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PDB ID	:	6YAN
EMDB ID	:	EMD-10762
Title	:	Mammalian 48S late-stage translation initiation complex with histone 4 mRNA
Authors	:	Bochler, A.; Simonetti, A.; Guca, E.; Hashem, Y.
Deposited on	:	2020-03-12
Resolution	:	3.48 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 43
Mogul	:	1.8.4, 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 (i)

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

The reported resolution of this entry is 3.48 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$		
Clashscore	158937	4297		
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  $\geq=3, 2, 1$  and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq=5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	1	25	88%	12%
2	С	208	93%	7%
3	D	215	93%	6% •
4	Е	226	95%	5%
5	F	227	90%	9% •
6	G	263	97%	•
7	Н	191	93%	7%



Continued from previous page... Chain Length Quality of chain Mol 8% 8 Ι 23793% 7% 17% 9 J 19089% 10% • 7% 10 Κ 206 . . 95%  $\mathbf{L}$ 18211 94% 6% 12% 12М 9812% • 87% 15% 13Ν 15892% 6% • 44% Ο 1412495% 5% 5% • Р 1515098% • Q 1361693% 7% • i.  $\mathbf{S}$ 1714190% 10% 8% Т . 18 12698% • V 1914194% 5%• 5% 20W 10493% 7% Х 82. 2198% 22Υ 129• 98% i. Ζ 23142• 96% 5% . . 24126 $\mathbf{a}$ 96% ÷ 99 25b • • 96% 10% 2684  $\mathbf{c}$ 5% • 94% 6% 27d 6494% 5%• • 2853е 87% 13% 45% f 297182% 17% . 7% 30 31396% • g 12% 75• 31 h 96% 22% 32 i 5986% 12%



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Mol	Chain	Length	Quality of chain		
33	2	1863	• 73%	18%	• 6%
			72%		
34	3	36	42% 56%		•
			82%		
35	А	266	88%		8% ••
			100%		
36	В	422	91%		9%
37	U	142	86%		11% ••
			13%		
38	R	135	79%	16	5% • •
			43%		
39	1	75	69%	21%	9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	C4J	2	1244	Х	-	-	-



## 2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 84251 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 protein called 60s ribosomal protein l41.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
1	1	25	Total 240	C 145	N 64	O 28	${ m S} { m 3}$	0	0

• Molecule 2 is a protein called 40S ribosomal protein SA.

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

• Molecule 3 is a protein called ribosomal protein eS1.

Mol	Chain	Residues		At		AltConf	Trace		
3	D	215	Total 1742	C 1107	N 309	0 311	S 15	0	0

• Molecule 4 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues		Ate		AltConf	Trace		
4	Е	226	Total 1743	C 1127	N 300	O 307	S 9	0	0

• Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues		Ate		AltConf	Trace		
5	F	227	Total 1765	C 1124	N 317	0 316	S 8	0	0

• Molecule 6 is a protein called 40S ribosomal protein S4.

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



• Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	Н	191	Total 1509	C 943	N 286	0 273	${ m S} 7$	0	0

• Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
8	Ι	237	Total 1924	C 1200	N 387	O 330	S 7	0	0

• Molecule 9 is a protein called ribosomal protein eS7.

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

• Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues		Ate			AltConf	Trace	
10	K	206	Total 1680	C 1054	N 329	O 292	${ m S}{ m 5}$	0	0

• Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues		At	oms			AltConf	Trace
11	L	182	Total 1499	C 952	N 300	0 245	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 12 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues		At	oms	AltConf	Trace		
12	М	98	Total 828	C 539	N 148	0 135	S 6	0	0

• Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues		Atoms					Trace
13	Ν	158	Total 1296	C 827	N 241	0 221	${f S}{7}$	0	0

• Molecule 14 is a protein called 40S ribosomal protein S12.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	0	124	Total 958	C 600	N 170	O 179	S 9	0	0

• Molecule 15 is a protein called ribosomal protein uS15.

Mol	Chain	Residues		Atoms					Trace
15	Р	150	Total 1208	С 773	N 229	O 205	S 1	0	0

• Molecule 16 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	Q	136	Total 1016	C 621	N 199	O 190	S 6	0	0

• Molecule 17 is a protein called ribosomal protein uS9.

Mol	Chain	Residues		At	oms			AltConf	Trace
17	S	141	Total 1123	C 715	N 212	O 193	${ m S} { m 3}$	0	0

• Molecule 18 is a protein called ribosomal protein eS17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	Т	126	Total 1020	C 639	N 188	0 188	${ m S}{ m 5}$	0	0

• Molecule 19 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	V	141	Total 1113	C 701	N 213	0 196	${ m S} { m 3}$	0	0

• Molecule 20 is a protein called Ribosomal\_S10 domain-containing protein.

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	W	104	Total 822	C 514	N 156	0 148	${f S}$ $4$	0	0

• Molecule 21 is a protein called 40S ribosomal protein S21.



Mol	Chain	Residues		At	oms	AltConf	Trace		
21	Х	82	Total 620	$\begin{array}{c} \mathrm{C} \\ 378 \end{array}$	N 117	O 120	${ m S}{ m 5}$	0	0

• Molecule 22 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	Y	129	Total 1034	C 659	N 193	0 176	S 6	0	0

• Molecule 23 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues		At	oms	AltConf	Trace		
23	Z	142	Total 1107	C 698	N 220	0 185	$\frac{S}{4}$	0	0

• Molecule 24 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	a	126	Total 1022	C 645	N 198	0 174	${ m S}{ m 5}$	0	0

• Molecule 25 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues		At	oms	AltConf	Trace		
25	b	99	Total 790	C 491	N 162	0 131	S 6	0	0

• Molecule 26 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	С	84	Total 659	C 413	N 122	0 116	S 8	0	0

• Molecule 27 is a protein called ribosomal protein eS28.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
27	d	64	Total 507	C 308	N 102	O 95	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 28 is a protein called ribosomal protein uS14.



Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
28	е	53	Total 445	C 278	N 90	0 72	${ m S}{ m 5}$	0	0

• Molecule 29 is a protein called ribosomal protein eS31.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
29	f	71	Total 582	$\begin{array}{c} \mathrm{C} \\ 367 \end{array}$	N 109	O 99	${ m S} 7$	0	0

• Molecule 30 is a protein called ribosomal protein RACK1.

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

• Molecule 31 is a protein called ribosomal protein eS25.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	h	75	Total 599	C 382	N 111	O 105	S 1	0	0

• Molecule 32 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues		At	oms			AltConf	Trace
32	i	59	Total 473	C 293	N 104	O 75	S 1	0	0

• Molecule 33 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues		1	Atoms			AltConf	Trace
33	2	1744	Total 37202	C 16613	N 6663	0 12186	Р 1740	0	0

• Molecule 34 is a RNA chain called histone 4 (H4) mRNA.

Mol	Chain	Residues		A	toms			AltConf	Trace
34	3	36	Total 774	C 346	N 144	0 249	Р 35	0	0

• Molecule 35 is a protein called Eukaryotic translation initiation factor 2 subunit 1.



Mol	Chain	Residues		At	oms			AltConf	Trace
35	А	266	Total 2147	C 1354	N 376	O 406	S 11	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
36	В	422	Total 3214	C 2044	N 561	O 592	S 17	0	0

• Molecule 37 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues		At	oms			AltConf	Trace
37	U	142	Total 1172	С 733	N 239	O 199	S 1	0	0

• Molecule 38 is a protein called Ribosomal protein S15.

Mol	Chain	Residues		At	oms			AltConf	Trace
38	R	135	Total 1111	C 704	N 211	0 189	S 7	0	0

• Molecule 39 is a RNA chain called initiator methionylated tRNA.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
39	1	75	Total 1614	С 722	N 299	O 519	Р 74	0	0



### 3 Residue-property plots (i)

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

• Molecule 1: 60s ribosomal protein l41





• Molecule 12: 40S ribosomal protein eS10







• Molecule 19: 40S ribosomal protein eS19

Chain V:	94%	5% •
V4 K27 L28 V34 K38 K38 L39 A40 L45 L45 V48 Y48 S90 S90	D116	
• Molecule 20: Ribosom	al_S10 domain-containing protein	
Chain W:	93%	7%
A16 120 770 671 671 671 872 872 8105 1106 1107	1116 A117 A119 A119	
• Molecule 21: 40S ribo	somal protein S21	
Chain X:	98%	·
M1 E7 D10 K41 K41 H82		
• Molecule 22: Ribosom	al protein S15a	
Chain Y:	98%	<del>.</del>
N2 N9 A66 F130		
• Molecule 23: 40S ribo	somal protein uS12	
Chain Z:	96%	•
M1 L32 F41 F41 F41 A126 A126 A126 A126 A126 A126 A126 A126 A126		
• Molecule 24: 40S ribo	somal protein S24	
Chain a:	96%	•••
B3 14 14 13 13 13 13 13 13 13 13 13 13 13 13 13	G128	
• Molecule 25: 40S ribo	somal protein eS26	



Chain b:	96%	••
12 NB A11 B33 B33 B33 B32 B46		
• Molecule 26: 40S	b ribosomal protein S27	
Chain c:	94%	5% •
M1 R17 P34 Y41 Y42 I43 C59 S60	G76 773 778 881 483 483 483 484	
• Molecule 27: ribe	osomal protein eS28	
Chain d:	94%	5% •
RIS VIG 1037 138 1339 1339 1339 1338 1466 1466 1466 1466 1466 1466 1466 146		
• Molecule 28: ribe	osomal protein uS14	
Chain e:	87%	13%
48 48 48 54 48 42 42 63 150 451		
• Molecule 29: ribe	osomal protein eS31	
Chain f:	45% 82%	17% •
K82 K83 84 84 84 785 785 788 788 788 788 789 8091	Kist Kist Kist Kist Kist Kist Kist Kist	C1120 C1121 2123 2123 2123 0123 C126 0127 C145 C145 C145 C145 C145 C145 C145 C146 C145 C145 C146
• Molecule 30: ribe	osomal protein RACK1	
Chain g:	96%	•
T2         E3         E3         64         04         69         69         69         613         150         T50         N51	F101 F101 H104 H104 F101 F113 N159 S161 N159 S161 S161 S161 S161 C190 C190 C190 C190 C190 C190 C190 C19	233 233 233 223 223 2246 263 226 263 2275 2275 8277 82779 82279 82279 82279 82279 82279 82279 82279 82279 82279 82279 82279 82279 82279 82279 82279 82273 82778 82
• Molecule 31: ribe	osomal protein eS25	
Chain h:	96%	· ·
R41 D42 K43 L44 N45 L49 K49 Y65 Y109	TII0 NII1 TII3 KII4 G115 G115	
	WORLDWIDE PROTEIN DATA BANK	

• Molecule 32: 40S ribosomal protein eS30 22% Chain i: 86% 12% • • • • 678 879 882 V83 V83 C84 C84 K85 K85 V86 • Molecule 33: 18S ribosomal RNA Chain 2: • 6% 73% 18% A61 G62 U63 A64 C65 G66 C67 149 150 151 152 152 153 153 U239 C240 186 187 188 189 190 191 2012 3272 G303
 G304
 A304
 U305
 U305
 C306
 C308
 C312
 C312 C313 3337 338 339 339 1341 1342 1342 3373 1379 1380 138 39 3426 3427 3428 4429 4429 3430 2431 2432 445 447 448 3449 1450 1451 453 454 455 0486 0487 0488 0488 0488 1489 0490 0491 3555 3555 3555 3557 3555 3555 3555 3562 3562 3562 3563 4566 4565 4566 4566 3601 3602 3603 3604 3605 3605 3607 3687 0000 000040004



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U	IJ.	00	5 0	) <del>'</del>	<mark>U728</mark>	C729	0230	C731	C732	G733	C734	C735	C736	C737	11738	0010	6510	C741	C742	U743	C744	U745	C746	G747	G748	C749	G750	C751	C752	υυ	00	D Z	0 5	Å	D	, U	D	, D	n ·	A G	U	D	Þ ٩	IJ	סט	• 0	ບບ	ບອບ
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IJ	IJ	G784	G785	C786	C787	C788	G789	A790	A791	G792	0193	U795	U796	797U	A798	C799	0000		G803	A804	A805	A806	A808	<b>A809</b>	U810	U811 1811	G813	A814	G815	0120	U818	U819 7070	0020 4821	A822	A823 G824	C825	A826 G827	G828	C829	C831	<mark>G832</mark>	A833	G834	C835	G837	C838	U840	<mark>6841</mark>
																										•					•	•							•									
G842	A843	U844	A 845 C 846	C847	G848	C849	A850	C852	<b>U853</b>	A854	G855 0010	1856 1057	A007 A858	U859	A860	A861	<b>U862</b>	G863	0864 1865	A866	<b>U867</b>	A868	G869 G870	4871	C872	C873	G874	C875	G877 G877	<b>U878</b>	U879	C880	0881 4882	U883	U884 U885	<b>U886</b>	G887 11000	0000 U889	G890	G891	U893	<b>U894</b>	U895	G897	0.898 1.000	A899 A900	C901	
<b>U902</b>	G903	A904	6906 6906	C907	<mark>C908</mark>	A909	0910	4911 A912	U913	U914	A915	A916	4918	G919	<b>G920</b>	G921	A922	C923	G924 C075	C926	C927	G928	6929	G931	<mark>G932</mark>	C933	A934	0336 036	<mark>C937</mark>	G938 11020	0939 A940	<b>U941</b>	0942	C944	G945	C947	G948	U950	A951	6952 4953	G954	G955	0956 C957	A958	A959 A960	U961		
<b>U962</b>	C963	U964 1106 F	0300 0366	000D	A968	C969	C970	G972	C973	G974	C975	A976 A077	1.197.8	A979	C980	G981	G982	A983	C984 7085	0300 A986	G987	A988	6989 0000	6991	A992	A993	A994 7005	0006 0006	<u>A997</u>	0998 11000	01000	G1001	C1002	A1004	A1005	41006 A1007	A1008	G1010	U1011	U1012 11013	01014	C1015	A1016	U1018	A1019	0201A U1021		
C1022	A1023	A1024	61025 A1026	A1027	C1028	G1029	A1030	A1032	G1033	U1034	C1035	G1036	41038 A1038	G1039	G1040	U1041	U1042	C1043	G1044 A1045	A1046	G1047	A1048	C1049	41051 A1051	<b>U1052</b>	C1053	A1054 C1055	41056 A1056	U1057	A1058	C1060	G1061	U1062	G1064	U1065	A1 066 G1 067	U1068	C1070	C1071	G1072 A1073	C1074	C1075	A1076	A1078	A1079	C1081		
G1082	A1083	U1084	G1085 C1086	C1087	G1088	A1089	C1090	G1092	G1093	C1094	G1095	A1096	0109/ G1098	C1099	G1100	G1101	C1102	G1103	G1104 C1105	G1105 G1106	U1107	U1108	A1109	01110 01111	C1112	C1113	C1114 A1115	01115 01116	G1117	A1118	C11120 C1120	C1121	G1122 C1122	C1124	G1125	G1127 G1127	C1128	G1129 G1130	C1131	U1132 I1133	C1134	C1135	G1136 C1137	G1138	A1139	A1140 A1141		
C1142	C1143	A1144	A1145 A1146	G1147	U1148	C1149	U1150	01152 U1152	G1153	G1154	G1155	U1156 111155	0115/ C1158	C1159	G1160	G1161	G1162	G1163	G1164 C1165	A1166	G1167	U1168	A1169	G1171	G1172	U1173	01174 61176	C1176	A1177	A1178	G1180 G1180	C1181	U1182	A1184	A1185	A1160 C1187	U1188	01109 A1190	A1191	A1192 G1193	G1194	A1195	A1196 11197	U1198	G1199 A1200	C1201		
G1202	G1203	A1204	G1206 G1206	G1207	G1208	C1209	A1210	C1212	A1213	C1214	C1215	A1216	G1218	A1219	G1220	U1221	G1222	G1223	A1224	C1226	C1227	U1228	G1229	G1231	G1232	C1233	U1234 111235	01235 A1236	A1237	U1238	01233 U1240	G1241	A1242	C4J1244	C1245	A1240 A1247	C1248	A1249 C1250	G1251	G1252 G1253	A1254	A1255	A1256 C1257	C1258	U1259 C1260	01260 A1261		
C1262	C1263	C1264	G1266	C1267	C1268	C1269	G1270	A1272	C1273	A1274	C1275	G1276	41278 41278	C1279	A1280	G1281	G1282	A1283	U1284 111285	01285 G1286	A1287	C1288	A1289	A1291	U1292	U1293	G1294	01296 01296	A1297	G1298	U1300	C1301	U1302	U1304	C1305	01300 C1307	G1308	01310 U1310	U1311	C1312 111313	G1314	U1315	G1316 C1317	G1318	U1319	G1321		
U1322	G1323	G1324	01325 G1326	C1327	A1328	U1329	61330 61331	C1332	C1333	G1334	U1335	01336	01337 111338	U1339	A1340	G1341	<b>U1342</b>	U1343	G1344 C1345	U1346	G1347	G1348	A1349	C1351	G1352	A1353	U1354 11255	01355 U1356	<mark>G1357</mark>	U1358	U1360	G1361	G1362	U1364	A1365	A1300 U1367	U1368	C1370	G1371	A1372 111373	A1374	A1375	C1376 C1377	A1378	A1379	G1381		
A1382	G1383	A1384	01386 U1386	C1387	U1388	G1389	G1390	A1392	U1393	G1394	C1395	01396	A 1398	C1399	U1400	A1401	G1402	U1403	01404 01405	C1406	G1407	C1408	G1409	C1411	C1412	C1413	C1414	C1415	2171A	G1418	C1419	G1420	G1421	01422 C1423	G1424	G1425 C1426	G1427	01428 C1429	C1430	C1431	C1402	A1434	A1435	C1436 111437	U1438	C1439 111440	U1441	
A1442	G1443	A1444	G1445 G1446	G1447	A1448	C1449	A1450 A1451	G1452	U1453	G1454	G1455	C1456	11458 111458	01459 U1459	C1460	A1461	G1462	C1463	C1464 A1465	C1466	C1467	C1468	G1469	G1471	A1472	U1473	U1474	G1475 A1776	G1477	C1478	A1479 A1480	U1481	A1482	A1483 C1484	A1485	G1486 C1487	U1488	C1489 111 490	G1491	U1492	G1493 A1494	U1495	G1496	C1497 C1498	C1499	U1500 U1501		
A1502	G1503	A1504	G1506	U1507	C1508	G1509	G1510 C1511	G1512	C1513	U1514	G1515	C1516 A1517	A 151 / C1518	G1519	C1520	G1521	C1522	G1523	C1524 111525	A1526	C1527	A1528	C1529	G1531	A1532	C1533	01534 61535	G1536 G1536	C1537	U1538	A1540	G1541	C1542	U1544	G1545	01540 G1547	C1548	U1550	A1551	C1552 C1553	C1554	U1555	A1556 C1557	G1558	C1559 C1560	G1561		
G1562	C1563	A1564	G1566	C1567	G1568	C1569	G1570 C1571	G1572	U1573	A1574	A1575	C15/6	C1578	G1579	U1580	U1581	G1582	A1583	A1584 C1585	C1586	C1587	C1588	A1589 111600	U1591	C1592	<mark>G1593</mark>	01594	41596 A1596	<mark>U1597</mark>	G1598	G1600	G1601	A1602	C1604	G1605	G1607	G1608	A1609 U1610	U1611	G1612 C1613	A1614	A1615	01616 11617	A1618	U1619 114200	01620 C1621		
C1622	C1623	C1624	A1625 U1626	G1627	A1628	A1629	C1630	A1632	G1633	G1634	A1635	A1636	01637 11638	C1639	C1640	C1641	A1642	G1643	01644 A1645	A1646	G1647	U1648	G1649 C1650	G1651	G1652	G1653	U1654	C1055 A1656	U1657	A1658	G1660	C1661	U1662 111663	01000 G1664	C1665	01667 U1667	U1668	41670 A1670	U1671	01672 A1673	A1674	G1675	01676 C1677	C1678	C1679	01000 G1681		





• Molecule 35: Eukaryotic translation initiation factor 2 subunit 1



• Molecule 36: eukaryotic translation initiation factor 2 subunit gamma







# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	26	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0109	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor



## 5 Model quality (i)

#### 5.1 Standard geometry (i)

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

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 Chair		B	ond lengths	Bond angles		
1VIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	1	1.35	0/241	0.96	0/305	
2	С	0.97	0/1680	0.99	0/2283	
3	D	0.90	0/1770	1.02	2/2367~(0.1%)	
4	Ε	0.91	0/1779	0.99	5/2399~(0.2%)	
5	F	0.97	0/1793	1.03	1/2412~(0.0%)	
6	G	0.97	0/2125	1.00	0/2856	
7	Н	0.99	0/1531	0.97	0/2059	
8	Ι	1.07	0/1946	1.03	6/2587~(0.2%)	
9	J	0.96	0/1553	1.00	0/2079	
10	Κ	1.03	0/1709	1.05	5/2278~(0.2%)	
11	L	1.07	0/1523	0.98	2/2031~(0.1%)	
12	М	0.96	0/852	1.01	0/1147	
13	Ν	1.00	0/1319	1.01	0/1761	
14	0	0.90	0/968	1.04	2/1296~(0.2%)	
15	Р	0.97	0/1232	0.92	2/1656~(0.1%)	
16	Q	1.02	0/1029	1.05	2/1380~(0.1%)	
17	S	1.01	0/1141	1.01	0/1528	
18	Т	0.99	0/1032	0.99	0/1383	
19	V	0.98	0/1133	0.99	3/1517~(0.2%)	
20	W	0.96	0/832	1.02	0/1117	
21	Х	0.99	0/627	1.01	0/839	
22	Υ	0.99	0/1051	0.98	0/1406	
23	Ζ	0.99	0/1125	0.99	2/1500~(0.1%)	
24	a	1.01	0/1038	1.04	1/1377~(0.1%)	
25	b	1.06	0/803	1.03	1/1076~(0.1%)	
26	с	0.94	0/673	1.00	0/902	
27	d	1.13	0/509	1.02	0/680	
28	е	1.10	$0/\overline{455}$	1.05	$0/\overline{603}$	
29	f	0.98	0/594	1.07	0/786	
30	g	0.92	0/2494	1.10	$4\overline{/3394}~(0.1\%)$	
31	h	0.97	0/605	1.08	2/810~(0.2%)	
32	i	1.09	0/478	1.06	1/628 (0.2%)	



Mal	Chain	B	ond lengths	Bond angles		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
33	2	1.61	115/41562~(0.3%)	2.42	4485/64770~(6.9%)	
34	3	1.22	0/867	1.89	54/1352~(4.0%)	
35	А	1.00	0/2178	1.08	9/2935~(0.3%)	
36	В	0.92	0/3267	1.07	4/4415~(0.1%)	
37	U	1.01	0/1190	0.92	0/1592	
38	R	0.99	0/1132	0.99	3/1510~(0.2%)	
39	1	2.46	8/1770~(0.5%)	2.77	221/2759~(8.0%)	
All	All	1.35	123/89606~(0.1%)	1.90	4817/129775~(3.7%)	

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	<b>#Planarity outliers</b>
2	С	0	1
3	D	0	1
5	F	0	2
8	Ι	0	2
9	J	0	2
11	L	0	2
12	М	0	5
17	S	0	2
26	с	0	1
28	е	0	2
29	f	0	1
31	h	0	1
32	i	0	2
33	2	1	64
34	3	1	0
35	А	0	8
36	В	0	11
37	U	0	3
39	1	3	3
All	All	5	113

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
39	1	19	G	O3'-P	43.51	2.13	1.61
39	1	16	G	O3'-P	-39.18	1.14	1.61
39	1	17	С	O3'-P	32.10	1.99	1.61



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	1815	U	O3'-P	-29.22	1.26	1.61
39	1	17	С	C2'-O2'	-26.05	1.07	1.41
39	1	18	G	O3'-P	21.68	1.87	1.61
33	2	350	А	O3'-P	21.20	1.86	1.61
33	2	1172	G	O3'-P	-19.95	1.37	1.61
33	2	675	А	O3'-P	19.45	1.84	1.61
33	2	676	U	O3'-P	-19.09	1.38	1.61
39	1	18	G	C3'-O3'	-16.78	1.18	1.42
33	2	797	U	O3'-P	-14.47	1.43	1.61
33	2	351	U	O3'-P	-13.61	1.44	1.61
33	2	1170	U	O3'-P	-10.27	1.48	1.61
33	2	1171	G	O3'-P	-9.29	1.50	1.61
39	1	18	G	C1'-N9	-7.93	1.35	1.46
33	2	916	А	N7-C5	-7.78	1.34	1.39
33	2	1816	А	O3'-P	-7.72	1.51	1.61
33	2	1170	U	C2-N3	7.11	1.42	1.37
33	2	1809	А	N7-C5	-6.63	1.35	1.39
33	2	1186	А	N7-C5	-6.35	1.35	1.39
33	2	960	А	N7-C5	-6.33	1.35	1.39
33	2	1141	А	N7-C5	-6.32	1.35	1.39
33	2	1023	А	N7-C5	-6.24	1.35	1.39
33	2	1283	А	N7-C5	-6.08	1.35	1.39
33	2	304	А	N7-C5	-6.07	1.35	1.39
33	2	1730	А	N7-C5	-6.07	1.35	1.39
33	2	1192	А	N7-C5	-6.04	1.35	1.39
33	2	1045	А	N7-C5	-6.03	1.35	1.39
33	2	1200	А	N7-C5	-6.02	1.35	1.39
33	2	1170	U	C1'-N1	6.02	1.57	1.48
33	2	1066	А	N7-C5	-5.99	1.35	1.39
33	2	619	А	N7-C5	-5.98	1.35	1.39
33	2	1178	А	N7-C5	-5.91	1.35	1.39
33	2	994	А	N7-C5	-5.90	1.35	1.39
33	2	102	А	N7-C5	-5.87	1.35	1.39
33	2	1139	А	N7-C5	-5.87	1.35	1.39
33	2	1645	А	N7-C5	-5.85	1.35	1.39
33	2	1353	А	N7-C5	-5.84	1.35	1.39
33	2	170	А	N7-C5	-5.82	1.35	1.39
33	2	171	A	N7-C5	-5.82	1.35	1.39
33	2	1646	A	N7-C5	-5.82	1.35	1.39
33	2	577	А	N7-C5	-5.81	1.35	1.39
33	2	1146	A	N7-C5	-5.81	1.35	1.39
33	2	437	А	N7-C5	-5.80	1.35	1.39



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	1140	А	N7-C5	-5.80	1.35	1.39
33	2	1184	А	N7-C5	-5.77	1.35	1.39
33	2	822	А	N7-C5	-5.73	1.35	1.39
33	2	1584	А	N7-C5	-5.72	1.35	1.39
33	2	474	А	N7-C5	-5.68	1.35	1.39
33	2	206	А	N7-C5	-5.67	1.35	1.39
33	2	391	А	N7-C5	-5.66	1.35	1.39
33	2	177	G	C2-N3	5.66	1.37	1.32
33	2	1629	А	N7-C5	-5.64	1.35	1.39
39	1	17	С	C3'-O3'	-5.64	1.34	1.42
33	2	1828	А	N7-C5	-5.61	1.35	1.39
33	2	1615	А	N7-C5	-5.60	1.35	1.39
33	2	1019	А	N7-C5	-5.59	1.35	1.39
33	2	968	А	N7-C5	-5.58	1.35	1.39
33	2	584	А	N7-C5	-5.58	1.35	1.39
33	2	1169	А	N7-C5	-5.58	1.35	1.39
33	2	1185	А	N7-C5	-5.56	1.35	1.39
33	2	1046	А	N7-C5	-5.54	1.35	1.39
33	2	1378	А	N7-C5	-5.53	1.35	1.39
33	2	423	А	N7-C5	-5.52	1.35	1.39
33	2	1740	А	N7-C5	-5.48	1.35	1.39
33	2	92	А	N7-C5	-5.46	1.35	1.39
33	2	1628	А	N7-C5	-5.45	1.35	1.39
33	2	317	G	C2-N3	5.43	1.37	1.32
33	2	1024	А	N7-C5	-5.41	1.36	1.39
33	2	1784	А	N7-C5	-5.41	1.36	1.39
33	2	439	А	N7-C5	-5.41	1.36	1.39
33	2	1479	А	N7-C5	-5.41	1.36	1.39
33	2	1785	A	N7-C5	-5.36	1.36	1.39
33	2	66	G	N7-C5	-5.36	1.36	1.39
33	2	1461	A	N7-C5	-5.36	1.36	1.39
33	2	1635	А	N7-C5	-5.35	1.36	1.39
33	2	594	A	N7-C5	-5.32	1.36	1.39
33	2	227	A	N7-C5	-5.32	1.36	1.39
33	2	99	A	N7-C5	-5.31	1.36	1.39
33	2	273	G	C2-N3	5.28	1.36	1.32
33	2	843	A	N7-C5	-5.27	1.36	1.39
33	2	643	A	N7-C5	-5.27	1.36	1.39
33	2	1196	A	N7-C5	-5.26	1.36	1.39
33	2	546	U	C2-N3	5.25	1.41	1.37
33	2	661	A	N7-C5	-5.21	1.36	1.39
33	2	1825	A	N7-C5	-5.21	1.36	1.39



Mol	Choin	<b>P</b> og	Tuno	Atoma	7	Observed(Å)	$Ideal(\lambda)$
22	Onam	1945	Type	Atoms N7 OF	<b>L</b>	Ubserveu(A)	$1 \frac{1}{20}$
<u>- 33</u>	2	1840	A	N7-C5	-0.21	1.30	1.39
33	2	821	A	N7-C5	-5.20	1.30	1.39
33	2		A	N7-C5	-5.19	1.30	1.39
33	2	1177	A	N7-C5	-5.19	1.36	1.39
33	2	19	A	N7-C5	-5.18	1.36	1.39
33	2	554	A	N7-C5	-5.17	1.36	1.39
33	2	537	G	C2-N3	5.17	1.36	1.32
33	2	1794	A	N7-C5	-5.17	1.36	1.39
33	2	1287	A	N7-C5	-5.16	1.36	1.39
33	2	149	A	N7-C5	-5.15	1.36	1.39
33	2	476	А	N7-C5	-5.15	1.36	1.39
33	2	436	G	C2-N3	5.15	1.36	1.32
33	2	229	А	N7-C5	-5.13	1.36	1.39
33	2	940	А	N7-C5	-5.13	1.36	1.39
33	2	1714	А	N7-C5	-5.13	1.36	1.39
33	2	1079	А	N7-C5	-5.13	1.36	1.39
33	2	1418	G	C2-N3	5.13	1.36	1.32
33	2	1303	U	C2-N3	5.13	1.41	1.37
33	2	402	G	N7-C5	-5.12	1.36	1.39
33	2	1349	А	N7-C5	-5.11	1.36	1.39
33	2	964	U	C2-N3	5.09	1.41	1.37
33	2	640	А	N7-C5	-5.08	1.36	1.39
33	2	630	А	N7-C5	-5.08	1.36	1.39
33	2	436	G	N7-C5	-5.07	1.36	1.39
33	2	832	G	C2-N3	5.05	1.36	1.32
33	2	1080	А	N7-C5	-5.05	1.36	1.39
33	2	1078	А	N7-C5	-5.04	1.36	1.39
33	2	1170	U	C5-C6	5.04	1.38	1.34
33	2	934	A	N7-C5	-5.04	1.36	1.39
33	2	319	G	C2-N3	5.03	1.36	1.32
33	2	1030	A	N7-C5	-5.03	1.36	1.39
33	2	1210	А	N7-C5	-5.02	1.36	1.39
33	2	1556	A	N7-C5	-5.02	1.36	1.39
33	2	976	A	N7-C5	-5.02	1.36	1.39
33	2	1328	A	N7-C5	-5.02	1.36	1.39
33	2	1170	U	N1-C2	-5.00	1.34	1.38

