98%)	85 (87%)	11 (11%)	2 (2%)	7	38
22	AV	101/104 (97%)	89 (88%)	11 (11%)	1 (1%)	15	55
23	AW	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	6	35
24	AX	82/85 (96%)	67 (82%)	12 (15%)	3 (4%)	3	24
25	AY	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	5	31
26	AZ	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	2	20
27	Aa	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	8	40
28	Ab	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	10	46
29	Ac	54/57 (95%)	47 (87%)	5 (9%)	2 (4%)	3	24
30	Ad	52/55 (94%)	45 (86%)	7 (14%)	0	100	100
31	Ae	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
32	Af	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	Ag	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	30
36	BC	391/393 (100%)	368 (94%)	20 (5%)	3 (1%)	19	60
38	BF	238/241 (99%)	215 (90%)	20 (8%)	3 (1%)	12	48
39	BG	230/233 (99%)	211 (92%)	17 (7%)	2 (1%)	17	57
40	BH	203/206 (98%)	191 (94%)	10 (5%)	2 (1%)	15	55
41	BI	164/167 (98%)	144 (88%)	17 (10%)	3 (2%)	8	40
42	BJ	133/135 (98%)	128 (96%)	3 (2%)	2 (2%)	10	46
43	BK	176/179 (98%)	160 (91%)	14 (8%)	2 (1%)	14	52
44	BL	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	9	44
45	BM	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	9	44
46	BN	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	BO	126/129 (98%)	113 (90%)	11 (9%)	2 (2%)	9	44
48	BP	121/124 (98%)	104 (86%)	12 (10%)	5 (4%)	3	23
49	BQ	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
50	BR	98/101 (97%)	83 (85%)	8 (8%)	7 (7%)	1	14
51	BS	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
52	BT	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
53	BU	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
54	BV	72/75 (96%)	65 (90%)	5 (7%)	2 (3%)	5	30
55	BW	89/92 (97%)	80 (90%)	9 (10%)	0	100	100
56	BX	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
57	BY	68/71 (96%)	60 (88%)	7 (10%)	1 (2%)	10	46
All	All	6548/6682 (98%)	5904 (90%)	536 (8%)	108 (2%)	13	44

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AD	260	LYS
5	AE	122	VAL
5	AE	150	GLN
5	AE	170	VAL
9	AI	23	ALA
14	AN	36	VAL
16	AP	68	LYS
19	AS	91	GLN
22	AV	6	ARG
26	AZ	46	VAL
29	Ac	26	SER
40	BH	18	LEU
45	BM	3	ASN
46	BN	74	VAL
47	BO	118	ASN
48	BP	86	VAL
50	BR	37	ASP
50	BR	70	HIS
57	BY	3	ILE
3	AC	217	THR
3	AC	229	LEU
4	AD	119	VAL

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Mol	Chain	Res	Type
4	AD	237	ARG
5	AE	43	ASP
7	AG	148	VAL
13	AM	36	LYS
18	AR	104	ALA
24	AX	9	THR
24	AX	72	GLY
25	AY	27	ARG
25	AY	62	GLY
26	AZ	23	ARG
27	Aa	9	THR
29	Ac	39	ARG
36	BC	21	ASP
36	BC	60	ILE
38	BF	41	ASN
41	BI	77	ASN
43	BK	55	LYS
54	BV	11	ARG
4	AD	193	GLU
4	AD	240	GLY
5	AE	41	ALA
5	AE	137	SER
6	AF	62	GLN
8	AH	50	THR
8	AH	164	ALA
12	AL	70	ARG
33	Ag	4	ARG
41	BI	43	GLY
41	BI	162	GLU
43	BK	116	ALA
46	BN	90	LEU
47	BO	74	LYS
48	BP	75	GLU
50	BR	61	ASN
50	BR	73	LEU
4	AD	140	VAL
4	AD	190	THR
12	AL	3	GLN
19	AS	53	PHE
19	AS	80	ARG
21	AU	69	ARG
23	AW	85	LYS

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Mol	Chain	Res	Type
38	BF	132	GLU
42	BJ	92	THR
45	BM	13	SER
48	BP	24	GLU
50	BR	32	ASP
50	BR	35	ALA
54	BV	3	TYR
6	AF	66	GLY
8	AH	8	VAL
14	AN	106	ASP
15	AO	81	ASN
36	BC	9	LYS
39	BG	14	VAL
42	BJ	100	SER
46	BN	42	LEU
48	BP	21	PRO
48	BP	43	LYS
3	AC	73	VAL
4	AD	141	HIS
6	AF	71	GLY
7	AG	73	VAL
9	AI	28	ASN
10	AJ	90	GLY
21	AU	23	ALA
26	AZ	17	GLU
38	BF	149	GLY
13	AM	20	GLY
14	AN	23	GLY
39	BG	8	GLY
46	BN	57	VAL
9	AI	118	PRO
9	AI	121	VAL
17	AQ	22	GLY
23	AW	65	VAL
40	BH	27	ILE
28	Ab	36	VAL
44	BL	81	GLY
44	BL	125	ILE
50	BR	30	ILE
9	AI	94	ILE
17	AQ	32	VAL
19	AS	101	ILE

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Mol	Chain	Res	Type
20	AT	80	PRO
24	AX	36	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	181/181 (100%)	171 (94%)	10 (6%)	21	47
4	AD	217/218 (100%)	204 (94%)	13 (6%)	19	44
5	AE	164/164 (100%)	154 (94%)	10 (6%)	18	44
6	AF	165/165 (100%)	158 (96%)	7 (4%)	30	54
7	AG	149/150 (99%)	138 (93%)	11 (7%)	13	38
8	AH	137/138 (99%)	125 (91%)	12 (9%)	10	31
9	AI	114/114 (100%)	106 (93%)	8 (7%)	15	40
10	AJ	109/110 (99%)	105 (96%)	4 (4%)	34	58
11	AK	116/116 (100%)	113 (97%)	3 (3%)	46	66
12	AL	104/104 (100%)	94 (90%)	10 (10%)	8	27
13	AM	103/103 (100%)	99 (96%)	4 (4%)	32	56
14	AN	109/109 (100%)	103 (94%)	6 (6%)	21	47
15	AO	103/103 (100%)	101 (98%)	2 (2%)	57	75
16	AP	87/87 (100%)	80 (92%)	7 (8%)	12	35
17	AQ	99/100 (99%)	91 (92%)	8 (8%)	11	35
18	AR	89/90 (99%)	82 (92%)	7 (8%)	12	35
19	AS	84/84 (100%)	78 (93%)	6 (7%)	14	39
20	AT	93/93 (100%)	89 (96%)	4 (4%)	29	53
21	AU	84/84 (100%)	79 (94%)	5 (6%)	19	44
22	AV	84/85 (99%)	81 (96%)	3 (4%)	35	59
23	AW	78/78 (100%)	72 (92%)	6 (8%)	13	37
24	AX	62/63 (98%)	60 (97%)	2 (3%)	39	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AY	67/68 (98%)	67 (100%)	0	100	100
26	AZ	55/55 (100%)	49 (89%)	6 (11%)	6	23
27	Aa	48/49 (98%)	45 (94%)	3 (6%)	18	43
28	Ab	62/62 (100%)	58 (94%)	4 (6%)	17	42
29	Ac	47/48 (98%)	43 (92%)	4 (8%)	10	33
30	Ad	48/49 (98%)	46 (96%)	2 (4%)	30	54
31	Ae	38/38 (100%)	35 (92%)	3 (8%)	12	35
32	Af	51/52 (98%)	50 (98%)	1 (2%)	55	74
33	Ag	34/34 (100%)	33 (97%)	1 (3%)	42	64
36	BC	326/326 (100%)	316 (97%)	10 (3%)	40	62
38	BF	198/199 (100%)	188 (95%)	10 (5%)	24	48
39	BG	189/190 (100%)	176 (93%)	13 (7%)	15	40
40	BH	172/173 (99%)	164 (95%)	8 (5%)	26	51
41	BI	125/126 (99%)	118 (94%)	7 (6%)	21	46
42	BJ	116/116 (100%)	111 (96%)	5 (4%)	29	53
43	BK	146/147 (99%)	139 (95%)	7 (5%)	25	51
44	BL	104/105 (99%)	98 (94%)	6 (6%)	20	45
45	BM	106/107 (99%)	98 (92%)	8 (8%)	13	38
46	BN	90/90 (100%)	80 (89%)	10 (11%)	6	22
47	BO	98/99 (99%)	94 (96%)	4 (4%)	30	55
48	BP	103/104 (99%)	100 (97%)	3 (3%)	42	64
49	BQ	95/96 (99%)	91 (96%)	4 (4%)	30	54
50	BR	83/84 (99%)	76 (92%)	7 (8%)	11	33
51	BS	76/77 (99%)	75 (99%)	1 (1%)	69	81
52	BT	65/65 (100%)	63 (97%)	2 (3%)	40	62
53	BU	77/78 (99%)	75 (97%)	2 (3%)	46	66
54	BV	64/65 (98%)	56 (88%)	8 (12%)	4	19
55	BW	78/79 (99%)	74 (95%)	4 (5%)	24	48
56	BX	65/66 (98%)	63 (97%)	2 (3%)	40	62
57	BY	60/61 (98%)	55 (92%)	5 (8%)	11	34
All	All	5417/5447 (99%)	5119 (94%)	298 (6%)	25	47

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	11	ILE
3	AC	60	ARG
3	AC	85	GLU
3	AC	98	GLU
3	AC	164	ARG
3	AC	165	ASN
3	AC	167	LYS
3	AC	174	THR
3	AC	203	GLN
3	AC	218	MET
4	AD	6	LYS
4	AD	17	LYS
4	AD	43	ASN
4	AD	59	GLN
4	AD	62	ARG
4	AD	90	ILE
4	AD	129	LEU
4	AD	132	ARG
4	AD	145	MET
4	AD	200	MET
4	AD	222	THR
4	AD	231	HIS
4	AD	270	ARG
5	AE	36	GLN
5	AE	40	LEU
5	AE	74	GLU
5	AE	86	GLU
5	AE	89	GLU
5	AE	122	VAL
5	AE	148	GLN
5	AE	159	LYS
5	AE	168	GLU
5	AE	183	GLU
6	AF	78	TRP
6	AF	79	ARG
6	AF	122	GLU
6	AF	134	LEU
6	AF	155	GLU
6	AF	157	LEU
6	AF	165	HIS
7	AG	21	TYR
7	AG	22	ASN

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Mol	Chain	Res	Type
7	AG	25	MET
7	AG	41	GLU
7	AG	46	LYS
7	AG	79	ARG
7	AG	91	ARG
7	AG	109	ARG
7	AG	129	MET
7	AG	132	ARG
7	AG	149	ARG
8	AH	5	LYS
8	AH	26	LYS
8	AH	34	ARG
8	AH	38	ASP
8	AH	40	VAL
8	AH	41	GLU
8	AH	84	LYS
8	AH	94	ARG
8	AH	98	LYS
8	AH	102	ILE
8	AH	133	LYS
8	AH	169	ARG
9	AI	8	LYS
9	AI	17	ASP
9	AI	25	TYR
9	AI	53	GLU
9	AI	75	LEU
9	AI	87	GLU
9	AI	109	GLU
9	AI	116	ARG
10	AJ	9	LYS
10	AJ	39	LYS
10	AJ	49	GLU
10	AJ	106	GLN
11	AK	120	ARG
11	AK	129	GLU
11	AK	136	GLN
12	AL	17	ARG
12	AL	20	MET
12	AL	45	GLU
12	AL	73	ASP
12	AL	78	ARG
12	AL	106	GLU

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Mol	Chain	Res	Type
12	AL	110	GLU
12	AL	112	PHE
12	AL	113	MET
12	AL	114	LYS
13	AM	2	ARG
13	AM	10	GLU
13	AM	30	THR
13	AM	103	ILE
14	AN	6	ARG
14	AN	28	PHE
14	AN	36	VAL
14	AN	47	GLU
14	AN	59	ARG
14	AN	100	LYS
15	AO	114	GLU
15	AO	127	GLU
16	AP	7	ARG
16	AP	16	ARG
16	AP	36	TYR
16	AP	76	LYS
16	AP	94	ARG
16	AP	98	GLN
16	AP	112	GLU
17	AQ	31	VAL
17	AQ	33	GLU
17	AQ	39	LEU
17	AQ	54	LEU
17	AQ	98	TYR
17	AQ	100	ARG
17	AQ	109	ILE
17	AQ	114	ASN
18	AR	5	ARG
18	AR	43	GLN
18	AR	70	GLN
18	AR	77	LYS
18	AR	91	ARG
18	AR	102	LYS
18	AR	110	GLU
19	AS	6	GLN
19	AS	10	LYS
19	AS	16	GLU
19	AS	22	LEU

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Mol	Chain	Res	Type
19	AS	37	GLU
19	AS	70	GLU
20	AT	28	LYS
20	AT	59	GLU
20	AT	66	ILE
20	AT	86	MET
21	AU	6	ARG
21	AU	9	LYS
21	AU	24	MET
21	AU	26	LYS
21	AU	73	ARG
22	AV	46	LYS
22	AV	85	ARG
22	AV	91	LYS
23	AW	11	GLU
23	AW	34	LYS
23	AW	51	GLN
23	AW	55	GLU
23	AW	79	ARG
23	AW	90	ASP
24	AX	31	LEU
24	AX	69	GLU
26	AZ	5	GLU
26	AZ	7	ARG
26	AZ	24	GLU
26	AZ	30	MET
26	AZ	31	GLN
26	AZ	60	LYS
27	Aa	5	LYS
27	Aa	38	GLU
27	Aa	58	GLU
28	Ab	56	ARG
28	Ab	59	ARG
28	Ab	62	LYS
28	Ab	65	ASN
29	Ac	3	GLN
29	Ac	9	ARG
29	Ac	12	ARG
29	Ac	47	TYR
30	Ad	29	LYS
30	Ad	34	GLU
31	Ae	3	ARG

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Mol	Chain	Res	Type
31	Ae	34	ARG
31	Ae	41	ARG
32	Af	63	TYR
33	Ag	1	MET
36	BC	11	HIS
36	BC	74	ARG
36	BC	155	GLU
36	BC	204	ARG
36	BC	236	ILE
36	BC	279	ARG
36	BC	326	TYR
36	BC	349	MET
36	BC	351	MET
36	BC	378	GLU
38	BF	8	MET
38	BF	9	LEU
38	BF	17	HIS
38	BF	20	ARG
38	BF	51	GLU
38	BF	77	GLU
38	BF	80	LYS
38	BF	117	GLU
38	BF	224	ARG
38	BF	234	GLU
39	BG	40	GLN
39	BG	55	VAL
39	BG	61	LYS
39	BG	68	HIS
39	BG	71	ARG
39	BG	79	LYS
39	BG	85	LYS
39	BG	109	GLU
39	BG	120	THR
39	BG	143	LEU
39	BG	167	TYR
39	BG	203	LYS
39	BG	228	ARG
40	BH	12	ARG
40	BH	20	LEU
40	BH	35	GLN
40	BH	80	ARG
40	BH	123	MET

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Mol	Chain	Res	Type
40	BH	131	ILE
40	BH	142	VAL
40	BH	184	LYS
41	BI	11	GLN
41	BI	13	LYS
41	BI	49	TYR
41	BI	92	ARG
41	BI	95	MET
41	BI	143	LEU
41	BI	150	GLU
42	BJ	13	ASP
42	BJ	16	GLU
42	BJ	23	GLU
42	BJ	37	HIS
42	BJ	113	ARG
43	BK	105	GLU
43	BK	122	GLU
43	BK	129	ASN
43	BK	138	GLU
43	BK	148	LYS
43	BK	161	PHE
43	BK	164	GLN
44	BL	2	MET
44	BL	14	ARG
44	BL	41	GLU
44	BL	59	GLU
44	BL	117	GLN
44	BL	127	TYR
45	BM	12	LYS
45	BM	36	GLN
45	BM	40	ARG
45	BM	58	GLU
45	BM	65	THR
45	BM	91	GLU
45	BM	94	ARG
45	BM	105	ARG
46	BN	1	MET
46	BN	7	ARG
46	BN	10	LEU
46	BN	15	HIS
46	BN	31	ARG
46	BN	37	ARG

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Mol	Chain	Res	Type
46	BN	46	LYS
46	BN	54	SER
46	BN	82	LYS
46	BN	99	GLN
47	BO	6	ARG
47	BO	82	GLU
47	BO	93	GLU
47	BO	124	LYS
48	BP	81	ILE
48	BP	85	ARG
48	BP	113	ARG
49	BQ	16	ILE
49	BQ	26	LYS
49	BQ	61	LYS
49	BQ	85	TYR
50	BR	20	PHE
50	BR	29	ILE
50	BR	33	VAL
50	BR	41	TRP
50	BR	66	THR
50	BR	70	HIS
50	BR	84	ARG
51	BS	13	GLU
52	BT	5	ARG
52	BT	67	ILE
53	BU	17	GLU
53	BU	54	ILE
54	BV	5	ARG
54	BV	6	ARG
54	BV	8	LYS
54	BV	11	ARG
54	BV	34	GLU
54	BV	42	ARG
54	BV	47	ARG
54	BV	69	TYR
55	BW	5	LYS
55	BW	28	LYS
55	BW	76	THR
55	BW	80	ARG
56	BX	57	VAL
56	BX	73	ARG
57	BY	15	LEU

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Mol	Chain	Res	Type
57	BY	36	PHE
57	BY	38	GLU
57	BY	39	LYS
57	BY	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	119/120 (99%)	15 (12%)	3 (2%)
2	AB	2898/2904 (99%)	396 (13%)	130 (4%)
34	BA	1538/1542 (99%)	192 (12%)	77 (5%)
35	BB	73/76 (96%)	12 (16%)	2 (2%)
35	BE	73/76 (96%)	12 (16%)	6 (8%)
37	BD	24/24 (100%)	4 (16%)	5 (20%)
All	All	4725/4742 (99%)	631 (13%)	223 (4%)

All (631) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	13	G
1	AA	15	A
1	AA	16	G
1	AA	36	C
1	AA	38	C
1	AA	42	C
1	AA	45	A
1	AA	57	A
1	AA	58	A
1	AA	68	C
1	AA	71	C
1	AA	88	C
1	AA	90	C
1	AA	109	A
2	AB	11	C
2	AB	13	A
2	AB	14	A
2	AB	28	A

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Mol	Chain	Res	Type
2	AB	52	A
2	AB	61	C
2	AB	64	A
2	AB	65	U
2	AB	71	A
2	AB	72	U
2	AB	75	G
2	AB	91	A
2	AB	101	A
2	AB	102	U
2	AB	118	A
2	AB	119	A
2	AB	120	U
2	AB	125	A
2	AB	126	A
2	AB	128	C
2	AB	138	U
2	AB	142	A
2	AB	149	A
2	AB	154	U
2	AB	165	A
2	AB	196	A
2	AB	204	A
2	AB	205	G
2	AB	215	G
2	AB	216	A
2	AB	221	A
2	AB	222	A
2	AB	223	A
2	AB	226	A
2	AB	248	G
2	AB	265	A
2	AB	266	G
2	AB	269	C
2	AB	270	A
2	AB	271	G
2	AB	272	A
2	AB	277	G
2	AB	279	A
2	AB	294	A
2	AB	302	C
2	AB	323	C

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Mol	Chain	Res	Type
2	AB	324	A
2	AB	330	A
2	AB	331	C
2	AB	338	G
2	AB	346	A
2	AB	373	U
2	AB	383	C
2	AB	386	G
2	AB	391	A
2	AB	411	G
2	AB	418	C
2	AB	432	A
2	AB	444	C
2	AB	447	A
2	AB	448	U
2	AB	451	U
2	AB	456	C
2	AB	457	A
2	AB	458	G
2	AB	459	U
2	AB	479	A
2	AB	480	A
2	AB	481	G
2	AB	482	A
2	AB	504	A
2	AB	505	A
2	AB	508	A
2	AB	509	C
2	AB	527	C
2	AB	529	A
2	AB	530	G
2	AB	531	C
2	AB	532	A
2	AB	533	G
2	AB	546	U
2	AB	547	A
2	AB	548	G
2	AB	549	G
2	AB	563	A
2	AB	573	U
2	AB	574	A
2	AB	575	A

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Mol	Chain	Res	Type
2	AB	586	A
2	AB	588	U
2	AB	603	A
2	AB	607	U
2	AB	637	A
2	AB	645	C
2	AB	654	A
2	AB	655	A
2	AB	656	G
2	AB	669	G
2	AB	670	A
2	AB	686	U
2	AB	715	A
2	AB	717	C
2	AB	728	G
2	AB	730	A
2	AB	736	C
2	AB	737	C
2	AB	740	C
2	AB	747	5MU
2	AB	748	G
2	AB	753	A
2	AB	764	A
2	AB	775	G
2	AB	776	G
2	AB	782	A
2	AB	784	G
2	AB	786	C
2	AB	790	U
2	AB	791	C
2	AB	792	A
2	AB	793	A
2	AB	805	G
2	AB	812	C
2	AB	828	U
2	AB	910	A
2	AB	914	G
2	AB	931	U
2	AB	941	A
2	AB	945	A
2	AB	946	C
2	AB	959	A

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Mol	Chain	Res	Type
2	AB	962	G
2	AB	974	G
2	AB	980	A
2	AB	984	A
2	AB	995	C
2	AB	996	A
2	AB	1012	U
2	AB	1013	C
2	AB	1016	G
2	AB	1022	G
2	AB	1025	G
2	AB	1026	G
2	AB	1033	U
2	AB	1034	G
2	AB	1047	G
2	AB	1048	A
2	AB	1056	G
2	AB	1067	A
2	AB	1069	A
2	AB	1070	A
2	AB	1079	C
2	AB	1086	A
2	AB	1088	A
2	AB	1095	A
2	AB	1110	G
2	AB	1112	G
2	AB	1128	G
2	AB	1129	A
2	AB	1130	U
2	AB	1132	U
2	AB	1133	A
2	AB	1134	A
2	AB	1135	C
2	AB	1136	G
2	AB	1143	A
2	AB	1170	C
2	AB	1175	A
2	AB	1177	G
2	AB	1184	U
2	AB	1185	G
2	AB	1186	G
2	AB	1206	G