All (4817) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
39	1	19	G	O3'-P-O5'	31.90	164.60	104.00
39	1	16	G	P-O3'-C3'	23.25	147.60	119.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	351	U	P-O3'-C3'	18.59	142.01	119.70
33	2	797	U	O3'-P-O5'	-17.82	70.15	104.00
33	2	676	U	O3'-P-O5'	-17.57	70.62	104.00
33	2	1817	А	P-O3'-C3'	-17.39	98.83	119.70
39	1	19	G	OP1-P-O3'	-17.13	67.51	105.20
39	1	17	С	C4'-C3'-O3'	16.30	145.59	113.00
39	1	54	А	N1-C6-N6	14.70	127.42	118.60
33	2	1007	А	N1-C6-N6	14.15	127.09	118.60
33	2	1556	A	N1-C6-N6	14.07	127.04	118.60
33	2	545	А	N1-C6-N6	13.94	126.96	118.60
33	2	519	А	N1-C6-N6	13.86	126.92	118.60
33	2	1032	А	N1-C6-N6	13.86	126.92	118.60
33	2	1575	А	N1-C6-N6	13.83	126.90	118.60
39	1	17	С	O3'-P-O5'	13.83	130.28	104.00
39	1	8	G	P-O3'-C3'	13.82	136.28	119.70
33	2	1027	А	N1-C6-N6	13.78	126.86	118.60
33	2	1200	А	N1-C6-N6	13.77	126.86	118.60
33	2	173	А	N1-C6-N6	13.72	126.83	118.60
33	2	1405	А	N1-C6-N6	13.70	126.82	118.60
33	2	976	А	N1-C6-N6	13.63	126.78	118.60
39	1	15	А	N1-C6-N6	13.62	126.77	118.60
33	2	640	А	N1-C6-N6	13.59	126.75	118.60
33	2	1854	А	P-O3'-C3'	13.50	135.91	119.70
39	1	7	А	N1-C6-N6	13.49	126.70	118.60
39	1	50	А	N1-C6-N6	13.41	126.64	118.60
33	2	1417	А	N1-C6-N6	13.39	126.63	118.60
39	1	18	G	O3'-P-O5'	13.39	129.44	104.00
33	2	68	А	N1-C6-N6	13.37	126.62	118.60
33	2	1378	А	N1-C6-N6	13.28	126.57	118.60
33	2	554	А	N1-C6-N6	13.26	126.55	118.60
33	2	1854	А	N1-C6-N6	13.24	126.54	118.60
39	1	38	А	N1-C6-N6	13.21	126.53	118.60
39	1	60	А	N1-C6-N6	13.20	126.52	118.60
33	2	1190	А	N1-C6-N6	13.16	126.50	118.60
39	1	2	А	N1-C6-N6	13.15	126.49	118.60
33	2	643	А	N1-C6-N6	13.12	126.47	118.60
39	1	63	A	N1-C6-N6	13.12	126.47	118.60
33	2	997	A	N1-C6-N6	13.12	126.47	118.60
33	2	1813	A	N1-C6-N6	13.11	126.47	118.60
33	2	423	A	N1-C6-N6	13.03	126.42	118.60
33	2	1825	A	N1-C6-N6	13.03	126.42	118.60
33	2	1636	A	N1-C6-N6	13.01	126.41	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	940	А	N1-C6-N6	12.99	126.40	118.60
33	2	535	А	N1-C6-N6	12.99	126.39	118.60
33	2	1177	А	N1-C6-N6	12.99	126.39	118.60
33	2	1526	А	N1-C6-N6	12.99	126.39	118.60
33	2	1839	А	N1-C6-N6	12.98	126.39	118.60
33	2	458	А	N1-C6-N6	12.98	126.39	118.60
33	2	977	А	N1-C6-N6	12.96	126.38	118.60
33	2	550	А	N1-C6-N6	12.96	126.37	118.60
33	2	425	A	N1-C6-N6	12.93	126.36	118.60
33	2	1853	А	N1-C6-N6	12.93	126.36	118.60
33	2	1016	А	N1-C6-N6	12.92	126.35	118.60
33	2	1609	А	N1-C6-N6	12.92	126.35	118.60
33	2	510	А	N1-C6-N6	12.91	126.35	118.60
34	3	52	А	N1-C6-N6	12.91	126.34	118.60
33	2	1349	А	N1-C6-N6	12.85	126.31	118.60
33	2	445	А	N1-C6-N6	12.85	126.31	118.60
33	2	1646	А	N1-C6-N6	12.83	126.30	118.60
33	2	1726	А	N1-C6-N6	12.80	126.28	118.60
33	2	91	А	N1-C6-N6	12.79	126.28	118.60
33	2	1144	А	N1-C6-N6	12.79	126.28	118.60
33	2	1289	А	N1-C6-N6	12.79	126.27	118.60
33	2	404	А	N1-C6-N6	12.78	126.27	118.60
33	2	388	A	N1-C6-N6	12.77	126.26	118.60
33	2	1710	A	N1-C6-N6	12.77	126.26	118.60
33	2	798	А	N1-C6-N6	12.76	126.26	118.60
33	2	854	А	N1-C6-N6	12.75	126.25	118.60
33	2	882	А	N1-C6-N6	12.75	126.25	118.60
33	2	1109	А	N1-C6-N6	12.75	126.25	118.60
33	2	288	А	N1-C6-N6	12.73	126.24	118.60
33	2	1224	А	N1-C6-N6	12.72	126.23	118.60
33	2	479	А	N1-C6-N6	12.71	126.22	118.60
33	2	986	А	N1-C6-N6	12.70	126.22	118.60
33	2	50	А	N1-C6-N6	12.70	126.22	118.60
33	2	309	А	N1-C6-N6	12.69	126.22	118.60
33	2	858	А	N1-C6-N6	12.69	126.21	118.60
33	2	988	A	N1-C6-N6	12.69	126.22	118.60
33	2	232	А	N1-C6-N6	12.69	126.21	118.60
33	2	366	А	N1-C6-N6	12.68	126.20	118.60
33	2	382	A	N1-C6-N6	12.67	126.20	118.60
33	2	509	A	N1-C6-N6	12.66	126.20	118.60
33	2	1089	A	N1-C6-N6	12.65	126.19	118.60
33	2	951	A	N1-C6-N6	12.64	126.19	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1632	А	N1-C6-N6	12.63	126.18	118.60
33	2	1274	А	N1-C6-N6	12.62	126.17	118.60
33	2	1287	А	N1-C6-N6	12.62	126.17	118.60
33	2	904	А	N1-C6-N6	12.61	126.16	118.60
33	2	1479	А	N1-C6-N6	12.61	126.16	118.60
33	2	1800	А	N1-C6-N6	12.60	126.16	118.60
33	2	868	А	N1-C6-N6	12.60	126.16	118.60
33	2	1775	А	N1-C6-N6	12.60	126.16	118.60
33	2	228	А	N1-C6-N6	12.59	126.15	118.60
33	2	1618	А	N1-C6-N6	12.58	126.15	118.60
33	2	1141	А	N1-C6-N6	12.57	126.14	118.60
33	2	429	А	N1-C6-N6	12.57	126.14	118.60
33	2	1375	А	N1-C6-N6	12.57	126.14	118.60
33	2	1674	А	N1-C6-N6	12.57	126.14	118.60
33	2	1216	А	N1-C6-N6	12.57	126.14	118.60
33	2	826	А	N1-C6-N6	12.56	126.14	118.60
33	2	1740	А	N1-C6-N6	12.56	126.14	118.60
33	2	1564	А	N1-C6-N6	12.56	126.14	118.60
33	2	1410	А	N1-C6-N6	12.56	126.13	118.60
33	2	915	А	N1-C6-N6	12.55	126.13	118.60
33	2	164	А	N1-C6-N6	12.54	126.12	118.60
34	3	76	А	N1-C6-N6	12.54	126.12	118.60
33	2	1026	А	N1-C6-N6	12.51	126.10	118.60
33	2	630	А	N1-C6-N6	12.50	126.10	118.60
33	2	1844	А	N1-C6-N6	12.50	126.10	118.60
33	2	1280	А	N1-C6-N6	12.48	126.09	118.60
33	2	379	А	N1-C6-N6	12.47	126.08	118.60
33	2	1782	А	N1-C6-N6	12.47	126.08	118.60
33	2	450	А	N1-C6-N6	12.46	126.08	118.60
33	2	1366	А	N1-C6-N6	12.45	126.07	118.60
33	2	227	А	N1-C6-N6	12.43	126.06	118.60
33	2	214	А	N1-C6-N6	12.42	126.06	118.60
39	1	16	G	OP1-P-O3'	12.42	132.53	105.20
33	2	807	А	N1-C6-N6	12.42	126.05	118.60
33	2	1019	А	N1-C6-N6	12.41	126.05	118.60
33	2	624	А	N1-C6-N6	12.40	126.04	118.60
33	2	25	A	N1-C6-N6	12.40	126.04	118.60
33	2	1829	A	N1-C6-N6	12.37	126.02	118.60
33	2	1020	A	N1-C6-N6	12.36	126.01	118.60
33	2	1295	A	N1-C6-N6	12.36	126.01	118.60
33	2	1247	A	N1-C6-N6	12.35	$126.0\overline{1}$	118.60
33	2	40	А	N1-C6-N6	12.35	126.01	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1236	А	N1-C6-N6	12.35	126.01	118.60
33	2	1717	G	N1-C6-O6	12.35	127.31	119.90
33	2	22	А	N1-C6-N6	12.34	126.00	118.60
33	2	959	А	N1-C6-N6	12.34	126.00	118.60
33	2	809	А	N1-C6-N6	12.33	126.00	118.60
33	2	1532	А	N1-C6-N6	12.33	126.00	118.60
33	2	1379	А	N1-C6-N6	12.32	125.99	118.60
33	2	1714	А	N1-C6-N6	12.32	125.99	118.60
33	2	99	А	N1-C6-N6	12.32	125.99	118.60
33	2	1219	A	N1-C6-N6	12.31	125.99	118.60
33	2	293	А	N1-C6-N6	12.31	125.99	118.60
33	2	574	А	N1-C6-N6	12.31	125.98	118.60
33	2	845	А	N1-C6-N6	12.31	125.98	118.60
33	2	953	А	N1-C6-N6	12.29	125.97	118.60
33	2	1589	А	N1-C6-N6	12.29	125.97	118.60
33	2	589	А	N1-C6-N6	12.28	125.97	118.60
33	2	1172	G	P-O3'-C3'	12.28	134.43	119.70
33	2	333	А	N1-C6-N6	12.27	125.96	118.60
33	2	1803	A	N1-C6-N6	12.25	125.95	118.60
33	2	1038	А	N1-C6-N6	12.24	125.95	118.60
33	2	661	А	N1-C6-N6	12.24	125.94	118.60
33	2	1692	А	N1-C6-N6	12.23	125.94	118.60
33	2	544	А	N1-C6-N6	12.22	125.94	118.60
33	2	1083	А	N1-C6-N6	12.22	125.93	118.60
33	2	521	A	N1-C6-N6	12.21	125.93	118.60
33	2	38	А	N1-C6-N6	12.21	125.92	118.60
33	2	1205	А	N1-C6-N6	12.20	125.92	118.60
33	2	1213	А	N1-C6-N6	12.20	125.92	118.60
33	2	233	А	N1-C6-N6	12.19	125.91	118.60
33	2	1476	A	N1-C6-N6	12.19	125.91	118.60
33	2	466	A	N1-C6-N6	12.18	125.91	118.60
33	2	85	А	N1-C6-N6	12.16	125.89	118.60
33	2	1008	А	N1-C6-N6	12.16	125.89	118.60
33	2	638	А	N1-C6-N6	12.15	125.89	118.60
33	2	223	А	N1-C6-N6	12.15	125.89	118.60
33	2	513	А	N1-C6-N6	12.15	125.89	118.60
33	2	958	A	N1-C6-N6	12.15	125.89	118.60
33	2	1129	A	N1-C6-N6	12.15	125.89	118.60
33	2	361	A	N1-C6-N6	12.14	$125.8\overline{9}$	118.60
33	2	1031	A	N1-C6-N6	12.14	125.88	118.60
33	2	1272	A	N1-C6-N6	12.14	$125.8\overline{8}$	118.60
33	2	993	A	N1-C6-N6	12.12	125.88	118.60



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	994	А	N1-C6-N6	12.12	125.87	118.60
33	2	979	А	N1-C6-N6	12.12	125.87	118.60
33	2	1465	А	N1-C6-N6	12.11	125.87	118.60
33	2	103	А	N1-C6-N6	12.11	125.87	118.60
33	2	1249	А	N1-C6-N6	12.11	125.86	118.60
33	2	283	А	N1-C6-N6	12.11	125.86	118.60
33	2	808	А	N1-C6-N6	12.10	125.86	118.60
33	2	1444	А	N1-C6-N6	12.09	125.85	118.60
33	2	483	А	N1-C6-N6	12.08	125.85	118.60
33	2	518	А	N1-C6-N6	12.08	125.85	118.60
33	2	1204	А	N1-C6-N6	12.08	125.85	118.60
33	2	1372	А	N1-C6-N6	12.08	125.85	118.60
33	2	1118	А	N1-C6-N6	12.07	125.84	118.60
33	2	1382	А	N1-C6-N6	12.07	125.84	118.60
33	2	405	А	N1-C6-N6	12.07	125.84	118.60
33	2	918	А	N1-C6-N6	12.07	125.84	118.60
33	2	1196	А	N1-C6-N6	12.06	125.84	118.60
33	2	19	А	N1-C6-N6	12.06	125.83	118.60
33	2	660	А	N1-C6-N6	12.06	125.83	118.60
33	2	77	А	N1-C6-N6	12.05	125.83	118.60
33	2	633	А	N1-C6-N6	12.05	125.83	118.60
33	2	1054	А	N1-C6-N6	12.05	125.83	118.60
33	2	1625	А	N1-C6-N6	12.05	125.83	118.60
34	3	77	А	N1-C6-N6	12.05	125.83	118.60
33	2	1080	А	N1-C6-N6	12.05	125.83	118.60
33	2	523	А	N1-C6-N6	12.04	125.83	118.60
33	2	631	А	N1-C6-N6	12.04	125.83	118.60
33	2	850	А	N1-C6-N6	12.04	125.82	118.60
33	2	823	А	N1-C6-N6	12.04	125.82	118.60
33	2	339	А	N1-C6-N6	12.03	125.82	118.60
33	2	983	А	N1-C6-N6	12.03	125.82	118.60
33	2	475	А	N1-C6-N6	12.03	125.82	118.60
33	2	1673	А	N1-C6-N6	12.03	125.82	118.60
33	2	1596	А	N1-C6-N6	12.03	125.81	118.60
33	2	166	А	N1-C6-N6	12.02	125.81	118.60
33	2	2	А	N1-C6-N6	12.02	125.81	118.60
33	2	1169	A	N1-C6-N6	12.02	125.81	118.60
33	2	814	А	N1-C6-N6	12.02	125.81	118.60
33	2	1328	A	N1-C6-N6	12.01	125.81	118.60
33	2	1242	A	N1-C6-N6	12.01	125.81	118.60
33	2	912	A	N1-C6-N6	12.00	125.80	118.60
33	2	512	А	N1-C6-N6	11.99	125.80	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	54	А	N1-C6-N6	11.99	125.79	118.60
33	2	1291	А	N1-C6-N6	11.98	125.79	118.60
39	1	21	А	N1-C6-N6	11.98	125.79	118.60
33	2	490	А	N1-C6-N6	11.98	125.79	118.60
33	2	416	А	N1-C6-N6	11.98	125.79	118.60
33	2	1078	А	N1-C6-N6	11.98	125.79	118.60
33	2	1845	А	N1-C6-N6	11.97	125.78	118.60
33	2	1297	А	N1-C6-N6	11.97	125.78	118.60
33	2	1451	А	N1-C6-N6	11.97	125.78	118.60
39	1	35	А	N1-C6-N6	11.97	125.78	118.60
33	2	1472	А	N1-C6-N6	11.97	125.78	118.60
33	2	502	А	N1-C6-N6	11.96	125.78	118.60
33	2	1340	А	N1-C6-N6	11.96	125.78	118.60
33	2	1574	А	N1-C6-N6	11.96	125.78	118.60
33	2	595	А	N1-C6-N6	11.95	125.77	118.60
33	2	27	А	N1-C6-N6	11.95	125.77	118.60
33	2	459	А	N1-C6-N6	11.95	125.77	118.60
33	2	1004	А	N1-C6-N6	11.94	125.76	118.60
33	2	1073	А	N1-C6-N6	11.93	125.76	118.60
33	2	454	А	N1-C6-N6	11.93	125.76	118.60
33	2	463	А	N1-C6-N6	11.93	125.76	118.60
34	3	68	А	N1-C6-N6	11.93	125.76	118.60
33	2	1719	А	N1-C6-N6	11.93	125.76	118.60
33	2	1096	А	N1-C6-N6	11.92	125.75	118.60
33	2	1787	А	N1-C6-N6	11.92	125.75	118.60
33	2	922	А	N1-C6-N6	11.91	125.75	118.60
33	2	1707	А	N1-C6-N6	11.90	125.74	118.60
33	2	42	А	N1-C6-N6	11.90	125.74	118.60
33	2	290	А	N1-C6-N6	11.90	125.74	118.60
39	1	44	А	N1-C6-N6	11.90	125.74	118.60
33	2	559	А	N1-C6-N6	11.90	125.74	118.60
33	2	1146	А	N1-C6-N6	11.90	125.74	118.60
33	2	84	А	N1-C6-N6	11.89	125.74	118.60
33	2	1353	A	N1-C6-N6	11.89	125.74	118.60
33	2	45	A	N1-C6-N6	11.89	125.73	118.60
33	2	960	А	N1-C6-N6	11.89	125.73	118.60
33	2	221	А	N1-C6-N6	11.88	125.73	118.60
33	2	821	A	N1-C6-N6	11.88	$1\overline{25.73}$	118.60
33	2	64	A	N1-C6-N6	11.88	$1\overline{25.73}$	118.60
33	2	354	A	N1-C6-N6	11.88	125.73	118.60
33	2	566	A	N1-C6-N6	11.88	$1\overline{25.7}\overline{3}$	118.60
33	2	1502	A	N1-C6-N6	11.88	125.73	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	11	А	N1-C6-N6	11.86	125.72	118.60
33	2	833	А	N1-C6-N6	11.86	125.72	118.60
33	2	580	А	N1-C6-N6	11.86	125.71	118.60
33	2	968	А	N1-C6-N6	11.85	125.71	118.60
33	2	860	А	N1-C6-N6	11.84	125.71	118.60
39	1	59	А	N1-C6-N6	11.84	125.71	118.60
33	2	1470	А	N1-C6-N6	11.84	125.70	118.60
33	2	662	А	N1-C6-N6	11.84	125.70	118.60
33	2	1816	А	N1-C6-N6	11.84	125.70	118.60
33	2	1670	А	N1-C6-N6	11.83	125.70	118.60
33	2	1045	А	N1-C6-N6	11.82	125.69	118.60
33	2	147	А	N1-C6-N6	11.82	125.69	118.60
33	2	338	А	N1-C6-N6	11.81	125.69	118.60
33	2	1246	А	N1-C6-N6	11.80	125.68	118.60
33	2	1482	А	N1-C6-N6	11.80	125.68	118.60
33	2	644	А	N1-C6-N6	11.80	125.68	118.60
33	2	329	A	N1-C6-N6	11.79	125.68	118.60
33	2	899	A	N1-C6-N6	11.79	125.67	118.60
33	2	1145	А	N1-C6-N6	11.79	125.67	118.60
33	2	1448	А	N1-C6-N6	11.79	125.67	118.60
33	2	1374	А	N1-C6-N6	11.78	125.67	118.60
33	2	438	A	N1-C6-N6	11.78	125.67	118.60
33	2	1826	А	N1-C6-N6	11.77	125.66	118.60
39	1	20	A	N1-C6-N6	11.77	125.66	118.60
33	2	565	А	N1-C6-N6	11.77	125.66	118.60
33	2	871	А	N1-C6-N6	11.77	125.66	118.60
33	2	659	А	N1-C6-N6	11.76	125.66	118.60
33	2	1656	А	N1-C6-N6	11.76	125.66	118.60
33	2	812	A	N1-C6-N6	11.76	125.66	118.60
33	2	292	A	N1-C6-N6	11.75	125.65	118.60
33	2	934	А	N1-C6-N6	11.75	125.65	118.60
33	2	992	А	N1-C6-N6	11.75	125.65	118.60
33	2	111	А	N1-C6-N6	11.75	125.65	118.60
33	2	1056	А	N1-C6-N6	11.75	125.65	118.60
33	2	175	А	N1-C6-N6	11.74	125.64	118.60
35	А	54	ARG	C-N-CA	11.74	151.05	121.70
33	2	61	A	N1-C6-N6	11.74	$1\overline{25.64}$	118.60
33	2	1005	A	N1-C6-N6	11.73	125.64	118.60
33	2	1807	A	N1-C6-N6	11.73	$1\overline{25.64}$	118.60
33	2	1795	A	N1-C6-N6	11.73	$1\overline{25.64}$	118.60
33	2	1694	A	N1-C6-N6	11.71	125.63	118.60
33	2	1659	A	N1-C6-N6	11.71	125.62	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1384	А	N1-C6-N6	11.71	125.62	118.60
33	2	350	А	N1-C6-N6	11.70	125.62	118.60
33	2	141	А	N1-C6-N6	11.69	125.62	118.60
33	2	1483	А	N1-C6-N6	11.68	125.61	118.60
33	2	1551	А	N1-C6-N6	11.68	125.61	118.60
33	2	594	А	N1-C6-N6	11.68	125.61	118.60
33	2	1179	А	N1-C6-N6	11.68	125.61	118.60
33	2	865	А	N1-C6-N6	11.67	125.60	118.60
33	2	158	А	N1-C6-N6	11.67	125.60	118.60
33	2	645	А	N1-C6-N6	11.67	125.60	118.60
33	2	159	А	N1-C6-N6	11.66	125.60	118.60
33	2	857	А	N1-C6-N6	11.66	125.59	118.60
33	2	1690	А	N1-C6-N6	11.65	125.59	118.60
33	2	1048	А	N1-C6-N6	11.65	125.59	118.60
39	1	42	А	N1-C6-N6	11.65	125.59	118.60
33	2	218	А	N1-C6-N6	11.65	125.59	118.60
33	2	455	А	N1-C6-N6	11.64	125.58	118.60
33	2	609	А	N1-C6-N6	11.64	125.58	118.60
33	2	916	А	N1-C6-N6	11.64	125.58	118.60
33	2	1278	А	N1-C6-N6	11.64	125.58	118.60
33	2	1237	А	N1-C6-N6	11.64	125.58	118.60
33	2	511	А	N1-C6-N6	11.63	125.58	118.60
33	2	1023	А	N1-C6-N6	11.63	125.58	118.60
33	2	1485	А	N1-C6-N6	11.62	125.57	118.60
33	2	909	А	N1-C6-N6	11.62	125.57	118.60
33	2	1718	G	N1-C6-O6	11.61	126.87	119.90
34	3	67	А	N1-C6-N6	11.61	125.56	118.60
33	2	1614	А	N1-C6-N6	11.60	125.56	118.60
33	2	398	А	N1-C6-N6	11.57	125.54	118.60
33	2	618	А	N1-C6-N6	11.56	125.53	118.60
33	2	806	А	N1-C6-N6	11.56	125.53	118.60
33	2	1480	А	N1-C6-N6	11.56	125.53	118.60
33	2	1450	А	N1-C6-N6	11.54	125.53	118.60
33	2	1494	А	N1-C6-N6	11.55	125.53	118.60
33	2	1115	А	N1-C6-N6	11.54	125.52	118.60
33	2	1051	А	N1-C6-N6	11.53	125.52	118.60
33	2	476	А	N1-C6-N6	11.53	125.52	118.60
33	2	1076	A	N1-C6-N6	11.53	125.52	118.60
33	2	1583	A	N1-C6-N6	11.52	125.51	118.60
33	2	102	А	N1-C6-N6	11.51	125.51	118.60
33	2	181	А	N1-C6-N6	11.51	125.50	118.60
33	2	861	А	N1-C6-N6	11.50	125.50	118.60



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1139	А	N1-C6-N6	11.49	125.49	118.60
33	2	1434	А	N1-C6-N6	11.48	125.49	118.60
33	2	1186	А	N1-C6-N6	11.48	125.49	118.60
33	2	805	А	N1-C6-N6	11.48	125.49	118.60
33	2	39	А	N1-C6-N6	11.47	125.48	118.60
33	2	675	А	N1-C6-N6	11.46	125.47	118.60
33	2	427	G	N1-C6-O6	11.46	126.77	119.90
33	2	1195	А	N1-C6-N6	11.45	125.47	118.60
33	2	584	А	N1-C6-N6	11.44	125.47	118.60
33	2	1140	А	N1-C6-N6	11.44	125.47	118.60
33	2	900	А	N1-C6-N6	11.44	125.47	118.60
33	2	1397	А	N1-C6-N6	11.44	125.46	118.60
33	2	107	А	N1-C6-N6	11.43	125.46	118.60
33	2	1365	А	N1-C6-N6	11.43	125.46	118.60
33	2	408	А	N1-C6-N6	11.41	125.45	118.60
33	2	1730	А	N1-C6-N6	11.41	125.44	118.60
39	1	73	А	N1-C6-N6	11.39	125.43	118.60
33	2	1184	А	N1-C6-N6	11.39	125.43	118.60
33	2	1442	А	N1-C6-N6	11.38	125.43	118.60
33	2	573	А	N1-C6-N6	11.37	125.42	118.60
33	2	304	А	N1-C6-N6	11.36	125.42	118.60
33	2	1461	А	N1-C6-N6	11.36	125.41	118.60
33	2	435	А	N1-C6-N6	11.35	125.41	118.60
33	2	995	G	N1-C6-O6	11.33	126.70	119.90
33	2	1058	А	N1-C6-N6	11.33	125.40	118.60
33	2	619	А	N1-C6-N6	11.32	125.39	118.60
33	2	843	А	N1-C6-N6	11.27	125.36	118.60
33	2	564	А	N1-C6-N6	11.27	125.36	118.60
33	2	1857	А	N1-C6-N6	11.26	125.36	118.60
33	2	577	А	N1-C6-N6	11.26	125.36	118.60
39	1	5	А	N1-C6-N6	11.24	125.34	118.60
33	2	516	А	N1-C6-N6	11.23	125.34	118.60
33	2	1496	G	N1-C6-O6	11.23	126.64	119.90
33	2	654	А	N1-C6-N6	11.21	125.33	118.60
33	2	525	G	N1-C6-O6	11.20	126.62	119.90
33	2	804	А	N1-C6-N6	11.20	125.32	118.60
33	2	448	А	N1-C6-N6	11.18	125.31	118.60
33	2	1255	A	N1-C6-N6	11.18	125.31	118.60
33	2	1401	А	N1-C6-N6	11.16	125.30	118.60
33	2	1178	A	N1-C6-N6	11.16	125.30	118.60
33	2	60	А	N1-C6-N6	11.15	125.29	118.60
33	2	1809	A	N1-C6-N6	11.13	125.28	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	226	A	N1-C6-N6	11.12	125.27	118.60
33	2	1024	А	N1-C6-N6	11.12	125.27	118.60
33	2	551	А	N1-C6-N6	11.11	125.27	118.60
33	2	1794	А	N1-C6-N6	11.10	125.26	118.60
33	2	83	А	N1-C6-N6	11.07	125.25	118.60
33	2	326	А	N1-C6-N6	11.07	125.24	118.60
33	2	474	A	N1-C6-N6	11.07	125.24	118.60
33	2	1605	G	N1-C6-O6	11.05	126.53	119.90
33	2	1435	А	N1-C6-N6	11.04	125.22	118.60
33	2	437	A	N1-C6-N6	11.02	125.21	118.60
33	2	1628	А	N1-C6-N6	11.02	125.21	118.60
33	2	1066	А	N1-C6-N6	11.02	125.21	118.60
33	2	320	G	N1-C6-O6	10.98	126.49	119.90
33	2	1398	А	N1-C6-N6	10.95	125.17	118.60
33	2	149	А	N1-C6-N6	10.94	125.16	118.60
33	2	1266	G	N1-C6-O6	10.92	126.45	119.90
33	2	1635	А	N1-C6-N6	10.92	125.15	118.60
33	2	822	А	N1-C6-N6	10.92	125.15	118.60
33	2	1528	А	N1-C6-N6	10.92	125.15	118.60
33	2	1540	А	N1-C6-N6	10.91	125.15	118.60
33	2	866	А	N1-C6-N6	10.91	125.14	118.60
33	2	526	А	N1-C6-N6	10.91	125.14	118.60
33	2	600	G	N1-C6-O6	10.88	126.43	119.90
33	2	658	А	N1-C6-N6	10.87	125.12	118.60
33	2	506	А	N1-C6-N6	10.87	125.12	118.60
33	2	170	А	N1-C6-N6	10.84	125.11	118.60
33	2	1256	А	N1-C6-N6	10.83	125.10	118.60
33	2	229	А	N1-C6-N6	10.81	125.09	118.60
33	2	1629	А	N1-C6-N6	10.80	125.08	118.60
33	2	1812	А	N1-C6-N6	10.80	125.08	118.60
33	2	1283	А	N1-C6-N6	10.78	125.07	118.60
33	2	515	А	N1-C6-N6	10.77	125.06	118.60
33	2	123	G	N1-C6-O6	10.75	126.35	119.90
33	2	500	G	N1-C6-O6	10.73	126.34	119.90
33	2	1361	G	N1-C6-O6	10.72	126.33	119.90
33	2	1030	А	N1-C6-N6	10.71	125.03	118.60
33	2	401	G	N1-C6-O6	10.70	126.32	119.90
33	2	1743	G	N1-C6-O6	10.70	126.32	119.90
33	2	46	A	N1-C6-N6	10.69	125.01	118.60
33	2	62	G	N1-C6-O6	10.67	126.30	119.90
33	2	1137	G	N1-C6-06	10.66	126.30	119.90
39	1	76	A	N1-C6-N6	10.63	124.98	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	279	G	N1-C6-O6	10.62	126.27	119.90
33	2	146	G	N1-C6-O6	10.62	126.27	119.90
33	2	353	А	N1-C6-N6	10.60	124.96	118.60
33	2	1348	G	N1-C6-O6	10.60	126.26	119.90
33	2	1079	А	N1-C6-N6	10.58	124.95	118.60
39	1	19	G	P-O3'-C3'	10.58	132.40	119.70
33	2	212	G	N1-C6-O6	10.56	126.24	119.90
33	2	1828	А	N1-C6-N6	10.56	124.94	118.60
33	2	1837	G	N1-C6-O6	10.56	126.23	119.90
33	2	869	G	N1-C6-O6	10.54	126.22	119.90
33	2	1752	G	N1-C6-O6	10.54	126.22	119.90
33	2	6	G	N1-C6-O6	10.53	126.22	119.90
33	2	1784	А	N1-C6-N6	10.53	124.92	118.60
33	2	1770	G	N1-C6-O6	10.52	126.21	119.90
33	2	1816	А	P-O3'-C3'	-10.51	107.08	119.70
33	2	52	G	N1-C6-O6	10.51	126.20	119.90
39	1	29	G	N1-C6-O6	10.50	126.20	119.90
33	2	1823	G	N1-C6-O6	10.50	126.20	119.90
33	2	384	G	N1-C6-O6	10.49	126.20	119.90
33	2	1602	А	N1-C6-N6	10.49	124.90	118.60
33	2	1642	А	N1-C6-N6	10.49	124.89	118.60
33	2	1371	G	N1-C6-O6	10.49	126.19	119.90
33	2	1254	А	N1-C6-N6	10.48	124.89	118.60
33	2	156	G	N1-C6-O6	10.46	126.18	119.90
33	2	498	А	N1-C6-N6	10.46	124.88	118.60
33	2	289	G	N1-C6-O6	10.46	126.17	119.90
39	1	24	G	N1-C6-O6	10.45	126.17	119.90
33	2	300	G	N1-C6-O6	10.44	126.17	119.90
33	2	1160	G	N1-C6-O6	10.44	126.16	119.90
33	2	206	A	N1-C6-N6	10.43	124.86	118.60
33	2	579	G	N1-C6-O6	10.43	126.16	119.90
33	2	1606	G	N1-C6-O6	10.42	126.15	119.90
33	2	310	G	N1-C6-O6	10.41	126.14	119.90
33	2	1170	U	P-O3'-C3'	10.40	132.19	119.70
39	1	53	G	N1-C6-O6	10.40	126.14	119.90
33	2	670	G	N1-C6-O6	10.40	126.14	119.90
33	2	1732	G	N1-C6-O6	10.39	126.14	119.90
33	2	1653	G	N1-C6-O6	10.39	126.14	119.90
33	2	92	A	N1-C6-N6	10.38	124.83	118.60
33	2	887	G	N1-C6-O6	10.38	126.13	119.90
33	2	1171	G	O3'-P-O5'	10.38	123.73	104.00
33	2	167	G	N1-C6-O6	10.36	126.12	119.90

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	457	G	N1-C6-O6	10.35	126.11	119.90
33	2	1392	А	N1-C6-N6	10.35	124.81	118.60
33	2	1001	G	N1-C6-O6	10.34	126.11	119.90
33	2	1231	G	N1-C6-O6	10.34	126.10	119.90
33	2	1688	G	N1-C6-O6	10.34	126.10	119.90
33	2	1183	G	N1-C6-O6	10.32	126.09	119.90
33	2	1633	G	N1-C6-O6	10.31	126.09	119.90
33	2	427	G	C5-C6-O6	-10.31	122.41	128.60
33	2	1261	А	N1-C6-N6	10.31	124.79	118.60
33	2	1651	G	N1-C6-O6	10.30	126.08	119.90
33	2	1314	G	N1-C6-O6	10.29	126.08	119.90
39	1	31	G	N1-C6-O6	10.27	126.06	119.90
33	2	80	G	N1-C6-O6	10.25	126.05	119.90
33	2	536	G	N1-C6-O6	10.25	126.05	119.90
33	2	1202	G	N1-C6-O6	10.25	126.05	119.90
33	2	323	G	N1-C6-O6	10.24	126.05	119.90
33	2	421	G	N1-C6-O6	10.24	126.05	119.90
33	2	542	G	N1-C6-O6	10.23	126.04	119.90
33	2	827	G	N1-C6-O6	10.23	126.04	119.90
33	2	856	G	N1-C6-O6	10.23	126.04	119.90
33	2	7	G	N1-C6-O6	10.21	126.03	119.90
39	1	22	G	N1-C6-O6	10.21	126.03	119.90
33	2	1506	G	N1-C6-O6	10.19	126.02	119.90
33	2	303	G	N1-C6-O6	10.19	126.01	119.90
33	2	434	G	N1-C6-O6	10.19	126.01	119.90
33	2	1774	G	N1-C6-O6	10.19	126.01	119.90
33	2	606	А	N1-C6-N6	10.17	124.70	118.60
33	2	1744	G	N1-C6-O6	10.16	125.99	119.90
33	2	596	G	N1-C6-O6	10.15	125.99	119.90
33	2	1771	G	N1-C6-O6	10.15	125.99	119.90
33	2	1185	А	N1-C6-N6	10.15	124.69	118.60
33	2	1037	G	N1-C6-O6	10.14	125.98	119.90
33	2	208	G	N1-C6-O6	10.14	125.98	119.90
33	2	676	U	OP2-P-O3'	10.13	127.50	105.20
33	2	1799	G	N1-C6-O6	10.13	125.98	119.90
33	2	1786	G	N1-C6-O6	10.13	125.98	119.90
33	2	669	А	N1-C6-N6	10.13	124.68	118.60
39	1	49	G	N1-C6-O6	10.13	125.98	119.90
33	2	1820	G	N1-C6-O6	10.12	125.97	119.90
33	2	1645	А	N1-C6-N6	10.12	124.67	118.60
33	2	1840	G	N1-C6-O6	10.11	125.97	119.90