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Mol	Chain	Res	Type
2	AB	1211	C
2	AB	1212	G
2	AB	1213	A
2	AB	1249	U
2	AB	1250	G
2	AB	1255	U
2	AB	1256	G
2	AB	1266	G
2	AB	1271	G
2	AB	1272	A
2	AB	1286	A
2	AB	1287	A
2	AB	1296	G
2	AB	1300	G
2	AB	1301	A
2	AB	1365	A
2	AB	1378	A
2	AB	1379	U
2	AB	1391	U
2	AB	1416	G
2	AB	1417	C
2	AB	1427	A
2	AB	1440	U
2	AB	1452	G
2	AB	1453	A
2	AB	1455	G
2	AB	1458	U
2	AB	1459	G
2	AB	1460	U
2	AB	1462	C
2	AB	1482	G
2	AB	1493	C
2	AB	1509	A
2	AB	1510	G
2	AB	1523	U
2	AB	1558	C
2	AB	1566	A
2	AB	1569	A
2	AB	1584	U
2	AB	1585	C
2	AB	1596	A
2	AB	1607	C

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Mol	Chain	Res	Type
2	AB	1608	A
2	AB	1616	A
2	AB	1646	C
2	AB	1647	U
2	AB	1648	U
2	AB	1654	A
2	AB	1700	A
2	AB	1705	A
2	AB	1715	G
2	AB	1732	C
2	AB	1733	G
2	AB	1757	A
2	AB	1762	A
2	AB	1773	A
2	AB	1781	U
2	AB	1782	U
2	AB	1791	A
2	AB	1800	C
2	AB	1802	A
2	AB	1808	A
2	AB	1809	A
2	AB	1839	G
2	AB	1840	G
2	AB	1871	A
2	AB	1873	G
2	AB	1900	A
2	AB	1901	A
2	AB	1906	G
2	AB	1907	G
2	AB	1929	G
2	AB	1930	G
2	AB	1931	U
2	AB	1937	A
2	AB	1938	A
2	AB	1943	U
2	AB	1952	A
2	AB	1954	G
2	AB	1955	U
2	AB	1956	U
2	AB	1962	5MC
2	AB	1964	G
2	AB	1965	C

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Mol	Chain	Res	Type
2	AB	1966	A
2	AB	1970	A
2	AB	1971	U
2	AB	1972	G
2	AB	1981	A
2	AB	1992	G
2	AB	1993	U
2	AB	1997	C
2	AB	2003	A
2	AB	2021	C
2	AB	2023	C
2	AB	2032	G
2	AB	2042	A
2	AB	2043	C
2	AB	2056	G
2	AB	2059	A
2	AB	2061	G
2	AB	2068	U
2	AB	2076	U
2	AB	2092	U
2	AB	2112	G
2	AB	2119	A
2	AB	2120	G
2	AB	2127	G
2	AB	2129	C
2	AB	2131	U
2	AB	2132	U
2	AB	2133	G
2	AB	2135	A
2	AB	2140	G
2	AB	2147	A
2	AB	2158	A
2	AB	2159	G
2	AB	2172	U
2	AB	2173	A
2	AB	2174	C
2	AB	2179	C
2	AB	2199	A
2	AB	2203	U
2	AB	2212	A
2	AB	2213	U
2	AB	2214	C

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Mol	Chain	Res	Type
2	AB	2225	A
2	AB	2238	G
2	AB	2239	G
2	AB	2250	G
2	AB	2266	A
2	AB	2273	A
2	AB	2283	C
2	AB	2287	A
2	AB	2288	A
2	AB	2305	U
2	AB	2308	G
2	AB	2309	A
2	AB	2310	C
2	AB	2321	U
2	AB	2322	A
2	AB	2325	G
2	AB	2333	A
2	AB	2335	A
2	AB	2350	C
2	AB	2357	G
2	AB	2363	G
2	AB	2382	G
2	AB	2383	G
2	AB	2385	C
2	AB	2390	U
2	AB	2391	G
2	AB	2399	G
2	AB	2406	A
2	AB	2407	A
2	AB	2408	U
2	AB	2425	A
2	AB	2429	G
2	AB	2432	A
2	AB	2439	A
2	AB	2440	C
2	AB	2441	U
2	AB	2448	A
2	AB	2449	H2U
2	AB	2466	C
2	AB	2472	G
2	AB	2475	C
2	AB	2476	A

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Mol	Chain	Res	Type
2	AB	2478	A
2	AB	2491	U
2	AB	2501	C
2	AB	2502	G
2	AB	2504	PSU
2	AB	2506	U
2	AB	2507	C
2	AB	2530	A
2	AB	2543	G
2	AB	2566	A
2	AB	2567	G
2	AB	2573	C
2	AB	2574	G
2	AB	2578	G
2	AB	2586	U
2	AB	2599	G
2	AB	2610	C
2	AB	2613	U
2	AB	2615	U
2	AB	2629	U
2	AB	2630	G
2	AB	2639	A
2	AB	2655	G
2	AB	2685	G
2	AB	2689	U
2	AB	2690	U
2	AB	2699	C
2	AB	2700	A
2	AB	2714	G
2	AB	2726	A
2	AB	2732	G
2	AB	2733	A
2	AB	2751	G
2	AB	2752	C
2	AB	2756	U
2	AB	2765	A
2	AB	2766	A
2	AB	2778	A
2	AB	2780	G
2	AB	2791	G
2	AB	2792	A
2	AB	2799	A

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Mol	Chain	Res	Type
2	AB	2815	C
2	AB	2820	A
2	AB	2833	U
2	AB	2848	G
2	AB	2850	A
2	AB	2861	U
2	AB	2867	G
2	AB	2873	A
2	AB	2880	C
2	AB	2883	A
2	AB	2884	U
2	AB	2894	G
2	AB	2895	G
2	AB	2904	U
34	BA	9	G
34	BA	31	G
34	BA	32	A
34	BA	39	G
34	BA	40	C
34	BA	48	C
34	BA	49	U
34	BA	51	A
34	BA	60	A
34	BA	61	G
34	BA	66	A
34	BA	83	C
34	BA	86	G
34	BA	87	C
34	BA	88	U
34	BA	95	C
34	BA	109	A
34	BA	121	U
34	BA	130	A
34	BA	131	A
34	BA	164	G
34	BA	183	C
34	BA	184	G
34	BA	188	C
34	BA	247	G
34	BA	266	G
34	BA	275	G
34	BA	281	G

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Mol	Chain	Res	Type
34	BA	289	G
34	BA	293	G
34	BA	306	A
34	BA	328	C
34	BA	329	A
34	BA	331	G
34	BA	352	C
34	BA	353	A
34	BA	354	G
34	BA	366	A
34	BA	367	U
34	BA	368	U
34	BA	369	G
34	BA	370	C
34	BA	381	C
34	BA	388	G
34	BA	393	A
34	BA	397	A
34	BA	398	U
34	BA	406	G
34	BA	413	G
34	BA	414	A
34	BA	416	G
34	BA	424	G
34	BA	429	U
34	BA	439	U
34	BA	465	A
34	BA	466	A
34	BA	468	A
34	BA	478	A
34	BA	482	A
34	BA	484	G
34	BA	486	U
34	BA	495	A
34	BA	511	C
34	BA	512	U
34	BA	518	C
34	BA	521	G
34	BA	524	G
34	BA	525	C
34	BA	527	7MG
34	BA	531	U

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Mol	Chain	Res	Type
34	BA	532	A
34	BA	547	A
34	BA	559	A
34	BA	564	C
34	BA	566	G
34	BA	570	G
34	BA	572	A
34	BA	573	A
34	BA	576	C
34	BA	632	U
34	BA	653	U
34	BA	665	A
34	BA	687	A
34	BA	690	G
34	BA	691	G
34	BA	694	A
34	BA	695	A
34	BA	700	G
34	BA	724	G
34	BA	734	G
34	BA	746	A
34	BA	749	A
34	BA	755	G
34	BA	793	U
34	BA	794	A
34	BA	796	C
34	BA	811	C
34	BA	815	A
34	BA	817	C
34	BA	818	G
34	BA	819	A
34	BA	820	U
34	BA	821	G
34	BA	827	U
34	BA	828	U
34	BA	841	C
34	BA	843	U
34	BA	846	G
34	BA	864	A
34	BA	867	G
34	BA	872	A
34	BA	884	U

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Mol	Chain	Res	Type
34	BA	885	G
34	BA	889	A
34	BA	890	G
34	BA	899	C
34	BA	922	G
34	BA	934	C
34	BA	935	A
34	BA	941	G
34	BA	949	A
34	BA	960	U
34	BA	961	U
34	BA	966	2MG
34	BA	968	A
34	BA	969	A
34	BA	975	A
34	BA	993	G
34	BA	1004	A
34	BA	1041	G
34	BA	1064	G
34	BA	1065	U
34	BA	1066	C
34	BA	1085	U
34	BA	1094	G
34	BA	1101	A
34	BA	1129	C
34	BA	1130	A
34	BA	1138	G
34	BA	1139	G
34	BA	1152	A
34	BA	1159	U
34	BA	1189	U
34	BA	1190	G
34	BA	1196	A
34	BA	1202	U
34	BA	1212	U
34	BA	1213	A
34	BA	1214	C
34	BA	1225	A
34	BA	1226	C
34	BA	1227	A
34	BA	1241	G
34	BA	1250	A

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Mol	Chain	Res	Type
34	BA	1256	A
34	BA	1278	G
34	BA	1279	G
34	BA	1280	A
34	BA	1285	A
34	BA	1298	U
34	BA	1299	A
34	BA	1300	G
34	BA	1301	U
34	BA	1303	C
34	BA	1317	C
34	BA	1320	C
34	BA	1322	C
34	BA	1338	G
34	BA	1340	A
34	BA	1341	U
34	BA	1343	G
34	BA	1346	A
34	BA	1359	C
34	BA	1360	A
34	BA	1379	G
34	BA	1381	U
34	BA	1382	C
34	BA	1397	C
34	BA	1399	C
34	BA	1432	G
34	BA	1447	A
34	BA	1494	G
34	BA	1505	G
34	BA	1506	U
34	BA	1517	G
34	BA	1529	G
34	BA	1530	G
34	BA	1534	A
34	BA	1535	C
34	BA	1537	U
34	BA	1539	C
34	BA	1542	A
35	BB	7	A
35	BB	8	4SU
35	BB	10	G
35	BB	16	H2U

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Mol	Chain	Res	Type
35	BB	18	G
35	BB	19	G
35	BB	20	H2U
35	BB	46	7MG
35	BB	48	C
35	BB	49	C
35	BB	59	U
35	BB	60	U
37	BD	25	U
37	BD	26	U
37	BD	36	U
37	BD	40	G
35	BE	10	G
35	BE	16	H2U
35	BE	17	C
35	BE	18	G
35	BE	20	H2U
35	BE	56	C
35	BE	57	G
35	BE	58	A
35	BE	73	A
35	BE	74	C
35	BE	75	C
35	BE	76	A

All (223) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	15	A
1	AA	77	U
1	AA	109	A
2	AB	13	A
2	AB	72	U
2	AB	75	G
2	AB	125	A
2	AB	164	C
2	AB	194	G
2	AB	196	A
2	AB	221	A
2	AB	222	A
2	AB	227	A
2	AB	277	G

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Mol	Chain	Res	Type
2	AB	331	C
2	AB	332	A
2	AB	345	A
2	AB	372	G
2	AB	380	G
2	AB	448	U
2	AB	479	A
2	AB	503	A
2	AB	504	A
2	AB	529	A
2	AB	532	A
2	AB	545	U
2	AB	586	A
2	AB	615	U
2	AB	669	G
2	AB	671	C
2	AB	673	C
2	AB	720	U
2	AB	729	G
2	AB	736	C
2	AB	743	A
2	AB	786	C
2	AB	790	U
2	AB	791	C
2	AB	805	G
2	AB	810	U
2	AB	827	U
2	AB	979	A
2	AB	995	C
2	AB	1032	A
2	AB	1033	U
2	AB	1045	C
2	AB	1046	A
2	AB	1068	G
2	AB	1069	A
2	AB	1084	A
2	AB	1087	G
2	AB	1109	C
2	AB	1112	G
2	AB	1128	G
2	AB	1132	U
2	AB	1133	A

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Mol	Chain	Res	Type
2	AB	1134	A
2	AB	1142	A
2	AB	1185	G
2	AB	1210	G
2	AB	1241	A
2	AB	1248	G
2	AB	1254	A
2	AB	1262	A
2	AB	1286	A
2	AB	1288	G
2	AB	1305	C
2	AB	1365	A
2	AB	1383	A
2	AB	1390	U
2	AB	1407	G
2	AB	1420	A
2	AB	1451	C
2	AB	1458	U
2	AB	1508	A
2	AB	1552	A
2	AB	1602	U
2	AB	1608	A
2	AB	1614	A
2	AB	1616	A
2	AB	1646	C
2	AB	1647	U
2	AB	1649	G
2	AB	1674	G
2	AB	1714	U
2	AB	1732	C
2	AB	1761	C
2	AB	1816	C
2	AB	1839	G
2	AB	1847	A
2	AB	1870	C
2	AB	1887	C
2	AB	1900	A
2	AB	1930	G
2	AB	1952	A
2	AB	1955	U
2	AB	1969	A
2	AB	2020	A

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Mol	Chain	Res	Type
2	AB	2021	C
2	AB	2119	A
2	AB	2130	U
2	AB	2172	U
2	AB	2309	A
2	AB	2339	C
2	AB	2357	G
2	AB	2380	C
2	AB	2389	G
2	AB	2390	U
2	AB	2391	G
2	AB	2448	A
2	AB	2465	C
2	AB	2500	U
2	AB	2542	A
2	AB	2581	G
2	AB	2584	U
2	AB	2602	A
2	AB	2619	C
2	AB	2654	A
2	AB	2655	G
2	AB	2662	A
2	AB	2667	C
2	AB	2696	U
2	AB	2717	C
2	AB	2726	A
2	AB	2732	G
2	AB	2744	G
2	AB	2751	G
2	AB	2791	G
2	AB	2838	G
2	AB	2866	U
2	AB	2870	C
2	AB	2872	A
2	AB	2894	G
34	BA	31	G
34	BA	52	C
34	BA	56	U
34	BA	59	A
34	BA	60	A
34	BA	65	A
34	BA	70	U

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Mol	Chain	Res	Type
34	BA	85	U
34	BA	86	G
34	BA	100	G
34	BA	193	C
34	BA	194	C
34	BA	209	U
34	BA	318	G
34	BA	365	U
34	BA	367	U
34	BA	368	U
34	BA	369	G
34	BA	385	C
34	BA	403	C
34	BA	415	A
34	BA	425	G
34	BA	438	U
34	BA	451	A
34	BA	465	A
34	BA	484	G
34	BA	489	C
34	BA	494	G
34	BA	524	G
34	BA	531	U
34	BA	570	G
34	BA	620	C
34	BA	641	U
34	BA	674	G
34	BA	690	G
34	BA	694	A
34	BA	753	A
34	BA	785	G
34	BA	793	U
34	BA	794	A
34	BA	815	A
34	BA	817	C
34	BA	824	G
34	BA	843	U
34	BA	884	U
34	BA	889	A
34	BA	899	C
34	BA	934	C
34	BA	968	A

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Mol	Chain	Res	Type
34	BA	975	A
34	BA	1065	U
34	BA	1104	G
34	BA	1112	C
34	BA	1124	G
34	BA	1129	C
34	BA	1131	G
34	BA	1212	U
34	BA	1213	A
34	BA	1227	A
34	BA	1257	A
34	BA	1278	G
34	BA	1279	G
34	BA	1280	A
34	BA	1298	U
34	BA	1299	A
34	BA	1300	G
34	BA	1302	C
34	BA	1312	G
34	BA	1323	G
34	BA	1340	A
34	BA	1347	G
34	BA	1377	A
34	BA	1399	C
34	BA	1441	A
34	BA	1529	G
34	BA	1534	A
34	BA	1536	C
35	BB	9	A
35	BB	45	U
37	BD	24	A
37	BD	25	U
37	BD	29	G
37	BD	42	U
37	BD	45	G
35	BE	3	C
35	BE	9	A
35	BE	18	G
35	BE	20	H2U
35	BE	56	C
35	BE	73	A

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

55 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
2	1MG	AB	745	2	18,26,27	1.16	2 (11%)	19,39,42	1.34	2 (10%)
2	PSU	AB	2605	2	18,21,22	0.91	0	22,30,33	0.94	1 (4%)
35	7MG	BB	46	35	22,26,27	4.67	2 (9%)	29,39,42	1.34	2 (6%)
2	PSU	AB	2457	2	18,21,22	0.98	1 (5%)	22,30,33	1.37	3 (13%)
35	PSU	BE	55	35	18,21,22	1.00	1 (5%)	22,30,33	0.94	1 (4%)
2	PSU	AB	1917	2	18,21,22	0.92	0	22,30,33	0.72	1 (4%)
2	7MG	AB	2069	2	22,26,27	4.64	1 (4%)	29,39,42	1.34	1 (3%)
2	OMG	AB	2251	2	18,26,27	1.11	2 (11%)	19,38,41	0.90	0
2	3TD	AB	1915	2	18,22,23	0.80	0	22,32,35	0.93	1 (4%)
2	PSU	AB	746	2	18,21,22	1.00	1 (5%)	22,30,33	1.31	2 (9%)
34	7MG	BA	527	34	22,26,27	4.60	1 (4%)	29,39,42	1.40	3 (10%)
35	5MU	BE	54	35	19,22,23	0.67	0	28,32,35	1.15	3 (10%)
35	4SU	BB	8	35	18,21,22	1.41	1 (5%)	26,30,33	1.15	3 (11%)
2	5MU	AB	1939	2	19,22,23	0.66	0	28,32,35	1.25	3 (10%)
2	6MZ	AB	2030	2	18,25,26	0.97	1 (5%)	16,36,39	1.39	3 (18%)
2	OMC	AB	2498	2	19,22,23	0.56	0	26,31,34	0.87	0
34	MA6	BA	1519	34	19,26,27	1.05	1 (5%)	18,38,41	1.21	2 (11%)
34	5MC	BA	967	34	18,22,23	0.65	0	26,32,35	0.84	1 (3%)
35	H2U	BE	16	35	18,21,22	0.84	0	21,30,33	1.07	1 (4%)
35	7MG	BE	46	35	22,26,27	4.63	2 (9%)	29,39,42	1.40	2 (6%)
34	PSU	BA	516	34	18,21,22	0.93	1 (5%)	22,30,33	1.11	1 (4%)
2	2MG	AB	2445	2	18,26,27	1.21	2 (11%)	16,38,41	0.77	0
35	5MU	BB	54	35	19,22,23	0.66	0	28,32,35	1.23	3 (10%)
34	UR3	BA	1498	34	19,22,23	0.72	0	26,32,35	0.92	1 (3%)
35	H2U	BB	16	35	18,21,22	0.82	0	21,30,33	1.08	1 (4%)
2	PSU	AB	1911	2	18,21,22	0.90	0	22,30,33	0.81	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	3AU	BB	47	-	25,28,29	0.88	1 (4%)	32,40,43	0.90	1 (3%)
35	PSU	BB	32	35	18,21,22	0.95	1 (5%)	22,30,33	1.09	2 (9%)
2	6MZ	AB	1618	2	18,25,26	0.98	1 (5%)	16,36,39	1.32	2 (12%)
35	PSU	BB	39	35	18,21,22	0.86	0	22,30,33	0.94	1 (4%)
35	H2U	BE	20	35	18,21,22	0.81	0	21,30,33	1.26	2 (9%)
35	MIA	BE	37	35	24,31,32	1.10	3 (12%)	26,44,47	1.56	4 (15%)
2	5MC	AB	1962	2	18,22,23	0.56	0	26,32,35	1.17	3 (11%)
2	PSU	AB	955	2	18,21,22	0.88	0	22,30,33	1.08	1 (4%)
2	CH	AB	2575	2	16,21,22	1.03	1 (6%)	20,30,33	1.26	2 (10%)
35	PSU	BE	32	35	18,21,22	0.96	1 (5%)	22,30,33	1.08	2 (9%)
35	MIA	BB	37	35	24,31,32	1.09	3 (12%)	26,44,47	1.72	5 (19%)
2	OMU	AB	2552	2	19,22,23	0.71	0	26,31,34	0.95	2 (7%)
35	4SU	BE	8	35	18,21,22	1.40	1 (5%)	26,30,33	1.64	6 (23%)
34	2MG	BA	966	34	18,26,27	1.17	1 (5%)	16,38,41	1.31	3 (18%)
34	2MG	BA	1516	34	18,26,27	1.21	3 (16%)	16,38,41	0.83	1 (6%)
35	3AU	BE	47	-	25,28,29	0.90	1 (4%)	32,40,43	1.22	4 (12%)
2	2MA	AB	2503	2	17,25,26	1.17	2 (11%)	17,37,40	1.33	2 (11%)
2	PSU	AB	2580	2	18,21,22	0.96	0	22,30,33	1.24	2 (9%)
34	5MC	BA	1407	34	18,22,23	0.65	0	26,32,35	0.93	1 (3%)
2	H2U	AB	2449	2	18,21,22	0.81	0	21,30,33	0.91	1 (4%)
34	2MG	BA	1207	34	18,26,27	1.20	1 (5%)	16,38,41	0.95	0
34	4OC	BA	1402	34	20,23,24	0.71	0	26,32,35	1.08	2 (7%)
2	PSU	AB	2504	2	18,21,22	1.09	2 (11%)	22,30,33	1.30	2 (9%)
35	PSU	BE	39	35	18,21,22	0.93	1 (5%)	22,30,33	1.00	1 (4%)
35	H2U	BB	20	35	18,21,22	0.81	0	21,30,33	1.00	1 (4%)
2	5MU	AB	747	2	19,22,23	0.71	0	28,32,35	1.39	3 (10%)
34	MA6	BA	1518	34	19,26,27	1.06	2 (10%)	18,38,41	0.74	0
35	PSU	BB	55	35	18,21,22	0.93	1 (5%)	22,30,33	1.04	1 (4%)
2	2MG	AB	1835	2	18,26,27	1.16	2 (11%)	16,38,41	1.00	1 (6%)