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N1-C6-O6

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1232	G	N1-C6-O6	10.11	125.96	119.90
33	2	932	G	N1-C6-O6	10.10	125.96	119.90
39	1	58	А	N1-C6-N6	10.10	124.66	118.60
33	2	1790	G	N1-C6-O6	10.10	125.96	119.90
33	2	1615	А	N1-C6-N6	10.09	124.65	118.60
33	2	320	G	C5-C6-O6	-10.08	122.55	128.60
39	1	6	G	N1-C6-O6	10.08	125.95	119.90
33	2	1223	G	N1-C6-O6	10.07	125.94	119.90
33	2	1785	А	N1-C6-N6	10.07	124.64	118.60
33	2	1290	G	N1-C6-O6	10.07	125.94	119.90
33	2	1571	G	N1-C6-O6	10.07	125.94	119.90
33	2	1286	G	N1-C6-O6	10.07	125.94	119.90
33	2	601	G	N1-C6-O6	10.05	125.93	119.90
33	2	1605	G	C5-C6-O6	-10.05	122.57	128.60
33	2	1046	А	N1-C6-N6	10.05	124.63	118.60
33	2	274	G	N1-C6-O6	10.05	125.93	119.90
33	2	204	G	N1-C6-O6	10.04	125.93	119.90
33	2	337	G	N1-C6-O6	10.04	125.92	119.90
33	2	1701	G	N1-C6-O6	10.04	125.92	119.90
33	2	1658	А	N1-C6-N6	10.03	124.62	118.60
33	2	190	А	N1-C6-N6	10.02	124.61	118.60
33	2	41	G	N1-C6-O6	10.01	125.91	119.90
33	2	1101	G	N1-C6-O6	10.01	125.91	119.90
33	2	1100	G	N1-C6-O6	10.01	125.90	119.90
33	2	403	G	N1-C6-O6	10.00	125.90	119.90
33	2	1565	G	N1-C6-O6	10.00	125.90	119.90
33	2	95	G	N1-C6-O6	9.99	125.89	119.90
33	2	578	G	N1-C6-O6	9.98	125.89	119.90
33	2	1566	G	N1-C6-O6	9.98	125.89	119.90
33	2	1509	G	N1-C6-O6	9.98	125.89	119.90
33	2	1519	G	N1-C6-O6	9.98	125.89	119.90
33	2	79	А	N1-C6-N6	9.96	124.58	118.60
33	2	394	G	N1-C6-O6	9.96	125.88	119.90
33	2	663	G	N1-C6-O6	9.96	125.87	119.90
33	2	1445	G	N1-C6-O6	9.95	125.87	119.90
33	2	534	G	N1-C6-O6	9.93	125.86	119.90
33	2	1852	G	N1-C6-O6	9.93	125.86	119.90
33	2	1572	G	N1-C6-O6	9.92	125.85	119.90
33	2	88	G	N1-C6-O6	9.92	125.85	119.90
33	2	104	А	N1-C6-N6	9.91	124.55	118.60
33	2	1424	G	N1-C6-O6	9.91	125.84	119.90
33	2	1547	G	N1-C6-O6	9.91	$1\overline{25.84}$	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	978	G	N1-C6-O6	9.90	125.84	119.90
33	2	1598	G	N1-C6-O6	9.90	125.84	119.90
33	2	1362	G	N1-C6-O6	9.90	125.84	119.90
33	2	1455	G	N1-C6-O6	9.89	125.84	119.90
33	2	1849	G	N1-C6-O6	9.89	125.83	119.90
33	2	1192	А	N1-C6-N6	9.89	124.53	118.60
33	2	1515	G	N1-C6-O6	9.88	125.83	119.90
33	2	649	G	N1-C6-O6	9.88	125.83	119.90
33	2	1044	G	N1-C6-O6	9.88	125.83	119.90
33	2	1136	G	N1-C6-O6	9.87	125.82	119.90
33	2	1470	А	P-O3'-C3'	9.87	131.55	119.70
33	2	870	G	N1-C6-O6	9.87	125.82	119.90
33	2	367	G	N1-C6-O6	9.85	125.81	119.90
33	2	1033	G	N1-C6-O6	9.84	125.81	119.90
33	2	945	G	N1-C6-O6	9.84	125.81	119.90
33	2	1669	G	N1-C6-O6	9.84	125.80	119.90
33	2	1072	G	N1-C6-O6	9.83	125.80	119.90
33	2	271	G	N1-C6-O6	9.83	125.80	119.90
33	2	319	G	N1-C6-O6	9.82	125.79	119.90
33	2	952	G	N1-C6-O6	9.82	125.79	119.90
33	2	1781	G	N1-C6-O6	9.82	125.79	119.90
33	2	464	G	N1-C6-O6	9.81	125.78	119.90
33	2	1210	А	N1-C6-N6	9.80	124.48	118.60
33	2	1454	G	N1-C6-O6	9.80	125.78	119.90
33	2	503	G	N1-C6-O6	9.79	125.78	119.90
39	1	8	G	N1-C6-O6	9.79	125.77	119.90
33	2	108	G	N1-C6-O6	9.77	125.77	119.90
33	2	1229	G	N1-C6-O6	9.77	125.76	119.90
33	2	183	G	N1-C6-O6	9.76	125.76	119.90
33	2	274	G	C5-C6-O6	-9.76	122.74	128.60
39	1	70	G	N1-C6-O6	9.76	125.75	119.90
33	2	122	G	N1-C6-O6	9.75	125.75	119.90
33	2	1721	G	N1-C6-O6	9.75	125.75	119.90
33	2	1851	G	N1-C6-O6	9.75	125.75	119.90
33	2	201	G	N1-C6-O6	9.73	125.74	119.90
33	2	47	G	N1-C6-O6	9.73	125.74	119.90
33	2	400	G	N1-C6-O6	9.73	125.74	119.90
33	2	890	G	N1-C6-O6	9.73	125.74	119.90
33	2	1122	G	N1-C6-O6	9.73	125.73	119.90
33	2	1718	G	C5-C6-O6	-9.72	122.77	128.60
33	2	360	G	N1-C6-O6	9.71	125.72	119.90
33	2	1731	G	N1-C6-O6	9.71	125.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
39	1	11	G	N1-C6-O6	9.70	125.72	119.90
33	2	1535	G	N1-C6-O6	9.70	125.72	119.90
33	2	146	G	C5-C6-O6	-9.70	122.78	128.60
33	2	1334	G	N1-C6-O6	9.67	125.70	119.90
33	2	1531	G	N1-C6-O6	9.67	125.70	119.90
33	2	1855	G	N1-C6-O6	9.67	125.70	119.90
33	2	145	G	N1-C6-O6	9.66	125.70	119.90
33	2	634	G	N1-C6-O6	9.66	125.70	119.90
33	2	1208	G	N1-C6-O6	9.66	125.69	119.90
33	2	1477	G	N1-C6-O6	9.66	125.70	119.90
33	2	542	G	C5-C6-O6	-9.66	122.81	128.60
33	2	525	G	C5-C6-O6	-9.65	122.81	128.60
33	2	919	G	N1-C6-O6	9.65	125.69	119.90
33	2	1619	U	O4'-C1'-N1	9.65	115.92	108.20
33	2	29	G	N1-C6-O6	9.64	125.69	119.90
33	2	943	G	N1-C6-O6	9.64	125.68	119.90
33	2	197	U	O4'-C1'-N1	9.63	115.91	108.20
33	2	1510	G	N1-C6-O6	9.62	125.67	119.90
33	2	1675	G	N1-C6-O6	9.62	125.67	119.90
33	2	1584	А	N1-C6-N6	9.62	124.37	118.60
33	2	925	G	N1-C6-O6	9.61	125.66	119.90
33	2	1649	G	N1-C6-O6	9.61	125.66	119.90
33	2	1810	G	N1-C6-O6	9.60	125.66	119.90
33	2	591	G	N1-C6-O6	9.60	125.66	119.90
33	2	1036	G	N1-C6-O6	9.60	125.66	119.90
39	1	18	G	O4'-C1'-N9	9.60	115.88	108.20
33	2	62	G	C5-C6-O6	-9.59	122.84	128.60
33	2	1061	G	N1-C6-O6	9.59	125.66	119.90
33	2	385	G	N1-C6-O6	9.59	125.65	119.90
33	2	279	G	C5-C6-O6	-9.59	122.85	128.60
33	2	345	G	N1-C6-O6	9.58	125.65	119.90
33	2	1608	G	N1-C6-O6	9.56	125.64	119.90
33	2	863	G	N1-C6-O6	9.56	125.64	119.90
33	2	500	G	C5-C6-O6	-9.56	122.87	128.60
33	2	828	G	N1-C6-O6	9.56	125.63	119.90
33	2	1717	G	C5-C6-O6	-9.56	122.87	128.60
33	2	1600	G	N1-C6-O6	9.55	125.63	119.90
33	2	409	G	N1-C6-O6	9.55	125.63	119.90
33	2	1025	G	N1-C6-O6	9.55	125.63	119.90
39	1	57	G	N1-C6-O6	9.55	125.63	119.90
33	2	203	G	N1-C6-O6	9.55	125.63	119.90
33	2	1164	G	N1-C6-O6	9.54	125.62	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1180	G	N1-C6-O6	9.54	125.62	119.90
33	2	607	G	N1-C6-O6	9.54	125.62	119.90
33	2	995	G	C5-C6-O6	-9.54	122.88	128.60
33	2	1416	G	N1-C6-O6	9.53	125.62	119.90
39	1	13	G	N1-C6-O6	9.53	125.61	119.90
33	2	1341	G	N1-C6-O6	9.52	125.61	119.90
39	1	52	G	N1-C6-O6	9.52	125.61	119.90
33	2	66	G	N1-C6-O6	9.52	125.61	119.90
33	2	971	G	N1-C6-O6	9.52	125.61	119.90
33	2	1117	G	N1-C6-O6	9.52	125.61	119.90
33	2	1265	G	N1-C6-O6	9.51	125.60	119.90
33	2	1536	G	N1-C6-O6	9.50	125.60	119.90
33	2	1561	G	N1-C6-O6	9.50	125.60	119.90
33	2	903	G	N1-C6-O6	9.49	125.60	119.90
33	2	855	G	N1-C6-O6	9.49	125.59	119.90
33	2	1345	G	N1-C6-O6	9.49	125.59	119.90
33	2	981	G	N1-C6-O6	9.48	125.59	119.90
33	2	1137	G	C5-C6-O6	-9.48	122.91	128.60
33	2	1599	G	N1-C6-O6	9.48	125.59	119.90
33	2	499	G	N1-C6-O6	9.48	125.59	119.90
33	2	1218	G	N1-C6-O6	9.48	125.59	119.90
39	1	30	G	N1-C6-O6	9.47	125.58	119.90
33	2	1294	G	N1-C6-O6	9.46	125.58	119.90
33	2	1316	G	N1-C6-O6	9.45	125.57	119.90
39	1	24	G	C5-C6-O6	-9.45	122.93	128.60
33	2	1055	G	N1-C6-O6	9.45	125.57	119.90
33	2	1496	G	C5-C6-O6	-9.45	122.93	128.60
33	2	1770	G	C5-C6-O6	-9.44	122.93	128.60
33	2	127	С	O4'-C1'-N1	9.44	115.75	108.20
33	2	1166	А	N1-C6-N6	9.44	124.26	118.60
33	2	880	С	O4'-C1'-N1	9.44	115.75	108.20
33	2	1486	G	N1-C6-O6	9.43	125.56	119.90
33	2	307	G	N1-C6-O6	9.43	125.56	119.90
33	2	1085	G	N1-C6-O6	9.42	125.55	119.90
33	2	1206	G	N1-C6-O6	9.42	125.55	119.90
33	2	1331	G	N1-C6-O6	9.42	125.55	119.90
33	2	1006	G	N1-C6-O6	9.41	125.55	119.90
33	2	1462	G	N1-C6-O6	9.41	125.55	119.90
39	1	16	G	N1-C6-O6	9.41	$1\overline{25.55}$	119.90
33	2	1232	G	C5-C6-O6	-9.41	122.96	128.60
33	2	56	G	N1-C6-O6	9.40	$1\overline{25.5}4$	119.90
33	2	1271	G	N1-C6-O6	9.40	125.54	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1789	G	N1-C6-O6	9.40	125.54	119.90
33	2	1748	G	N1-C6-O6	9.39	125.53	119.90
33	2	1814	G	N1-C6-O6	9.39	125.53	119.90
33	2	322	G	O4'-C1'-N9	9.38	115.71	108.20
33	2	588	G	N1-C6-O6	9.38	125.53	119.90
33	2	906	G	N1-C6-O6	9.38	125.53	119.90
33	2	1010	G	N1-C6-O6	9.38	125.53	119.90
33	2	1050	G	N1-C6-O6	9.38	125.53	119.90
33	2	636	G	N1-C6-O6	9.37	125.52	119.90
39	1	3	G	N1-C6-O6	9.37	125.52	119.90
33	2	411	G	N1-C6-O6	9.37	125.52	119.90
33	2	1320	G	N1-C6-O6	9.37	125.52	119.90
33	2	974	G	N1-C6-O6	9.36	125.52	119.90
33	2	1104	G	N1-C6-O6	9.36	125.52	119.90
33	2	1047	G	N1-C6-O6	9.36	125.52	119.90
33	2	1347	G	N1-C6-O6	9.36	125.52	119.90
33	2	1324	G	N1-C6-O6	9.36	125.51	119.90
33	2	1751	G	N1-C6-O6	9.35	125.51	119.90
33	2	1407	G	P-O3'-C3'	9.34	130.91	119.70
33	2	1092	G	N1-C6-O6	9.34	125.50	119.90
33	2	1162	G	N1-C6-O6	9.33	125.50	119.90
33	2	931	G	N1-C6-O6	9.33	125.50	119.90
33	2	1266	G	C5-C6-O6	-9.33	123.00	128.60
33	2	393	G	N1-C6-O6	9.32	125.49	119.90
33	2	1558	G	N1-C6-O6	9.32	125.49	119.90
33	2	1447	G	N1-C6-O6	9.32	125.49	119.90
33	2	472	G	N1-C6-O6	9.31	125.49	119.90
33	2	1427	G	N1-C6-O6	9.31	125.49	119.90
33	2	186	G	N1-C6-O6	9.31	125.49	119.90
33	2	920	G	N1-C6-O6	9.30	125.48	119.90
33	2	351	U	OP1-P-O3'	-9.30	84.74	105.20
33	2	1487	G	N1-C6-O6	9.30	125.48	119.90
33	2	1612	G	N1-C6-O6	9.30	125.48	119.90
33	2	33	G	N1-C6-O6	9.30	125.48	119.90
33	2	189	G	N1-C6-O6	9.29	125.48	119.90
33	2	1570	G	N1-C6-O6	9.29	125.47	119.90
33	2	1160	G	C5-C6-O6	-9.29	123.03	128.60
33	2	494	G	N1-C6-O6	9.28	125.47	119.90
33	2	948	G	N1-C6-O6	9.28	125.47	119.90
33	2	1383	G	N1-C6-O6	9.28	125.47	119.90
33	2	1361	G	C5-C6-O6	-9.27	123.04	128.60
33	2	1452	G	N1-C6-O6	9.27	125.46	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1664	G	N1-C6-O6	9.27	125.46	119.90
33	2	524	G	N1-C6-O6	9.24	125.44	119.90
33	2	613	G	N1-C6-O6	9.24	125.44	119.90
33	2	1697	G	N1-C6-O6	9.23	125.44	119.90
33	2	1171	G	N1-C6-O6	9.23	125.44	119.90
33	2	470	G	N1-C6-O6	9.23	125.44	119.90
33	2	864	G	N1-C6-O6	9.23	125.44	119.90
33	2	555	G	N1-C6-O6	9.22	125.43	119.90
33	2	1752	G	C5-C6-O6	-9.22	123.07	128.60
33	2	1125	G	N1-C6-O6	9.21	125.43	119.90
33	2	1308	G	N1-C6-O6	9.21	125.43	119.90
33	2	1241	G	N1-C6-O6	9.21	125.42	119.90
33	2	939	U	O4'-C1'-N1	9.21	115.56	108.20
33	2	1067	G	N1-C6-O6	9.21	125.42	119.90
33	2	457	G	C5-C6-O6	-9.20	123.08	128.60
33	2	212	G	C5-C6-O6	-9.20	123.08	128.60
33	2	1381	G	N1-C6-O6	9.20	125.42	119.90
33	2	592	G	N1-C6-O6	9.19	125.41	119.90
33	2	1727	G	N1-C6-O6	9.19	125.41	119.90
33	2	1773	G	N1-C6-O6	9.18	125.41	119.90
33	2	238	G	N1-C6-O6	9.18	125.41	119.90
33	2	397	G	N1-C6-O6	9.18	125.41	119.90
33	2	1323	G	N1-C6-O6	9.18	125.41	119.90
33	2	1130	G	N1-C6-O6	9.18	125.41	119.90
33	2	1153	G	N1-C6-O6	9.17	125.41	119.90
33	2	1545	G	N1-C6-O6	9.17	125.40	119.90
33	2	456	G	N1-C6-O6	9.16	125.40	119.90
33	2	1199	G	N1-C6-O6	9.16	125.40	119.90
33	2	1443	G	N1-C6-O6	9.15	125.39	119.90
33	2	1729	G	N1-C6-O6	9.15	125.39	119.90
33	2	1722	G	N1-C6-O6	9.15	125.39	119.90
33	2	430	G	N1-C6-O6	9.15	125.39	119.90
33	2	1172	G	N1-C6-O6	9.14	125.39	119.90
33	2	424	G	N1-C6-O6	9.14	125.38	119.90
33	2	1766	С	O4'-C1'-N1	9.14	115.51	108.20
33	2	1811	G	N1-C6-O6	9.13	125.38	119.90
33	2	987	G	N1-C6-O6	9.12	$1\overline{25.37}$	119.90
33	2	1064	G	N1-C6-O6	9.12	125.37	119.90
33	2	418	U	04'-C1'-N1	9.12	115.49	108.20
33	2	505	G	N1-C6-O6	9.12	125.37	119.90
33	2	1309	A	N1-C6-N6	9.12	124.07	118.60
33	2	1394	G	N1-C6-O6	9.12	125.37	119.90



 $Ideal(^{o})$ 

119.90

119.90

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$
33	2	930	G	N1-C6-O6	9.11	125.36
33	2	1220	G	N1-C6-O6	9.11	125.36
33	2	972	G	N1-C6-O6	9.11	125.36
33	2	1253	G	N1-C6-O6	9.11	125.36
33	2	1841	G	N1-C6-O6	9.11	125.36
33	2	932	G	C5-C6-O6	-9.10	123.14
33	2	1837	G	C5-C6-O6	-9.10	123.14
39	1	19	G	OP2-P-O3'	-9.10	85.19
33	2	1225	G	N1-C6-O6	9.09	125.35
33	2	1772	С	O4'-C1'-N1	9.09	115.47
33	2	966	G	N1-C6-O6	9.09	125.35
33	2	1568	G	N1-C6-O6	9.09	125.35
33	2	468	G	N1-C6-O6	9.08	125.35
33	2	874	G	N1-C6-O6	9.08	125.35
33	2	1469	G	N1-C6-O6	9.08	125.35
33	2	1607	G	N1-C6-O6	9.07	125.34
33	2	323	G	C5-C6-O6	-9.07	123.16
39	1	22	G	C5-C6-O6	-9.07	123.16
33	2	803	G	N1-C6-O6	9.07	125.34
33	2	898	G	N1-C6-O6	9.07	125.34
- 33	2	1371	G	C5-C6-O6	-9.06	123.16

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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	972	G	N1-C6-O6	9.11	125.36	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1253	G	N1-C6-O6	9.11	125.36	119.90
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	33	2	1841	G	N1-C6-O6	9.11	125.36	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	932	G	C5-C6-O6	-9.10	123.14	128.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1837	G	C5-C6-O6	-9.10	123.14	128.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	39	1	19	G	OP2-P-O3'	-9.10	85.19	105.20
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1225	G	N1-C6-O6	9.09	125.35	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1772	С	O4'-C1'-N1	9.09	115.47	108.20
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	966	G	N1-C6-O6	9.09	125.35	119.90
332468GN1-C6-O69.08125.35119.90332874GN1-C6-O69.08125.35119.903321469GN1-C6-O69.08125.35119.903321607GN1-C6-O69.07125.34119.90332323GC5-C6-O6-9.07123.16128.6039122GC5-C6-O6-9.07125.34119.90332803GN1-C6-O69.07125.34119.90332898GN1-C6-O69.07125.34119.903321523GN1-C6-O69.06123.16128.603321523GN1-C6-O69.06125.33119.9034365GN1-C6-O69.06125.33119.903321765GN1-C6-O69.05125.33119.903321765GN1-C6-O69.05125.33119.903321566GC5-C6-O6-9.04125.17128.603321566GC5-C6-O6-9.04125.32119.903321566GC5-C6-O6-9.04125.32119.903321246GN1-C6-O69.04125.32119.903321246GN1-C6-O69.04125.32119.90 <td< td=""><td>33</td><td>2</td><td>1568</td><td>G</td><td>N1-C6-O6</td><td>9.09</td><td>125.35</td><td>119.90</td></td<>	33	2	1568	G	N1-C6-O6	9.09	125.35	119.90
332874GN1-C6-O69.08125.35119.903321469GN1-C6-O69.08125.35119.903321607GN1-C6-O69.07125.34119.90332323GC5-C6-O6-9.07123.16128.6039122GC5-C6-O6-9.07123.16128.60332803GN1-C6-O69.07125.34119.90332898GN1-C6-O69.07125.34119.903321371GC5-C6-O6-9.06125.33119.903321523GN1-C6-O69.06125.33119.9034365GN1-C6-O69.05125.33119.903321418GN1-C6-O69.05125.33119.90332165GN1-C6-O69.05125.33119.90332166GC5-C6-O6-9.05123.17128.603321566GC5-C6-O6-9.04123.17128.603321566GC5-C6-O6-9.04125.32119.903321344GN1-C6-O69.04125.32119.903321246GN1-C6-O69.04125.32119.903321344GN1-C6-O69.04125.32119.90 <td< td=""><td>33</td><td>2</td><td>468</td><td>G</td><td>N1-C6-O6</td><td>9.08</td><td>125.35</td><td>119.90</td></td<>	33	2	468	G	N1-C6-O6	9.08	125.35	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	874	G	N1-C6-O6	9.08	125.35	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1469	G	N1-C6-O6	9.08	125.35	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1607	G	N1-C6-O6	9.07	125.34	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	323	G	C5-C6-O6	-9.07	123.16	128.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	39	1	22	G	C5-C6-O6	-9.07	123.16	128.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	803	G	N1-C6-O6	9.07	125.34	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	898	G	N1-C6-O6	9.07	125.34	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1371	G	C5-C6-O6	-9.06	123.16	128.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1523	G	N1-C6-O6	9.06	125.33	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	34	3	65	G	N1-C6-O6	9.06	125.33	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1418	G	N1-C6-O6	9.05	125.33	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1765	G	N1-C6-O6	9.05	125.33	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	381	С	O4'-C1'-N1	9.05	115.44	108.20
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1566	G	C5-C6-O6	-9.05	123.17	128.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	653	С	O4'-C1'-N1	9.04	115.44	108.20
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	6	G	C5-C6-O6	-9.04	123.17	128.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1103	G	N1-C6-O6	9.04	125.32	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	426	G	N1-C6-O6	9.04	125.32	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1222	G	N1-C6-O6	9.04	125.32	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1344	G	N1-C6-O6	9.04	125.32	119.90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	33	2	1851	G	C5-C6-O6	-9.04	123.18	128.60
33 2 1753 G N1-C6-O6 9.02 125.31 119.90   33 2 123 G C5-C6-O6 -9.02 123.19 128.60   33 2 23 G N1-C6-O6 9.02 125.31 119.90   33 2 23 G N1-C6-O6 9.02 125.31 119.90   33 2 837 G O4'-C1'-N9 9.01 115.41 108.20   33 2 856 G C5-C6-O6 -9.01 123.19 128.60   33 2 1823 G C5-C6-O6 -9.01 123.19 128.60   33 2 1823 G C5-C6-O6 -9.01 123.19 128.60   39 1 10 G N1-C6-O6 9.01 125.31 119.90	33	2	1840	G	C5-C6-O6	-9.03	123.18	128.60
33 2 123 G C5-C6-O6 -9.02 123.19 128.60   33 2 23 G N1-C6-O6 9.02 125.31 119.90   33 2 837 G O4'-C1'-N9 9.01 115.41 108.20   33 2 856 G C5-C6-O6 -9.01 123.19 128.60   33 2 1823 G C5-C6-O6 -9.01 123.19 128.60   33 2 1823 G C5-C6-O6 -9.01 123.19 128.60   33 1 10 G N1-C6-O6 9.01 123.19 128.60	33	2	1753	G	N1-C6-O6	9.02	125.31	119.90
33 2 23 G N1-C6-O6 9.02 125.31 119.90   33 2 837 G O4'-C1'-N9 9.01 115.41 108.20   33 2 856 G C5-C6-O6 -9.01 123.19 128.60   33 2 1823 G C5-C6-O6 -9.01 123.19 128.60   39 1 10 G N1-C6-O6 9.01 125.31 119.90	33	2	123	G	C5-C6-O6	-9.02	123.19	128.60
33 2 837 G O4'-C1'-N9 9.01 115.41 108.20   33 2 856 G C5-C6-O6 -9.01 123.19 128.60   33 2 1823 G C5-C6-O6 -9.01 123.19 128.60   39 1 10 G N1-C6-O6 9.01 125.31 119.90	33	2	23	G	N1-C6-O6	9.02	125.31	119.90
33 2 856 G C5-C6-O6 -9.01 123.19 128.60   33 2 1823 G C5-C6-O6 -9.01 123.19 128.60   39 1 10 G N1-C6-O6 9.01 125.31 119.90	33	2	837	G	O4'-C1'-N9	9.01	115.41	108.20
33 2 1823 G C5-C6-O6 -9.01 123.19 128.60   39 1 10 G N1-C6-O6 9.01 125.31 119.90	33	2	856	G	C5-C6-O6	-9.01	123.19	128.60
39 1 10 G N1-C6-O6 9.01 125.31 119.90	33	2	1823	G	C5-C6-O6	-9.01	123.19	128.60
	39	1	10	G	N1-C6-O6	9.01	125.31	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
34	3	64	G	N1-C6-O6	9.01	125.31	119.90
33	2	1332	С	O4'-C1'-N1	9.01	115.41	108.20
33	2	1562	G	N1-C6-O6	9.01	125.30	119.90
33	2	1511	G	N1-C6-O6	9.00	125.30	119.90
33	2	625	G	N1-C6-O6	9.00	125.30	119.90
33	2	114	G	N1-C6-O6	9.00	125.30	119.90
33	2	911	G	N1-C6-O6	9.00	125.30	119.90
33	2	1633	G	C5-C6-O6	-9.00	123.20	128.60
33	2	1475	G	N1-C6-O6	9.00	125.30	119.90
33	2	1294	G	O4'-C1'-N9	8.99	115.39	108.20
33	2	1808	G	N1-C6-O6	8.99	125.30	119.90
34	3	71	G	N1-C6-O6	8.99	125.29	119.90
33	2	938	G	N1-C6-O6	8.99	125.29	119.90
33	2	1191	А	N1-C6-N6	8.99	123.99	118.60
33	2	587	G	N1-C6-O6	8.98	125.29	119.90
33	2	1743	G	C5-C6-O6	-8.98	123.21	128.60
39	1	49	G	C5-C6-O6	-8.98	123.21	128.60
33	2	375	G	N1-C6-O6	8.98	125.29	119.90
33	2	967	G	N1-C6-O6	8.98	125.29	119.90
33	2	1147	G	N1-C6-O6	8.98	125.29	119.90
33	2	1127	G	N1-C6-O6	8.97	125.28	119.90
33	2	16	G	N1-C6-O6	8.97	125.28	119.90
33	2	75	G	N1-C6-O6	8.97	125.28	119.90
33	2	827	G	C5-C6-O6	-8.97	123.22	128.60
33	2	1100	G	C5-C6-O6	-8.97	123.22	128.60
33	2	991	G	N1-C6-O6	8.97	125.28	119.90
33	2	1093	G	N1-C6-O6	8.96	125.28	119.90
33	2	921	G	N1-C6-O6	8.96	125.28	119.90
33	2	1786	G	C5-C6-O6	-8.96	123.23	128.60
33	2	1411	С	O4'-C1'-N1	8.95	115.36	108.20
33	2	1835	С	O4'-C1'-N1	8.95	115.36	108.20
33	2	113	G	N1-C6-O6	8.94	125.26	119.90
39	1	43	G	N1-C6-O6	8.93	125.26	119.90
33	2	1175	G	N1-C6-O6	8.93	125.26	119.90
33	2	205	G	N1-C6-O6	8.93	125.25	119.90
33	2	1521	G	N1-C6-O6	8.91	125.25	119.90
33	2	167	G	C5-C6-O6	-8.91	123.25	128.60
33	2	1165	G	N1-C6-O6	8.90	125.24	119.90
33	2	319	G	C5-C6-O6	-8.90	123.26	128.60
33	2	153	G	N1-C6-O6	8.90	125.24	119.90
33	2	883	U	O4'-C1'-N1	8.90	115.32	108.20
33	2	670	G	C5-C6-O6	-8.90	123.26	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	928	G	N1-C6-O6	8.90	125.24	119.90
33	2	1778	G	N1-C6-O6	8.89	125.24	119.90
33	2	1231	G	C5-C6-O6	-8.89	123.27	128.60
33	2	1163	G	N1-C6-O6	8.89	125.23	119.90
33	2	1276	G	N1-C6-O6	8.89	125.23	119.90
33	2	1314	G	C5-C6-O6	-8.89	123.27	128.60
33	2	1414	С	C2-N1-C1'	8.89	128.57	118.80
33	2	310	G	C5-C6-O6	-8.88	123.27	128.60
33	2	163	U	O4'-C1'-N1	8.88	115.30	108.20
33	2	496	G	N1-C6-O6	8.88	125.23	119.90
33	2	1776	G	N1-C6-O6	8.88	125.23	119.90
33	2	289	G	C5-C6-O6	-8.87	123.28	128.60
33	2	1503	G	N1-C6-O6	8.87	125.22	119.90
33	2	1321	G	N1-C6-O6	8.87	125.22	119.90
33	2	1793	G	N1-C6-O6	8.87	125.22	119.90
33	2	1425	G	N1-C6-O6	8.87	125.22	119.90
33	2	52	G	C5-C6-O6	-8.86	123.28	128.60
33	2	616	G	N1-C6-O6	8.85	125.21	119.90
33	2	1565	G	C5-C6-O6	-8.85	123.29	128.60
33	2	155	G	N1-C6-O6	8.84	125.20	119.90
33	2	370	G	N1-C6-O6	8.84	125.20	119.90
33	2	1001	G	C5-C6-O6	-8.84	123.30	128.60
33	2	522	С	O4'-C1'-N1	8.84	115.27	108.20
33	2	1774	G	C5-C6-O6	-8.84	123.30	128.60
33	2	1126	G	N1-C6-O6	8.83	125.20	119.90
33	2	1360	U	O4'-C1'-N1	8.83	115.26	108.20
33	2	199	G	N1-C6-O6	8.82	125.19	119.90
33	2	1106	G	N1-C6-O6	8.82	125.19	119.90
33	2	1094	С	O4'-C1'-N1	8.82	115.26	108.20
33	2	1509	G	C5-C6-O6	-8.82	123.31	128.60
33	2	1541	G	N1-C6-O6	8.82	125.19	119.90
33	2	1317	G	N1-C6-O6	8.82	125.19	119.90
33	2	461	G	N1-C6-O6	8.82	125.19	119.90
33	2	1251	G	N1-C6-O6	8.82	125.19	119.90
33	2	403	G	C5-C6-O6	-8.81	123.31	128.60
33	2	832	G	N1-C6-O6	8.81	125.19	119.90
33	2	1704	G	N1-C6-O6	8.81	125.19	119.90
33	2	180	G	N1-C6-O6	8.80	125.18	119.90
33	2	1515	G	C5-C6-O6	-8.80	123.32	128.60
33	2	1390	G	N1-C6-O6	8.80	125.18	119.90
33	2	1267	С	O4'-C1'-N1	8.79	115.23	108.20
33	2	402	G	N1-C6-O6	8.79	125.17	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	955	G	N1-C6-O6	8.79	125.17	119.90
33	2	1039	G	N1-C6-O6	8.79	125.17	119.90
33	2	222	G	N1-C6-O6	8.78	125.17	119.90
33	2	1678	С	O4'-C1'-N1	8.78	115.22	108.20
33	2	1830	G	N1-C6-O6	8.78	125.17	119.90
33	2	1767	С	O4'-C1'-N1	8.78	115.22	108.20
39	1	31	G	C5-C6-O6	-8.78	123.33	128.60
33	2	401	G	C5-C6-O6	-8.77	123.34	128.60
33	2	1088	G	N1-C6-O6	8.77	125.17	119.90
33	2	891	G	N1-C6-O6	8.77	125.16	119.90
33	2	299	G	N1-C6-O6	8.77	125.16	119.90
33	2	945	G	C5-C6-O6	-8.77	123.34	128.60
33	2	1593	G	N1-C6-O6	8.77	125.16	119.90
33	2	328	G	N1-C6-O6	8.76	125.16	119.90
33	2	1420	G	N1-C6-O6	8.75	125.15	119.90
33	2	1738	G	N1-C6-O6	8.75	125.15	119.90
33	2	1681	G	N1-C6-O6	8.75	125.15	119.90
33	2	1660	G	N1-C6-O6	8.74	125.14	119.90
33	2	422	G	N1-C6-O6	8.74	125.14	119.90
33	2	901	C	O4'-C1'-N1	8.74	115.19	108.20
39	1	9	U	O4'-C1'-N1	8.74	115.19	108.20
33	2	322	G	N1-C6-O6	8.74	125.14	119.90
33	2	410	G	N1-C6-O6	8.74	125.14	119.90
33	2	508	G	N1-C6-O6	8.74	125.14	119.90
33	2	568	С	O4'-C1'-N1	8.73	115.18	108.20
33	2	495	G	N1-C6-O6	8.72	125.13	119.90
33	2	655	G	N1-C6-O6	8.72	125.13	119.90
33	2	877	G	N1-C6-O6	8.72	125.13	119.90
33	2	400	G	C5-C6-O6	-8.72	123.37	128.60
33	2	579	G	C5-C6-O6	-8.71	123.37	128.60
33	2	596	G	C5-C6-O6	-8.71	123.37	128.60
33	2	345	G	C5-C6-O6	-8.71	123.38	128.60
33	2	1095	G	N1-C6-O6	8.70	125.12	119.90
33	2	395	G	N1-C6-O6	8.70	125.12	119.90
33	2	156	G	C5-C6-O6	-8.70	123.38	128.60
33	2	1183	G	C5-C6-O6	-8.70	123.38	128.60
33	2	303	G	C5-C6-O6	-8.70	123.38	128.60
33	2	1846	C	O4'-C1'-N1	8.70	115.16	108.20
33	2	460	G	N1-C6-O6	8.69	125.11	119.90
33	2	1571	G	C5-C6-O6	-8.69	123.39	128.60
33	2	300	G	C5-C6-O6	-8.69	123.39	128.60
33	2	80	G	C5-C6-O6	-8.68	123.39	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	82	G	N1-C6-O6	8.68	125.11	119.90
33	2	646	G	N1-C6-O6	8.68	125.11	119.90
33	2	1229	G	C5-C6-O6	-8.68	123.39	128.60
33	2	1187	С	O4'-C1'-N1	8.68	115.14	108.20
33	2	813	G	N1-C6-O6	8.68	125.11	119.90
33	2	875	С	O4'-C1'-N1	8.68	115.14	108.20
33	2	929	G	N1-C6-O6	8.68	125.11	119.90
33	2	165	G	N1-C6-O6	8.67	125.10	119.90
33	2	537	G	N1-C6-O6	8.67	125.10	119.90
34	3	73	G	N1-C6-O6	8.67	125.10	119.90
33	2	421	G	C5-C6-O6	-8.67	123.40	128.60
33	2	817	G	N1-C6-O6	8.67	125.10	119.90
33	2	1037	G	C5-C6-O6	-8.67	123.40	128.60
33	2	1739	G	N1-C6-O6	8.67	125.10	119.90
33	2	1506	G	C5-C6-O6	-8.66	123.40	128.60
33	2	29	G	C5-C6-O6	-8.66	123.41	128.60
33	2	957	G	N1-C6-O6	8.65	125.09	119.90
33	2	842	G	N1-C6-O6	8.65	125.09	119.90
33	2	1040	G	N1-C6-O6	8.65	125.09	119.90
33	2	20	G	N1-C6-O6	8.64	125.09	119.90
33	2	538	С	O4'-C1'-N1	8.64	115.11	108.20
33	2	1783	G	N1-C6-O6	8.64	125.09	119.90
33	2	1113	С	O4'-C1'-N1	8.64	115.11	108.20
33	2	1631	G	N1-C6-O6	8.64	125.08	119.90
33	2	1125	G	C5-C6-O6	-8.63	123.42	128.60
33	2	1270	G	N1-C6-O6	8.63	125.08	119.90
33	2	1666	G	N1-C6-O6	8.63	125.08	119.90
33	2	1749	С	O4'-C1'-N1	8.63	115.10	108.20
33	2	1389	G	N1-C6-O6	8.62	125.08	119.90
33	2	1768	С	O4'-C1'-N1	8.62	115.10	108.20
39	1	17	С	P-O3'-C3'	8.62	130.04	119.70
33	2	415	G	N1-C6-O6	8.62	125.07	119.90
33	2	48	С	O4'-C1'-N1	8.62	115.09	108.20
33	2	649	G	C5-C6-O6	-8.62	123.43	128.60
33	2	905	G	N1-C6-O6	8.62	125.07	119.90
33	2	1519	G	C5-C6-O6	-8.61	123.43	128.60
34	3	69	G	N1-C6-O6	8.61	125.07	119.90
33	2	581	U	P-O3'-C3'	8.61	130.03	119.70
33	2	436	G	N1-C6-O6	8.60	125.06	119.90
33	2	441	G	N1-C6-O6	8.60	125.06	119.90
33	2	1781	G	C5-C6-O6	-8.60	123.44	128.60
39	1	46	G	N1-C6-O6	8.60	125.06	119.90



33

2

1318

G

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	373	G	N1-C6-O6	8.60	125.06	119.90
33	2	590	G	N1-C6-O6	8.59	125.06	119.90
33	2	1510	G	C5-C6-O6	-8.59	123.44	128.60
33	2	1286	G	C5-C6-O6	-8.59	123.45	128.60
33	2	1402	G	N1-C6-O6	8.59	125.05	119.90
33	2	906	G	C5-C6-O6	-8.58	123.45	128.60
33	2	1535	G	C5-C6-O6	-8.57	123.46	128.60
33	2	1446	G	N1-C6-O6	8.57	125.04	119.90
34	3	62	G	N1-C6-O6	8.57	125.04	119.90
33	2	553	G	C5-C6-O6	-8.57	123.46	128.60
33	2	1265	G	C5-C6-O6	-8.57	123.46	128.60
33	2	325	G	N1-C6-O6	8.56	125.04	119.90
33	2	1290	G	C5-C6-O6	-8.56	123.46	128.60
33	2	576	G	N1-C6-O6	8.56	125.03	119.90
33	2	74	G	O4'-C1'-N9	8.55	115.04	108.20
33	2	394	G	C5-C6-O6	-8.55	123.47	128.60
33	2	820	С	O4'-C1'-N1	8.55	115.04	108.20
39	1	57	G	C5-C6-O6	-8.54	123.47	128.60
33	2	1841	G	C5-C6-O6	-8.54	123.48	128.60
33	2	74	G	N1-C6-O6	8.54	125.02	119.90
33	2	897	G	N1-C6-O6	8.53	125.02	119.90
33	2	70	G	N1-C6-O6	8.53	125.02	119.90
33	2	1701	G	C5-C6-O6	-8.53	123.48	128.60
33	2	533	С	O4'-C1'-N1	8.52	115.01	108.20
33	2	982	G	N1-C6-O6	8.52	125.01	119.90
33	2	1029	G	N1-C6-O6	8.52	125.01	119.90
33	2	1348	G	C5-C6-O6	-8.51	123.49	128.60
33	2	184	G	N1-C6-O6	8.51	125.00	119.90
33	2	1357	G	N1-C6-O6	8.51	125.00	119.90
33	2	434	G	C5-C6-O6	-8.50	123.50	128.60
33	2	673	G	N1-C6-O6	8.49	125.00	119.90
33	2	1010	G	C5-C6-O6	-8.49	123.51	128.60
33	2	1072	G	C5-C6-O6	-8.49	123.51	128.60
33	2	1207	G	N1-C6-O6	8.49	124.99	119.90
33	2	69	С	O4'-C1'-N1	8.49	114.99	108.20
33	2	71	G	N1-C6-O6	8.48	124.99	119.90
33	2	204	G	C5-C6-O6	-8.48	123.51	128.60
33	2	1326	G	N1-C6-O6	8.48	124.99	119.90
33	2	1512	G	N1-C6-O6	8.48	124.99	119.90
33	2	1744	G	C5-C6-O6	-8.48	123.51	128.60
33	2	1856	G	N1-C6-O6	8.48	124.99	119.90