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
2	1MG	AB	745	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	2605	2	-	0/7/25/26	0/2/2/2
35	7MG	BB	46	35	-	1/7/37/38	0/3/3/3
2	PSU	AB	2457	2	-	0/7/25/26	0/2/2/2
35	PSU	BE	55	35	-	1/7/25/26	0/2/2/2
2	PSU	AB	1917	2	-	0/7/25/26	0/2/2/2
2	7MG	AB	2069	2	-	0/7/37/38	0/3/3/3
2	OMG	AB	2251	2	-	0/5/27/28	0/3/3/3
2	3TD	AB	1915	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	746	2	-	2/7/25/26	0/2/2/2
34	7MG	BA	527	34	-	1/7/37/38	0/3/3/3
35	5MU	BE	54	35	-	0/7/25/26	0/2/2/2
35	4SU	BB	8	35	-	0/7/25/26	0/2/2/2
2	5MU	AB	1939	2	-	0/7/25/26	0/2/2/2
2	6MZ	AB	2030	2	-	1/5/27/28	0/3/3/3
2	OMC	AB	2498	2	-	1/9/27/28	0/2/2/2
34	MA6	BA	1519	34	-	0/7/29/30	0/3/3/3
34	5MC	BA	967	34	-	0/7/25/26	0/2/2/2
35	H2U	BE	16	35	-	0/7/38/39	0/2/2/2
35	7MG	BE	46	35	-	0/7/37/38	0/3/3/3
34	PSU	BA	516	34	-	0/7/25/26	0/2/2/2
2	2MG	AB	2445	2	-	0/5/27/28	0/3/3/3
35	5MU	BB	54	35	-	0/7/25/26	0/2/2/2
34	UR3	BA	1498	34	-	0/7/25/26	0/2/2/2
35	H2U	BB	16	35	-	1/7/38/39	0/2/2/2
2	PSU	AB	1911	2	-	0/7/25/26	0/2/2/2
35	3AU	BB	47	-	-	2/16/34/35	0/2/2/2
35	PSU	BB	32	35	-	2/7/25/26	0/2/2/2
2	6MZ	AB	1618	2	-	0/5/27/28	0/3/3/3
35	PSU	BB	39	35	-	0/7/25/26	0/2/2/2
35	H2U	BE	20	35	-	0/7/38/39	0/2/2/2
35	MIA	BE	37	35	-	0/11/33/34	0/3/3/3
2	5MC	AB	1962	2	-	5/7/25/26	0/2/2/2
2	PSU	AB	955	2	-	0/7/25/26	0/2/2/2
2	CH	AB	2575	2	-	1/5/25/26	0/2/2/2
35	PSU	BE	32	35	-	0/7/25/26	0/2/2/2
35	MIA	BB	37	35	-	1/11/33/34	0/3/3/3
2	OMU	AB	2552	2	-	0/9/27/28	0/2/2/2
35	4SU	BE	8	35	-	0/7/25/26	0/2/2/2
34	2MG	BA	966	34	-	0/5/27/28	0/3/3/3
34	2MG	BA	1516	34	-	0/5/27/28	0/3/3/3
35	3AU	BE	47	-	-	5/16/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2MA	AB	2503	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	2580	2	-	0/7/25/26	0/2/2/2
34	5MC	BA	1407	34	-	0/7/25/26	0/2/2/2
2	H2U	AB	2449	2	-	0/7/38/39	0/2/2/2
34	2MG	BA	1207	34	-	0/5/27/28	0/3/3/3
34	4OC	BA	1402	34	-	0/9/29/30	0/2/2/2
2	PSU	AB	2504	2	-	2/7/25/26	0/2/2/2
35	PSU	BE	39	35	-	0/7/25/26	0/2/2/2
35	H2U	BB	20	35	-	1/7/38/39	0/2/2/2
2	5MU	AB	747	2	-	4/7/25/26	0/2/2/2
34	MA6	BA	1518	34	-	0/7/29/30	0/3/3/3
35	PSU	BB	55	35	-	1/7/25/26	0/2/2/2
2	2MG	AB	1835	2	-	0/5/27/28	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BB	46	7MG	C8-N9	-21.59	1.33	1.46
2	AB	2069	7MG	C8-N9	-21.49	1.34	1.46
35	BE	46	7MG	C8-N9	-21.44	1.34	1.46
34	BA	527	7MG	C8-N9	-21.30	1.34	1.46
35	BB	8	4SU	C5-C4	-5.01	1.36	1.42
35	BE	8	4SU	C5-C4	-4.95	1.36	1.42
2	AB	2575	CH	C5-C4	3.29	1.44	1.39
2	AB	745	1MG	C8-N7	-2.71	1.30	1.35
35	BE	37	MIA	C2-S10	2.61	1.77	1.75
34	BA	1207	2MG	C8-N7	-2.61	1.30	1.35
2	AB	2445	2MG	C8-N7	-2.60	1.30	1.35
34	BA	1516	2MG	C8-N7	-2.59	1.30	1.35
34	BA	1518	MA6	C8-N7	-2.55	1.30	1.34
2	AB	2030	6MZ	C8-N7	-2.53	1.30	1.34
34	BA	966	2MG	C8-N7	-2.53	1.30	1.35
2	AB	2251	OMG	C8-N7	-2.52	1.30	1.35
2	AB	2503	2MA	C8-N7	-2.51	1.30	1.35
35	BB	37	MIA	C2-S10	2.47	1.77	1.75
2	AB	1835	2MG	C8-N7	-2.38	1.31	1.35
34	BA	1519	MA6	C8-N7	-2.33	1.30	1.34
2	AB	1618	6MZ	C8-N7	-2.31	1.30	1.34
2	AB	2504	PSU	O4'-C1'	-2.30	1.40	1.43
35	BB	37	MIA	C8-N7	-2.27	1.30	1.34
35	BB	55	PSU	C2-N1	2.27	1.39	1.36
35	BE	37	MIA	C8-N7	-2.25	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BE	37	MIA	C6-N1	2.20	1.35	1.32
35	BE	47	3AU	O31-C13	-2.20	1.23	1.30
35	BB	47	3AU	O31-C13	-2.18	1.23	1.30
2	AB	745	1MG	C5-C4	-2.18	1.37	1.43
2	AB	2457	PSU	C2-N1	2.16	1.39	1.36
35	BB	32	PSU	C2-N1	2.14	1.39	1.36
2	AB	746	PSU	C2-N1	2.13	1.39	1.36
35	BB	37	MIA	C6-N1	2.11	1.35	1.32
35	BE	46	7MG	C5-N7	2.11	1.38	1.35
34	BA	516	PSU	C2-N1	2.09	1.39	1.36
35	BE	39	PSU	C2-N1	2.09	1.39	1.36
34	BA	1516	2MG	C5-C6	-2.09	1.43	1.47
35	BE	32	PSU	C2-N1	2.09	1.39	1.36
35	BE	55	PSU	C2-N1	2.08	1.39	1.36
34	BA	1516	2MG	C5-C4	-2.06	1.37	1.43
35	BB	46	7MG	C5-N7	2.06	1.38	1.35
2	AB	1835	2MG	C5-C4	-2.05	1.37	1.43
2	AB	2504	PSU	C2-N1	2.04	1.39	1.36
2	AB	2445	2MG	C5-C4	-2.03	1.37	1.43
34	BA	1518	MA6	C6-N1	2.01	1.36	1.33
2	AB	2251	OMG	C5-C4	-2.00	1.38	1.43
2	AB	2503	2MA	C5-C4	-2.00	1.38	1.43

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	37	MIA	C11-S10-C2	5.98	106.73	102.27
35	BE	46	7MG	N9-C8-N7	5.91	111.82	103.38
2	AB	2069	7MG	N9-C8-N7	5.82	111.70	103.38
34	BA	527	7MG	N9-C8-N7	5.72	111.56	103.38
35	BB	46	7MG	N9-C8-N7	5.60	111.39	103.38
35	BE	37	MIA	C11-S10-C2	4.78	105.84	102.27
2	AB	745	1MG	C2-N1-C6	4.18	124.34	120.95
2	AB	2457	PSU	C6-C5-C4	4.12	121.08	118.20
2	AB	746	PSU	C6-C5-C4	3.96	120.97	118.20
2	AB	2580	PSU	C6-C5-C4	3.86	120.90	118.20
34	BA	516	PSU	C6-C5-C4	3.81	120.86	118.20
2	AB	747	5MU	C6-C5-C4	3.77	121.18	118.03
2	AB	2504	PSU	C6-C5-C4	3.62	120.73	118.20
35	BE	8	4SU	C4-N3-C2	-3.61	123.83	127.34
35	BB	32	PSU	C6-C5-C4	3.59	120.71	118.20
35	BE	32	PSU	C6-C5-C4	3.58	120.70	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	955	PSU	C6-C5-C4	3.44	120.60	118.20
35	BE	39	PSU	C6-C5-C4	3.41	120.58	118.20
35	BE	47	3AU	O4'-C1'-N1	3.39	116.10	108.36
35	BE	16	H2U	O4'-C1'-N1	3.28	113.77	109.30
2	AB	1939	5MU	C6-C5-C4	3.26	120.75	118.03
35	BB	37	MIA	C5-C6-N1	-3.23	118.13	120.81
35	BB	54	5MU	C6-C5-C4	3.21	120.72	118.03
35	BB	55	PSU	C6-C5-C4	3.18	120.42	118.20
35	BE	37	MIA	C5-C6-N1	-3.17	118.18	120.81
2	AB	2575	CH	C4'-O4'-C1'	-3.15	106.85	109.85
35	BB	8	4SU	C5-C4-N3	3.11	117.57	114.69
35	BB	39	PSU	C6-C5-C4	3.08	120.36	118.20
35	BE	8	4SU	C5'-C4'-C3'	3.07	126.70	115.18
35	BE	54	5MU	C6-C5-C4	3.05	120.58	118.03
34	BA	1519	MA6	O3'-C3'-C2'	2.98	121.47	111.82
2	AB	1618	6MZ	C2-N1-C6	2.97	119.14	116.59
2	AB	2503	2MA	N1-C2-N3	2.96	127.97	123.06
35	BE	55	PSU	C6-C5-C4	2.91	120.23	118.20
2	AB	1915	3TD	C6-C5-C4	2.91	120.23	118.22
2	AB	2504	PSU	C3'-C2'-C1'	2.86	104.96	101.64
2	AB	2580	PSU	O4'-C1'-C2'	2.85	109.16	105.14
2	AB	2030	6MZ	C2'-C3'-C4'	-2.82	97.16	102.64
2	AB	1962	5MC	CM5-C5-C6	-2.81	119.09	122.85
2	AB	2575	CH	C5-C4-N3	2.78	119.62	118.04
35	BB	8	4SU	C4-N3-C2	-2.76	124.66	127.34
2	AB	1618	6MZ	C9-N6-C6	2.75	125.24	122.87
35	BE	8	4SU	O3'-C3'-C4'	2.75	119.00	111.05
2	AB	2503	2MA	C5-C6-N1	2.75	118.76	114.02
35	BE	47	3AU	C4'-O4'-C1'	-2.74	103.44	109.47
35	BB	37	MIA	C2-N3-C4	-2.72	111.57	115.32
2	AB	1939	5MU	O4'-C1'-N1	2.72	114.58	108.36
35	BB	54	5MU	C5M-C5-C6	-2.72	119.22	122.85
2	AB	2030	6MZ	C2-N1-C6	2.70	118.91	116.59
35	BE	37	MIA	C2-N3-C4	-2.66	111.66	115.32
35	BE	20	H2U	O4'-C1'-N1	2.64	112.90	109.30
34	BA	966	2MG	C2'-C3'-C4'	-2.63	97.53	102.64
35	BE	8	4SU	C5-C4-N3	2.63	117.13	114.69
35	BB	16	H2U	O3'-C3'-C4'	-2.60	103.52	111.05
35	BE	37	MIA	C12-C13-C14	-2.60	122.08	127.14
34	BA	527	7MG	O5'-C5'-C4'	2.58	117.78	108.99
35	BE	8	4SU	C6-N1-C2	-2.57	117.70	120.99
2	AB	2457	PSU	C3'-C2'-C1'	2.56	104.62	101.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1498	UR3	O4'-C1'-N1	2.52	114.13	108.36
35	BE	54	5MU	C5'-C4'-C3'	-2.48	105.87	115.18
35	BE	54	5MU	C5M-C5-C6	-2.47	119.55	122.85
35	BB	20	H2U	O4'-C1'-N1	2.46	112.65	109.30
2	AB	747	5MU	O4'-C4'-C5'	2.46	117.48	109.37
2	AB	2605	PSU	C6-C5-C4	2.44	119.91	118.20
2	AB	1835	2MG	O3'-C3'-C2'	2.43	119.69	111.82
35	BB	37	MIA	C12-N6-C6	2.42	126.13	122.55
2	AB	1911	PSU	C6-C5-C4	2.41	119.89	118.20
2	AB	2030	6MZ	O3'-C3'-C4'	-2.41	104.08	111.05
34	BA	1402	4OC	C2'-C1'-N1	-2.36	109.65	114.22
2	AB	2457	PSU	O4'-C1'-C2'	2.35	108.46	105.14
34	BA	1519	MA6	O4'-C1'-C2'	2.34	110.34	106.93
35	BE	47	3AU	O4'-C4'-C3'	2.24	109.56	105.11
34	BA	967	5MC	CM5-C5-C6	-2.24	119.85	122.85
2	AB	1939	5MU	C5M-C5-C6	-2.24	119.86	122.85
35	BB	47	3AU	O4-C4-N3	2.24	121.84	119.16
2	AB	746	PSU	O3'-C3'-C2'	2.24	119.06	111.82
35	BE	8	4SU	C1'-N1-C6	2.24	125.72	120.84
2	AB	2449	H2U	C4-N3-C2	2.23	127.64	125.79
34	BA	966	2MG	O3'-C3'-C4'	2.23	117.50	111.05
2	AB	1962	5MC	C3'-C2'-C1'	-2.23	97.19	101.43
35	BE	47	3AU	O4-C4-N3	2.22	121.81	119.16
2	AB	1917	PSU	C6-C5-C4	2.22	119.75	118.20
35	BB	8	4SU	S4-C4-N3	-2.21	118.04	120.21
35	BE	20	H2U	O4'-C4'-C3'	2.20	109.47	105.11
35	BB	54	5MU	O3'-C3'-C2'	2.19	118.92	111.82
2	AB	747	5MU	O3'-C3'-C2'	2.17	118.86	111.82
34	BA	1402	4OC	O4'-C1'-N1	2.17	113.33	108.36
2	AB	745	1MG	O3'-C3'-C2'	-2.17	104.79	111.82
35	BB	37	MIA	C12-C13-C14	-2.16	122.94	127.14
35	BB	46	7MG	C2'-C3'-C4'	-2.16	98.45	102.64
35	BB	32	PSU	O4'-C1'-C2'	2.08	108.08	105.14
34	BA	1407	5MC	O4'-C4'-C5'	2.07	116.20	109.37
2	AB	1962	5MC	O3'-C3'-C2'	-2.07	105.14	111.82
35	BE	32	PSU	O4'-C1'-C2'	2.06	108.05	105.14
2	AB	2552	OMU	C5'-C4'-C3'	-2.06	107.48	115.18
34	BA	966	2MG	O6-C6-C5	2.03	128.33	124.37
2	AB	2552	OMU	C2'-C3'-C4'	-2.01	97.62	101.99
34	BA	527	7MG	C5'-C4'-C3'	-2.01	107.64	115.18
35	BE	46	7MG	C5-C4-N9	2.01	108.96	106.35
34	BA	1516	2MG	O6-C6-C5	2.00	128.28	124.37

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AB	747	5MU	C2'-C1'-N1-C2
34	BA	527	7MG	C4'-C5'-O5'-P
35	BB	37	MIA	N6-C12-C13-C14
35	BB	46	7MG	C4'-C5'-O5'-P
2	AB	1962	5MC	C2'-C1'-N1-C6
2	AB	747	5MU	C2'-C1'-N1-C6
35	BE	47	3AU	O4'-C1'-N1-C6
35	BB	47	3AU	O4'-C4'-C5'-O5'
35	BB	47	3AU	C3'-C4'-C5'-O5'
2	AB	747	5MU	O4'-C1'-N1-C6
2	AB	1962	5MC	O4'-C1'-N1-C2
35	BE	47	3AU	O4'-C1'-N1-C2
2	AB	1962	5MC	O4'-C1'-N1-C6
2	AB	1962	5MC	C2'-C1'-N1-C2
35	BE	47	3AU	N40-C12-C13-O31
2	AB	746	PSU	O4'-C1'-C5-C4
2	AB	2504	PSU	O4'-C1'-C5-C4
35	BB	32	PSU	O4'-C1'-C5-C4
2	AB	747	5MU	O4'-C1'-N1-C2
35	BE	47	3AU	N40-C12-C13-O30
2	AB	746	PSU	O4'-C1'-C5-C6
35	BB	32	PSU	O4'-C1'-C5-C6
35	BB	55	PSU	O4'-C1'-C5-C6
35	BE	55	PSU	O4'-C1'-C5-C6
2	AB	2575	CH	O4'-C1'-N1-C2
2	AB	2030	6MZ	O4'-C4'-C5'-O5'
2	AB	2504	PSU	O4'-C4'-C5'-O5'
35	BB	16	H2U	O4'-C4'-C5'-O5'
35	BB	20	H2U	O4'-C4'-C5'-O5'
35	BE	47	3AU	O4'-C4'-C5'-O5'
2	AB	2498	OMC	C4'-C5'-O5'-P
2	AB	1962	5MC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

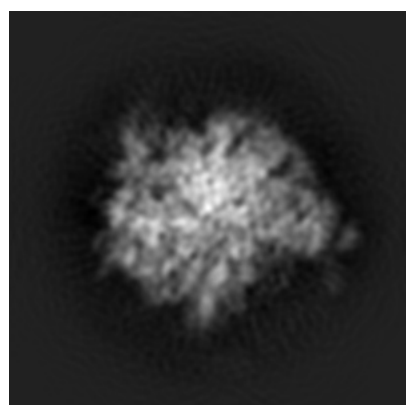
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1849. These allow visual inspection of the internal detail of the map and identification of artifacts.

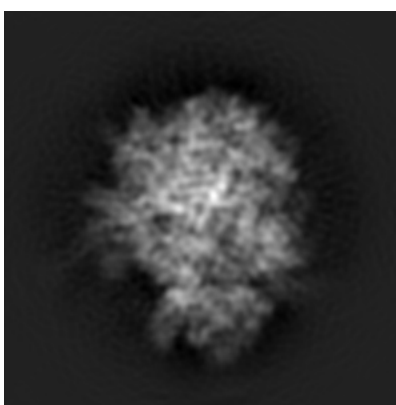
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

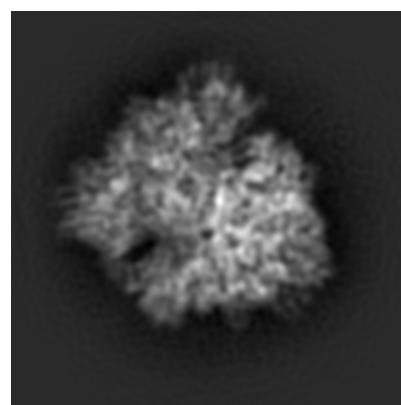
6.1.1 Primary map



X



Y

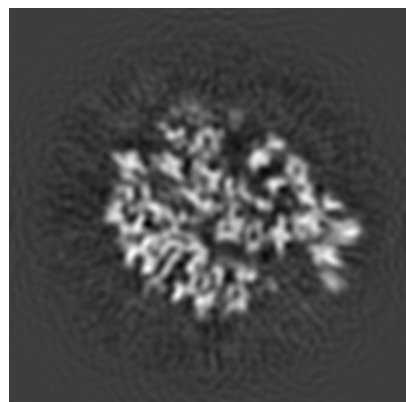


Z

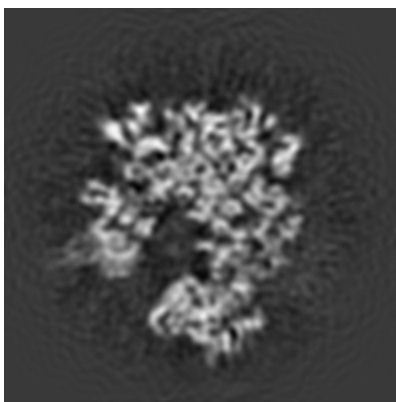
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

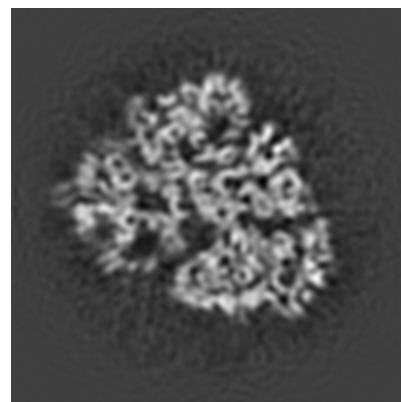
6.2.1 Primary map



X Index: 125



Y Index: 125

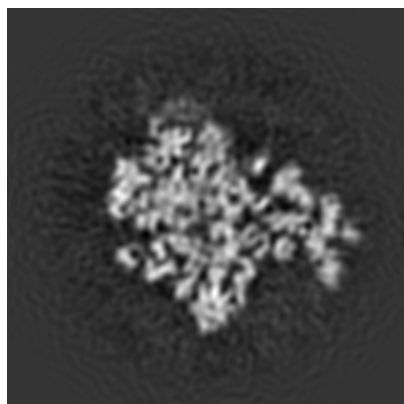


Z Index: 125

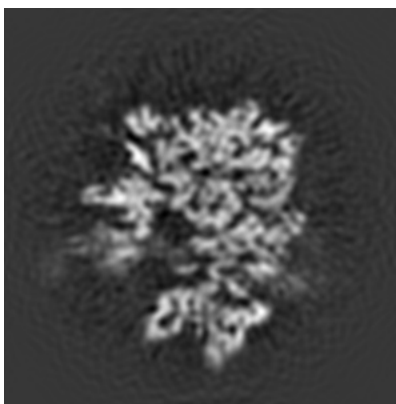
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