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124.99

119.90



8.48

N1-C6-O6

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	7	G	C5-C6-O6	-8.48	123.51	128.60
33	2	601	G	C5-C6-O6	-8.47	123.52	128.60
33	2	1105	С	O4'-C1'-N1	8.47	114.98	108.20
33	2	634	G	C5-C6-O6	-8.47	123.52	128.60
33	2	497	G	N1-C6-O6	8.47	124.98	119.90
33	2	1708	С	O4'-C1'-N1	8.47	114.97	108.20
33	2	975	С	O4'-C1'-N1	8.46	114.97	108.20
33	2	1362	G	C5-C6-O6	-8.46	123.52	128.60
39	1	29	G	C5-C6-O6	-8.46	123.52	128.60
33	2	954	G	N1-C6-O6	8.46	124.97	119.90
33	2	1407	G	N1-C6-O6	8.46	124.97	119.90
33	2	1154	G	N1-C6-O6	8.46	124.97	119.90
33	2	1227	С	O4'-C1'-N1	8.45	114.96	108.20
33	2	1552	С	O4'-C1'-N1	8.45	114.96	108.20
33	2	208	G	C5-C6-O6	-8.44	123.53	128.60
33	2	154	U	O4'-C1'-N1	8.44	114.95	108.20
33	2	464	G	C5-C6-O6	-8.44	123.53	128.60
33	2	550	А	O4'-C1'-N9	8.44	114.95	108.20
33	2	600	G	C5-C6-O6	-8.44	123.53	128.60
33	2	237	G	N1-C6-O6	8.44	124.96	119.90
33	2	280	G	N1-C6-O6	8.44	124.96	119.90
33	2	210	G	N1-C6-O6	8.43	124.96	119.90
33	2	220	С	O4'-C1'-N1	8.43	114.94	108.20
33	2	1155	G	N1-C6-O6	8.43	124.96	119.90
33	2	1377	G	N1-C6-O6	8.43	124.96	119.90
33	2	1383	G	C5-C6-O6	-8.43	123.54	128.60
33	2	1731	G	C5-C6-O6	-8.43	123.55	128.60
33	2	1852	G	C5-C6-O6	-8.42	123.55	128.60
33	2	834	G	N1-C6-O6	8.41	124.95	119.90
33	2	1277	G	N1-C6-O6	8.41	124.95	119.90
33	2	830	С	O4'-C1'-N1	8.41	114.93	108.20
33	2	1138	G	N1-C6-O6	8.41	124.95	119.90
33	2	1649	G	C5-C6-O6	-8.41	123.55	128.60
33	2	273	G	N1-C6-O6	8.40	124.94	119.90
33	2	1298	G	N1-C6-O6	8.40	124.94	119.90
33	2	534	G	C5-C6-O6	-8.40	123.56	128.60
33	2	1082	G	N1-C6-O6	8.40	124.94	119.90
33	2	824	G	N1-C6-O6	8.40	124.94	119.90
33	2	876	G	O4'-C1'-N9	8.40	114.92	108.20
33	2	1572	G	C5-C6-O6	-8.40	123.56	128.60
33	2	1006	G	C5-C6-O6	-8.39	123.56	128.60
33	2	1843	G	N1-C6-O6	8.39	124.93	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1202	G	C5-C6-O6	-8.38	123.57	128.60
33	2	1430	С	O4'-C1'-N1	8.38	114.91	108.20
33	2	118	С	O4'-C1'-N1	8.38	114.91	108.20
34	3	63	U	O4'-C1'-N1	8.38	114.91	108.20
39	1	19	G	N1-C6-O6	8.38	124.93	119.90
33	2	663	G	C5-C6-O6	-8.38	123.57	128.60
33	2	1606	G	C5-C6-O6	-8.38	123.57	128.60
33	2	183	G	C5-C6-O6	-8.37	123.58	128.60
33	2	380	С	O4'-C1'-N1	8.37	114.90	108.20
33	2	1754	G	N1-C6-O6	8.37	124.92	119.90
33	2	1099	С	O4'-C1'-N1	8.37	114.89	108.20
33	2	1455	G	C5-C6-O6	-8.37	123.58	128.60
33	2	1454	G	C5-C6-O6	-8.36	123.58	128.60
33	2	1582	G	N1-C6-O6	8.36	124.92	119.90
39	1	11	G	C5-C6-O6	-8.36	123.58	128.60
33	2	1595	G	N1-C6-O6	8.36	124.92	119.90
33	2	177	G	N1-C6-O6	8.36	124.91	119.90
33	2	815	G	N1-C6-O6	8.36	124.91	119.90
33	2	90	G	N1-C6-O6	8.35	124.91	119.90
33	2	327	С	O4'-C1'-N1	8.35	114.88	108.20
33	2	275	С	O4'-C1'-N1	8.35	114.88	108.20
33	2	375	G	C5-C6-O6	-8.35	123.59	128.60
33	2	1112	С	O4'-C1'-N1	8.35	114.88	108.20
33	2	270	G	N1-C6-O6	8.34	124.91	119.90
33	2	1608	G	C5-C6-O6	-8.34	123.59	128.60
33	2	896	С	O4'-C1'-N1	8.34	114.87	108.20
33	2	1647	G	N1-C6-O6	8.33	124.90	119.90
33	2	1543	G	N1-C6-O6	8.33	124.90	119.90
33	2	835	С	O4'-C1'-N1	8.33	114.86	108.20
33	2	360	G	C5-C6-O6	-8.33	123.60	128.60
33	2	193	С	O4'-C1'-N1	8.32	114.86	108.20
33	2	428	G	N1-C6-O6	8.32	124.89	119.90
33	2	674	G	N1-C6-O6	8.32	124.89	119.90
33	2	384	G	C5-C6-O6	-8.32	123.61	128.60
33	2	667	G	N1-C6-O6	8.32	124.89	119.90
33	2	1333	С	O4'-C1'-N1	8.31	114.84	108.20
33	2	47	G	C5-C6-O6	-8.30	123.62	128.60
33	2	273	G	C5-C6-O6	-8.30	123.62	128.60
33	2	1688	G	C5-C6-O6	-8.30	123.62	128.60
33	2	1651	G	C5-C6-O6	-8.30	123.62	128.60
33	2	1409	G	N1-C6-O6	8.30	124.88	119.90
33	2	122	G	C5-C6-O6	-8.29	123.62	128.60



33

2

1043

С

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	367	G	C5-C6-O6	-8.29	123.62	128.60
33	2	1119	С	O4'-C1'-N1	8.29	114.83	108.20
33	2	1536	G	C5-C6-O6	-8.29	123.62	128.60
33	2	1601	G	N1-C6-O6	8.29	124.88	119.90
33	2	1655	С	C2-N1-C1'	8.29	127.92	118.80
39	1	8	G	C5-C6-O6	-8.29	123.62	128.60
33	2	615	G	N1-C6-O6	8.29	124.87	119.90
33	2	1201	С	O4'-C1'-N1	8.29	114.83	108.20
33	2	1634	G	N1-C6-O6	8.29	124.87	119.90
33	2	1002	С	O4'-C1'-N1	8.28	114.83	108.20
33	2	1131	С	O4'-C1'-N1	8.28	114.83	108.20
34	3	70	G	N1-C6-O6	8.28	124.87	119.90
33	2	548	G	N1-C6-O6	8.28	124.87	119.90
33	2	1324	G	C5-C6-O6	-8.28	123.63	128.60
33	2	1419	С	O4'-C1'-N1	8.28	114.82	108.20
33	2	1493	G	N1-C6-O6	8.28	124.87	119.90
33	2	1330	G	N1-C6-O6	8.28	124.87	119.90
33	2	1653	G	C5-C6-O6	-8.27	123.64	128.60
33	2	307	G	C5-C6-O6	-8.27	123.64	128.60
33	2	870	G	C5-C6-O6	-8.27	123.64	128.60
33	2	629	С	O4'-C1'-N1	8.27	114.81	108.20
33	2	317	G	N1-C6-O6	8.26	124.86	119.90
33	2	1416	G	C5-C6-O6	-8.26	123.65	128.60
33	2	1194	G	N1-C6-O6	8.25	124.85	119.90
33	2	337	G	C5-C6-O6	-8.25	123.65	128.60
33	2	1445	G	C5-C6-O6	-8.25	123.65	128.60
33	2	201	G	C5-C6-O6	-8.24	123.66	128.60
33	2	1167	G	N1-C6-O6	8.24	124.84	119.90
33	2	1181	С	O4'-C1'-N1	8.24	114.79	108.20
33	2	1771	G	C5-C6-O6	-8.24	123.66	128.60
33	2	1675	G	C5-C6-O6	-8.24	123.66	128.60
33	2	385	G	C5-C6-O6	-8.23	123.66	128.60
33	2	1098	G	N1-C6-O6	8.23	124.84	119.90
33	2	1604	С	O4'-C1'-N1	8.23	114.78	108.20
33	2	952	G	C5-C6-O6	-8.22	123.67	128.60
33	2	1136	G	C5-C6-O6	-8.22	123.67	128.60
10	K	149	TYR	CB-CG-CD1	8.21	125.93	121.00
33	2	1217	G	N1-C6-O6	8.22	124.83	119.90
33	2	1334	G	C5-C6-O6	-8.21	123.67	128.60
33	2	1790	G	C5-C6-O6	-8.21	123.67	128.60
39	1	39	С	O4'-C1'-N1	8.21	114.77	108.20

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108.20

114.77



8.21

O4'-C1'-N1

 $Observed(^{o}) | Ideal(^{o})$ 

108.20

114.77

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Mol	Chain	Res	Type	Atoms	Z
33	2	937	С	O4'-C1'-N1	8.21
33	2	1466	С	O4'-C1'-N1	8.21
33	2	1471	G	N1-C6-O6	8.21
33	2	1497	С	O4'-C1'-N1	8.21
33	2	1627	G	N1-C6-O6	8.21
33	2	837	G	N1-C6-O6	8.21
33	2	1193	G	N1-C6-O6	8.21
33	2	605	С	O4'-C1'-N1	8.20
33	2	1370	С	O4'-C1'-N1	8.21
33	2	1745	С	O4'-C1'-N1	8 20

33	2	1466	С	O4'-C1'-N1	8.21	114.77	108.20
33	2	1471	G	N1-C6-O6	8.21	124.83	119.90
33	2	1497	С	O4'-C1'-N1	8.21	114.77	108.20
33	2	1627	G	N1-C6-O6	8.21	124.82	119.90
33	2	837	G	N1-C6-O6	8.21	124.82	119.90
33	2	1193	G	N1-C6-O6	8.21	124.82	119.90
33	2	605	С	O4'-C1'-N1	8.20	114.76	108.20
33	2	1370	С	O4'-C1'-N1	8.21	114.76	108.20
33	2	1745	С	O4'-C1'-N1	8.20	114.76	108.20
33	2	469	С	O4'-C1'-N1	8.20	114.76	108.20
33	2	209	С	O4'-C1'-N1	8.20	114.76	108.20
33	2	298	G	N1-C6-O6	8.20	124.82	119.90
33	2	1427	G	C5-C6-O6	-8.19	123.69	128.60
39	1	13	G	C5-C6-O6	-8.19	123.69	128.60
33	2	352	С	O4'-C1'-N1	8.18	114.75	108.20
33	2	558	С	O4'-C1'-N1	8.18	114.74	108.20
33	2	94	G	N1-C6-O6	8.18	124.81	119.90
33	2	560	С	O4'-C1'-N1	8.18	114.74	108.20
33	2	1779	С	O4'-C1'-N1	8.17	114.74	108.20
39	1	6	G	C5-C6-O6	-8.17	123.70	128.60
33	2	387	G	N1-C6-O6	8.16	124.80	119.90
10	Κ	149	TYR	CB-CG-CD2	-8.16	116.10	121.00
33	2	1135	С	O4'-C1'-N1	8.16	114.73	108.20
33	2	1101	G	C5-C6-O6	-8.16	123.70	128.60
33	2	145	G	C5-C6-O6	-8.16	123.71	128.60
33	2	178	С	O4'-C1'-N1	8.15	114.72	108.20
33	2	1669	G	C5-C6-O6	-8.15	123.71	128.60
33	2	351	U	O3'-P-O5'	8.15	119.48	104.00
33	2	1268	С	O4'-C1'-N1	8.14	114.72	108.20
33	2	1732	G	C5-C6-O6	-8.14	123.71	128.60
33	2	885	U	O4'-C1'-N1	8.14	114.72	108.20
33	2	1054	А	O4'-C1'-N9	8.14	114.71	108.20
33	2	56	G	C5-C6-O6	-8.14	123.72	128.60
39	1	53	G	C5-C6-O6	-8.14	123.72	128.60
33	2	597	U	04'-C1'-N1	8.14	114.71	108.20
39	1	45	G	N1-C6-O6	8.13	124.78	119.90
33	2	192	U	O4'-C1'-N1	8.13	114.70	108.20
33	2	890	G	C5-C6-O6	-8.13	123.72	128.60
33	2	1250	С	O4'-C1'-N1	8.12	114.70	108.20
33	2	420	С	O4'-C1'-N1	8.12	114.70	108.20
33	2	828	G	C5-C6-O6	-8.12	123.73	128.60



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
39	1	26	G	N1-C6-O6	8.12	124.77	119.90
33	2	1776	G	C5-C6-O6	-8.12	123.73	128.60
33	2	1579	G	N1-C6-O6	8.12	124.77	119.90
33	2	1350	G	N1-C6-O6	8.11	124.77	119.90
33	2	1468	С	O4'-C1'-N1	8.11	114.69	108.20
33	2	341	G	N1-C6-O6	8.11	124.77	119.90
33	2	943	G	C5-C6-O6	-8.11	123.73	128.60
33	2	848	G	O4'-C1'-N9	8.11	114.68	108.20
33	2	1176	С	O4'-C1'-N1	8.11	114.69	108.20
33	2	879	U	O4'-C1'-N1	8.10	114.68	108.20
33	2	1421	G	N1-C6-O6	8.10	124.76	119.90
33	2	1607	G	C5-C6-O6	-8.10	123.74	128.60
39	1	30	G	C5-C6-O6	-8.10	123.74	128.60
33	2	95	G	C5-C6-O6	-8.10	123.74	128.60
33	2	1252	G	N1-C6-O6	8.10	124.76	119.90
33	2	841	G	N1-C6-O6	8.10	124.76	119.90
33	2	1652	G	N1-C6-O6	8.10	124.76	119.90
19	V	48	TYR	CB-CG-CD2	-8.09	116.14	121.00
33	2	364	G	N1-C6-O6	8.09	124.75	119.90
33	2	1778	G	C5-C6-O6	-8.09	123.74	128.60
33	2	284	С	O4'-C1'-N1	8.09	114.67	108.20
33	2	1562	G	O4'-C1'-N9	8.09	114.67	108.20
33	2	1047	G	C5-C6-O6	-8.08	123.75	128.60
33	2	442	G	N1-C6-O6	8.08	124.75	119.90
33	2	1616	U	O4'-C1'-N1	8.07	114.66	108.20
33	2	1111	U	O4'-C1'-N1	8.07	114.65	108.20
33	2	1639	С	O4'-C1'-N1	8.07	114.65	108.20
33	2	10	G	N1-C6-O6	8.06	124.74	119.90
33	2	431	С	O4'-C1'-N1	8.06	114.64	108.20
33	2	876	G	N1-C6-O6	8.06	124.73	119.90
39	1	52	G	C5-C6-O6	-8.06	123.77	128.60
33	2	1226	С	O4'-C1'-N1	8.05	114.64	108.20
33	2	1847	$\mathbf{C}$	O4'-C1'-N1	8.05	114.64	108.20
33	2	1343	U	O4'-C1'-N1	8.05	114.64	108.20
33	2	1676	U	O4'-C1'-N1	8.05	114.64	108.20
33	2	37	С	O4'-C1'-N1	8.05	114.64	108.20
33	2	494	G	C5-C6-O6	-8.05	123.77	128.60
33	2	536	G	C5-C6-O6	-8.04	123.78	128.60
33	2	555	G	C5-C6-O6	-8.04	123.78	128.60
33	2	729	C	O4'-C1'-N1	8.04	114.63	108.20
33	2	$59\overline{2}$	G	$C5-C6-\overline{O6}$	-8.03	$123.7\overline{8}$	128.60
33	2	1522	$\mathbf{C}$	O4'-C1'-N1	8.03	114.62	108.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1621	С	O4'-C1'-N1	8.03	114.62	108.20
34	3	74	G	N1-C6-O6	8.03	124.72	119.90
33	2	917	G	N1-C6-O6	8.03	124.72	119.90
33	2	1553	С	O4'-C1'-N1	8.02	114.62	108.20
33	2	1748	G	C5-C6-O6	-8.02	123.79	128.60
33	2	1801	С	O4'-C1'-N1	8.02	114.62	108.20
33	2	931	G	C5-C6-O6	-8.02	123.79	128.60
34	3	68	А	O4'-C1'-N9	8.02	114.61	108.20
33	2	503	G	C5-C6-O6	-8.01	123.79	128.60
33	2	1061	G	C5-C6-O6	-8.01	123.79	128.60
33	2	41	G	C5-C6-O6	-8.01	123.80	128.60
33	2	1599	G	C5-C6-O6	-8.01	123.80	128.60
33	2	1206	G	C5-C6-O6	-8.00	123.80	128.60
33	2	294	С	O4'-C1'-N1	8.00	114.60	108.20
33	2	1561	G	C5-C6-O6	-8.00	123.80	128.60
33	2	1736	U	O4'-C1'-N1	8.00	114.60	108.20
33	2	369	С	O4'-C1'-N1	8.00	114.60	108.20
33	2	1352	G	N1-C6-O6	8.00	124.70	119.90
33	2	1531	G	C5-C6-O6	-8.00	123.80	128.60
33	2	849	С	C2-N1-C1'	8.00	127.60	118.80
33	2	1053	С	O4'-C1'-N1	8.00	114.60	108.20
33	2	1315	U	O4'-C1'-N1	7.99	114.59	108.20
33	2	626	С	O4'-C1'-N1	7.99	114.59	108.20
33	2	1467	С	O4'-C1'-N1	7.99	114.59	108.20
33	2	1487	G	C5-C6-O6	-7.99	123.81	128.60
33	2	591	G	C5-C6-O6	-7.99	123.81	128.60
33	2	924	G	N1-C6-O6	7.98	124.69	119.90
33	2	88	G	C5-C6-O6	-7.98	123.81	128.60
33	2	545	А	P-O3'-C3'	7.98	129.28	119.70
33	2	543	U	O4'-C1'-N1	7.97	114.58	108.20
33	2	1311	U	O4'-C1'-N1	7.97	114.58	108.20
33	2	1504	А	N1-C6-N6	7.97	123.38	118.60
33	2	1414	С	C6-N1-C1'	-7.96	111.24	120.80
33	2	837	G	C5-C6-O6	-7.96	123.82	128.60
33	2	439	А	N1-C6-N6	7.96	123.38	118.60
33	2	115	U	O4'-C1'-N1	7.96	114.57	108.20
33	2	613	G	C5-C6-O6	-7.96	123.82	128.60
34	3	72	U	O4'-C1'-N1	7.96	114.57	108.20
33	2	1122	G	C5-C6-O6	-7.95	123.83	128.60
33	2	1643	G	N1-C6-O6	7.95	124.67	119.90
33	2	607	G	$C5-C6-\overline{O6}$	-7.94	123.83	128.60
33	2	851	G	N1-C6-O6	7.94	124.67	119.90



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А

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal $(^{o})$
33	2	1586	С	O4'-C1'-N1	7.94	114.55	108.20
33	2	426	G	C5-C6-O6	-7.94	123.84	128.60
33	2	126	G	N1-C6-O6	7.94	124.66	119.90
33	2	1033	G	C5-C6-O6	-7.94	123.84	128.60
33	2	1208	G	C5-C6-O6	-7.94	123.84	128.60
33	2	282	G	N1-C6-O6	7.93	124.66	119.90
33	2	430	G	C5-C6-O6	-7.93	123.84	128.60
33	2	839	С	O4'-C1'-N1	7.93	114.55	108.20
33	2	893	U	O4'-C1'-N1	7.93	114.55	108.20
33	2	1638	U	O4'-C1'-N1	7.93	114.55	108.20
33	2	1547	G	C5-C6-O6	-7.93	123.84	128.60
33	2	1598	G	C5-C6-O6	-7.93	123.84	128.60
33	2	549	G	N1-C6-O6	7.92	124.66	119.90
33	2	1753	G	C5-C6-O6	-7.92	123.84	128.60
33	2	1524	С	O4'-C1'-N1	7.92	114.54	108.20
33	2	1746	С	O4'-C1'-N1	7.92	114.54	108.20
33	2	1705	С	O4'-C1'-N1	7.92	114.53	108.20
33	2	75	G	O4'-C1'-N9	7.92	114.53	108.20
33	2	569	С	O4'-C1'-N1	7.92	114.53	108.20
33	2	1281	G	N1-C6-O6	7.92	124.65	119.90
33	2	1443	G	C5-C6-O6	-7.91	123.85	128.60
39	1	32	С	O4'-C1'-N1	7.91	114.53	108.20
33	2	625	G	C5-C6-O6	-7.91	123.85	128.60
39	1	3	G	C5-C6-O6	-7.91	123.85	128.60
33	2	1477	G	C5-C6-O6	-7.91	123.86	128.60
33	2	946	С	O4'-C1'-N1	7.90	114.52	108.20
33	2	200	U	O4'-C1'-N1	7.90	114.52	108.20
33	2	1341	G	C5-C6-O6	-7.90	123.86	128.60
33	2	1849	G	C5-C6-O6	-7.90	123.86	128.60
33	2	336	С	O4'-C1'-N1	7.89	114.52	108.20
33	2	1209	С	O4'-C1'-N1	7.89	114.51	108.20
39	1	66	С	O4'-C1'-N1	7.89	114.51	108.20
33	2	484	С	O4'-C1'-N1	7.89	114.51	108.20
33	2	1103	G	C5-C6-O6	-7.89	123.86	128.60
33	2	1036	G	C5-C6-O6	-7.89	123.87	128.60
39	1	54	А	C5-C6-N6	-7.89	117.39	123.70
33	2	1713	G	N1-C6-O6	7.88	124.63	119.90
33	2	499	G	C5-C6-O6	-7.88	123.87	128.60
33	2	846	С	O4'-C1'-N1	7.88	114.51	108.20
39	1	62	С	O4'-C1'-N1	7.88	114.50	108.20
33	2	186	G	C5-C6-O6	-7.88	123.87	128.60

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123.70

117.40



-7.88

C5-C6-N6

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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1426	С	O4'-C1'-N1	7.88	114.50	108.20
33	2	628	С	O4'-C1'-N1	7.88	114.50	108.20
33	2	1727	G	C5-C6-O6	-7.87	123.88	128.60
33	2	140	U	O4'-C1'-N1	7.87	114.49	108.20
33	2	409	G	C5-C6-O6	-7.87	123.88	128.60
33	2	1282	G	N1-C6-O6	7.87	124.62	119.90
33	2	1093	G	C5-C6-O6	-7.86	123.89	128.60
33	2	191	С	O4'-C1'-N1	7.86	114.48	108.20
33	2	911	G	O4'-C1'-N9	7.85	114.48	108.20
33	2	81	U	O4'-C1'-N1	7.85	114.48	108.20
33	2	332	С	O4'-C1'-N1	7.85	114.48	108.20
33	2	1735	С	O4'-C1'-N1	7.85	114.48	108.20
33	2	1457	G	N1-C6-O6	7.85	124.61	119.90
39	1	23	С	O4'-C1'-N1	7.85	114.48	108.20
33	2	1345	G	C5-C6-O6	-7.84	123.89	128.60
33	2	947	С	O4'-C1'-N1	7.84	114.47	108.20
33	2	1830	G	C5-C6-O6	-7.84	123.90	128.60
33	2	424	G	C5-C6-O6	-7.84	123.90	128.60
33	2	1007	А	C5-C6-N6	-7.83	117.43	123.70
33	2	529	С	O4'-C1'-N1	7.83	114.47	108.20
33	2	578	G	C5-C6-O6	-7.83	123.90	128.60
33	2	355	С	O4'-C1'-N1	7.83	114.46	108.20
33	2	1697	G	C5-C6-O6	-7.83	123.90	128.60
39	1	27	С	O4'-C1'-N1	7.83	114.46	108.20
33	2	926	С	O4'-C1'-N1	7.82	114.46	108.20
33	2	972	G	C5-C6-O6	-7.82	123.91	128.60
33	2	1279	С	O4'-C1'-N1	7.82	114.46	108.20
33	2	1709	U	O4'-C1'-N1	7.82	114.46	108.20
33	2	604	G	N1-C6-O6	7.82	124.59	119.90
33	2	1323	G	C5-C6-O6	-7.82	123.91	128.60
33	2	1733	С	O4'-C1'-N1	7.82	114.45	108.20
33	2	376	С	O4'-C1'-N1	7.82	114.45	108.20
33	2	392	С	O4'-C1'-N1	7.82	114.45	108.20
33	2	1810	G	C5-C6-O6	-7.82	123.91	128.60
33	2	1105	С	C2-N1-C1'	7.81	127.39	118.80
33	2	1499	С	O4'-C1'-N1	7.81	114.44	108.20
33	2	980	С	O4'-C1'-N1	7.80	114.44	108.20
33	2	803	G	C5-C6-O6	-7.80	123.92	128.60
33	2	1214	С	O4'-C1'-N1	7.80	114.44	108.20
33	2	1542	С	O4'-C1'-N1	7.80	114.44	108.20
33	2	639	U	O4'-C1'-N1	7.80	114.44	108.20
33	2	1679	С	O4'-C1'-N1	7.80	114.44	108.20



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1722	G	C5-C6-O6	-7.80	123.92	128.60
33	2	1248	С	O4'-C1'-N1	7.79	114.44	108.20
33	2	1456	С	O4'-C1'-N1	7.79	114.44	108.20
33	2	981	G	C5-C6-O6	-7.79	123.93	128.60
33	2	1130	G	C5-C6-O6	-7.79	123.93	128.60
39	1	70	G	C5-C6-O6	-7.79	123.93	128.60
33	2	432	С	O4'-C1'-N1	7.78	114.42	108.20
33	2	1070	С	O4'-C1'-N1	7.78	114.42	108.20
33	2	1128	С	O4'-C1'-N1	7.78	114.42	108.20
33	2	1153	G	C5-C6-O6	-7.78	123.93	128.60
33	2	1498	С	O4'-C1'-N1	7.77	114.42	108.20
33	2	1025	G	C5-C6-O6	-7.77	123.94	128.60
33	2	916	А	C4-C5-C6	7.77	120.89	117.00
33	2	1090	С	O4'-C1'-N1	7.77	114.42	108.20
33	2	1711	С	O4'-C1'-N1	7.77	114.42	108.20
33	2	974	G	C5-C6-O6	-7.77	123.94	128.60
33	2	1121	С	O4'-C1'-N1	7.76	114.41	108.20
33	2	1275	С	O4'-C1'-N1	7.76	114.41	108.20
33	2	271	G	C5-C6-O6	-7.76	123.95	128.60
33	2	664	С	O4'-C1'-N1	7.75	114.40	108.20
33	2	954	G	O4'-C1'-N9	7.75	114.40	108.20
33	2	1106	G	C5-C6-O6	-7.75	123.95	128.60
33	2	1135	С	C2-N1-C1'	7.75	127.33	118.80
33	2	165	G	O4'-C1'-N9	7.75	114.40	108.20
33	2	162	С	O4'-C1'-N1	7.75	114.40	108.20
33	2	1613	С	O4'-C1'-N1	7.74	114.39	108.20
33	2	330	С	O4'-C1'-N1	7.74	114.39	108.20
33	2	489	G	N1-C6-O6	7.74	124.55	119.90
33	2	948	G	C5-C6-O6	-7.74	123.96	128.60
33	2	1102	С	O4'-C1'-N1	7.74	114.39	108.20
33	2	925	G	C5-C6-O6	-7.74	123.96	128.60
33	2	650	С	O4'-C1'-N1	7.73	114.39	108.20
33	2	1077	U	O4'-C1'-N1	7.73	114.39	108.20
33	2	1271	G	C5-C6-O6	-7.73	123.96	128.60
33	2	1147	G	C5-C6-O6	-7.72	123.97	128.60
33	2	1850	С	O4'-C1'-N1	7.72	114.38	108.20
33	2	1223	G	C5-C6-O6	-7.72	123.97	128.60
33	2	1559	С	O4'-C1'-N1	7.72	114.38	108.20
33	2	517	С	04'-C1'-N1	7.72	114.38	108.20
33	2	306	С	O4'-C1'-N1	7.72	114.37	108.20
33	2	1164	G	C5-C6-O6	-7.72	123.97	128.60
33	2	913	U	O4'-C1'-N1	7.71	114.37	108.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1624	С	O4'-C1'-N1	7.71	114.37	108.20
33	2	933	С	O4'-C1'-N1	7.70	114.36	108.20
33	2	1380	С	O4'-C1'-N1	7.70	114.36	108.20
33	2	971	G	C5-C6-O6	-7.70	123.98	128.60
33	2	407	С	O4'-C1'-N1	7.70	114.36	108.20
33	2	89	С	O4'-C1'-N1	7.69	114.35	108.20
33	2	507	С	O4'-C1'-N1	7.69	114.35	108.20
33	2	567	U	O4'-C1'-N1	7.69	114.35	108.20
33	2	1486	G	C5-C6-O6	-7.69	123.99	128.60
33	2	1831	G	N1-C6-O6	7.69	124.51	119.90
33	2	1855	G	C5-C6-O6	-7.69	123.99	128.60
33	2	881	U	O4'-C1'-N1	7.69	114.35	108.20
33	2	1429	С	O4'-C1'-N1	7.69	114.35	108.20
33	2	112	U	O4'-C1'-N1	7.69	114.35	108.20
33	2	446	С	O4'-C1'-N1	7.68	114.35	108.20
33	2	1028	С	O4'-C1'-N1	7.68	114.35	108.20
33	2	1683	С	O4'-C1'-N1	7.68	114.35	108.20
19	V	48	TYR	CB-CG-CD1	7.68	125.61	121.00
33	2	324	С	O4'-C1'-N1	7.68	114.34	108.20
33	2	174	С	O4'-C1'-N1	7.68	114.34	108.20
33	2	989	G	N1-C6-O6	7.67	124.50	119.90
33	2	1702	U	O4'-C1'-N1	7.67	114.34	108.20
33	2	1447	G	C5-C6-O6	-7.67	124.00	128.60
33	2	1750	С	O4'-C1'-N1	7.67	114.34	108.20
33	2	467	G	N1-C6-O6	7.67	124.50	119.90
33	2	1563	С	O4'-C1'-N1	7.67	114.34	108.20
33	2	1802	U	O4'-C1'-N1	7.67	114.34	108.20
33	2	530	U	O4'-C1'-N1	7.67	114.33	108.20
33	2	236	С	O4'-C1'-N1	7.66	114.33	108.20
33	2	348	С	O4'-C1'-N1	7.66	114.33	108.20
33	2	443	С	O4'-C1'-N1	7.66	114.32	108.20
33	2	1543	G	C5-C6-O6	-7.65	124.01	128.60
33	2	587	G	C5-C6-O6	-7.65	124.01	128.60
33	2	886	U	O4'-C1'-N1	7.65	114.32	108.20
33	2	1087	С	O4'-C1'-N1	7.65	114.32	108.20
33	2	235	C	N3-C4-N4	7.65	$1\overline{23.3}\overline{5}$	118.00
33	2	1218	G	C5-C6-O6	-7.65	124.01	128.60
33	2	286	C	O4'-C1'-N1	7.64	114.32	108.20
39	1	10	G	C5-C6-O6	-7.64	124.01	128.60
33	2	1492	U	O4'-C1'-N1	7.64	114.31	108.20
4	Ε	251	TYR	CB-CG-CD2	-7.64	116.42	121.00
33	2	848	G	N1-C6-O6	7.63	124.48	119.90



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1207	G	C5-C6-O6	-7.63	124.02	128.60
33	2	1415	С	O4'-C1'-N1	7.63	114.31	108.20
33	2	635	С	O4'-C1'-N1	7.63	114.31	108.20
39	1	12	С	O4'-C1'-N1	7.63	114.31	108.20
33	2	217	U	O4'-C1'-N1	7.63	114.30	108.20
33	2	1585	С	O4'-C1'-N1	7.63	114.30	108.20
33	2	105	U	O4'-C1'-N1	7.63	114.30	108.20
33	2	1478	С	O4'-C1'-N1	7.62	114.30	108.20
33	2	929	G	C5-C6-O6	-7.62	124.03	128.60
33	2	1789	G	C5-C6-O6	-7.62	124.03	128.60
33	2	894	U	O4'-C1'-N1	7.62	114.30	108.20
33	2	887	G	C5-C6-O6	-7.62	124.03	128.60
39	1	40	С	O4'-C1'-N1	7.62	114.30	108.20
33	2	481	С	O4'-C1'-N1	7.62	114.29	108.20
33	2	1053	С	C2-N1-C1'	7.62	127.18	118.80
33	2	1403	U	O4'-C1'-N1	7.62	114.29	108.20
33	2	582	С	O4'-C1'-N1	7.61	114.29	108.20
33	2	1820	G	C5-C6-O6	-7.61	124.03	128.60
33	2	1423	С	O4'-C1'-N1	7.61	114.28	108.20
39	1	4	С	O4'-C1'-N1	7.61	114.28	108.20
33	2	468	G	O4'-C1'-N9	7.60	114.28	108.20
33	2	1501	U	O4'-C1'-N1	7.60	114.28	108.20
33	2	666	С	O4'-C1'-N1	7.60	114.28	108.20
33	2	969	С	O4'-C1'-N1	7.60	114.28	108.20
33	2	24	С	O4'-C1'-N1	7.60	114.28	108.20
33	2	677	С	O3'-P-O5'	7.60	118.44	104.00
33	2	847	С	O4'-C1'-N1	7.60	114.28	108.20
33	2	1520	С	O4'-C1'-N1	7.60	114.28	108.20
33	2	914	U	O4'-C1'-N1	7.59	114.28	108.20
33	2	1050	G	C5-C6-O6	-7.59	124.04	128.60
33	2	1741	U	O4'-C1'-N1	7.59	114.28	108.20
33	2	557	С	O4'-C1'-N1	7.59	114.27	108.20
33	2	422	G	C5-C6-O6	-7.59	124.05	128.60
33	2	1475	G	C5-C6-O6	-7.59	124.05	128.60
33	2	1650	С	O4'-C1'-N1	7.58	114.27	108.20
33	2	1788	С	O4'-C1'-N1	7.58	114.27	108.20
33	2	106	С	O4'-C1'-N1	7.58	114.27	108.20
33	2	731	С	O4'-C1'-N1	7.58	114.27	108.20
33	2	1149	С	O4'-C1'-N1	7.58	114.27	108.20
33	2	1511	G	C5-C6-O6	-7.58	124.05	128.60
33	2	119	U	04'-C1'-N1	7.58	114.26	108.20
33	2	227	A	C4-C5-C6	7.58	120.79	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	187	С	O4'-C1'-N1	7.57	114.26	108.20
33	2	561	U	O4'-C1'-N1	7.57	114.26	108.20
33	2	849	С	C6-N1-C1'	-7.57	111.71	120.80
33	2	1822	С	O4'-C1'-N1	7.57	114.26	108.20
33	2	1545	G	C5-C6-O6	-7.57	124.06	128.60
33	2	944	С	O4'-C1'-N1	7.57	114.25	108.20
33	2	1273	С	O4'-C1'-N1	7.57	114.25	108.20
33	2	532	U	O4'-C1'-N1	7.56	114.25	108.20
33	2	898	G	C5-C6-O6	-7.56	124.06	128.60
33	2	1703	С	O4'-C1'-N1	7.56	114.25	108.20
33	2	1588	С	O4'-C1'-N1	7.56	114.25	108.20
33	2	414	С	O4'-C1'-N1	7.56	114.24	108.20
33	2	1143	С	O4'-C1'-N1	7.56	114.25	108.20
33	2	552	U	O4'-C1'-N1	7.55	114.24	108.20
33	2	1661	С	O4'-C1'-N1	7.55	114.24	108.20
33	2	1473	U	O4'-C1'-N1	7.55	114.24	108.20
33	2	1549	С	O4'-C1'-N1	7.55	114.24	108.20
33	2	903	G	C5-C6-O6	-7.55	124.07	128.60
33	2	1523	G	C5-C6-O6	-7.55	124.07	128.60
33	2	352	С	N3-C4-C5	-7.54	118.88	121.90
33	2	33	G	C5-C6-O6	-7.54	124.08	128.60
33	2	1806	U	O4'-C1'-N1	7.54	114.23	108.20
33	2	18	С	O4'-C1'-N1	7.54	114.23	108.20
33	2	53	С	O4'-C1'-N1	7.54	114.23	108.20
33	2	973	С	O4'-C1'-N1	7.54	114.23	108.20
33	2	1664	G	C5-C6-O6	-7.53	124.08	128.60
33	2	1331	G	C5-C6-O6	-7.52	124.09	128.60
33	2	1537	С	O4'-C1'-N1	7.52	114.22	108.20
33	2	1600	G	C5-C6-O6	-7.52	124.09	128.60
33	2	1044	G	C5-C6-O6	-7.52	124.09	128.60
33	2	1257	С	O4'-C1'-N1	7.52	114.21	108.20
33	2	1376	С	O4'-C1'-N1	7.52	114.21	108.20
39	1	68	С	O4'-C1'-N1	7.52	114.21	108.20
33	2	838	С	O4'-C1'-N1	7.51	114.21	108.20
33	2	919	G	C5-C6-O6	-7.51	124.09	128.60
33	2	1294	G	C5-C6-O6	-7.51	124.09	128.60
33	2	923	С	O4'-C1'-N1	7.51	114.21	108.20
33	2	1312	С	04'-C1'-N1	7.51	114.21	108.20
33	2	117	C	O4'-C1'-N1	7.51	114.21	108.20
33	2	17	C	O4'-C1'-N1	7.51	114.20	108.20
33	2	495	G	C5-C6-O6	-7.50	124.10	128.60
- 33	2	470	G	C5-C6-O6	-7.50	124.10	128.60