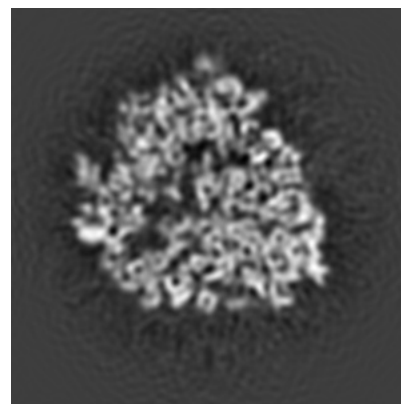
6.3.1 Primary map



X Index: 130



Y Index: 130

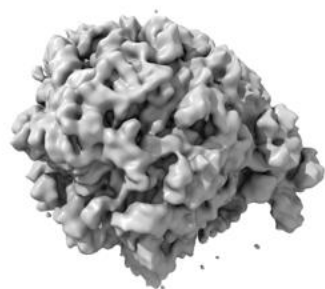


Z Index: 117

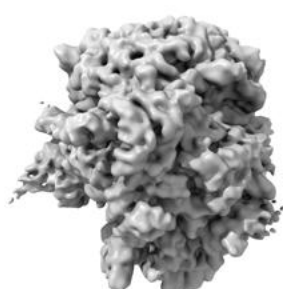
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

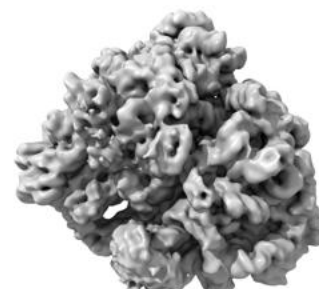
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 32.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

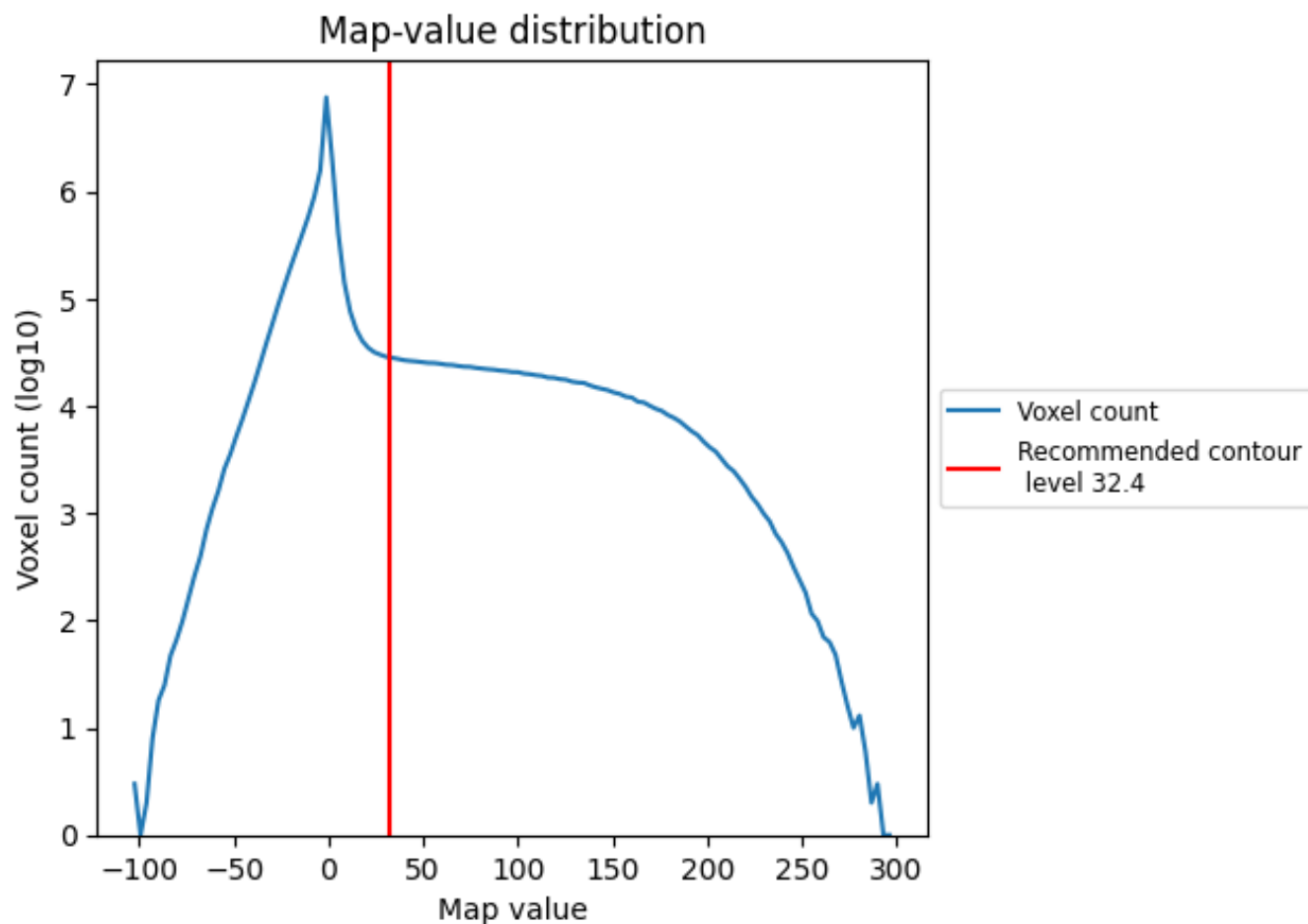
6.5 Mask visualisation

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

7 Map analysis [i](#)

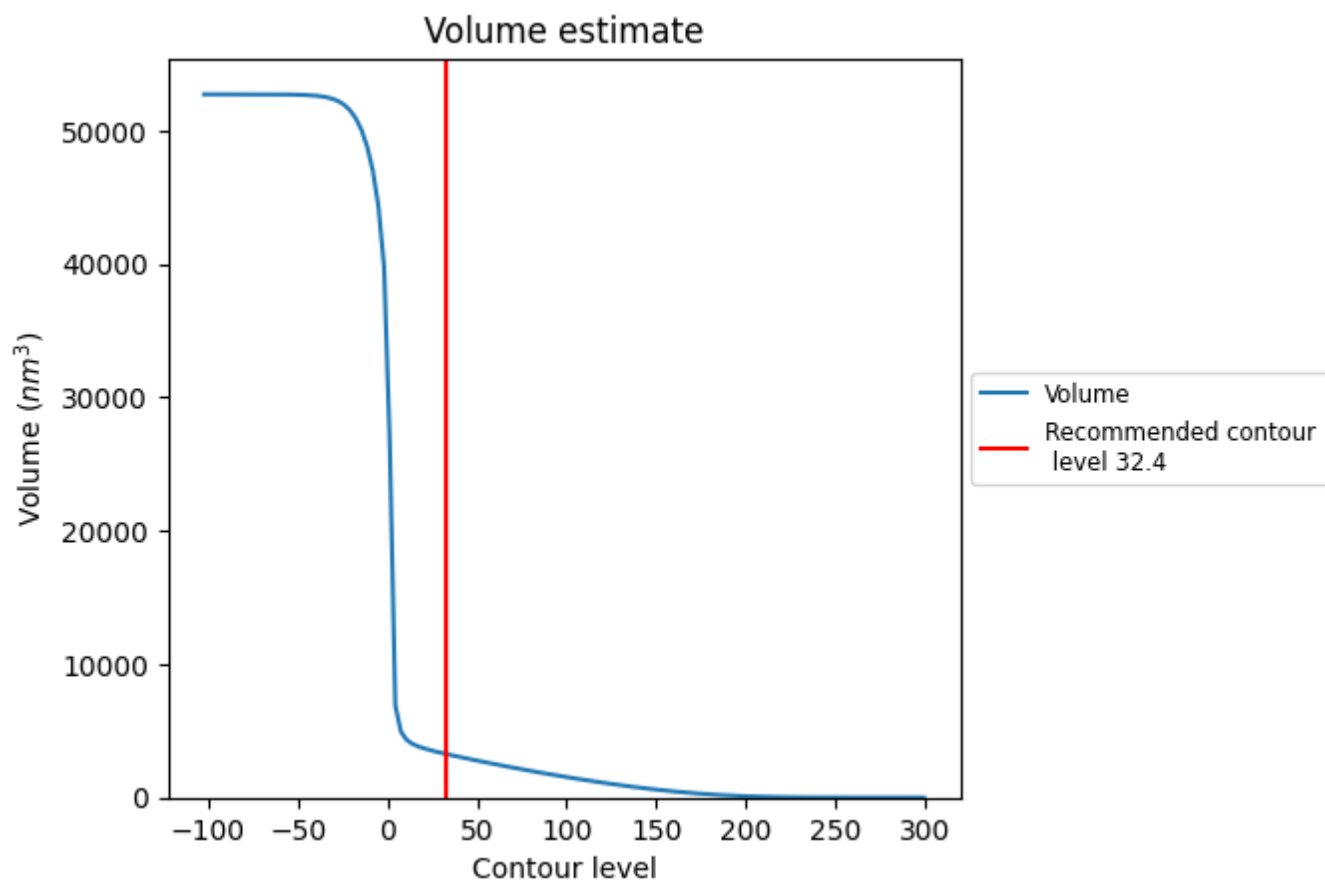
This section contains the results of statistical analysis of the map.

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.

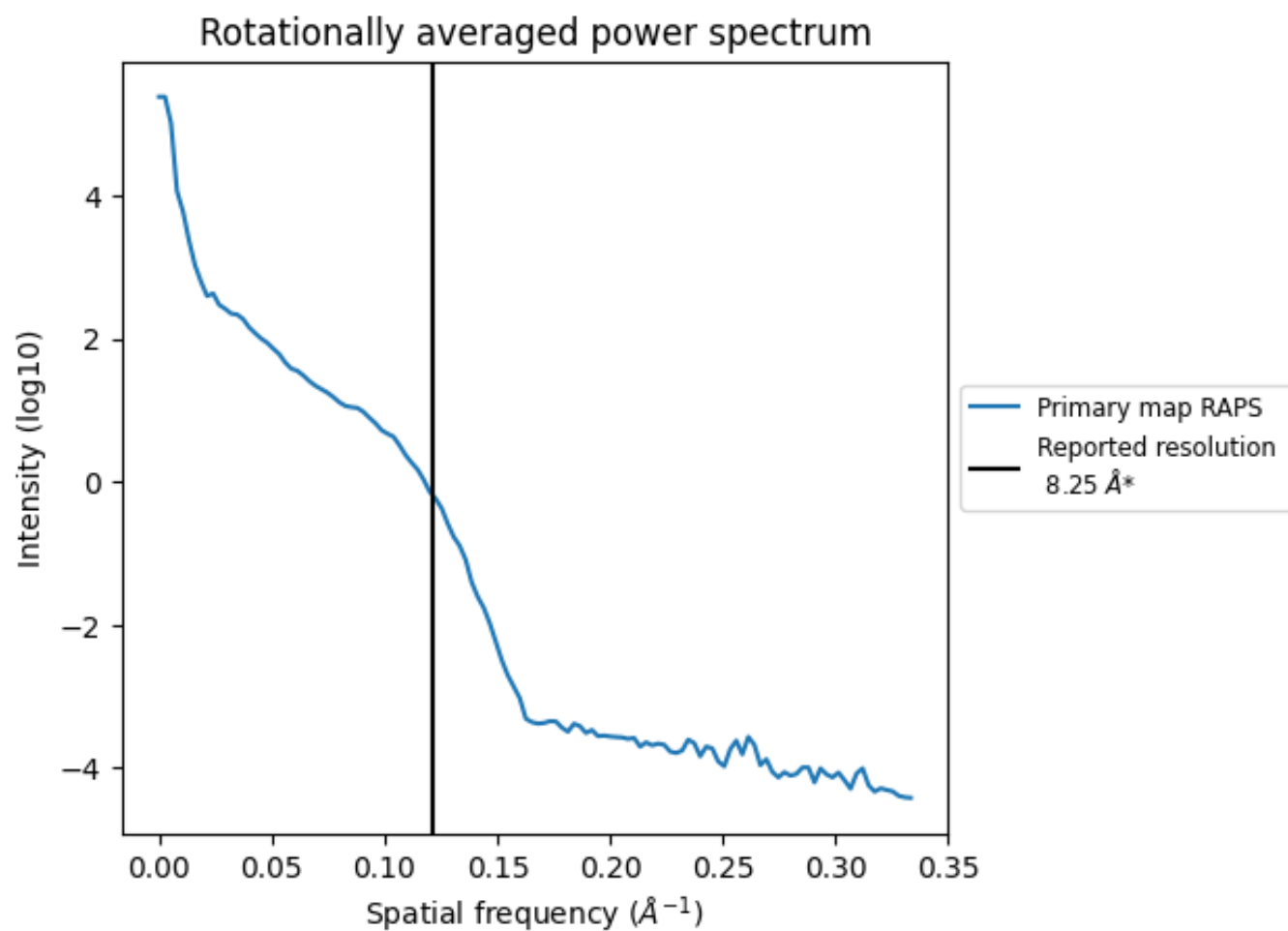
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3278 nm³; this corresponds to an approximate mass of 2961 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 0.121 Å⁻¹