108.20

108.20

108.20

108.20

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	1500	U	O4'-C1'-N1	7.50	114.20	108.20
33	2	1836	С	O4'-C1'-N1	7.50	114.20	108.20
33	2	1071	С	O4'-C1'-N1	7.49	114.19	108.20
33	2	1815	U	O4'-C1'-N1	7.49	114.19	108.20
33	2	1452	G	C5-C6-O6	-7.49	124.11	128.60
33	2	898	G	O4'-C1'-N9	7.49	114.19	108.20
33	2	151	С	O4'-C1'-N1	7.49	114.19	108.20
33	2	585	U	O4'-C1'-N1	7.48	114.19	108.20
33	2	1385	С	O4'-C1'-N1	7.48	114.19	108.20
33	2	15	U	O4'-C1'-N1	7.48	114.18	108.20
33	2	970	С	O4'-C1'-N1	7.48	114.18	108.20
33	2	1085	G	C5-C6-O6	-7.48	124.11	128.60
33	2	1092	G	C5-C6-O6	-7.48	124.11	128.60
33	2	1347	G	C5-C6-O6	-7.48	124.11	128.60
33	2	999	U	O4'-C1'-N1	7.48	114.18	108.20
33	2	1123	С	O4'-C1'-N1	7.47	114.18	108.20
33	2	411	G	C5-C6-O6	-7.47	124.12	128.60
33	2	906	G	O4'-C1'-N9	7.47	114.18	108.20
33	2	1814	G	C5-C6-O6	-7.47	124.12	128.60
33	2	928	G	C5-C6-O6	-7.47	124.12	128.60
33	2	869	G	C5-C6-O6	-7.47	124.12	128.60
33	2	1000	U	O4'-C1'-N1	7.47	114.17	108.20
39	1	16	G	C5-C6-O6	-7.47	124.12	128.60
33	2	612	С	O4'-C1'-N1	7.47	114.17	108.20
33	2	978	G	C5-C6-O6	-7.46	124.12	128.60
33	2	1263	С	O4'-C1'-N1	7.46	114.17	108.20
33	2	1436	С	O4'-C1'-N1	7.46	114.17	108.20
33	2	1805	С	O4'-C1'-N1	7.46	114.17	108.20
33	2	1369	С	O4'-C1'-N1	7.46	114.17	108.20
34	3	61	С	O4'-C1'-N1	7.46	114.17	108.20
39	1	34	С	O4'-C1'-N1	7.46	114.17	108.20
33	2	935	U	O4'-C1'-N1	7.46	114.17	108.20
33	2	198	U	O4'-C1'-N1	7.46	114.17	108.20
33	2	863	G	C5-C6-O6	-7.46	124.13	128.60
33	2	1737	С	O4'-C1'-N1	7.46	114.17	108.20
33	2	372	С	O4'-C1'-N1	7.45	114.16	108.20
33	2	608	С	O4'-C1'-N1	7.45	114.16	108.20
33	2	1283	A	C4-C5-C6	7.45	120.73	117.00

С

С

С

U

O4'-C1'-N1

O4'-C1'-N1

O4'-C1'-N1

O4'-C1'-N1

1560

990

1700

1842

2

2

2

2

33

33

33 33

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114.16

114.16

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114.16



7.45

7.45

7.45

7.45

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal $(^{o})$
33	2	1670	А	O4'-C1'-N9	7.44	114.15	108.20
33	2	96	С	O4'-C1'-N1	7.44	114.15	108.20
33	2	984	С	O4'-C1'-N1	7.44	114.15	108.20
33	2	1319	U	O4'-C1'-N1	7.44	114.15	108.20
33	2	1191	А	O4'-C1'-N9	7.44	114.15	108.20
33	2	1698	С	O4'-C1'-N1	7.43	114.14	108.20
33	2	728	U	O4'-C1'-N1	7.43	114.14	108.20
33	2	524	G	C5-C6-O6	-7.43	124.14	128.60
33	2	802	U	O4'-C1'-N1	7.42	114.14	108.20
33	2	150	А	N1-C6-N6	7.42	123.05	118.60
33	2	508	G	C5-C6-O6	-7.42	124.15	128.60
33	2	393	G	C5-C6-O6	-7.42	124.15	128.60
33	2	570	U	O4'-C1'-N1	7.42	114.13	108.20
33	2	312	С	O4'-C1'-N1	7.41	114.13	108.20
33	2	1013	U	O4'-C1'-N1	7.41	114.13	108.20
33	2	1387	С	O4'-C1'-N1	7.41	114.13	108.20
33	2	1556	А	C5-C6-N6	-7.41	117.77	123.70
33	2	1827	С	O4'-C1'-N1	7.41	114.13	108.20
33	2	143	U	O4'-C1'-N1	7.41	114.13	108.20
33	2	1258	С	O4'-C1'-N1	7.41	114.13	108.20
33	2	1622	С	O4'-C1'-N1	7.41	114.13	108.20
33	2	1116	U	O4'-C1'-N1	7.41	114.12	108.20
33	2	496	G	C5-C6-O6	-7.40	124.16	128.60
33	2	806	А	O4'-C1'-N9	7.40	114.12	108.20
33	2	1747	С	O4'-C1'-N1	7.39	114.11	108.20
33	2	1734	С	O4'-C1'-N1	7.39	114.11	108.20
33	2	1301	С	O4'-C1'-N1	7.39	114.11	108.20
33	2	1381	G	C5-C6-O6	-7.38	124.17	128.60
33	2	1425	G	C5-C6-O6	-7.38	124.17	128.60
33	2	1208	G	O4'-C1'-N9	7.38	114.11	108.20
33	2	1684	С	O4'-C1'-N1	7.38	114.11	108.20
33	2	675	А	OP2-P-O3'	7.38	121.44	105.20
33	2	1307	С	O4'-C1'-N1	7.37	114.09	108.20
33	2	1673	А	O4'-C1'-N9	7.37	114.09	108.20
33	2	473	С	O4'-C1'-N1	7.37	114.09	108.20
33	2	1404	U	O4'-C1'-N1	7.36	114.09	108.20
33	2	1568	G	C5-C6-O6	-7.36	124.18	128.60
33	2	428	G	O4'-C1'-N9	7.36	114.09	108.20
33	2	395	G	C5-C6-O6	-7.36	124.19	128.60
33	2	71	G	O4'-C1'-N9	7.36	114.08	108.20
33	2	1746	С	N3-C4-N4	7.35	123.15	118.00
33	2	1320	G	C5-C6-O6	-7.35	124.19	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1233	С	O4'-C1'-N1	7.35	114.08	108.20
33	2	446	С	N3-C4-N4	7.34	123.14	118.00
33	2	797	U	OP2-P-O3'	7.34	121.36	105.20
33	2	987	G	C5-C6-O6	-7.34	124.19	128.60
33	2	1412	С	O4'-C1'-N1	7.34	114.07	108.20
33	2	1262	С	O4'-C1'-N1	7.34	114.07	108.20
33	2	468	G	C5-C6-O6	-7.33	124.20	128.60
33	2	1682	С	O4'-C1'-N1	7.33	114.07	108.20
33	2	173	А	C5-C6-N6	-7.33	117.83	123.70
33	2	235	С	O4'-C1'-N1	7.33	114.06	108.20
33	2	1310	U	O4'-C1'-N1	7.33	114.06	108.20
33	2	406	U	O4'-C1'-N1	7.33	114.06	108.20
33	2	1446	G	C5-C6-O6	-7.33	124.20	128.60
33	2	892	U	O4'-C1'-N1	7.33	114.06	108.20
33	2	1075	С	O4'-C1'-N1	7.33	114.06	108.20
33	2	616	G	C5-C6-O6	-7.33	124.20	128.60
33	2	1285	U	O4'-C1'-N1	7.33	114.06	108.20
33	2	86	С	O4'-C1'-N1	7.32	114.06	108.20
33	2	1423	С	N3-C4-N4	7.32	123.12	118.00
33	2	1554	С	O4'-C1'-N1	7.32	114.05	108.20
33	2	1122	G	O4'-C1'-N9	7.31	114.05	108.20
33	2	1776	G	O4'-C1'-N9	7.31	114.05	108.20
34	3	69	G	O4'-C1'-N9	7.31	114.05	108.20
33	2	611	С	O4'-C1'-N1	7.31	114.05	108.20
33	2	1577	С	O4'-C1'-N1	7.31	114.05	108.20
33	2	819	U	O4'-C1'-N1	7.31	114.05	108.20
33	2	1088	G	C5-C6-O6	-7.30	124.22	128.60
33	2	1162	G	C5-C6-O6	-7.30	124.22	128.60
33	2	1440	U	O4'-C1'-N1	7.30	114.04	108.20
33	2	586	U	O4'-C1'-N1	7.30	114.04	108.20
33	2	588	G	C5-C6-O6	-7.30	124.22	128.60
33	2	1655	С	C6-N1-C1'	-7.30	112.04	120.80
33	2	206	А	C4-C5-C6	7.29	120.65	117.00
33	2	668	U	O4'-C1'-N1	7.29	114.03	108.20
33	2	1811	G	C5-C6-O6	-7.29	124.22	128.60
33	2	1796	С	O4'-C1'-N1	7.29	114.03	108.20
33	2	21	U	O4'-C1'-N1	7.29	114.03	108.20
33	2	182	C	O4'-C1'-N1	7.29	114.03	108.20
33	2	216	U	O4'-C1'-N1	7.29	114.03	108.20
33	2	991	G	C5-C6-O6	-7.29	124.23	128.60
33	2	1724	U	O4'-C1'-N1	7.28	114.03	108.20
33	2	465	С	O4'-C1'-N1	7.28	114.03	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	929	G	O4'-C1'-N9	7.28	114.03	108.20
33	2	66	G	C5-C6-O6	-7.28	124.23	128.60
33	2	961	U	O4'-C1'-N1	7.28	114.02	108.20
33	2	1215	С	O4'-C1'-N1	7.28	114.02	108.20
33	2	872	С	N3-C4-N4	7.28	123.09	118.00
33	2	891	G	C5-C6-O6	-7.28	124.23	128.60
33	2	1067	G	C5-C6-O6	-7.27	124.24	128.60
33	2	456	G	C5-C6-O6	-7.27	124.24	128.60
33	2	93	U	O4'-C1'-N1	7.27	114.02	108.20
33	2	1104	G	C5-C6-O6	-7.27	124.24	128.60
33	2	938	G	C5-C6-O6	-7.26	124.24	128.60
31	h	65	TYR	CB-CG-CD1	7.26	125.36	121.00
33	2	1055	G	C5-C6-O6	-7.26	124.24	128.60
33	2	1141	А	C4-C5-C6	7.26	120.63	117.00
33	2	231	С	O4'-C1'-N1	7.26	114.01	108.20
33	2	1424	G	C5-C6-O6	-7.26	124.24	128.60
33	2	1769	U	O4'-C1'-N1	7.26	114.01	108.20
33	2	1792	С	O4'-C1'-N1	7.26	114.00	108.20
33	2	1836	С	N3-C4-N4	7.26	123.08	118.00
33	2	1854	А	C5-C6-N6	-7.26	117.89	123.70
33	2	834	G	O4'-C1'-N9	7.25	114.00	108.20
33	2	930	G	C5-C6-O6	-7.25	124.25	128.60
33	2	1065	U	O4'-C1'-N1	7.25	114.00	108.20
33	2	28	U	O4'-C1'-N1	7.25	114.00	108.20
33	2	1550	U	O4'-C1'-N1	7.25	114.00	108.20
33	2	1720	U	O4'-C1'-N1	7.25	114.00	108.20
33	2	1175	G	C5-C6-O6	-7.25	124.25	128.60
33	2	1754	G	C5-C6-O6	-7.25	124.25	128.60
33	2	1253	G	C5-C6-O6	-7.24	124.25	128.60
33	2	1558	G	C5-C6-O6	-7.24	124.25	128.60
33	2	491	С	O4'-C1'-N1	7.24	113.99	108.20
33	2	1003	С	O4'-C1'-N1	7.24	113.99	108.20
33	2	1751	G	C5-C6-O6	-7.24	124.26	128.60
33	2	412	U	O4'-C1'-N1	7.24	113.99	108.20
33	2	869	G	P-O3'-C3'	7.24	128.38	119.70
33	2	1409	G	C5-C6-O6	-7.24	124.26	128.60
33	2	1592	С	O4'-C1'-N1	7.24	113.99	108.20
33	2	1712	С	O4'-C1'-N1	7.23	113.99	108.20
33	2	180	G	C5-C6-O6	-7.23	124.26	128.60
33	2	527	С	O4'-C1'-N1	7.23	113.99	108.20
33	2	433	U	04'-C1'-N1	7.23	113.98	108.20
33	2	1325	U	O4'-C1'-N1	7.23	113.98	108.20



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Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	478	U	O4'-C1'-N1	7.22	113.98	108.20
39	1	51	U	O4'-C1'-N1	7.22	113.98	108.20
33	2	1527	С	O4'-C1'-N1	7.22	113.98	108.20
33	2	399	С	O4'-C1'-N1	7.22	113.98	108.20
33	2	189	G	C5-C6-O6	-7.22	124.27	128.60
33	2	419	С	O4'-C1'-N1	7.22	113.98	108.20
33	2	636	G	C5-C6-O6	-7.22	124.27	128.60
33	2	927	С	O4'-C1'-N1	7.22	113.98	108.20
33	2	1587	С	O4'-C1'-N1	7.22	113.97	108.20
33	2	519	А	C5-C6-N6	-7.22	117.93	123.70
33	2	1172	G	C5-C6-O6	-7.21	124.27	128.60
33	2	1225	G	C5-C6-O6	-7.21	124.27	128.60
33	2	471	С	O4'-C1'-N1	7.21	113.97	108.20
33	2	957	G	C5-C6-O6	-7.21	124.28	128.60
33	2	199	G	C5-C6-O6	-7.21	124.28	128.60
33	2	1681	G	C5-C6-O6	-7.21	124.28	128.60
33	2	1418	G	C5-C6-O6	-7.20	124.28	128.60
33	2	35	С	O4'-C1'-N1	7.20	113.96	108.20
33	2	1264	С	O4'-C1'-N1	7.20	113.96	108.20
33	2	1305	С	O4'-C1'-N1	7.20	113.96	108.20
33	2	1351	С	O4'-C1'-N1	7.20	113.96	108.20
33	2	325	G	C5-C6-O6	-7.20	124.28	128.60
33	2	590	G	C5-C6-O6	-7.20	124.28	128.60
33	2	1198	U	O4'-C1'-N1	7.20	113.96	108.20
33	2	1555	U	O4'-C1'-N1	7.20	113.96	108.20
33	2	368	U	O4'-C1'-N1	7.19	113.95	108.20
33	2	1039	G	C5-C6-O6	-7.19	124.29	128.60
33	2	1321	G	C5-C6-O6	-7.19	124.29	128.60
33	2	1729	G	C5-C6-O6	-7.19	124.29	128.60
33	2	1230	С	O4'-C1'-N1	7.19	113.95	108.20
39	1	65	С	O4'-C1'-N1	7.19	113.95	108.20
33	2	1373	U	O4'-C1'-N1	7.18	113.95	108.20
33	2	1672	U	O4'-C1'-N1	7.18	113.95	108.20
34	3	65	G	C5-C6-O6	-7.18	124.29	128.60
33	2	213	С	O4'-C1'-N1	7.18	113.95	108.20
33	2	397	G	C5-C6-O6	-7.18	124.29	128.60
33	2	447	С	O4'-C1'-N1	7.18	113.94	108.20
33	2	575	C	O4'-C1'-N1	7.18	113.94	108.20
33	2	864	G	C5-C6-O6	-7.18	124.29	128.60
33	2	215	U	O4'-C1'-N1	7.18	113.94	108.20
33	2	$14\overline{64}$	C	O4'-C1'-N1	7.18	113.94	108.20
33	2	1793	G	C5-C6-O6	-7.17	124.30	128.60



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
39	1	72	U	O4'-C1'-N1	7.17	113.94	108.20
33	2	30	С	O4'-C1'-N1	7.17	113.94	108.20
33	2	989	G	C5-C6-O6	-7.17	124.30	128.60
33	2	343	С	O4'-C1'-N1	7.17	113.93	108.20
31	h	65	TYR	CB-CG-CD2	-7.16	116.70	121.00
33	2	108	G	C5-C6-O6	-7.16	124.30	128.60
33	2	1184	А	C4-C5-C6	7.16	120.58	117.00
33	2	347	С	O4'-C1'-N1	7.16	113.93	108.20
33	2	994	А	C4-C5-C6	7.16	120.58	117.00
33	2	1120	С	O4'-C1'-N1	7.16	113.93	108.20
33	2	1041	U	O4'-C1'-N1	7.16	113.92	108.20
33	2	1180	G	C5-C6-O6	-7.16	124.31	128.60
33	2	1481	U	O4'-C1'-N1	7.16	113.92	108.20
33	2	1376	С	N3-C4-N4	7.15	123.01	118.00
33	2	593	С	O4'-C1'-N1	7.15	113.92	108.20
33	2	1117	G	C5-C6-O6	-7.14	124.31	128.60
33	2	849	С	O4'-C1'-N1	7.14	113.92	108.20
33	2	1640	С	O4'-C1'-N1	7.14	113.91	108.20
33	2	840	U	O4'-C1'-N1	7.13	113.91	108.20
33	2	36	U	O4'-C1'-N1	7.13	113.91	108.20
33	2	671	U	O4'-C1'-N1	7.13	113.91	108.20
33	2	287	U	O4'-C1'-N1	7.13	113.91	108.20
33	2	328	G	C5-C6-O6	-7.13	124.32	128.60
33	2	844	U	O4'-C1'-N1	7.13	113.91	108.20
33	2	1316	G	C5-C6-O6	-7.13	124.32	128.60
33	2	637	U	O4'-C1'-N1	7.13	113.90	108.20
33	2	1395	С	O4'-C1'-N1	7.13	113.90	108.20
39	1	12	С	N3-C4-N4	7.13	122.99	118.00
33	2	334	U	O4'-C1'-N1	7.12	113.90	108.20
33	2	1765	G	C5-C6-O6	-7.12	124.33	128.60
39	1	61	С	O4'-C1'-N1	7.12	113.90	108.20
33	2	1391	С	O4'-C1'-N1	7.12	113.89	108.20
33	2	197	U	C2-N1-C1'	7.12	126.24	117.70
39	1	64	U	O4'-C1'-N1	7.11	113.89	108.20
33	2	1158	С	O4'-C1'-N1	7.11	113.89	108.20
33	2	1557	С	O4'-C1'-N1	7.11	113.89	108.20
33	2	1681	G	O4'-C1'-N9	7.11	113.89	108.20
33	2	1755	U	O4'-C1'-N1	7.11	113.89	108.20
33	2	1834	U	O4'-C1'-N1	7.11	113.89	108.20
33	2	1655	С	O4'-C1'-N1	7.11	113.88	108.20
33	2	377	С	O4'-C1'-N1	7.10	113.88	108.20
33	2	599	U	04'-C1'-N1	7.10	113.88	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°)
33	2	1570	G	C5-C6-O6	-7.10	124.34	128.60
33	2	374	U	O4'-C1'-N1	7.10	113.88	108.20
39	1	43	G	C5-C6-O6	-7.10	124.34	128.60
33	2	513	А	O4'-C1'-N9	7.10	113.88	108.20
33	2	544	А	O4'-C1'-N9	7.10	113.88	108.20
33	2	1063	С	O4'-C1'-N1	7.10	113.88	108.20
33	2	1178	А	C4-C5-C6	7.10	120.55	117.00
33	2	1665	С	O4'-C1'-N1	7.10	113.88	108.20
33	2	1567	С	O4'-C1'-N1	7.10	113.88	108.20
33	2	1671	U	O4'-C1'-N1	7.10	113.88	108.20
33	2	480	С	O4'-C1'-N1	7.09	113.88	108.20
33	2	1239	U	O4'-C1'-N1	7.09	113.88	108.20
33	2	114	G	C5-C6-O6	-7.09	124.34	128.60
33	2	623	С	O4'-C1'-N1	7.09	113.88	108.20
33	2	1474	U	O4'-C1'-N1	7.09	113.87	108.20
33	2	1298	G	C5-C6-O6	-7.09	124.35	128.60
33	2	1773	G	C5-C6-O6	-7.09	124.35	128.60
33	2	1774	G	O4'-C1'-N9	7.09	113.87	108.20
33	2	1170	U	O4'-C1'-N1	7.08	113.87	108.20
33	2	391	А	N1-C6-N6	7.08	122.85	118.60
33	2	730	С	O4'-C1'-N1	7.08	113.86	108.20
33	2	1159	С	O4'-C1'-N1	7.08	113.86	108.20
33	2	1533	С	O4'-C1'-N1	7.08	113.86	108.20
33	2	1612	G	C5-C6-O6	-7.08	124.36	128.60
33	2	1402	G	C5-C6-O6	-7.07	124.36	128.60
33	2	1569	С	O4'-C1'-N1	7.07	113.86	108.20
39	1	23	С	N3-C4-N4	7.07	122.95	118.00
33	2	224	U	P-O3'-C3'	7.07	128.19	119.70
33	2	1809	A	C4-C5-C6	7.07	120.53	117.00
33	2	415	G	C5-C6-O6	-7.07	124.36	128.60
33	2	815	G	C5-C6-O6	-7.07	124.36	128.60
33	2	949	С	O4'-C1'-N1	7.07	113.85	108.20
33	2	373	G	C5-C6-O6	-7.07	124.36	128.60
33	2	1750	С	N3-C4-N4	7.07	122.95	118.00
33	2	1848	U	O4'-C1'-N1	7.06	113.85	108.20
33	2	171	A	N1-C6-N6	7.06	122.84	118.60
33	2	505	G	C5-C6-O6	-7.06	124.36	128.60
33	2	966	G	C5-C6-O6	-7.06	124.36	128.60
33	2	181	A	C4-C5-C6	7.06	120.53	117.00
33	2	545	A	C5-C6-N6	-7.06	118.05	123.70
33	2	211	U	O4'-C1'-N1	7.06	113.84	108.20
33	2	1556	A	C4-C5-C6	7.06	120.53	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal $(^{o})$
33	2	1111	U	C2-N1-C1'	7.05	126.16	117.70
33	2	1335	U	O4'-C1'-N1	7.05	113.84	108.20
33	2	1680	U	O4'-C1'-N1	7.05	113.84	108.20
33	2	413	U	O4'-C1'-N1	7.05	113.84	108.20
33	2	895	U	O4'-C1'-N1	7.05	113.84	108.20
33	2	34	U	O4'-C1'-N1	7.04	113.84	108.20
33	2	321	С	O4'-C1'-N1	7.04	113.84	108.20
33	2	1562	G	C5-C6-O6	-7.04	124.37	128.60
33	2	349	U	O4'-C1'-N1	7.04	113.83	108.20
33	2	219	U	O4'-C1'-N1	7.04	113.83	108.20
33	2	317	G	O4'-C1'-N9	7.04	113.83	108.20
33	2	472	G	C5-C6-O6	-7.04	124.38	128.60
33	2	474	А	C4-C5-C6	7.04	120.52	117.00
33	2	588	G	O4'-C1'-N9	7.04	113.83	108.20
33	2	635	С	N3-C4-N4	7.04	122.93	118.00
33	2	17	С	N3-C4-N4	7.04	122.92	118.00
33	2	1046	А	O4'-C1'-N9	7.04	113.83	108.20
34	3	64	G	C5-C6-O6	-7.04	124.38	128.60
33	2	238	G	C5-C6-O6	-7.03	124.38	128.60
33	2	1045	А	C4-C5-C6	7.03	120.52	117.00
33	2	655	G	C5-C6-O6	-7.03	124.38	128.60
33	2	1721	G	C5-C6-O6	-7.03	124.38	128.60
39	1	71	С	N3-C4-N4	7.03	122.92	118.00
33	2	1704	G	C5-C6-O6	-7.03	124.38	128.60
33	2	541	U	O4'-C1'-N1	7.03	113.82	108.20
33	2	1308	G	C5-C6-O6	-7.03	124.38	128.60
33	2	1200	А	C5-C6-N6	-7.03	118.08	123.70
33	2	1405	А	C5-C6-N6	-7.03	118.08	123.70
33	2	878	U	O4'-C1'-N1	7.02	113.82	108.20
33	2	1240	U	O4'-C1'-N1	7.02	113.82	108.20
33	2	1490	U	O4'-C1'-N1	7.02	113.82	108.20
39	1	41	С	O4'-C1'-N1	7.02	113.82	108.20
33	2	449	С	O4'-C1'-N1	7.02	113.81	108.20
33	2	536	G	P-O3'-C3'	7.02	128.12	119.70
33	2	602	U	O4'-C1'-N1	7.02	113.81	108.20
33	2	49	С	O4'-C1'-N1	7.01	113.81	108.20
33	2	322	G	C5-C6-O6	-7.01	124.39	128.60
33	2	402	G	C5-C6-O6	-7.01	124.39	128.60
33	2	1355	U	O4'-C1'-N1	7.01	113.81	108.20
33	2	549	G	O4'-C1'-N9	7.01	113.81	108.20
33	2	730	С	N3-C4-N4	7.01	122.91	118.00
33	2	1808	G	C5-C6-O6	-7.01	124.39	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	460	G	C5-C6-O6	-7.01	124.39	128.60
33	2	1647	G	C5-C6-O6	-7.01	124.39	128.60
33	2	207	U	O4'-C1'-N1	7.00	113.80	108.20
33	2	229	А	C4-C5-C6	7.00	120.50	117.00
33	2	1603	U	O4'-C1'-N1	7.00	113.80	108.20
33	2	1628	А	C4-C5-C6	7.00	120.50	117.00
33	2	462	С	O4'-C1'-N1	7.00	113.80	108.20
33	2	1462	G	C5-C6-O6	-7.00	124.40	128.60
33	2	31	U	O4'-C1'-N1	7.00	113.80	108.20
33	2	101	U	O4'-C1'-N1	7.00	113.80	108.20
33	2	1241	G	C5-C6-O6	-6.99	124.40	128.60
33	2	321	С	N3-C4-N4	6.99	122.89	118.00
33	2	1357	G	C5-C6-O6	-6.99	124.41	128.60
33	2	1513	С	O4'-C1'-N1	6.99	113.79	108.20
33	2	963	С	O4'-C1'-N1	6.99	113.79	108.20
33	2	1306	U	O4'-C1'-N1	6.98	113.79	108.20
33	2	1032	А	C5-C6-N6	-6.98	118.11	123.70
33	2	331	С	O4'-C1'-N1	6.98	113.78	108.20
33	2	1637	U	O4'-C1'-N1	6.98	113.78	108.20
33	2	20	G	C5-C6-O6	-6.98	124.41	128.60
33	2	1074	С	O4'-C1'-N1	6.98	113.78	108.20
33	2	86	С	N3-C4-N4	6.98	122.88	118.00
33	2	520	U	O4'-C1'-N1	6.98	113.78	108.20
33	2	1471	G	C5-C6-O6	-6.98	124.41	128.60
33	2	1559	С	N3-C4-N4	6.97	122.88	118.00
8	Ι	28	TYR	CB-CG-CD2	-6.97	116.82	121.00
33	2	1624	С	N3-C4-N4	6.97	122.88	118.00
33	2	116	U	O4'-C1'-N1	6.96	113.77	108.20
33	2	153	G	C5-C6-O6	-6.96	124.42	128.60
33	2	1409	G	O4'-C1'-N9	6.96	113.77	108.20
33	2	1858	U	O4'-C1'-N1	6.96	113.77	108.20
33	2	311	С	N3-C4-N4	6.96	122.87	118.00
33	2	1668	U	O4'-C1'-N1	6.96	113.77	108.20
33	2	210	G	C5-C6-O6	-6.96	124.42	128.60
33	2	100	U	O4'-C1'-N1	6.96	113.76	108.20
33	2	1252	G	C5-C6-O6	-6.96	124.43	128.60
33	2	936	U	04'-C1'-N1	6.95	113.76	108.20
33	2	1326	G	C5-C6-O6	-6.95	124.43	128.60
33	2	1482	A	O4'-C1'-N9	6.95	113.76	108.20
33	2	1715	U	04'-C1'-N1	6.95	113.76	108.20
33	2	378	U	04'-C1'-N1	6.95	113.76	108.20
33	2	1023	A	C4-C5-C6	6.95	120.47	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
30	g	101	PHE	CB-CG-CD1	6.95	125.66	120.80
33	2	1056	А	O4'-C1'-N9	6.95	113.76	108.20
33	2	1188	U	O4'-C1'-N1	6.95	113.76	108.20
33	2	1666	G	C5-C6-O6	-6.95	124.43	128.60
33	2	1346	U	O4'-C1'-N1	6.94	113.75	108.20
33	2	301	С	O4'-C1'-N1	6.94	113.75	108.20
33	2	1200	А	C4-C5-C6	6.94	120.47	117.00
33	2	1453	U	O4'-C1'-N1	6.94	113.75	108.20
33	2	1015	С	O4'-C1'-N1	6.94	113.75	108.20
33	2	1173	U	O4'-C1'-N1	6.93	113.75	108.20
39	1	71	С	O4'-C1'-N1	6.93	113.75	108.20
33	2	152	U	O4'-C1'-N1	6.93	113.75	108.20
33	2	960	А	C4-C5-C6	6.93	120.47	117.00
33	2	1493	G	C5-C6-O6	-6.93	124.44	128.60
39	1	63	А	C5-C6-N6	-6.93	118.15	123.70
39	1	36	U	O4'-C1'-N1	6.93	113.75	108.20
33	2	891	G	O4'-C1'-N9	6.93	113.74	108.20
33	2	1516	С	N3-C4-N4	6.92	122.85	118.00
33	2	1623	С	O4'-C1'-N1	6.92	113.74	108.20
33	2	874	G	C5-C6-O6	-6.92	124.45	128.60
33	2	808	А	C5-C6-N6	-6.92	118.16	123.70
33	2	577	А	C4-C5-C6	6.92	120.46	117.00
33	2	1394	G	C5-C6-O6	-6.92	124.45	128.60
33	2	665	U	O4'-C1'-N1	6.92	113.73	108.20
33	2	1503	G	C5-C6-O6	-6.92	124.45	128.60
33	2	977	А	C5-C6-N6	-6.92	118.17	123.70
33	2	370	G	C5-C6-O6	-6.91	124.45	128.60
33	2	1163	G	C5-C6-O6	-6.91	124.45	128.60
33	2	1414	С	O4'-C1'-N1	6.91	113.73	108.20
33	2	1620	U	O4'-C1'-N1	6.91	113.73	108.20
33	2	672	U	O4'-C1'-N1	6.91	113.73	108.20
33	2	1228	U	O4'-C1'-N1	6.91	113.73	108.20
39	1	18	G	P-O3'-C3'	6.91	127.99	119.70
33	2	222	G	C5-C6-O6	-6.91	124.46	128.60
33	2	305	U	O4'-C1'-N1	6.91	113.73	108.20
33	2	603	С	O4'-C1'-N1	6.91	113.72	108.20
33	2	1276	G	C5-C6-O6	-6.91	124.46	128.60
33	2	1768	С	N3-C4-N4	6.90	122.83	118.00
33	2	341	G	O4'-C1'-N9	$6.9\overline{0}$	$113.7\overline{2}$	108.20
4	Е	251	TYR	CB-CG-CD1	6.90	125.14	121.00
33	2	799	C	O4'-C1'-N1	$6.9\overline{0}$	$113.7\overline{2}$	108.20
33	2	1165	G	C5-C6-O6	-6.90	124.46	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1396	U	O4'-C1'-N1	6.90	113.72	108.20
33	2	1833	U	O4'-C1'-N1	6.90	113.72	108.20
33	2	383	U	O4'-C1'-N1	6.90	113.72	108.20
33	2	615	G	C5-C6-O6	-6.90	124.46	128.60
33	2	524	G	O4'-C1'-N9	6.90	113.72	108.20
33	2	910	U	O4'-C1'-N1	6.90	113.72	108.20
33	2	437	А	C4-C5-C6	6.89	120.45	117.00
33	2	955	G	C5-C6-O6	-6.89	124.46	128.60
33	2	1646	А	C4-C5-C6	6.89	120.45	117.00
33	2	537	G	C5-C6-O6	-6.89	124.47	128.60
33	2	1222	G	C5-C6-O6	-6.89	124.47	128.60
33	2	1700	С	N3-C4-N4	6.89	122.82	118.00
33	2	1469	G	C5-C6-O6	-6.88	124.47	128.60
39	1	55	U	O4'-C1'-N1	6.88	113.71	108.20
33	2	16	G	C5-C6-O6	-6.88	124.47	128.60
33	2	194	С	O4'-C1'-N1	6.88	113.70	108.20
33	2	1009	U	O4'-C1'-N1	6.88	113.70	108.20
33	2	1042	U	O4'-C1'-N1	6.88	113.70	108.20
33	2	1086	С	O4'-C1'-N1	6.88	113.70	108.20
39	1	14	С	O4'-C1'-N1	6.88	113.70	108.20
33	2	1525	U	O4'-C1'-N1	6.88	113.70	108.20
33	2	286	С	N3-C4-N4	6.88	122.81	118.00
33	2	486	С	O4'-C1'-N1	6.87	113.70	108.20
33	2	1197	U	O4'-C1'-N1	6.87	113.70	108.20
33	2	1742	С	O4'-C1'-N1	6.87	113.70	108.20
33	2	14	С	O4'-C1'-N1	6.87	113.69	108.20
33	2	465	С	N3-C4-N4	6.87	122.81	118.00
39	1	50	А	C5-C6-N6	-6.87	118.20	123.70
33	2	173	А	C4-C5-C6	6.87	120.43	117.00
33	2	51	U	O4'-C1'-N1	6.86	113.69	108.20
33	2	501	U	O4'-C1'-N1	6.86	113.69	108.20
39	1	18	G	OP1-P-O3'	-6.86	90.11	105.20
33	2	1584	А	C4-C5-C6	6.86	120.43	117.00
33	2	921	G	C5-C6-O6	-6.86	124.48	128.60
33	2	1463	С	O4'-C1'-N1	6.86	113.69	108.20
33	2	124	U	O4'-C1'-N1	6.86	113.68	108.20
33	2	230	С	04'-C1'-N1	6.86	113.68	108.20
33	2	1220	G	C5-C6-O6	-6.86	124.49	128.60
33	2	1353	A	C4-C5-C6	6.86	120.43	117.00
33	2	1730	A	C4-C5-C6	6.86	120.43	117.00
33	2	842	G	C5-C6-O6	-6.85	124.49	128.60
- 33	2	153	G	O4'-C1'-N9	6.85	113.68	108.20


Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	26	U	O4'-C1'-N1	6.85	113.68	108.20
33	2	967	G	C5-C6-O6	-6.85	124.49	128.60
33	2	1035	С	O4'-C1'-N1	6.85	113.68	108.20
33	2	1287	А	C4-C5-C6	6.85	120.42	117.00
33	2	852	С	O4'-C1'-N1	6.84	113.68	108.20
33	2	1021	U	O4'-C1'-N1	6.84	113.68	108.20
39	1	33	С	O4'-C1'-N1	6.84	113.68	108.20
33	2	75	G	C5-C6-O6	-6.84	124.49	128.60
33	2	168	С	O4'-C1'-N1	6.84	113.67	108.20
33	2	1199	G	C5-C6-O6	-6.84	124.49	128.60
33	2	1049	С	O4'-C1'-N1	6.84	113.67	108.20
33	2	1578	С	O4'-C1'-N1	6.84	113.67	108.20
39	1	47	U	O4'-C1'-N1	6.84	113.67	108.20
33	2	554	А	C5-C6-N6	-6.83	118.23	123.70
33	2	583	С	O4'-C1'-N1	6.83	113.67	108.20
33	2	962	U	O4'-C1'-N1	6.83	113.67	108.20
33	2	1243	С	O4'-C1'-N1	6.83	113.67	108.20
39	1	48	С	N3-C4-C5	-6.83	119.17	121.90
33	2	504	U	O4'-C1'-N1	6.83	113.67	108.20
33	2	888	U	O4'-C1'-N1	6.83	113.67	108.20
33	2	1171	G	C5-C6-O6	-6.83	124.50	128.60
33	2	1618	А	O4'-C1'-N9	6.83	113.66	108.20
33	2	480	С	N3-C4-N4	6.82	122.78	118.00
33	2	998	U	O4'-C1'-N1	6.82	113.66	108.20
34	3	62	G	C5-C6-O6	-6.82	124.51	128.60
33	2	627	U	O4'-C1'-N1	6.82	113.66	108.20
33	2	99	А	C4-C5-C6	6.82	120.41	117.00
33	2	414	С	N3-C4-N4	6.82	122.77	118.00
33	2	933	С	N3-C4-N4	6.82	122.77	118.00
33	2	1788	C	N3-C4-N4	6.82	122.77	118.00
33	2	614	С	O4'-C1'-N1	6.82	113.65	108.20
33	2	1406	С	O4'-C1'-N1	6.82	113.65	108.20
33	2	1575	A	C5-C6-N6	-6.82	118.25	123.70
33	2	109	U	O4'-C1'-N1	6.82	113.65	108.20
33	2	1095	G	C5-C6-O6	-6.82	124.51	128.60
33	2	1804	U	O4'-C1'-N1	6.82	113.65	108.20
33	2	1217	G	C5-C6-O6	-6.81	124.51	128.60
33	2	104	А	C4-C5-C6	6.81	120.41	117.00
33	2	417	U	O4'-C1'-N1	6.81	113.65	108.20
33	2	556	U	O4'-C1'-N1	6.81	113.65	108.20
33	2	835	C	$C2-N1-\overline{C1'}$	$6.8\overline{1}$	126.29	118.80
-33	2	466	A	C5-C6-N6	-6.81	118.25	123.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	563	U	O4'-C1'-N1	6.81	113.64	108.20
33	2	673	G	C5-C6-O6	-6.81	124.52	128.60
33	2	1186	А	C4-C5-C6	6.80	120.40	117.00
33	2	1298	G	O4'-C1'-N9	6.80	113.64	108.20
33	2	364	G	C5-C6-O6	-6.80	124.52	128.60
33	2	1431	С	N3-C4-N4	6.80	122.76	118.00
33	2	576	G	C5-C6-O6	-6.80	124.52	128.60
39	1	28	U	O4'-C1'-N1	6.80	113.64	108.20
33	2	642	U	O4'-C1'-N1	6.79	113.64	108.20
33	2	87	U	O4'-C1'-N1	6.79	113.64	108.20
33	2	205	G	C5-C6-O6	-6.79	124.52	128.60
33	2	317	G	C5-C6-O6	-6.79	124.52	128.60
33	2	1108	U	O4'-C1'-N1	6.79	113.63	108.20
33	2	1349	А	C5-C6-N6	-6.79	118.27	123.70
33	2	344	U	O4'-C1'-N1	6.79	113.63	108.20
33	2	430	G	O4'-C1'-N9	6.79	113.63	108.20
33	2	1610	U	O4'-C1'-N1	6.79	113.63	108.20
33	2	1631	G	C5-C6-O6	-6.79	124.53	128.60
33	2	1213	А	C4-C5-C6	6.79	120.39	117.00
33	2	1114	С	O4'-C1'-N1	6.78	113.63	108.20
33	2	1154	G	C5-C6-O6	-6.78	124.53	128.60
39	1	38	А	C5-C6-N6	-6.78	118.28	123.70
33	2	868	А	O4'-C1'-N9	6.78	113.62	108.20
33	2	1292	U	O4'-C1'-N1	6.78	113.62	108.20
33	2	184	G	C5-C6-O6	-6.78	124.53	128.60
33	2	362	U	O4'-C1'-N1	6.77	113.62	108.20
33	2	1390	G	C5-C6-O6	-6.77	124.53	128.60
33	2	452	С	O4'-C1'-N1	6.77	113.62	108.20
33	2	1771	G	O4'-C1'-N9	6.77	113.62	108.20
33	2	1124	С	O4'-C1'-N1	6.77	113.62	108.20
39	1	54	А	C4-C5-C6	6.77	120.39	117.00
33	2	428	G	C5-C6-O6	-6.77	124.54	128.60
33	2	647	U	O4'-C1'-N1	6.77	113.62	108.20
33	2	1740	А	C4-C5-C6	6.77	120.39	117.00
39	1	14	С	N3-C4-N4	6.77	122.74	118.00
33	2	461	G	C5-C6-O6	-6.76	124.54	128.60
33	2	1634	G	C5-C6-O6	-6.76	124.54	128.60
33	2	641	U	O4'-C1'-N1	6.76	113.61	108.20
33	2	1626	U	O4'-C1'-N1	6.76	113.61	108.20
33	2	675	А	P-O3'-C3'	-6.76	111.59	119.70
33	2	1297	A	O4'-C1'-N9	6.76	113.61	108.20
33	2	1754	G	O4'-C1'-N9	6.76	113.61	108.20



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
33	2	23	G	C5-C6-O6	-6.76	124.54	128.60
33	2	68	А	C5-C6-N6	-6.76	118.29	123.70
33	2	1527	С	N3-C4-N4	6.76	122.73	118.00
33	2	1155	G	C5-C6-O6	-6.76	124.55	128.60
33	2	1825	А	C4-C5-C6	6.76	120.38	117.00
33	2	488	С	O4'-C1'-N1	6.75	113.60	108.20
33	2	832	G	C5-C6-O6	-6.75	124.55	128.60
33	2	1597	U	O4'-C1'-N1	6.75	113.60	108.20
33	2	551	А	O4'-C1'-N9	6.75	113.60	108.20
33	2	799	С	N3-C4-N4	6.75	122.72	118.00
39	1	31	G	O4'-C1'-N9	6.75	113.60	108.20
33	2	877	G	C5-C6-O6	-6.75	124.55	128.60
33	2	1593	G	C5-C6-O6	-6.75	124.55	128.60
33	2	272	С	N3-C4-N4	6.74	122.72	118.00
33	2	1389	G	C5-C6-O6	-6.74	124.55	128.60
33	2	1027	А	C5-C6-N6	-6.74	118.31	123.70
33	2	1420	G	C5-C6-O6	-6.74	124.56	128.60
33	2	90	G	C5-C6-O6	-6.74	124.56	128.60
33	2	1144	А	O4'-C1'-N9	6.74	113.59	108.20
33	2	442	G	C5-C6-O6	-6.73	124.56	128.60
33	2	571	U	O4'-C1'-N1	6.73	113.59	108.20
33	2	9	U	O4'-C1'-N1	6.73	113.58	108.20
33	2	1299	С	C2-N1-C1'	6.73	126.20	118.80
33	2	487	С	O4'-C1'-N1	6.72	113.58	108.20
33	2	528	U	O4'-C1'-N1	6.72	113.58	108.20
33	2	1297	А	C4-C5-C6	6.72	120.36	117.00
33	2	195	С	O4'-C1'-N1	6.72	113.57	108.20
33	2	458	А	C5-C6-N6	-6.72	118.33	123.70
33	2	275	С	C2-N1-C1'	6.71	126.19	118.80
33	2	97	U	O4'-C1'-N1	6.71	113.57	108.20
33	2	113	G	C5-C6-O6	-6.71	124.57	128.60
33	2	817	G	C5-C6-O6	-6.71	124.57	128.60
33	2	1156	U	O4'-C1'-N1	6.71	113.57	108.20
33	2	1713	G	N3-C2-N2	6.71	124.60	119.90
33	2	336	С	N3-C4-N4	6.71	122.70	118.00
33	2	485	U	O4'-C1'-N1	6.71	113.57	108.20
33	2	1234	U	O4'-C1'-N1	6.71	113.57	108.20
33	2	587	G	O4'-C1'-N9	6.71	113.56	108.20
33	2	797	U	O4'-C1'-N1	6.71	113.56	108.20
33	2	920	G	C5-C6-O6	-6.71	124.58	128.60
39	1	15	A	C5-C6-N6	-6.70	118.34	123.70
39	1	25	U	O4'-C1'-N1	6.70	113.56	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	811	U	O4'-C1'-N1	6.70	113.56	108.20
33	2	622	С	O4'-C1'-N1	6.70	113.56	108.20
33	2	548	G	C5-C6-O6	-6.70	124.58	128.60
33	2	1224	А	C4-C5-C6	6.70	120.35	117.00
33	2	882	А	C5-C6-N6	-6.69	118.34	123.70
33	2	18	С	N3-C4-N4	6.69	122.69	118.00
33	2	410	G	C5-C6-O6	-6.69	124.58	128.60
33	2	997	А	C5-C6-N6	-6.69	118.35	123.70
39	1	2	А	C5-C6-N6	-6.69	118.35	123.70
33	2	911	G	C5-C6-O6	-6.69	124.59	128.60
33	2	120	U	O4'-C1'-N1	6.69	113.55	108.20
33	2	829	С	N3-C4-N4	6.69	122.68	118.00
33	2	1058	A	C4-C5-C6	6.69	120.34	117.00
33	2	1068	U	O4'-C1'-N1	6.69	113.55	108.20
33	2	1388	U	O4'-C1'-N1	6.69	113.55	108.20
33	2	876	G	C5-C6-O6	-6.68	124.59	128.60
33	2	1138	G	C5-C6-O6	-6.68	124.59	128.60
39	1	40	С	N3-C4-N4	6.68	122.68	118.00
33	2	392	С	N3-C4-N4	6.68	122.68	118.00
33	2	1022	С	N3-C4-N4	6.68	122.68	118.00
33	2	1460	С	O4'-C1'-N1	6.68	113.55	108.20
33	2	1607	G	O4'-C1'-N9	6.68	113.55	108.20
34	3	71	G	C5-C6-O6	-6.68	124.59	128.60
33	2	646	G	C5-C6-O6	-6.68	124.59	128.60
34	3	75	U	O4'-C1'-N1	6.68	113.54	108.20
33	2	540	С	N3-C4-N4	6.67	122.67	118.00
33	2	974	G	O4'-C1'-N9	6.67	113.54	108.20
33	2	1091	U	O4'-C1'-N1	6.67	113.54	108.20
33	2	467	G	O4'-C1'-N9	6.67	113.54	108.20
33	2	1029	G	C5-C6-O6	-6.67	124.60	128.60
33	2	1082	G	C5-C6-O6	-6.67	124.60	128.60
33	2	1360	U	C2-N1-C1'	6.67	125.70	117.70
33	2	80	G	O4'-C1'-N9	6.67	113.53	108.20
33	2	291	U	O4'-C1'-N1	6.67	113.53	108.20
33	2	907	С	O4'-C1'-N1	6.67	113.53	108.20
33	2	1142	С	O4'-C1'-N1	6.67	113.53	108.20
33	2	510	A	O4'-C1'-N9	6.67	113.53	108.20
33	2	1224	A	C5-C6-N6	-6.67	118.37	123.70
33	2	1472	A	C4-C5-C6	6.66	120.33	117.00
33	2	177	G	N3-C2-N2	6.66	124.56	119.90
33	2	965	U	O4'-C1'-N1	6.66	113.53	108.20
39	1	7	A	C5-C6-N6	-6.66	118.37	123.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	12	U	O4'-C1'-N1	6.66	113.53	108.20
33	2	164	А	C4-C5-C6	6.66	120.33	117.00
33	2	964	U	O4'-C1'-N1	6.66	113.53	108.20
33	2	1130	G	O4'-C1'-N9	6.66	113.53	108.20
33	2	1609	А	C5-C6-N6	-6.66	118.37	123.70
33	2	121	U	O4'-C1'-N1	6.66	113.52	108.20
33	2	855	G	C5-C6-O6	-6.66	124.61	128.60
33	2	1775	А	C5-C6-N6	-6.66	118.38	123.70
33	2	1816	А	O3'-P-O5'	-6.66	91.36	104.00
33	2	1838	U	O4'-C1'-N1	6.66	113.53	108.20
33	2	231	С	N3-C4-N4	6.65	122.66	118.00
33	2	907	С	N3-C4-N4	6.65	122.66	118.00
33	2	1654	U	O4'-C1'-N1	6.65	113.52	108.20
33	2	1853	А	C5-C6-N6	-6.65	118.38	123.70
33	2	357	U	O4'-C1'-N1	6.65	113.52	108.20
33	2	373	G	O4'-C1'-N9	6.65	113.52	108.20
33	2	1040	G	C5-C6-O6	-6.65	124.61	128.60
33	2	1441	U	O4'-C1'-N1	6.65	113.52	108.20
33	2	1201	С	N3-C4-N4	6.65	122.66	118.00
33	2	1738	G	C5-C6-O6	-6.65	124.61	128.60
33	2	1839	А	C5-C6-N6	-6.65	118.38	123.70
33	2	177	G	C5-C6-O6	-6.65	124.61	128.60
39	1	30	G	O4'-C1'-N9	6.65	113.52	108.20
33	2	1591	U	O4'-C1'-N1	6.65	113.52	108.20
33	2	976	А	C5-C6-N6	-6.64	118.38	123.70
33	2	1001	G	O4'-C1'-N9	6.64	113.52	108.20
33	2	1843	G	O4'-C1'-N9	6.64	113.51	108.20
33	2	512	А	O4'-C1'-N9	6.64	113.51	108.20
33	2	909	А	O4'-C1'-N9	6.64	113.51	108.20
33	2	1142	С	N3-C4-N4	6.64	122.65	118.00
33	2	441	G	C5-C6-O6	-6.64	124.62	128.60
33	2	900	А	O4'-C1'-N9	6.64	113.51	108.20
33	2	1378	А	C5-C6-N6	-6.64	118.39	123.70
33	2	1548	С	O4'-C1'-N1	6.64	113.51	108.20
33	2	1656	А	C4-C5-C6	6.64	120.32	117.00
33	2	833	А	C4-C5-C6	6.64	120.32	117.00
33	2	1169	А	C4-C5-C6	6.64	120.32	117.00
33	2	1157	U	O4'-C1'-N1	6.63	113.51	108.20
33	2	1596	А	C4-C5-C6	6.63	120.32	117.00
33	2	233	А	C5-C6-N6	-6.63	118.39	123.70
33	2	1299	С	O4'-C1'-N1	6.63	113.50	108.20

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108.20

113.50



6.63

O4'-C1'-N1

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1521	G	C5-C6-O6	-6.63	124.62	128.60
33	2	1329	U	O4'-C1'-N1	6.63	113.50	108.20
33	2	1797	U	O4'-C1'-N1	6.63	113.50	108.20
33	2	1515	G	C4-N9-C1'	6.62	135.11	126.50
33	2	1856	G	C5-C6-O6	-6.62	124.63	128.60
33	2	1052	U	O4'-C1'-N1	6.62	113.50	108.20
33	2	1105	С	C6-N1-C1'	-6.62	112.86	120.80
33	2	1623	С	N3-C4-N4	6.62	122.64	118.00
33	2	889	U	O4'-C1'-N1	6.62	113.50	108.20
33	2	280	G	C5-C6-O6	-6.62	124.63	128.60
33	2	954	G	C5-C6-O6	-6.62	124.63	128.60
33	2	970	С	N3-C4-N4	6.62	122.63	118.00
33	2	1817	А	OP2-P-O3'	6.62	119.76	105.20
33	2	1723	U	O4'-C1'-N1	6.62	113.49	108.20
33	2	69	С	N3-C4-N4	6.61	122.63	118.00
33	2	432	С	N3-C4-N4	6.61	122.63	118.00
33	2	966	G	O4'-C1'-N9	6.61	113.49	108.20
33	2	525	G	O4'-C1'-N9	6.61	113.49	108.20
33	2	1728	U	O4'-C1'-N1	6.61	113.49	108.20
33	2	1438	U	O4'-C1'-N1	6.61	113.49	108.20
33	2	281	U	O4'-C1'-N1	6.61	113.49	108.20
33	2	387	G	C5-C6-O6	-6.61	124.64	128.60
36	В	137	PHE	CB-CG-CD1	6.61	125.42	120.80
33	2	179	С	O4'-C1'-N1	6.60	113.48	108.20
33	2	80	G	P-O3'-C3'	6.60	127.62	119.70
33	2	1002	С	N3-C4-N4	6.60	122.62	118.00
33	2	1317	G	C5-C6-O6	-6.60	124.64	128.60
33	2	452	С	N3-C4-N4	6.60	122.62	118.00
33	2	176	U	O4'-C1'-N1	6.60	113.48	108.20
33	2	1270	G	C5-C6-O6	-6.60	124.64	128.60
33	2	471	С	N3-C4-N4	6.60	122.62	118.00
33	2	337	G	O4'-C1'-N9	6.59	113.48	108.20
33	2	1028	С	N3-C4-N4	6.59	122.61	118.00
33	2	1263	С	N3-C4-N4	6.59	122.62	118.00
33	2	13	С	O4'-C1'-N1	6.59	113.47	108.20
33	2	1508	С	O4'-C1'-N1	6.59	113.47	108.20
33	2	1352	G	C5-C6-O6	-6.59	124.64	128.60
33	2	5	U	O4'-C1'-N1	6.59	113.47	108.20
33	2	1753	G	O4'-C1'-N9	6.59	113.47	108.20
33	2	1185	А	C4-C5-C6	6.58	120.29	117.00
33	2	237	G	C5-C6-O6	-6.58	124.65	128.60
- 33	2	1625	А	C5-C6-N1	-6.58	114.41	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1127	G	C5-C6-O6	-6.58	124.65	128.60
33	2	1182	U	O4'-C1'-N1	6.58	113.47	108.20
33	2	1791	U	O4'-C1'-N1	6.58	113.46	108.20
33	2	1251	G	C5-C6-O6	-6.58	124.65	128.60
33	2	1463	С	N3-C4-N4	6.58	122.61	118.00
33	2	868	А	C4-C5-C6	6.58	120.29	117.00
33	2	996	С	O4'-C1'-N1	6.58	113.46	108.20
33	2	1582	G	C5-C6-O6	-6.58	124.66	128.60
16	Q	34	PHE	CB-CG-CD2	-6.57	116.20	120.80
33	2	38	А	O4'-C1'-N9	6.57	113.46	108.20
33	2	572	U	O4'-C1'-N1	6.57	113.46	108.20
33	2	1177	A	C5-C6-N6	-6.57	118.44	123.70
39	1	16	G	O4'-C1'-N9	6.57	113.46	108.20
34	3	68	А	C4-C5-C6	6.57	120.29	117.00
33	2	82	G	C5-C6-O6	-6.57	124.66	128.60
33	2	539	С	O4'-C1'-N1	6.57	113.45	108.20
33	2	1054	А	C4-C5-C6	6.57	120.28	117.00
33	2	516	А	O4'-C1'-N9	6.56	113.45	108.20
33	2	824	G	C5-C6-O6	-6.56	124.66	128.60
33	2	1293	U	O4'-C1'-N1	6.56	113.45	108.20
33	2	1428	U	O4'-C1'-N1	6.56	113.45	108.20
33	2	1687	U	O4'-C1'-N1	6.56	113.45	108.20
33	2	225	С	O4'-C1'-N1	6.56	113.45	108.20
33	2	299	G	C5-C6-O6	-6.56	124.67	128.60
33	2	1136	G	O4'-C1'-N9	6.56	113.44	108.20
33	2	1810	G	O4'-C1'-N9	6.56	113.45	108.20
33	2	1375	A	C4-C5-C6	6.56	120.28	117.00
33	2	1611	U	O4'-C1'-N1	6.56	113.44	108.20
33	2	859	U	O4'-C1'-N1	6.55	113.44	108.20
33	2	1359	С	N3-C4-N4	6.55	122.59	118.00
33	2	1458	U	O4'-C1'-N1	6.55	113.44	108.20
33	2	1630	C	O4'-C1'-N1	6.55	113.44	108.20
33	2	1107	U	O4'-C1'-N1	6.55	113.44	108.20
33	2	1354	U	O4'-C1'-N1	6.55	113.44	108.20
33	2	1843	G	C5-C6-O6	-6.55	124.67	128.60
33	2	91	A	C4-C5-C6	6.55	120.28	117.00
33	2	843	A	C4-C5-C6	6.55	120.28	117.00
33	2	858	A	C4-C5-C6	6.55	120.28	117.00
33	2	1083	A	C4-C5-C6	6.55	120.27	117.00
33	2	1167	G	C5-C6-O6	-6.55	124.67	128.60
33	2	1714	A	$C4-C5-\overline{C6}$	$6.5\overline{5}$	$120.2\overline{7}$	117.00
33	2	40	A	C4-C5-C6	6.55	120.27	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	813	G	C5-C6-O6	-6.55	124.67	128.60
33	2	1060	С	N3-C4-N4	6.55	122.58	118.00
33	2	1066	А	C4-C5-C6	6.55	120.27	117.00
33	2	155	G	C5-C6-O6	-6.54	124.67	128.60
33	2	421	G	O4'-C1'-N9	6.54	113.44	108.20
33	2	544	А	C4-C5-C6	6.54	120.27	117.00
33	2	968	А	C4-C5-C6	6.54	120.27	117.00
33	2	645	А	C4-C5-C6	6.54	120.27	117.00
33	2	1539	С	N3-C4-N4	6.54	122.58	118.00
33	2	82	G	N3-C2-N2	6.54	124.48	119.90
33	2	654	А	O4'-C1'-N9	6.54	113.43	108.20
33	2	657	U	O4'-C1'-N1	6.54	113.43	108.20
33	2	164	А	C5-C6-N6	-6.54	118.47	123.70
33	2	548	G	O4'-C1'-N9	6.54	113.43	108.20
34	3	73	G	C5-C6-O6	-6.54	124.68	128.60
33	2	386	U	O4'-C1'-N1	6.54	113.43	108.20
38	R	37	TYR	CB-CG-CD2	-6.54	117.08	121.00
33	2	451	U	O4'-C1'-N1	6.54	113.43	108.20
33	2	594	А	C4-C5-C6	6.53	120.27	117.00
33	2	1132	U	O4'-C1'-N1	6.53	113.43	108.20
33	2	1172	G	O4'-C1'-N9	6.53	113.43	108.20
33	2	1507	U	O4'-C1'-N1	6.53	113.43	108.20
33	2	1673	А	C4-C5-C6	6.53	120.27	117.00
33	2	1779	С	N3-C4-N4	6.53	122.57	118.00
33	2	1799	G	C5-C6-O6	-6.53	124.68	128.60
33	2	1479	А	C4-C5-C6	6.53	120.27	117.00
39	1	60	А	C5-C6-N6	-6.53	118.47	123.70
33	2	1047	G	O4'-C1'-N9	6.53	113.42	108.20
33	2	1245	С	O4'-C1'-N1	6.53	113.42	108.20
33	2	1539	С	O4'-C1'-N1	6.53	113.42	108.20
33	2	63	U	O4'-C1'-N1	6.53	113.42	108.20
33	2	1629	А	C4-C5-C6	6.53	120.26	117.00
33	2	923	С	N3-C4-N4	6.52	122.57	118.00
33	2	1368	U	O4'-C1'-N1	6.52	113.42	108.20
34	3	52	А	C5-C6-N6	-6.52	118.48	123.70
33	2	1706	U	O4'-C1'-N1	6.52	113.42	108.20
33	2	1662	U	O4'-C1'-N1	6.52	113.42	108.20
33	2	1407	G	O4'-C1'-N9	6.52	113.42	108.20
39	1	46	G	C5-C6-O6	-6.52	124.69	128.60
33	2	839	С	N3-C4-N4	6.52	122.56	118.00
33	2	872	С	O4'-C1'-N1	6.52	113.41	108.20
33	2	1825	А	C5-C6-N6	-6.52	118.48	123.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	439	А	C4-C5-C6	6.52	120.26	117.00
35	А	54	ARG	O-C-N	-6.52	112.27	122.70
33	2	342	U	O4'-C1'-N1	6.51	113.41	108.20
33	2	1422	U	O4'-C1'-N1	6.51	113.41	108.20
33	2	1800	А	C5-C6-N6	-6.51	118.49	123.70
33	2	1635	А	C4-C5-C6	6.51	120.26	117.00
33	2	1660	G	C5-C6-O6	-6.51	124.69	128.60
33	2	1796	С	N3-C4-N4	6.51	122.56	118.00
33	2	363	G	N1-C6-O6	6.51	123.81	119.90
33	2	1417	А	C4-C5-C6	6.51	120.25	117.00
33	2	996	С	N3-C4-N4	6.51	122.56	118.00
33	2	1689	U	O4'-C1'-N1	6.51	113.41	108.20
33	2	1725	U	O4'-C1'-N1	6.51	113.41	108.20
33	2	32	U	O4'-C1'-N1	6.51	113.41	108.20
33	2	1595	G	C5-C6-O6	-6.50	124.70	128.60
33	2	356	U	O4'-C1'-N1	6.50	113.40	108.20
33	2	497	G	C5-C6-O6	-6.50	124.70	128.60
33	2	1146	А	C4-C5-C6	6.50	120.25	117.00
33	2	170	А	C4-C5-C6	6.50	120.25	117.00
33	2	1295	А	C4-C5-C6	6.50	120.25	117.00
33	2	1512	G	C5-C6-O6	-6.50	124.70	128.60
33	2	187	С	N3-C4-N4	6.50	122.55	118.00
33	2	228	А	C4-C5-C6	6.50	120.25	117.00
33	2	1699	С	O4'-C1'-N1	6.50	113.40	108.20
33	2	514	U	O4'-C1'-N1	6.50	113.40	108.20
39	1	19	G	C5-C6-O6	-6.50	124.70	128.60
33	2	619	А	C4-C5-C6	6.50	120.25	117.00
33	2	74	G	C5-C6-O6	-6.49	124.70	128.60
33	2	308	С	N3-C4-N4	6.49	122.55	118.00
33	2	982	G	C5-C6-O6	-6.49	124.70	128.60
33	2	102	А	C4-C5-C6	6.49	120.25	117.00
33	2	1489	С	N3-C4-N4	6.49	122.54	118.00
33	2	806	А	C4-C5-C6	6.49	120.24	117.00
33	2	979	А	O4'-C1'-N9	6.49	113.39	108.20
33	2	1255	А	C4-C5-C6	6.49	120.24	117.00
33	2	800	U	04'-C1'-N1	6.49	113.39	108.20
33	2	1069	U	O4'-C1'-N1	6.49	113.39	108.20
33	2	489	G	C5-C6-O6	-6.48	124.71	128.60
33	2	1513	С	C2-N1-C1'	6.48	125.93	118.80
33	2	1783	G	C5-C6-O6	-6.48	124.71	128.60
33	2	$17\overline{49}$	C	N3-C4-N4	$6.\overline{48}$	122.54	118.00
33	2	425	A	C5-C6-N6	-6.48	118.52	123.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1498	С	N3-C4-N4	6.48	122.53	118.00
33	2	382	А	O4'-C1'-N9	6.47	113.38	108.20
33	2	550	А	C5-C6-N6	-6.47	118.52	123.70
33	2	972	G	O4'-C1'-N9	6.47	113.38	108.20
33	2	1516	С	O4'-C1'-N1	6.47	113.38	108.20
33	2	78	С	C2-N1-C1'	6.47	125.92	118.80
33	2	236	С	N3-C4-N4	6.47	122.53	118.00
33	2	270	G	C5-C6-O6	-6.47	124.72	128.60
33	2	436	G	C5-C6-O6	-6.47	124.72	128.60
33	2	1082	G	O4'-C1'-N9	6.47	113.38	108.20
33	2	1011	U	O4'-C1'-N1	6.47	113.37	108.20
33	2	1168	U	O4'-C1'-N1	6.47	113.37	108.20
33	2	1511	G	O4'-C1'-N9	6.47	113.37	108.20
33	2	1719	А	O4'-C1'-N9	6.47	113.37	108.20
33	2	57	U	O4'-C1'-N1	6.46	113.37	108.20
33	2	162	С	N3-C4-N4	6.46	122.53	118.00
33	2	927	С	N3-C4-N4	6.46	122.53	118.00
33	2	1135	С	C6-N1-C1'	-6.46	113.04	120.80
33	2	1143	С	N3-C4-N4	6.46	122.53	118.00
33	2	420	С	N3-C4-N4	6.46	122.52	118.00
33	2	829	С	O4'-C1'-N1	6.46	113.37	108.20
33	2	915	А	C4-C5-C6	6.46	120.23	117.00
33	2	977	А	C4-C5-C6	6.46	120.23	117.00
33	2	1429	С	N3-C4-N4	6.46	122.52	118.00
33	2	1386	U	O4'-C1'-N1	6.46	113.37	108.20
33	2	1618	А	C4-C5-C6	6.46	120.23	117.00
33	2	522	С	N3-C4-N4	6.46	122.52	118.00
33	2	851	G	C5-C6-O6	-6.46	124.73	128.60
33	2	1410	А	C5-C6-N6	-6.46	118.53	123.70
33	2	1609	А	C4-C5-C6	6.46	120.23	117.00
33	2	1733	С	N3-C4-N4	6.46	122.52	118.00
33	2	1739	G	C5-C6-O6	-6.46	124.73	128.60
33	2	902	U	O4'-C1'-N1	6.46	113.36	108.20
33	2	1331	G	N3-C2-N2	6.46	124.42	119.90
33	2	1139	А	C4-C5-C6	6.45	120.23	117.00
33	2	1464	С	N3-C4-N4	6.45	122.52	118.00
33	2	1538	U	O4'-C1'-N1	6.45	113.36	108.20
33	2	371	С	04'-C1'-N1	6.45	113.36	108.20
33	2	1742	С	N3-C4-N4	6.45	122.52	118.00
33	2	1148	U	O4'-C1'-N1	6.45	113.36	108.20
33	2	94	G	C5-C6-O6	-6.45	$1\overline{24.7}\overline{3}$	128.60
33	2	674	G	C5-C6-O6	-6.45	124.73	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal $(^{o})$
33	2	1767	С	N3-C4-N4	6.45	122.51	118.00
33	2	454	А	C4-C5-C6	6.44	120.22	117.00
33	2	640	А	C5-C6-N6	-6.44	118.55	123.70
33	2	867	U	O4'-C1'-N1	6.44	113.35	108.20
33	2	1732	G	O4'-C1'-N9	6.44	113.35	108.20
33	2	309	А	C5-C6-N6	-6.44	118.55	123.70
33	2	396	U	O4'-C1'-N1	6.44	113.35	108.20
33	2	1330	G	O4'-C1'-N9	6.44	113.35	108.20
33	2	675	А	O3'-P-O5'	-6.43	91.78	104.00
33	2	925	G	O4'-C1'-N9	6.43	113.35	108.20
33	2	1262	С	N3-C4-N4	6.43	122.50	118.00
33	2	350	А	C4-C5-C6	6.43	120.22	117.00
33	2	1272	А	C4-C5-C6	6.43	120.22	117.00
34	3	69	G	C5-C6-O6	-6.43	124.74	128.60
33	2	1211	С	N3-C4-N4	6.43	122.50	118.00
33	2	1318	G	C5-C6-O6	-6.43	124.74	128.60
33	2	861	А	C4-C5-C6	6.43	120.21	117.00
33	2	1344	G	C5-C6-O6	-6.43	124.74	128.60
33	2	651	U	O4'-C1'-N1	6.43	113.34	108.20
33	2	1408	С	N3-C4-N4	6.43	122.50	118.00
33	2	1685	U	O4'-C1'-N1	6.43	113.34	108.20
33	2	1449	С	C2-N1-C1'	6.43	125.87	118.80
33	2	1582	G	O4'-C1'-N9	6.43	113.34	108.20
33	2	1801	С	N3-C4-N4	6.43	122.50	118.00
33	2	575	С	N3-C4-N4	6.42	122.50	118.00
33	2	1275	С	N3-C4-N4	6.42	122.50	118.00
33	2	1560	С	N3-C4-N4	6.42	122.50	118.00
33	2	366	А	C5-C6-N6	-6.42	118.56	123.70
33	2	203	G	C5-C6-O6	-6.42	124.75	128.60
33	2	834	G	C5-C6-O6	-6.42	124.75	128.60
33	2	643	A	C5-C6-N6	-6.42	118.57	123.70
33	2	1062	U	O4'-C1'-N1	6.42	113.33	108.20
33	2	1377	G	C5-C6-O6	-6.42	124.75	128.60
33	2	1379	А	C4-C5-C6	6.42	120.21	117.00
33	2	308	С	O4'-C1'-N1	6.42	113.33	108.20
33	2	444	U	O4'-C1'-N1	6.42	113.33	108.20
33	2	1016	А	C4-C5-C6	6.41	120.21	117.00
33	2	1115	А	C4-C5-C6	6.41	120.21	117.00
33	2	1219	A	C4-C5-C6	6.41	120.21	117.00
33	2	1233	С	N3-C4-N4	6.41	122.49	118.00
33	2	1313	U	O4'-C1'-N1	6.41	113.33	108.20
33	2	1543	G	O4'-C1'-N9	6.41	113.33	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	149	А	O4'-C1'-N9	6.41	113.33	108.20
33	2	1432	С	N3-C4-N4	6.41	122.49	118.00
33	2	310	G	O4'-C1'-N9	6.41	113.32	108.20
33	2	447	С	N3-C4-N4	6.41	122.48	118.00
34	3	70	G	C5-C6-O6	-6.41	124.76	128.60
33	2	816	U	O4'-C1'-N1	6.40	113.32	108.20
33	2	1034	U	O4'-C1'-N1	6.40	113.32	108.20
33	2	402	G	N3-C2-N2	6.40	124.38	119.90
33	2	942	U	O4'-C1'-N1	6.40	113.32	108.20
33	2	1318	G	O4'-C1'-N9	6.40	113.32	108.20
33	2	1627	G	C5-C6-O6	-6.40	124.76	128.60
33	2	1845	А	C4-C5-C6	6.40	120.20	117.00
33	2	1064	G	C5-C6-O6	-6.40	124.76	128.60
33	2	1103	G	O4'-C1'-N9	6.40	113.32	108.20
33	2	1828	А	C4-C5-C6	6.40	120.20	117.00
33	2	1277	G	C5-C6-O6	-6.40	124.76	128.60
33	2	1016	А	C5-C6-N6	-6.39	118.58	123.70
33	2	1067	G	O4'-C1'-N9	6.39	113.32	108.20
33	2	1602	А	C4-C5-C6	6.39	120.20	117.00
33	2	1722	G	O4'-C1'-N9	6.39	113.31	108.20
33	2	165	G	C5-C6-O6	-6.39	124.76	128.60
33	2	562	U	O4'-C1'-N1	6.39	113.31	108.20
33	2	1014	U	O4'-C1'-N1	6.39	113.31	108.20
33	2	899	A	O4'-C1'-N9	6.39	113.31	108.20
33	2	1465	A	C4-C5-C6	6.39	120.19	117.00
33	2	340	С	O4'-C1'-N1	6.39	113.31	108.20
33	2	1532	А	C4-C5-C6	6.39	120.19	117.00
39	1	68	С	N3-C4-N4	6.38	122.47	118.00
33	2	1177	A	C4-C5-C6	6.38	120.19	117.00
33	2	1221	U	O4'-C1'-N1	6.38	113.31	108.20
33	2	53	С	N3-C4-N4	6.38	122.47	118.00
33	2	1249	А	C4-C5-C6	6.38	120.19	117.00
33	2	1366	А	C4-C5-C6	6.38	120.19	117.00
33	2	1541	G	C5-C6-O6	-6.38	124.77	128.60
33	2	538	С	N3-C4-N4	6.38	122.47	118.00
33	2	1577	С	N3-C4-N4	6.38	122.46	118.00
33	2	160	U	O4'-C1'-N1	6.38	113.30	108.20
33	2	960	A	C5-C6-N1	-6.38	114.51	117.70
33	2	1044	G	N3-C2-N2	6.38	124.36	119.90
33	2	365	U	O4'-C1'-N1	6.37	113.30	108.20
33	2	482	C	O4'-C1'-N1	6.37	113.30	108.20
33	2	1847	C	N3-C4-N4	6.37	122.46	118.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	862	U	O4'-C1'-N1	6.37	113.30	108.20
33	2	1124	С	N3-C4-N4	6.37	122.46	118.00
33	2	1813	А	C4-C5-C6	6.37	120.18	117.00
33	2	488	С	N3-C4-N4	6.37	122.46	118.00
33	2	11	А	C4-C5-C6	6.37	120.18	117.00
33	2	416	А	C4-C5-C6	6.37	120.18	117.00
33	2	951	А	C5-C6-N6	-6.37	118.61	123.70
33	2	1150	U	O4'-C1'-N1	6.36	113.29	108.20
33	2	1648	U	O4'-C1'-N1	6.36	113.29	108.20
34	3	76	А	C5-C6-N6	-6.36	118.61	123.70
33	2	1115	А	O4'-C1'-N9	6.36	113.29	108.20
33	2	1230	С	N3-C4-N4	6.36	122.45	118.00
33	2	1336	U	O4'-C1'-N1	6.36	113.29	108.20
33	2	986	А	C4-C5-C6	6.36	120.18	117.00
33	2	1798	U	O4'-C1'-N1	6.36	113.28	108.20
33	2	71	G	C5-C6-O6	-6.35	124.79	128.60
33	2	166	А	O4'-C1'-N9	6.35	113.28	108.20
33	2	531	U	O4'-C1'-N1	6.35	113.28	108.20
33	2	1236	А	C5-C6-N6	-6.35	118.62	123.70
33	2	202	U	O4'-C1'-N1	6.35	113.28	108.20
33	2	1588	С	N3-C4-N4	6.35	122.44	118.00
33	2	312	С	N3-C4-N4	6.35	122.44	118.00
33	2	425	А	C4-C5-C6	6.35	120.17	117.00
33	2	527	С	N3-C4-N4	6.35	122.44	118.00
33	2	1218	G	O4'-C1'-N9	6.34	113.28	108.20
33	2	476	А	C4-C5-C6	6.34	120.17	117.00
33	2	1614	А	C4-C5-C6	6.34	120.17	117.00
33	2	918	А	C4-C5-C6	6.34	120.17	117.00
33	2	1392	А	C4-C5-C6	6.34	120.17	117.00
33	2	1727	G	O4'-C1'-N9	6.34	113.27	108.20
33	2	299	G	O4'-C1'-N9	6.34	113.27	108.20
33	2	1280	А	C4-C5-C6	6.34	120.17	117.00
33	2	1372	А	C4-C5-C6	6.34	120.17	117.00
33	2	1621	С	N3-C4-N4	6.34	122.44	118.00
33	2	394	G	O4'-C1'-N9	6.33	113.27	108.20
33	2	917	G	C5-C6-O6	-6.33	124.80	128.60
33	2	905	G	C5-C6-O6	-6.33	124.80	128.60
33	2	1554	C	N3-C4-N4	6.33	122.43	118.00
33	2	331	С	N3-C4-N4	6.33	122.43	118.00
33	2	397	G	O4'-C1'-N9	6.33	113.26	108.20
33	2	673	G	04'-C1'-N9	6.33	113.27	108.20
33	2	858	A	C5-C6-N6	-6.33	118.64	123.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	873	С	C2-N1-C1'	6.33	125.76	118.80
33	2	1652	G	C5-C6-O6	-6.33	124.80	128.60
33	2	1805	С	N3-C4-N4	6.33	122.43	118.00
39	1	2	А	C4-C5-C6	6.33	120.17	117.00
33	2	352	С	N3-C4-N4	6.33	122.43	118.00
33	2	1247	А	C4-C5-C6	6.33	120.16	117.00
39	1	3	G	O4'-C1'-N9	6.33	113.26	108.20
33	2	35	С	N3-C4-N4	6.33	122.43	118.00
33	2	1078	А	C4-C5-C6	6.33	120.16	117.00
33	2	1846	С	N3-C4-N4	6.33	122.43	118.00
33	2	329	А	C4-C5-C6	6.32	120.16	117.00
39	1	29	G	O4'-C1'-N9	6.32	113.26	108.20
33	2	1471	G	O4'-C1'-N9	6.32	113.26	108.20
33	2	1030	А	C4-C5-C6	6.32	120.16	117.00
33	2	1196	А	C4-C5-C6	6.32	120.16	117.00
33	2	1279	С	N3-C4-N4	6.32	122.42	118.00
33	2	10	G	C5-C6-O6	-6.32	124.81	128.60
33	2	111	А	C5-C6-N1	-6.32	114.54	117.70
33	2	510	А	C5-C6-N6	-6.32	118.65	123.70
33	2	1072	G	O4'-C1'-N9	6.32	113.25	108.20
33	2	1117	G	O4'-C1'-N9	6.32	113.25	108.20
33	2	1314	G	O4'-C1'-N9	6.32	113.25	108.20
33	2	1787	А	O4'-C1'-N9	6.32	113.25	108.20
33	2	1854	А	C4-C5-C6	6.32	120.16	117.00
33	2	42	A	C4-C5-C6	6.32	120.16	117.00
33	2	175	A	O4'-C1'-N9	6.32	113.25	108.20
33	2	845	А	C4-C5-C6	6.31	120.16	117.00
33	2	584	А	C4-C5-C6	6.31	120.16	117.00
33	2	1363	U	O4'-C1'-N1	6.31	113.25	108.20
33	2	479	A	C4-C5-C6	6.31	120.16	117.00
39	1	17	С	OP2-P-O3'	-6.31	91.31	105.20
33	2	589	A	C4-C5-C6	6.31	120.15	117.00
33	2	1020	А	C4-C5-C6	6.31	120.15	117.00
33	2	495	G	O4'-C1'-N9	6.31	113.25	108.20
33	2	848	G	P-O3'-C3'	6.30	127.27	119.70
33	2	1302	U	O4'-C1'-N1	6.30	113.24	108.20
33	2	1451	А	C4-C5-C6	6.30	120.15	117.00
33	2	1615	A	C4-C5-C6	6.30	120.15	117.00
33	2	50	A	C4-C5-C6	6.30	120.15	117.00
33	2	988	A	C5-C6-N6	-6.30	118.66	123.70
33	2	1342	U	O4'-C1'-N1	6.30	113.24	108.20
33	2	232	А	C5-C6-N6	-6.30	118.66	123.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	77	А	C4-C5-C6	6.30	120.15	117.00
33	2	213	С	N3-C4-N4	6.30	122.41	118.00
33	2	340	С	N3-C4-N4	6.30	122.41	118.00
33	2	1570	G	O4'-C1'-N9	6.30	113.24	108.20
33	2	1853	А	C4-C5-C6	6.29	120.15	117.00
34	3	77	А	C4-C5-C6	6.29	120.15	117.00
33	2	144	U	O4'-C1'-N1	6.29	113.23	108.20
34	3	74	G	C5-C6-O6	-6.29	124.83	128.60
33	2	614	С	N3-C4-N4	6.29	122.40	118.00
35	А	131	PHE	CB-CG-CD2	-6.29	116.40	120.80
33	2	382	А	C4-C5-C6	6.28	120.14	117.00
33	2	304	А	C4-C5-C6	6.28	120.14	117.00
33	2	513	А	C4-C5-C6	6.28	120.14	117.00
33	2	986	А	C5-C6-N6	-6.28	118.68	123.70
33	2	1632	А	C4-C5-C6	6.28	120.14	117.00
33	2	1775	А	O4'-C1'-N9	6.28	113.22	108.20
33	2	518	А	C5-C6-N6	-6.28	118.68	123.70
33	2	1636	А	C5-C6-N6	-6.28	118.68	123.70
34	3	63	U	C2-N1-C1'	6.28	125.23	117.70
33	2	909	А	P-O3'-C3'	6.28	127.23	119.70
33	2	1214	С	N3-C4-N4	6.28	122.39	118.00
33	2	1495	U	O4'-C1'-N1	6.28	113.22	108.20
33	2	1752	G	O4'-C1'-N9	6.28	113.22	108.20
33	2	1330	G	C5-C6-O6	-6.27	124.84	128.60
33	2	1691	С	O4'-C1'-N1	6.27	113.22	108.20
34	3	52	А	C4-C5-C6	6.27	120.14	117.00
39	1	69	U	O4'-C1'-N1	6.27	113.22	108.20
33	2	1551	A	O4'-C1'-N9	6.27	113.22	108.20
33	2	388	А	C5-C6-N6	-6.27	118.68	123.70
33	2	798	A	C4-C5-C6	6.27	120.14	117.00
33	2	429	A	C4-C5-C6	6.27	120.13	117.00
33	2	1019	A	C4-C5-C6	6.27	120.13	117.00
33	2	1172	G	OP2-P-O3'	-6.27	91.41	105.20
33	2	1667	U	O4'-C1'-N1	6.27	113.21	108.20
39	1	65	С	N3-C4-N4	6.27	122.39	118.00
33	2	1144	A	C4-C5-C6	6.27	120.13	117.00
33	2	1839	A	C4-C5-C6	6.27	120.13	117.00
33	2	664	C	N3-C4-C5	-6.26	119.39	121.90
33	2	1092	G	O4'-C1'-N9	6.26	113.21	108.20
33	2	1109	A	C4-C5-C6	6.26	120.13	117.00
33	2	418	U	C2-N1-C1'	6.26	125.22	117.70
33	2	306	C	N3-C4-N4	6.26	122.38	118.00