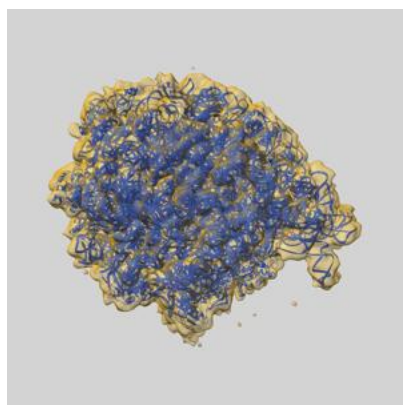
8 Fourier-Shell correlation

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

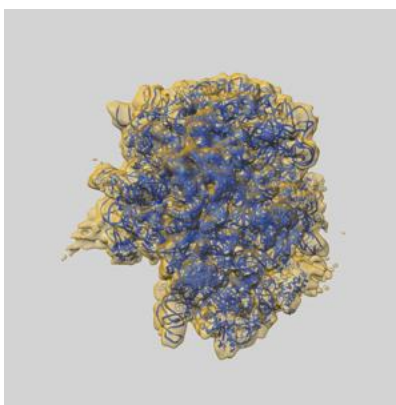
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1849 and PDB model 4V6K. Per-residue inclusion information can be found in section 3 on page 14.

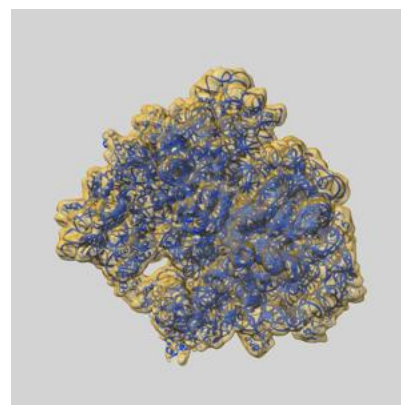
9.1 Map-model overlay [i](#)



X



Y



Z

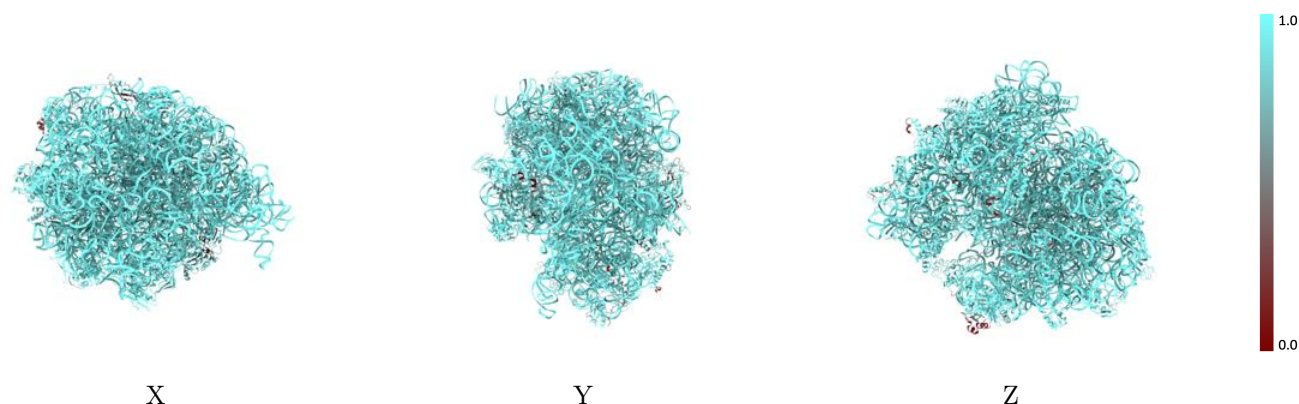
The images above show the 3D surface view of the map at the recommended contour level 32.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



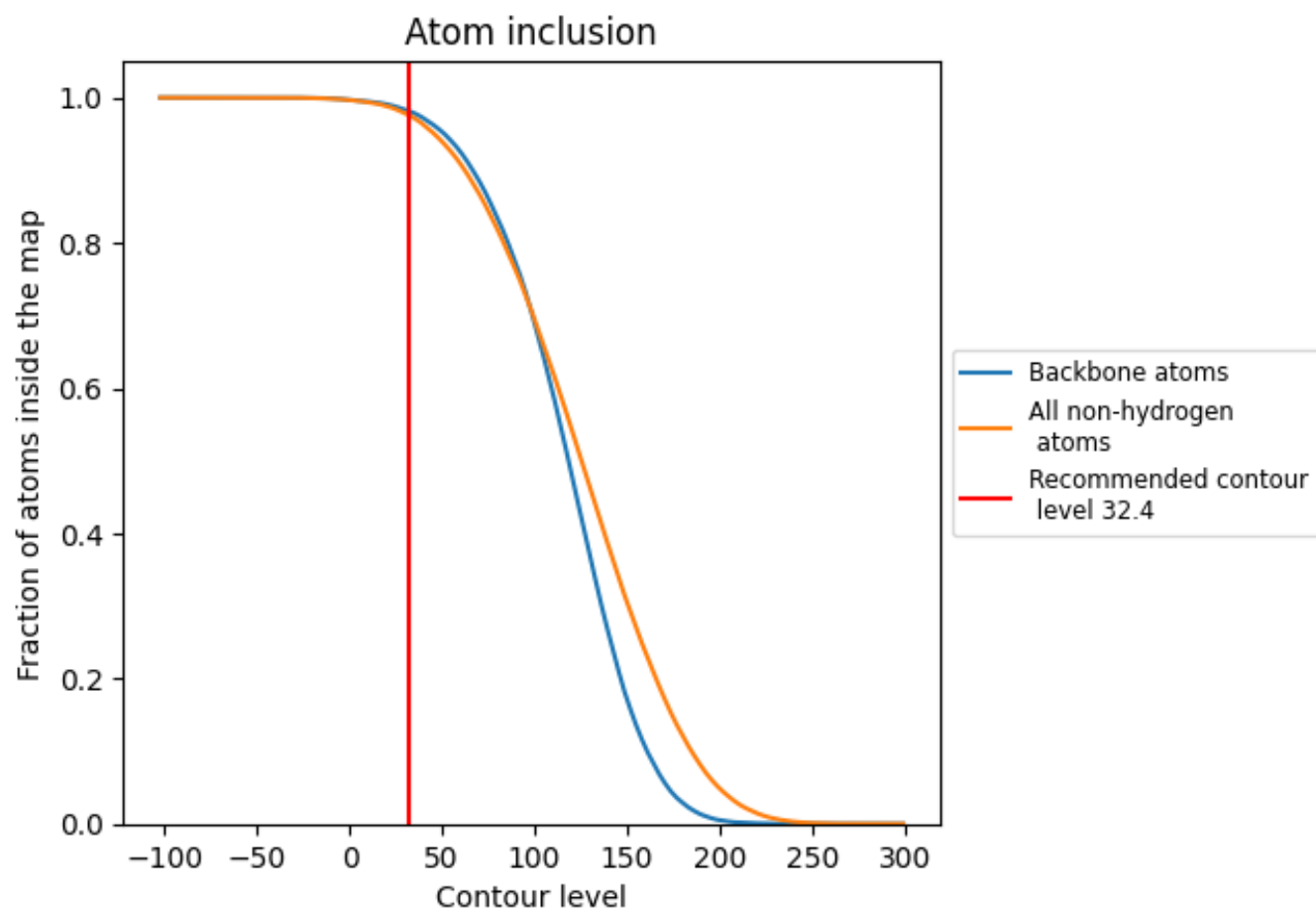
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (32.4).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 98% 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 (32.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9754	 0.1600
AA	 0.9981	 0.1930
AB	 0.9959	 0.1830
AC	 0.7851	 0.0430
AD	 0.9684	 0.1080
AE	 0.9694	 0.1100
AF	 0.9618	 0.1180
AG	 0.9740	 0.1250
AH	 0.9830	 0.1540
AI	 0.7901	 0.1140
AJ	 0.9599	 0.0990
AK	 0.9327	 0.1130
AL	 0.9501	 0.1230
AM	 0.9668	 0.1220
AN	 0.9607	 0.1210
AO	 0.9804	 0.1190
AP	 0.9897	 0.1380
AQ	 0.9414	 0.1510
AR	 0.9570	 0.1030
AS	 0.9435	 0.1270
AT	 0.9701	 0.1360
AU	 0.9702	 0.1300
AV	 0.9820	 0.1410
AW	 0.9851	 0.1560
AX	 0.8981	 0.0680
AY	 0.9517	 0.1110
AZ	 0.9517	 0.1250
Aa	 0.9794	 0.1460
Ab	 0.8829	 0.0890
Ac	 0.9860	 0.0910
Ad	 0.9607	 0.1000
Ae	 0.9746	 0.0930
Af	 0.9796	 0.1240
Ag	 0.9658	 0.0680
BA	 0.9963	 0.1780



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Chain	Atom inclusion	Q-score
BB	 0.9315	 0.1780
BC	 0.8140	 0.1240
BD	 0.9778	 0.1760
BE	 0.9804	 0.1800
BF	 0.9337	 0.1320
BG	 0.9012	 0.1260
BH	 0.9428	 0.1040
BI	 0.9244	 0.1220
BJ	 0.8731	 0.1110
BK	 0.9653	 0.1270
BL	 0.9812	 0.1450
BM	 0.9688	 0.1090
BN	 0.9250	 0.0960
BO	 0.9390	 0.1190
BP	 0.9501	 0.1150
BQ	 0.9784	 0.1320
BR	 0.9793	 0.1030
BS	 0.9855	 0.1310
BT	 0.9697	 0.1100
BU	 0.9787	 0.1210
BV	 0.9883	 0.1210
BW	 0.9058	 0.0800
BX	 0.9847	 0.1370
BY	 0.8661	 0.0860