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	946	С	N3-C4-N4	6.26	122.38	118.00
33	2	181	А	O4'-C1'-N9	6.26	113.21	108.20
33	2	1097	U	O4'-C1'-N1	6.26	113.21	108.20
33	2	1442	А	C4-C5-C6	6.26	120.13	117.00
38	R	37	TYR	CB-CG-CD1	6.26	124.76	121.00
33	2	288	А	C4-C5-C6	6.26	120.13	117.00
30	g	101	PHE	CB-CG-CD2	-6.26	116.42	120.80
33	2	335	U	O4'-C1'-N1	6.26	113.20	108.20
33	2	467	G	C5-C6-O6	-6.25	124.85	128.60
33	2	19	А	O4'-C1'-N9	6.25	113.20	108.20
33	2	659	А	C4-C5-C6	6.25	120.13	117.00
33	2	941	U	O4'-C1'-N1	6.25	113.20	108.20
33	2	988	А	C4-C5-C6	6.25	120.13	117.00
33	2	1526	А	C5-C6-N6	-6.25	118.70	123.70
33	2	1613	С	N3-C4-N4	6.25	122.38	118.00
33	2	54	А	C4-C5-C6	6.25	120.13	117.00
33	2	1118	А	C4-C5-C6	6.25	120.12	117.00
33	2	1457	G	C5-C6-O6	-6.25	124.85	128.60
33	2	1192	А	C4-C5-C6	6.25	120.12	117.00
33	2	1444	А	C4-C5-C6	6.25	120.12	117.00
33	2	1747	С	N3-C4-N4	6.25	122.37	118.00
33	2	1780	U	O4'-C1'-N1	6.25	113.20	108.20
33	2	450	А	C5-C6-N6	-6.25	118.70	123.70
33	2	676	U	O4'-C1'-N1	6.25	113.20	108.20
33	2	1035	С	N3-C4-N4	6.25	122.37	118.00
33	2	1382	A	C4-C5-C6	6.24	120.12	117.00
33	2	1079	A	C4-C5-C6	6.24	120.12	117.00
33	2	278	U	O4'-C1'-N1	6.24	113.19	108.20
33	2	1301	С	N3-C4-N4	6.24	122.37	118.00
33	2	1646	A	C5-C6-N6	-6.24	118.71	123.70
33	2	333	А	C4-C5-C6	6.24	120.12	117.00
33	2	1007	A	C4-C5-C6	6.24	120.12	117.00
33	2	1154	G	O4'-C1'-N9	6.24	113.19	108.20
33	2	629	C	N3-C4-N4	6.24	122.37	118.00
33	2	1421	G	C5-C6-O6	-6.24	124.86	128.60
33	2	838	С	N3-C4-N4	6.24	122.36	118.00
33	2	1273	С	N3-C4-N4	6.24	122.36	118.00
33	2	1279	C	N3-C4-C5	-6.24	119.41	121.90
33	2	377	C	N3-C4-N4	6.23	122.36	118.00
33	2	626	С	N3-C4-N4	6.23	122.36	118.00
33	2	666	С	N3-C4-N4	6.23	122.36	118.00
33	2	979	A	C4-C5-C6	6.23	120.11	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	979	А	C5-C6-N6	-6.23	118.72	123.70
33	2	1264	С	N3-C4-N4	6.23	122.36	118.00
33	2	1737	С	N3-C4-N4	6.23	122.36	118.00
33	2	1772	С	N3-C4-N4	6.23	122.36	118.00
33	2	458	А	O4'-C1'-N9	6.23	113.18	108.20
33	2	590	G	O4'-C1'-N9	6.23	113.18	108.20
33	2	1714	А	C5-C6-N6	-6.23	118.72	123.70
30	g	113	PHE	CB-CG-CD1	6.23	125.16	120.80
33	2	831	С	O4'-C1'-N1	6.23	113.18	108.20
33	2	1365	А	C4-C5-C6	6.23	120.11	117.00
33	2	1520	С	N3-C4-N4	6.23	122.36	118.00
33	2	1587	С	N3-C4-N4	6.23	122.36	118.00
33	2	1661	С	N3-C4-N4	6.23	122.36	118.00
39	1	34	С	N3-C4-N4	6.23	122.36	118.00
33	2	529	С	N3-C4-N4	6.23	122.36	118.00
33	2	419	С	N3-C4-N4	6.22	122.36	118.00
33	2	1850	С	N3-C4-N4	6.22	122.36	118.00
33	2	1726	А	C5-C6-N6	-6.22	118.72	123.70
33	2	379	А	C5-C6-N6	-6.22	118.72	123.70
33	2	423	А	C5-C6-N1	-6.22	114.59	117.70
33	2	475	А	C4-C5-C6	6.22	120.11	117.00
33	2	823	А	C4-C5-C6	6.22	120.11	117.00
33	2	1231	G	O4'-C1'-N9	6.22	113.18	108.20
33	2	1219	А	O4'-C1'-N9	6.21	113.17	108.20
33	2	1636	А	C4-C5-C6	6.21	120.11	117.00
33	2	479	А	C5-C6-N6	-6.21	118.73	123.70
33	2	70	G	C5-C6-O6	-6.21	124.87	128.60
33	2	220	С	N3-C4-N4	6.21	122.35	118.00
33	2	511	А	C4-C5-C6	6.21	120.11	117.00
33	2	551	А	C4-C5-C6	6.21	120.11	117.00
33	2	653	С	N3-C4-N4	6.21	122.35	118.00
33	2	1320	G	O4'-C1'-N9	6.21	113.17	108.20
33	2	151	С	N3-C4-N4	6.21	122.34	118.00
33	2	283	А	C4-C5-C6	6.21	120.10	117.00
33	2	398	А	C4-C5-C6	6.21	120.10	117.00
33	2	598	С	O4'-C1'-N1	6.21	113.17	108.20
33	2	1295	А	C5-C6-N6	-6.21	118.73	123.70
33	2	1439	C	O4'-C1'-N1	6.21	113.17	108.20
33	2	1712	C	N3-C4-N4	6.21	122.35	118.00
8	Ι	28	TYR	CB-CG-CD1	6.21	124.72	121.00
33	2	338	A	O4'-C1'-N9	6.21	113.16	108.20
33	2	84	A	C4-C5-C6	6.21	120.10	117.00



$\mathbf{Mol}$	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	490	А	C4-C5-C6	6.21	120.10	117.00
33	2	361	А	C4-C5-C6	6.20	120.10	117.00
33	2	1497	С	N3-C4-N4	6.20	122.34	118.00
34	3	53	U	O4'-C1'-N1	6.20	113.16	108.20
39	1	50	А	C4-C5-C6	6.20	120.10	117.00
33	2	175	А	C4-C5-C6	6.20	120.10	117.00
33	2	348	С	N3-C4-N4	6.20	122.34	118.00
33	2	922	А	C5-C6-N6	-6.20	118.74	123.70
33	2	147	А	C4-C5-C6	6.20	120.10	117.00
33	2	463	A	O4'-C1'-N9	6.20	113.16	108.20
33	2	827	G	O4'-C1'-N9	6.20	113.16	108.20
33	2	1020	А	C5-C6-N6	-6.20	118.74	123.70
33	2	1491	G	N1-C6-O6	6.20	123.62	119.90
33	2	1803	А	O4'-C1'-N9	6.20	113.16	108.20
33	2	1193	G	C5-C6-O6	-6.20	124.88	128.60
33	2	598	С	N3-C4-N4	6.20	122.34	118.00
33	2	1170	U	OP1-P-O3'	6.20	118.83	105.20
33	2	1532	А	C5-C6-N6	-6.20	118.74	123.70
33	2	422	G	O4'-C1'-N9	6.20	113.16	108.20
33	2	875	C	N3-C4-N4	6.20	122.34	118.00
33	2	1128	С	N3-C4-N4	6.20	122.34	118.00
33	2	535	А	C5-C6-N6	-6.19	118.75	123.70
33	2	841	G	C5-C6-O6	-6.19	124.89	128.60
33	2	934	A	C4-C5-C6	6.19	120.10	117.00
33	2	1622	С	N3-C4-N4	6.19	122.33	118.00
33	2	1630	С	N3-C4-N4	6.19	122.33	118.00
33	2	1740	A	C5-C6-N6	-6.19	118.75	123.70
33	2	301	С	N3-C4-N4	6.19	122.33	118.00
33	2	309	A	C4-C5-C6	6.19	120.10	117.00
33	2	1099	C	N3-C4-N4	6.19	122.33	118.00
33	2	67	С	N3-C4-N4	6.19	122.33	118.00
33	2	589	A	C5-C6-N6	-6.19	118.75	123.70
33	2	831	С	N3-C4-N4	6.19	122.33	118.00
33	2	1260	С	N3-C4-N4	6.19	122.33	118.00
39	1	20	А	C4-C5-C6	6.19	120.09	117.00
33	2	168	С	N3-C4-N4	6.19	122.33	118.00
33	2	841	G	O4'-C1'-N9	6.19	113.15	108.20
33	2	855	G	O4'-C1'-N9	6.19	113.15	108.20
33	2	1540	A	C4-C5-C6	6.18	120.09	117.00
33	2	1548	C	N3-C4-N4	6.18	122.33	118.00
39	1	4	С	N3-C4-N4	6.18	122.33	118.00
33	2	584	A	C5-C6-N1	-6.18	114.61	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	618	А	C4-C5-C6	6.18	120.09	117.00
33	2	78	С	O4'-C1'-N1	6.18	113.14	108.20
33	2	359	С	N3-C4-N4	6.18	122.33	118.00
33	2	367	G	O4'-C1'-N9	6.18	113.14	108.20
33	2	1665	С	N3-C4-N4	6.18	122.33	118.00
39	1	39	С	N3-C4-N4	6.18	122.33	118.00
33	2	388	А	C4-C5-C6	6.18	120.09	117.00
33	2	48	С	N3-C4-N4	6.18	122.32	118.00
33	2	282	G	C5-C6-O6	-6.18	124.89	128.60
33	2	554	А	C4-C5-C6	6.18	120.09	117.00
33	2	1003	С	N3-C4-N4	6.18	122.32	118.00
33	2	1235	U	O4'-C1'-N1	6.18	113.14	108.20
33	2	1585	С	N3-C4-N4	6.18	122.32	118.00
33	2	1751	G	O4'-C1'-N9	6.18	113.14	108.20
39	1	21	А	C4-C5-C6	6.18	120.09	117.00
39	1	60	А	C4-C5-C6	6.18	120.09	117.00
33	2	909	А	C4-C5-C6	6.17	120.09	117.00
33	2	1095	G	O4'-C1'-N9	6.17	113.14	108.20
33	2	1530	U	O4'-C1'-N1	6.17	113.14	108.20
33	2	126	G	C5-C6-O6	-6.17	124.90	128.60
33	2	313	С	N3-C4-N4	6.17	122.32	118.00
33	2	404	A	C4-C5-C6	6.17	120.09	117.00
33	2	1189	U	O4'-C1'-N1	6.17	113.14	108.20
33	2	1686	U	O4'-C1'-N1	6.17	113.14	108.20
33	2	1710	А	C5-C6-N6	-6.17	118.76	123.70
33	2	825	С	O4'-C1'-N1	6.17	113.14	108.20
33	2	405	А	C4-C5-C6	6.17	120.08	117.00
33	2	916	А	C5-C6-N1	-6.17	114.62	117.70
33	2	953	А	C4-C5-C6	6.17	120.08	117.00
33	2	1472	А	C5-C6-N1	-6.17	114.62	117.70
33	2	1682	С	N3-C4-N4	6.17	122.32	118.00
33	2	94	G	O4'-C1'-N9	6.17	113.13	108.20
33	2	123	G	O4'-C1'-N9	6.17	113.13	108.20
33	2	191	С	N3-C4-N4	6.17	122.32	118.00
33	2	339	А	C4-C5-C6	6.17	120.08	117.00
33	2	64	A	C4-C5-C6	6.17	120.08	117.00
33	2	1006	G	O4'-C1'-N9	6.17	113.13	108.20
33	2	1278	A	C4-C5-C6	6.17	120.08	117.00
33	2	159	A	C4-C5-C6	6.16	120.08	117.00
33	2	631	A	C4-C5-C6	6.16	120.08	117.00
33	2	1690	A	C4-C5-C6	6.16	120.08	117.00
33	2	107	A	C4-C5-C6	6.16	120.08	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal $(^{o})$
33	2	956	U	O4'-C1'-N1	6.16	113.13	108.20
33	2	1484	С	N3-C4-N4	6.16	122.31	118.00
33	2	209	С	N3-C4-N4	6.16	122.31	118.00
33	2	1165	G	N3-C2-N2	6.16	124.21	119.90
39	1	35	А	C4-C5-C6	6.16	120.08	117.00
33	2	346	С	O4'-C1'-N1	6.16	113.13	108.20
33	2	1266	G	O4'-C1'-N9	6.16	113.13	108.20
33	2	324	С	N3-C4-N4	6.16	122.31	118.00
33	2	1067	G	P-O3'-C3'	6.16	127.09	119.70
33	2	1513	С	C6-N1-C1'	-6.16	113.41	120.80
39	1	41	С	N3-C4-N4	6.16	122.31	118.00
33	2	994	А	C5-C6-N1	-6.15	114.62	117.70
33	2	201	G	O4'-C1'-N9	6.15	113.12	108.20
33	2	1029	G	N3-C2-N2	6.15	124.21	119.90
33	2	1553	С	N3-C4-N4	6.15	122.31	118.00
33	2	218	А	C4-C5-C6	6.15	120.08	117.00
33	2	332	С	N3-C4-N4	6.15	122.31	118.00
33	2	854	А	C4-C5-C6	6.15	120.08	117.00
33	2	1242	А	C4-C5-C6	6.15	120.08	117.00
33	2	1366	А	C5-C6-N6	-6.15	118.78	123.70
33	2	1643	G	C5-C6-O6	-6.15	124.91	128.60
33	2	1337	С	N3-C4-N4	6.15	122.30	118.00
33	2	1674	А	C5-C6-N6	-6.15	118.78	123.70
33	2	70	G	O4'-C1'-N9	6.14	113.12	108.20
33	2	1172	G	OP1-P-O3'	6.14	118.72	105.20
33	2	1407	G	C5-C6-O6	-6.14	124.91	128.60
33	2	379	А	C4-C5-C6	6.14	120.07	117.00
33	2	458	А	C4-C5-C6	6.14	120.07	117.00
33	2	1822	С	N3-C4-N4	6.14	122.30	118.00
16	Q	34	PHE	CB-CG-CD1	6.14	125.10	120.80
19	V	40	ALA	N-CA-CB	6.14	118.69	110.10
33	2	569	С	N3-C4-N4	6.14	122.30	118.00
33	2	463	A	C4-C5-C6	6.14	120.07	117.00
33	2	83	A	C4-C5-C6	6.13	120.07	117.00
33	2	214	А	C4-C5-C6	6.13	120.07	117.00
33	2	459	А	C4-C5-C6	6.13	120.07	117.00
33	2	670	G	O4'-C1'-N9	6.13	113.11	108.20
33	2	850	A	C4-C5-C6	6.13	120.07	117.00
33	2	1026	A	C5-C6-N6	-6.13	118.80	123.70
33	2	382	A	C5-C6-N6	-6.13	118.80	123.70
33	2	731	С	N3-C4-N4	6.13	122.29	118.00
33	2	866	A	C4-C5-C6	6.13	120.06	117.00

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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	148	U	O4'-C1'-N1	6.13	113.10	108.20
33	2	545	А	C4-C5-C6	6.13	120.06	117.00
33	2	649	G	O4'-C1'-N9	6.13	113.10	108.20
33	2	111	А	C4-C5-C6	6.12	120.06	117.00
33	2	475	А	C5-C6-N6	-6.12	118.80	123.70
33	2	580	А	C4-C5-C6	6.12	120.06	117.00
33	2	971	G	O4'-C1'-N9	6.12	113.10	108.20
33	2	1431	С	O4'-C1'-N1	6.12	113.10	108.20
33	2	1812	А	O4'-C1'-N9	6.12	113.10	108.20
36	В	137	PHE	CB-CG-CD2	-6.12	116.51	120.80
33	2	327	С	N3-C4-N4	6.12	122.28	118.00
33	2	481	С	N3-C4-N4	6.12	122.28	118.00
33	2	288	А	C5-C6-N6	-6.12	118.80	123.70
33	2	292	А	C4-C5-C6	6.12	120.06	117.00
33	2	624	А	C5-C6-N6	-6.12	118.81	123.70
33	2	580	А	O4'-C1'-N9	6.12	113.09	108.20
33	2	845	А	C5-C6-N6	-6.12	118.81	123.70
33	2	1190	А	C5-C6-N1	-6.12	114.64	117.70
33	2	1787	А	C5-C6-N1	-6.12	114.64	117.70
33	2	23	G	O4'-C1'-N9	6.11	113.09	108.20
33	2	142	С	C2-N1-C1'	6.11	125.53	118.80
33	2	366	А	C4-C5-C6	6.11	120.06	117.00
33	2	1254	А	C4-C5-C6	6.11	120.06	117.00
39	1	35	А	C5-C6-N1	-6.11	114.64	117.70
33	2	854	А	C5-C6-N1	-6.11	114.64	117.70
33	2	1162	G	O4'-C1'-N9	6.11	113.09	108.20
33	2	1249	А	C5-C6-N6	-6.11	118.81	123.70
33	2	1344	G	O4'-C1'-N9	6.11	113.09	108.20
33	2	973	С	N3-C4-N4	6.11	122.28	118.00
33	2	1835	С	N3-C4-N4	6.11	122.28	118.00
33	2	729	С	N3-C4-N4	6.11	122.28	118.00
33	2	1022	С	O4'-C1'-N1	6.11	113.08	108.20
33	2	1308	G	N3-C2-N2	6.11	124.18	119.90
33	2	1370	С	N3-C4-N4	6.11	122.28	118.00
33	2	1692	А	C4-C5-C6	6.11	120.05	117.00
33	2	1024	A	C4-C5-C6	6.11	120.05	117.00
33	2	1261	A	C4-C5-C6	6.11	120.05	117.00
33	2	1508	С	N3-C4-N4	6.11	122.27	118.00
33	2	1185	A	O4'-C1'-N9	6.10	113.08	108.20
33	2	1377	G	O4'-C1'-N9	6.10	113.08	108.20
33	2	976	A	C4-C5-C6	6.10	120.05	117.00
- 33	2	1650	C	N3-C4-N4	6.10	122.27	118.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	445	А	C5-C6-N1	-6.10	114.65	117.70
14	0	114	TYR	CB-CG-CD2	-6.10	117.34	121.00
33	2	239	U	O4'-C1'-N1	6.10	113.08	108.20
33	2	30	С	N3-C4-N4	6.10	122.27	118.00
33	2	443	С	N3-C4-N4	6.10	122.27	118.00
33	2	1102	С	N3-C4-N4	6.10	122.27	118.00
33	2	1246	А	C4-C5-C6	6.10	120.05	117.00
33	2	1781	G	O4'-C1'-N9	6.10	113.08	108.20
33	2	106	С	N3-C4-N4	6.10	122.27	118.00
33	2	487	С	N3-C4-N4	6.10	122.27	118.00
33	2	924	G	C5-C6-O6	-6.10	124.94	128.60
33	2	512	А	C4-C5-C6	6.09	120.05	117.00
33	2	564	А	C4-C5-C6	6.09	120.05	117.00
39	1	67	U	O4'-C1'-N1	6.09	113.08	108.20
33	2	358	U	O4'-C1'-N1	6.09	113.08	108.20
33	2	127	С	N3-C4-C5	-6.09	119.46	121.90
33	2	978	G	O4'-C1'-N9	6.09	113.07	108.20
33	2	1008	А	C4-C5-C6	6.09	120.05	117.00
33	2	1119	С	N3-C4-N4	6.09	122.26	118.00
33	2	1564	А	C4-C5-C6	6.09	120.05	117.00
33	2	1674	А	C4-C5-C6	6.09	120.05	117.00
35	А	56	ILE	C-N-CA	-6.09	106.47	121.70
33	2	2	А	C4-C5-C6	6.09	120.04	117.00
33	2	896	С	N3-C4-C5	-6.09	119.46	121.90
33	2	1303	U	C5-C4-O4	-6.09	122.25	125.90
33	2	1321	G	O4'-C1'-N9	6.09	113.07	108.20
39	1	63	А	C4-C5-C6	6.09	120.05	117.00
33	2	1450	А	C4-C5-C6	6.09	120.04	117.00
33	2	330	С	N3-C4-N4	6.09	122.26	118.00
33	2	429	А	C5-C6-N6	-6.09	118.83	123.70
33	2	1274	А	C4-C5-C6	6.09	120.04	117.00
33	2	1349	А	C4-C5-C6	6.09	120.04	117.00
33	2	1583	А	C4-C5-C6	6.09	120.04	117.00
33	2	1794	А	C4-C5-C6	6.09	120.04	117.00
39	1	76	А	O4'-C1'-N9	6.09	113.07	108.20
33	2	1232	G	04'-C1'-N9	6.08	113.07	108.20
39	1	74	C	N3-C4-N4	6.08	122.26	118.00
33	2	809	A	C4-C5-C6	6.08	120.04	117.00
33	2	469	C	N3-C4-N4	6.08	122.26	118.00
33	2	797	U	OP1-P-O3 <sup>7</sup>	6.08	118.58	105.20
33	2	$11\overline{40}$	A	C4-C5-C6	6.08	120.04	117.00
33	2	1096	А	C4-C5-C6	6.08	120.04	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1713	G	C5-C6-O6	-6.08	124.95	128.60
33	2	1406	С	N3-C4-N4	6.08	122.25	118.00
33	2	1564	A	C5-C6-N6	-6.08	118.84	123.70
33	2	1735	С	N3-C4-C5	-6.08	119.47	121.90
35	А	153	PHE	CB-CG-CD1	6.08	125.06	120.80
33	2	343	С	N3-C4-N4	6.08	122.25	118.00
33	2	625	G	O4'-C1'-N9	6.08	113.06	108.20
33	2	1418	G	O4'-C1'-N9	6.08	113.06	108.20
33	2	1829	А	C4-C5-C6	6.08	120.04	117.00
23	Ζ	41	PHE	CB-CG-CD1	6.07	125.05	120.80
33	2	50	А	O4'-C1'-N9	6.07	113.06	108.20
33	2	194	С	N3-C4-N4	6.07	122.25	118.00
33	2	884	U	O4'-C1'-N1	6.07	113.06	108.20
39	1	16	G	OP2-P-O3'	-6.07	91.84	105.20
33	2	1813	A	C5-C6-N6	-6.07	118.84	123.70
33	2	1580	U	O4'-C1'-N1	6.07	113.06	108.20
33	2	944	С	N3-C4-N4	6.07	122.25	118.00
33	2	1057	U	O4'-C1'-N1	6.07	113.05	108.20
33	2	1190	А	C5-C6-N6	-6.07	118.85	123.70
33	2	1645	А	C4-C5-C6	6.06	120.03	117.00
33	2	89	С	N3-C4-N4	6.06	122.24	118.00
33	2	361	A	C5-C6-N6	-6.06	118.85	123.70
33	2	638	A	C5-C6-N6	-6.06	118.85	123.70
33	2	1277	G	O4'-C1'-N9	6.06	113.05	108.20
33	2	22	А	C4-C5-C6	6.06	120.03	117.00
33	2	809	А	C5-C6-N6	-6.06	118.85	123.70
33	2	1031	A	C5-C6-N6	-6.06	118.85	123.70
33	2	58	С	N3-C4-N4	6.06	122.24	118.00
33	2	1216	A	C5-C6-N6	-6.06	118.85	123.70
33	2	206	A	C5-C6-N1	-6.06	114.67	117.70
33	2	638	A	C4-C5-C6	6.06	120.03	117.00
33	2	857	A	C4-C5-C6	6.06	120.03	117.00
33	2	897	G	O4'-C1'-N9	6.06	113.05	108.20
33	2	293	A	C4-C5-C6	6.06	120.03	117.00
33	2	1745	С	N3-C4-N4	6.05	122.24	118.00
33	2	990	C	N3-C4-N4	6.05	122.24	118.00
33	2	1213	A	C5-C6-N6	-6.05	118.86	123.70
33	2	272	C	O4'-C1'-N1	6.05	113.04	108.20
33	2	526	A	O4'-C1'-N9	6.05	113.04	108.20
33	2	664	C	N3-C4-N4	6.05	122.23	118.00
33	2	940	A	C5-C6-N6	-6.05	118.86	123.70
33	2	1053	С	C6-N1-C1'	-6.05	113.54	120.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1088	G	O4'-C1'-N9	6.05	113.04	108.20
33	2	1606	G	O4'-C1'-N9	6.05	113.04	108.20
33	2	103	А	C5-C6-N6	-6.05	118.86	123.70
33	2	1619	U	C2-N1-C1'	6.05	124.95	117.70
33	2	232	А	C4-C5-C6	6.04	120.02	117.00
33	2	1726	А	C4-C5-C6	6.04	120.02	117.00
39	1	45	G	C5-C6-O6	-6.04	124.97	128.60
33	2	40	А	C5-C6-N6	-6.04	118.86	123.70
33	2	60	А	C4-C5-C6	6.04	120.02	117.00
33	2	1134	С	O4'-C1'-N1	6.04	113.03	108.20
33	2	615	G	O4'-C1'-N9	6.04	113.03	108.20
33	2	826	А	C4-C5-C6	6.04	120.02	117.00
33	2	1380	С	N3-C4-N4	6.04	122.23	118.00
33	2	1418	G	N3-C2-N2	6.04	124.13	119.90
33	2	1807	А	C4-C5-C6	6.04	120.02	117.00
33	2	91	А	C5-C6-N6	-6.04	118.87	123.70
33	2	289	G	O4'-C1'-N9	6.04	113.03	108.20
33	2	957	G	O4'-C1'-N9	6.04	113.03	108.20
33	2	1859	С	O4'-C1'-N1	6.04	113.03	108.20
33	2	343	С	N3-C4-C5	-6.04	119.48	121.90
33	2	1051	А	C4-C5-C6	6.04	120.02	117.00
33	2	1169	А	C5-C6-N6	-6.04	118.87	123.70
33	2	1443	G	O4'-C1'-N9	6.04	113.03	108.20
39	1	66	С	N3-C4-N4	6.04	122.23	118.00
33	2	826	А	C5-C6-N6	-6.04	118.87	123.70
33	2	223	А	C4-C5-C6	6.04	120.02	117.00
33	2	1272	А	C5-C6-N6	-6.04	118.87	123.70
33	2	1437	U	O4'-C1'-N1	6.04	113.03	108.20
33	2	1792	С	N3-C4-N4	6.04	122.23	118.00
33	2	455	А	C4-C5-C6	6.03	120.02	117.00
33	2	807	А	C5-C6-N1	-6.03	114.68	117.70
33	2	882	А	C4-C5-C6	6.03	120.02	117.00
33	2	1127	G	O4'-C1'-N9	6.03	113.03	108.20
33	2	549	G	C5-C6-O6	-6.03	124.98	128.60
33	2	1813	А	C5-C6-N1	-6.03	114.68	117.70
33	2	1032	А	C4-C5-C6	6.03	120.02	117.00
33	2	1331	G	O4'-C1'-N9	6.03	113.03	108.20
33	2	1375	A	C5-C6-N6	-6.03	118.88	123.70
33	2	822	А	C4-C5-C6	6.03	120.01	117.00
33	2	56	G	O4'-C1'-N9	6.02	113.02	108.20
33	2	1059	C	N3-C4-N4	6.02	122.22	118.00
33	2	1571	G	O4'-C1'-N9	6.02	113.02	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1841	G	O4'-C1'-N9	6.02	113.02	108.20
33	2	1007	А	O4'-C1'-N9	6.02	113.02	108.20
33	2	1073	А	C4-C5-C6	6.02	120.01	117.00
33	2	1144	А	C5-C6-N6	-6.02	118.88	123.70
33	2	1194	G	C5-C6-O6	-6.02	124.99	128.60
33	2	1353	А	C5-C6-N1	-6.02	114.69	117.70
33	2	1485	А	C4-C5-C6	6.02	120.01	117.00
33	2	812	А	C4-C5-C6	6.02	120.01	117.00
33	2	1160	G	O4'-C1'-N9	6.02	113.02	108.20
33	2	304	А	C5-C6-N1	-6.02	114.69	117.70
33	2	1070	С	N3-C4-N4	6.02	122.21	118.00
33	2	1131	С	N3-C4-N4	6.02	122.21	118.00
33	2	1385	С	N3-C4-N4	6.02	122.21	118.00
39	1	27	С	N3-C4-N4	6.02	122.21	118.00
33	2	1204	А	C4-C5-C6	6.02	120.01	117.00
33	2	1483	А	C4-C5-C6	6.02	120.01	117.00
33	2	1821	U	O4'-C1'-N1	6.02	113.02	108.20
33	2	1405	А	C4-C5-C6	6.02	120.01	117.00
33	2	1694	A	C4-C5-C6	6.02	120.01	117.00
33	2	814	А	C5-C6-N6	-6.01	118.89	123.70
39	1	59	А	C4-C5-C6	6.01	120.01	117.00
33	2	851	G	O4'-C1'-N9	6.01	113.01	108.20
33	2	1714	A	O4'-C1'-N9	6.01	113.01	108.20
33	2	39	A	C4-C5-C6	6.01	120.00	117.00
33	2	404	А	C5-C6-N6	-6.01	118.89	123.70
33	2	640	А	C5-C6-N1	-6.01	114.69	117.70
33	2	1395	С	N3-C4-N4	6.01	122.21	118.00
33	2	1482	А	C4-C5-C6	6.01	120.00	117.00
33	2	1374	А	C4-C5-C6	6.01	120.00	117.00
33	2	1081	С	O4'-C1'-N1	6.01	113.01	108.20
33	2	1415	С	N3-C4-C5	-6.01	119.50	121.90
33	2	1629	А	O4'-C1'-N9	6.00	113.00	108.20
33	2	1642	А	C4-C5-C6	6.00	120.00	117.00
35	А	131	PHE	CB-CG-CD1	6.00	125.00	120.80
33	2	498	А	C4-C5-C6	6.00	120.00	117.00
33	2	675	А	C4-C5-C6	6.00	120.00	117.00
33	2	1434	А	C4-C5-C6	6.00	120.00	117.00
33	2	1575	A	C4-C5-C6	6.00	120.00	117.00
39	1	38	A	C4-C5-C6	6.00	120.00	117.00
33	2	225	С	N3-C4-N4	6.00	122.20	118.00
33	2	1145	A	C4-C5-C6	6.00	120.00	117.00
34	3	67	A	C4-C5-C6	6.00	120.00	117.00



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	147	А	O4'-C1'-N9	6.00	113.00	108.20
33	2	395	G	O4'-C1'-N9	6.00	113.00	108.20
33	2	1707	А	O4'-C1'-N9	6.00	113.00	108.20
33	2	65	С	N3-C4-N4	6.00	122.20	118.00
33	2	474	А	C5-C6-N1	-6.00	114.70	117.70
33	2	1364	U	O4'-C1'-N1	6.00	113.00	108.20
34	3	76	А	C4-C5-C6	6.00	120.00	117.00
33	2	1369	С	N3-C4-N4	6.00	122.20	118.00
33	2	1567	С	N3-C4-C5	-6.00	119.50	121.90
33	2	1782	А	C4-C5-C6	6.00	120.00	117.00
33	2	611	С	N3-C4-N4	6.00	122.20	118.00
33	2	1800	А	O4'-C1'-N9	6.00	113.00	108.20
33	2	993	А	O4'-C1'-N9	5.99	113.00	108.20
33	2	1023	А	C5-C6-N1	-5.99	114.70	117.70
33	2	19	А	C4-C5-C6	5.99	120.00	117.00
33	2	502	А	C4-C5-C6	5.99	120.00	117.00
33	2	897	G	C5-C6-O6	-5.99	125.00	128.60
33	2	1005	А	C5-C6-N6	-5.99	118.91	123.70
33	2	1080	А	C4-C5-C6	5.99	120.00	117.00
33	2	1476	А	C4-C5-C6	5.99	120.00	117.00
33	2	1478	С	N3-C4-N4	5.99	122.19	118.00
33	2	1589	А	C5-C6-N6	-5.99	118.91	123.70
33	2	1657	U	O4'-C1'-N1	5.99	112.99	108.20
33	2	597	U	C2-N1-C1'	5.99	124.89	117.70
39	1	13	G	O4'-C1'-N9	5.99	112.99	108.20
33	2	959	А	C5-C6-N6	-5.99	118.91	123.70
33	2	518	А	C4-C5-C6	5.99	119.99	117.00
33	2	959	А	C4-C5-C6	5.99	119.99	117.00
33	2	1829	А	C5-C6-N6	-5.99	118.91	123.70
39	1	62	С	N3-C4-N4	5.99	122.19	118.00
33	2	852	С	N3-C4-N4	5.98	122.19	118.00
33	2	1289	А	C5-C6-N6	-5.98	118.91	123.70
33	2	1425	G	O4'-C1'-N9	5.98	112.99	108.20
33	2	92	А	C4-C5-C6	5.98	119.99	117.00
33	2	1049	С	N3-C4-N4	5.98	122.19	118.00
33	2	1332	С	N3-C4-N4	5.98	122.19	118.00
33	2	1378	А	C4-C5-C6	5.98	119.99	117.00
33	2	1435	A	C4-C5-C6	5.98	119.99	117.00
33	2	865	A	C5-C6-N6	-5.98	118.92	123.70
33	2	1832	U	O4'-C1'-N1	5.98	112.98	108.20
33	2	640	A	C4-C5-C6	5.98	119.99	117.00
33	2	1126	G	C5-C6-O6	-5.98	125.01	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1529	С	O4'-C1'-N1	5.98	112.98	108.20
33	2	608	С	N3-C4-N4	5.98	122.19	118.00
33	2	1328	А	C4-C5-C6	5.98	119.99	117.00
33	2	511	А	O4'-C1'-N9	5.98	112.98	108.20
33	2	1109	А	C5-C6-N6	-5.98	118.92	123.70
33	2	630	А	C4-C5-C6	5.97	119.99	117.00
33	2	1031	А	C4-C5-C6	5.97	119.99	117.00
33	2	1663	U	O4'-C1'-N1	5.97	112.98	108.20
33	2	453	С	O4'-C1'-N1	5.97	112.98	108.20
33	2	1800	А	C4-C5-C6	5.97	119.99	117.00
33	2	46	А	C4-C5-C6	5.97	119.99	117.00
33	2	609	А	C4-C5-C6	5.97	119.98	117.00
33	2	821	А	C4-C5-C6	5.97	119.98	117.00
33	2	1015	С	N3-C4-C5	-5.97	119.51	121.90
33	2	1210	А	C4-C5-C6	5.97	119.98	117.00
33	2	1289	A	C4-C5-C6	5.97	119.98	117.00
33	2	1811	G	O4'-C1'-N9	5.97	112.97	108.20
33	2	1260	С	O4'-C1'-N1	5.97	112.97	108.20
33	2	228	А	C5-C6-N1	-5.97	114.72	117.70
33	2	483	А	C5-C6-N6	-5.97	118.93	123.70
33	2	1465	A	C5-C6-N6	-5.97	118.93	123.70
35	А	153	PHE	CB-CG-CD2	-5.97	116.62	120.80
33	2	521	A	C4-C5-C6	5.96	119.98	117.00
33	2	623	С	N3-C4-N4	5.96	122.17	118.00
33	2	1707	А	C4-C5-C6	5.96	119.98	117.00
33	2	1479	А	C5-C6-N6	-5.96	118.93	123.70
33	2	508	G	O4'-C1'-N9	5.96	112.97	108.20
33	2	559	А	C4-C5-C6	5.96	119.98	117.00
33	2	661	А	C5-C6-N1	-5.96	114.72	117.70
33	2	1340	A	C5-C6-N6	-5.96	118.93	123.70
33	2	459	A	O4'-C1'-N9	5.96	112.97	108.20
33	2	535	A	C4-C5-C6	5.96	119.98	117.00
33	2	661	A	C4-C5-C6	5.96	119.98	117.00
33	2	958	A	C4-C5-C6	5.96	119.98	117.00
33	2	1401	A	C4-C5-C6	5.96	119.98	117.00
33	2	1513	С	N3-C4-C5	-5.96	119.52	121.90
33	2	1669	G	N3-C2-N2	5.96	124.07	119.90
33	2	50	A	C5-C6-N6	-5.96	118.94	123.70
33	2	355	С	N3-C4-N4	5.96	122.17	118.00
33	2	1444	A	C5-C6-N1	-5.96	114.72	117.70
33	2	1695	С	N3-C4-N4	5.96	122.17	118.00
33	2	509	A	C5-C6-N1	-5.95	114.72	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal $(^{o})$
33	2	868	А	C5-C6-N6	-5.95	118.94	123.70
33	2	1510	G	O4'-C1'-N9	5.95	112.96	108.20
39	1	58	А	C4-C5-C6	5.95	119.98	117.00
33	2	99	А	C5-C6-N6	-5.95	118.94	123.70
33	2	807	А	C4-C5-C6	5.95	119.98	117.00
33	2	65	С	N3-C4-C5	-5.95	119.52	121.90
33	2	230	С	N3-C4-N4	5.95	122.17	118.00
33	2	341	G	C5-C6-O6	-5.95	125.03	128.60
33	2	1494	А	C4-C5-C6	5.95	119.97	117.00
33	2	1574	А	C5-C6-N6	-5.95	118.94	123.70
33	2	22	А	C5-C6-N1	-5.95	114.73	117.70
33	2	33	G	O4'-C1'-N9	5.95	112.96	108.20
33	2	164	А	O4'-C1'-N9	5.95	112.96	108.20
33	2	853	U	O4'-C1'-N1	5.95	112.96	108.20
39	1	58	А	C5-C6-N1	-5.95	114.73	117.70
33	2	4	С	O4'-C1'-N1	5.95	112.96	108.20
33	2	669	А	O4'-C1'-N9	5.95	112.96	108.20
33	2	438	А	C4-C5-C6	5.95	119.97	117.00
33	2	523	А	C5-C6-N1	-5.95	114.73	117.70
33	2	582	С	N3-C4-N4	5.95	122.16	118.00
33	2	912	А	C4-C5-C6	5.95	119.97	117.00
33	2	1413	С	N3-C4-N4	5.95	122.16	118.00
33	2	1446	G	O4'-C1'-N9	5.95	112.96	108.20
33	2	1461	А	C4-C5-C6	5.95	119.97	117.00
33	2	25	А	C5-C6-N6	-5.94	118.95	123.70
33	2	73	С	O4'-C1'-N1	5.94	112.95	108.20
33	2	808	А	O4'-C1'-N9	5.94	112.95	108.20
33	2	1193	G	O4'-C1'-N9	5.94	112.95	108.20
33	2	1274	А	C5-C6-N6	-5.94	118.95	123.70
33	2	1391	С	N3-C4-N4	5.94	122.16	118.00
33	2	1731	G	O4'-C1'-N9	5.94	112.95	108.20
33	2	953	А	C5-C6-N6	-5.94	118.95	123.70
33	2	1470	А	C5-C6-N6	-5.94	118.95	123.70
33	2	1608	G	O4'-C1'-N9	5.94	112.95	108.20
33	2	1618	А	C5-C6-N6	-5.94	118.95	123.70
33	2	221	А	O4'-C1'-N9	5.94	112.95	108.20
33	2	1601	G	C5-C6-O6	-5.94	125.04	128.60
33	2	61	А	C4-C5-C6	5.94	119.97	117.00
33	2	298	G	C5-C6-O6	-5.94	125.04	128.60
33	2	346	С	N3-C4-N4	5.94	122.16	118.00
33	2	660	A	C4-C5-C6	5.94	119.97	117.00
33	2	1579	G	C5-C6-O6	-5.94	125.04	128.60



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	439	А	O4'-C1'-N9	5.94	112.95	108.20
33	2	523	А	O4'-C1'-N9	5.94	112.95	108.20
33	2	1195	А	O4'-C1'-N9	5.94	112.95	108.20
33	2	408	А	O4'-C1'-N9	5.93	112.95	108.20
33	2	506	А	C4-C5-C6	5.93	119.97	117.00
33	2	984	С	N3-C4-N4	5.93	122.15	118.00
33	2	1205	А	C4-C5-C6	5.93	119.97	117.00
33	2	1268	С	N3-C4-N4	5.93	122.15	118.00
33	2	1397	А	C4-C5-C6	5.93	119.97	117.00
33	2	166	А	C4-C5-C6	5.93	119.97	117.00
33	2	948	G	O4'-C1'-N9	5.93	112.95	108.20
33	2	1777	С	O4'-C1'-N1	5.93	112.95	108.20
33	2	674	G	O4'-C1'-N9	5.93	112.94	108.20
33	2	1735	С	N3-C4-N4	5.93	122.15	118.00
33	2	622	С	N3-C4-N4	5.93	122.15	118.00
33	2	1019	А	C5-C6-N1	-5.93	114.73	117.70
33	2	1196	А	C5-C6-N6	-5.93	118.96	123.70
33	2	1468	С	N3-C4-N4	5.93	122.15	118.00
33	2	1488	U	O4'-C1'-N1	5.93	112.94	108.20
33	2	1684	С	N3-C4-N4	5.93	122.15	118.00
33	2	1844	А	O4'-C1'-N9	5.93	112.94	108.20
33	2	1356	U	O4'-C1'-N1	5.93	112.94	108.20
33	2	88	G	O4'-C1'-N9	5.93	112.94	108.20
33	2	158	А	O4'-C1'-N9	5.93	112.94	108.20
33	2	554	А	O4'-C1'-N9	5.93	112.94	108.20
33	2	558	С	N3-C4-N4	5.93	122.15	118.00
33	2	1451	А	C5-C6-N1	-5.93	114.74	117.70
33	2	1697	G	O4'-C1'-N9	5.93	112.94	108.20
33	2	326	А	O4'-C1'-N9	5.92	112.94	108.20
33	2	630	А	C5-C6-N6	-5.92	118.96	123.70
33	2	1094	С	N3-C4-N4	5.92	122.15	118.00
33	2	1140	А	C5-C6-N1	-5.92	114.74	117.70
33	2	1226	С	N3-C4-N4	5.92	122.15	118.00
33	2	1382	А	C5-C6-N6	-5.92	118.96	123.70
39	1	38	А	O4'-C1'-N9	5.92	112.94	108.20
33	2	1476	А	C5-C6-N6	-5.92	118.96	123.70
33	2	338	А	C4-C5-C6	5.92	119.96	117.00
33	2	1184	А	C5-C6-N1	-5.92	114.74	117.70
33	2	1434	А	O4'-C1'-N9	5.92	112.94	108.20
33	2	1799	G	O4'-C1'-N9	5.92	112.94	108.20
33	2	1485	А	O4'-C1'-N9	5.92	112.94	108.20
33	2	313	С	O4'-C1'-N1	5.92	112.94	108.20



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	445	А	C4-C5-C6	5.92	119.96	117.00
33	2	836	С	N3-C4-N4	5.92	122.14	118.00
33	2	1436	С	N3-C4-N4	5.92	122.14	118.00
33	2	408	А	C4-C5-C6	5.92	119.96	117.00
33	2	1710	А	C4-C5-C6	5.92	119.96	117.00
33	2	940	А	C5-C6-N1	-5.92	114.74	117.70
33	2	1187	С	N3-C4-N4	5.92	122.14	118.00
33	2	460	G	O4'-C1'-N9	5.91	112.93	108.20
33	2	492	С	O4'-C1'-N1	5.91	112.93	108.20
33	2	814	А	C4-C5-C6	5.91	119.96	117.00
33	2	1038	А	C5-C6-N6	-5.91	118.97	123.70
33	2	1181	С	N3-C4-N4	5.91	122.14	118.00
33	2	1632	А	C5-C6-N6	-5.91	118.97	123.70
39	1	52	G	O4'-C1'-N9	5.91	112.93	108.20
33	2	603	С	N3-C4-C5	-5.91	119.53	121.90
33	2	1118	А	C5-C6-N6	-5.91	118.97	123.70
33	2	186	G	O4'-C1'-N9	5.91	112.93	108.20
33	2	1480	А	C4-C5-C6	5.91	119.95	117.00
39	1	5	А	C4-C5-C6	5.91	119.95	117.00
33	2	1237	А	C4-C5-C6	5.91	119.95	117.00
33	2	1299	C	C6-N1-C1'	-5.91	113.71	120.80
33	2	1496	G	O4'-C1'-N9	5.91	112.93	108.20
39	1	42	А	C4-C5-C6	5.91	119.95	117.00
33	2	983	A	C4-C5-C6	5.91	119.95	117.00
33	2	798	A	C5-C6-N1	-5.91	114.75	117.70
33	2	1008	А	C5-C6-N6	-5.91	118.98	123.70
33	2	1089	А	C4-C5-C6	5.91	119.95	117.00
33	2	1534	U	O4'-C1'-N1	5.91	112.92	108.20
33	2	1431	С	N3-C4-C5	-5.90	119.54	121.90
33	2	1470	А	C4-C5-C6	5.90	119.95	117.00
33	2	1812	A	C4-C5-C6	5.90	119.95	117.00
33	2	24	С	N3-C4-C5	-5.90	119.54	121.90
33	2	401	G	O4'-C1'-N9	5.90	112.92	108.20
33	2	1063	С	N3-C4-N4	5.90	122.13	118.00
33	2	1241	G	O4'-C1'-N9	5.90	112.92	108.20
33	2	298	G	O4'-C1'-N9	5.90	112.92	108.20
32	i	131	ALA	N-CA-CB	5.90	118.36	110.10
33	2	190	A	C4-C5-C6	5.90	119.95	117.00
33	2	1384	A	C4-C5-C6	5.90	119.95	117.00
33	2	38	А	C5-C6-N6	-5.90	118.98	123.70
33	2	1236	А	C4-C5-C6	5.90	119.95	117.00
33	2	423	A	C5-C6-N6	-5.89	118.98	123.70



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	510	А	C4-C5-C6	5.89	119.95	117.00
33	2	1339	U	O4'-C1'-N1	5.89	112.92	108.20
33	2	1718	G	O4'-C1'-N9	5.89	112.92	108.20
33	2	1089	А	C5-C6-N6	-5.89	118.99	123.70
39	1	7	А	C4-C5-C6	5.89	119.95	117.00
33	2	326	А	C5-C6-N1	-5.89	114.75	117.70
33	2	667	G	C5-C6-O6	-5.89	125.06	128.60
33	2	662	А	C5-C6-N6	-5.89	118.99	123.70
33	2	218	А	O4'-C1'-N9	5.89	112.91	108.20
33	2	1337	С	O4'-C1'-N1	5.89	112.91	108.20
33	2	463	А	C5-C6-N6	-5.89	118.99	123.70
33	2	804	А	C4-C5-C6	5.89	119.94	117.00
33	2	1537	С	N3-C4-N4	5.89	122.12	118.00
39	1	26	G	C5-C6-O6	-5.89	125.07	128.60
33	2	14	С	N3-C4-C5	-5.88	119.55	121.90
33	2	565	А	C5-C6-N6	-5.88	118.99	123.70
33	2	1129	А	O4'-C1'-N9	5.88	112.91	108.20
33	2	1247	А	C5-C6-N6	-5.88	118.99	123.70
33	2	1548	С	N3-C4-C5	-5.88	119.55	121.90
33	2	1123	С	N3-C4-N4	5.88	122.12	118.00
33	2	1216	А	C4-C5-C6	5.88	119.94	117.00
33	2	1695	С	O4'-C1'-N1	5.88	112.91	108.20
33	2	339	А	C5-C6-N6	-5.88	118.99	123.70
33	2	574	А	C5-C6-N6	-5.88	119.00	123.70
33	2	798	А	C5-C6-N6	-5.88	119.00	123.70
33	2	1093	G	O4'-C1'-N9	5.88	112.91	108.20
33	2	1456	С	N3-C4-C5	-5.88	119.55	121.90
33	2	1225	G	O4'-C1'-N9	5.88	112.90	108.20
33	2	1287	А	C5-C6-N1	-5.88	114.76	117.70
33	2	1692	А	C5-C6-N6	-5.88	119.00	123.70
33	2	1707	А	C5-C6-N6	-5.88	119.00	123.70
33	2	644	А	C4-C5-C6	5.88	119.94	117.00
33	2	1827	С	N3-C4-N4	5.88	122.11	118.00
33	2	975	С	N3-C4-N4	5.88	122.11	118.00
33	2	1038	А	C4-C5-C6	5.88	119.94	117.00
33	2	1316	G	O4'-C1'-N9	5.88	112.90	108.20
33	2	280	G	O4'-C1'-N9	5.87	112.90	108.20
33	2	915	A	C5-C6-N6	-5.87	119.00	123.70
33	2	54	A	C5-C6-N6	-5.87	119.00	123.70
33	2	612	С	N3-C4-N4	5.87	122.11	118.00
33	2	963	С	N3-C4-N4	5.87	122.11	118.00
33	2	1104	G	O4'-C1'-N9	5.87	112.90	108.20



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1359	С	O4'-C1'-N1	5.87	112.90	108.20
33	2	604	G	C5-C6-O6	-5.87	125.08	128.60
33	2	1699	С	N3-C4-N4	5.87	122.11	118.00
33	2	1328	А	C5-C6-N6	-5.87	119.00	123.70
33	2	1384	А	O4'-C1'-N9	5.87	112.89	108.20
33	2	577	А	C5-C6-N1	-5.87	114.77	117.70
33	2	333	А	C5-C6-N1	-5.86	114.77	117.70
33	2	1096	А	C5-C6-N1	-5.86	114.77	117.70
33	2	1683	С	N3-C4-N4	5.86	122.11	118.00
33	2	1701	G	O4'-C1'-N9	5.86	112.89	108.20
33	2	566	А	C4-C5-C6	5.86	119.93	117.00
33	2	644	А	C5-C6-N6	-5.86	119.01	123.70
34	3	65	G	P-O3'-C3'	5.86	126.73	119.70
33	2	125	С	O4'-C1'-N1	5.86	112.89	108.20
33	2	1219	А	C5-C6-N6	-5.86	119.01	123.70
33	2	643	А	C4-C5-C6	5.86	119.93	117.00
33	2	1048	А	O4'-C1'-N9	5.86	112.89	108.20
39	1	7	А	O4'-C1'-N9	5.86	112.89	108.20
33	2	539	С	N3-C4-N4	5.86	122.10	118.00
33	2	1076	А	C4-C5-C6	5.86	119.93	117.00
33	2	1135	С	N3-C4-C5	-5.86	119.56	121.90
33	2	1255	А	C5-C6-N6	-5.86	119.01	123.70
33	2	141	А	C4-C5-C6	5.86	119.93	117.00
39	1	21	А	O4'-C1'-N9	5.86	112.88	108.20
33	2	1100	G	O4'-C1'-N9	5.85	112.88	108.20
33	2	380	С	N3-C4-N4	5.85	122.10	118.00
33	2	807	А	O4'-C1'-N9	5.85	112.88	108.20
33	2	1282	G	C5-C6-O6	-5.85	125.09	128.60
33	2	98	С	N3-C4-N4	5.85	122.09	118.00
33	2	169	U	O4'-C1'-N1	5.85	112.88	108.20
33	2	316	С	N3-C4-N4	5.85	122.09	118.00
33	2	874	G	O4'-C1'-N9	5.85	112.88	108.20
33	2	904	А	C5-C6-N6	-5.85	119.02	123.70
33	2	1276	G	O4'-C1'-N9	5.85	112.88	108.20
33	2	914	U	P-O3'-C3'	5.85	126.72	119.70
33	2	1171	G	O4'-C1'-N9	5.85	112.88	108.20
33	2	1402	G	O4'-C1'-N9	5.85	112.88	108.20
33	2	369	С	N3-C4-N4	5.84	122.09	118.00
33	2	1286	G	O4'-C1'-N9	5.84	112.88	108.20
33	2	1840	G	O4'-C1'-N9	5.84	112.88	108.20
33	2	1257	С	N3-C4-N4	5.84	122.09	118.00
33	2	1551	А	C4-C5-C6	5.84	119.92	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	1574	А	C4-C5-C6	5.84	119.92	117.00
33	2	1782	А	C5-C6-N6	-5.84	119.03	123.70
33	2	1046	А	C4-C5-C6	5.84	119.92	117.00
33	2	1060	С	O4'-C1'-N1	5.84	112.87	108.20
33	2	1299	С	N3-C4-C5	-5.84	119.56	121.90
33	2	1584	А	C5-C6-N1	-5.84	114.78	117.70
33	2	1090	С	N3-C4-N4	5.84	122.08	118.00
33	2	1795	А	C4-C5-C6	5.84	119.92	117.00
33	2	435	А	C4-C5-C6	5.83	119.92	117.00
33	2	832	G	O4'-C1'-N9	5.83	112.87	108.20
33	2	997	А	C4-C5-C6	5.83	119.92	117.00
33	2	1039	G	O4'-C1'-N9	5.83	112.87	108.20
33	2	1179	А	C4-C5-C6	5.83	119.92	117.00
33	2	1795	А	O4'-C1'-N9	5.83	112.87	108.20
33	2	27	А	C4-C5-C6	5.83	119.92	117.00
33	2	565	А	C4-C5-C6	5.83	119.92	117.00
33	2	1141	А	C5-C6-N1	-5.83	114.78	117.70
33	2	1280	А	C5-C6-N6	-5.83	119.03	123.70
33	2	1426	С	N3-C4-N4	5.83	122.08	118.00
33	2	98	С	O4'-C1'-N1	5.83	112.86	108.20
33	2	1161	G	O4'-C1'-N9	5.83	112.86	108.20
33	2	1030	А	O4'-C1'-N9	5.83	112.86	108.20
33	2	182	С	N3-C4-N4	5.83	122.08	118.00
33	2	937	С	N3-C4-N4	5.83	122.08	118.00
33	2	1350	G	C5-C6-O6	-5.83	125.11	128.60
33	2	1677	С	N3-C4-N4	5.83	122.08	118.00
33	2	796	U	O4'-C1'-N1	5.82	112.86	108.20
33	2	850	А	C5-C6-N1	-5.82	114.79	117.70
33	2	926	С	N3-C4-N4	5.82	122.08	118.00
33	2	1129	А	C5-C6-N6	-5.82	119.04	123.70
33	2	1659	А	O4'-C1'-N9	5.82	112.86	108.20
33	2	1679	С	N3-C4-N4	5.82	122.08	118.00
33	2	445	А	C5-C6-N6	-5.82	119.04	123.70
33	2	513	А	C5-C6-N6	-5.82	119.04	123.70
33	2	1408	С	N3-C4-C5	-5.82	119.57	121.90
33	2	221	А	C4-C5-C6	5.82	119.91	117.00
33	2	1324	G	O4'-C1'-N9	5.82	112.86	108.20
33	2	1379	A	C5-C6-N6	-5.82	119.04	123.70
33	2	916	A	O4'-C1'-N9	5.82	112.85	108.20
33	2	945	G	O4'-C1'-N9	5.82	112.85	108.20
33	2	1038	A	O4'-C1'-N9	5.82	112.85	108.20
33	2	1347	G	O4'-C1'-N9	5.82	112.85	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
39	1	73	А	C4-C5-C6	5.82	119.91	117.00
33	2	1146	А	C5-C6-N1	-5.81	114.79	117.70
33	2	1785	А	C4-C5-C6	5.81	119.91	117.00
33	2	1129	А	C4-C5-C6	5.81	119.91	117.00
33	2	1408	С	O4'-C1'-N1	5.81	112.85	108.20
33	2	1502	А	C4-C5-C6	5.81	119.91	117.00
33	2	170	А	C5-C6-N1	-5.81	114.79	117.70
33	2	662	А	C4-C5-C6	5.81	119.91	117.00
33	2	27	А	O4'-C1'-N9	5.81	112.85	108.20
33	2	922	А	C4-C5-C6	5.81	119.91	117.00
33	2	1066	А	O4'-C1'-N9	5.81	112.85	108.20
33	2	1659	А	C4-C5-C6	5.81	119.91	117.00
33	2	20	G	O4'-C1'-N9	5.81	112.85	108.20
33	2	1216	А	O4'-C1'-N9	5.81	112.85	108.20
33	2	908	С	N3-C4-C5	-5.81	119.58	121.90
33	2	922	А	O4'-C1'-N9	5.81	112.84	108.20
33	2	307	G	O4'-C1'-N9	5.80	112.84	108.20
33	2	1651	G	O4'-C1'-N9	5.80	112.84	108.20
33	2	877	G	O4'-C1'-N9	5.80	112.84	108.20
33	2	989	G	O4'-C1'-N9	5.80	112.84	108.20
33	2	68	А	C4-C5-C6	5.80	119.90	117.00
33	2	103	А	C4-C5-C6	5.80	119.90	117.00
33	2	1056	А	C4-C5-C6	5.80	119.90	117.00
33	2	1140	А	O4'-C1'-N9	5.80	112.84	108.20
33	2	1158	С	N3-C4-N4	5.80	122.06	118.00
39	1	76	А	C4-C5-C6	5.80	119.90	117.00
33	2	150	А	C4-C5-C6	5.80	119.90	117.00
33	2	470	G	O4'-C1'-N9	5.80	112.84	108.20
33	2	1552	С	N3-C4-C5	-5.80	119.58	121.90
33	2	1765	G	O4'-C1'-N9	5.80	112.84	108.20
33	2	1691	С	N3-C4-N4	5.80	122.06	118.00
33	2	59	U	O4'-C1'-N1	5.80	112.84	108.20
33	2	1027	А	C4-C5-C6	5.80	119.90	117.00
33	2	45	А	C4-C5-C6	5.79	119.90	117.00
33	2	303	G	O4'-C1'-N9	5.79	112.84	108.20
33	2	1071	С	N3-C4-N4	5.79	122.06	118.00
33	2	1134	C	N3-C4-N4	5.79	122.06	118.00
33	2	1467	С	N3-C4-N4	5.79	122.06	118.00
33	2	1844	A	C5-C6-N1	-5.79	114.80	117.70
33	2	1287	A	C5-C6-N6	-5.79	119.06	123.70
33	2	1291	A	C5-C6-N1	-5.79	114.80	117.70
33	2	1721	G	O4'-C1'-N9	5.79	112.83	108.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	108	G	O4'-C1'-N9	5.79	112.83	108.20
33	2	145	G	O4'-C1'-N9	5.79	112.83	108.20
33	2	171	А	C4-C5-C6	5.79	119.89	117.00
33	2	498	А	O4'-C1'-N9	5.79	112.83	108.20
33	2	900	А	C4-C5-C6	5.79	119.90	117.00
33	2	1159	С	N3-C4-N4	5.79	122.05	118.00
33	2	544	А	C5-C6-N6	-5.79	119.07	123.70
33	2	214	А	C5-C6-N1	-5.79	114.81	117.70
33	2	573	А	O4'-C1'-N9	5.79	112.83	108.20
33	2	1212	С	O4'-C1'-N1	5.79	112.83	108.20
33	2	1246	А	C5-C6-N6	-5.79	119.07	123.70
33	2	1524	С	N3-C4-N4	5.79	122.05	118.00
33	2	83	А	O4'-C1'-N9	5.79	112.83	108.20
33	2	193	С	N3-C4-N4	5.79	122.05	118.00
33	2	486	С	N3-C4-N4	5.79	122.05	118.00
33	2	934	А	C5-C6-N1	-5.79	114.81	117.70
33	2	1141	А	C5-C6-N6	-5.79	119.07	123.70
33	2	1589	А	C4-C5-C6	5.78	119.89	117.00
33	2	415	G	O4'-C1'-N9	5.78	112.82	108.20
33	2	580	А	C5-C6-N6	-5.78	119.08	123.70
33	2	1051	А	O4'-C1'-N9	5.78	112.82	108.20
33	2	900	А	C5-C6-N1	-5.78	114.81	117.70
33	2	660	А	C5-C6-N1	-5.78	114.81	117.70
33	2	1387	С	N3-C4-N4	5.78	122.04	118.00
33	2	1410	A	C4-C5-C6	5.78	119.89	117.00
33	2	1449	С	C6-N1-C1'	-5.78	113.87	120.80
33	2	1777	С	N3-C4-N4	5.78	122.04	118.00
33	2	234	С	N3-C4-N4	5.78	122.04	118.00
33	2	1048	A	C4-C5-C6	5.78	119.89	117.00
33	2	1170	U	N3-C4-O4	5.78	123.44	119.40
33	2	1305	С	N3-C4-N4	5.78	122.04	118.00
33	2	509	А	C5-C6-N6	-5.77	119.08	123.70
33	2	545	A	O4'-C1'-N9	5.77	112.82	108.20
33	2	1048	А	C5-C6-N6	-5.77	119.08	123.70
33	2	1289	A	C5-C6-N1	-5.77	114.81	117.70
33	2	354	А	C4-C5-C6	5.77	119.89	117.00
33	2	416	А	C5-C6-N6	-5.77	119.08	123.70
33	2	1227	С	N3-C4-N4	5.77	122.04	118.00
33	2	1362	G	O4'-C1'-N9	5.77	112.82	108.20
33	2	1708	С	N3-C4-N4	5.77	122.04	118.00
33	2	801	U	O4'-C1'-N1	5.77	112.82	108.20
33	2	904	A	C5-C6-N1	-5.77	114.81	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	25	А	C4-C5-C6	5.77	119.89	117.00
33	2	295	С	O4'-C1'-N1	5.77	112.82	108.20
33	2	515	А	C5-C6-N1	-5.77	114.81	117.70
33	2	992	А	C4-C5-C6	5.77	119.89	117.00
33	2	1098	G	C5-C6-O6	-5.77	125.14	128.60
39	1	33	С	N3-C4-C5	-5.77	119.59	121.90
33	2	392	С	N3-C4-C5	-5.77	119.59	121.90
33	2	1372	А	C5-C6-N6	-5.77	119.09	123.70
33	2	1719	А	C4-C5-C6	5.77	119.88	117.00
33	2	1470	А	O4'-C1'-N9	5.77	112.81	108.20
33	2	2	А	C5-C6-N6	-5.76	119.09	123.70
33	2	125	С	N3-C4-N4	5.76	122.03	118.00
33	2	158	А	C5-C6-N6	-5.76	119.09	123.70
33	2	1568	G	O4'-C1'-N9	5.76	112.81	108.20
33	2	521	А	C5-C6-N1	-5.76	114.82	117.70
33	2	517	С	N3-C4-N4	5.76	122.03	118.00
33	2	810	U	O4'-C1'-N1	5.76	112.81	108.20
33	2	904	А	C4-C5-C6	5.76	119.88	117.00
33	2	1803	А	C5-C6-N1	-5.76	114.82	117.70
33	2	79	А	C4'-C3'-C2'	-5.76	96.84	102.60
33	2	147	А	C5-C6-N6	-5.76	119.09	123.70
33	2	573	А	C5-C6-N6	-5.76	119.09	123.70
33	2	1089	А	C5-C6-N1	-5.76	114.82	117.70
33	2	1109	А	C5-C6-N1	-5.76	114.82	117.70
33	2	1145	А	C5-C6-N6	-5.76	119.09	123.70
33	2	1484	С	O4'-C1'-N1	5.76	112.81	108.20
33	2	1844	А	C5-C6-N6	-5.76	119.09	123.70
33	2	19	А	C5-C6-N6	-5.76	119.09	123.70
33	2	557	С	N3-C4-N4	5.76	122.03	118.00
33	2	870	G	O4'-C1'-N9	5.76	112.81	108.20
33	2	1340	А	C4-C5-C6	5.76	119.88	117.00
33	2	1466	С	N3-C4-N4	5.76	122.03	118.00
33	2	210	G	O4'-C1'-N9	5.75	112.80	108.20
33	2	1696	С	N3-C4-N4	5.75	122.03	118.00
33	2	122	G	O4'-C1'-N9	5.75	112.80	108.20
33	2	564	А	O4'-C1'-N9	5.75	112.80	108.20
33	2	1300	U	O4'-C1'-N1	5.75	112.80	108.20
33	2	1533	С	N3-C4-N4	5.75	122.03	118.00
33	2	1605	G	O4'-C1'-N9	5.75	112.80	108.20
33	2	1625	A	O4'-C1'-N9	5.75	112.80	108.20
33	2	636	G	O4'-C1'-N9	5.75	112.80	108.20
33	2	1083	А	C5-C6-N6	-5.75	119.10	123.70


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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	320	G	C5'-C4'-C3'	-5.75	106.80	116.00
33	2	559	А	C5-C6-N6	-5.75	119.10	123.70
33	2	1081	С	N3-C4-C5	-5.75	119.60	121.90
33	2	854	А	C5-C6-N6	-5.75	119.10	123.70
33	2	1027	А	C5-C6-N1	-5.75	114.83	117.70
33	2	1291	А	C4-C5-C6	5.75	119.87	117.00
30	g	113	PHE	CB-CG-CD2	-5.74	116.78	120.80
33	2	677	С	N3-C4-N4	5.74	122.02	118.00
33	2	1317	G	O4'-C1'-N9	5.74	112.79	108.20
33	2	1652	G	O4'-C1'-N9	5.74	112.80	108.20
33	2	229	А	O4'-C1'-N9	5.74	112.79	108.20
33	2	926	С	N3-C4-C5	-5.74	119.60	121.90
33	2	624	А	C4-C5-C6	5.74	119.87	117.00
33	2	1596	А	C5-C6-N6	-5.74	119.11	123.70
33	2	1715	U	P-O3'-C3'	5.74	126.59	119.70
33	2	73	С	N3-C4-N4	5.74	122.02	118.00
33	2	227	А	C5-C6-N1	-5.74	114.83	117.70
33	2	1081	С	N3-C4-N4	5.74	122.02	118.00
33	2	1112	С	N3-C4-N4	5.74	122.02	118.00
33	2	227	А	C5-C6-N6	-5.74	119.11	123.70
33	2	300	G	O4'-C1'-N9	5.74	112.79	108.20
33	2	976	А	C5-C6-N1	-5.74	114.83	117.70
33	2	1269	С	N3-C4-N4	5.73	122.01	118.00
33	2	197	U	C6-N1-C1'	-5.73	113.17	121.20
33	2	233	А	C4-C5-C6	5.73	119.87	117.00
33	2	534	G	O4'-C1'-N9	5.73	112.79	108.20
33	2	595	А	C4-C5-C6	5.73	119.87	117.00
33	2	821	А	C5-C6-N6	-5.73	119.11	123.70
33	2	993	А	C5-C6-N6	-5.73	119.11	123.70
33	2	1592	С	N3-C4-N4	5.73	122.01	118.00
33	2	1670	А	C4-C5-C6	5.73	119.87	117.00
33	2	228	А	C5-C6-N6	-5.73	119.11	123.70
33	2	1222	G	N3-C2-N2	5.73	123.91	119.90
33	2	1312	С	N3-C4-C5	-5.73	119.61	121.90
33	2	317	G	P-O3'-C3'	5.73	126.57	119.70
33	2	448	А	C4-C5-C6	5.73	119.86	117.00
33	2	633	А	C5-C6-N6	-5.73	119.12	123.70
33	2	662	А	O4'-C1'-N9	5.73	112.78	108.20
33	2	1161	G	N1-C6-O6	5.73	123.34	119.90
33	2	1192	А	C5-C6-N1	-5.72	114.84	117.70
33	2	1703	С	N3-C4-C5	-5.72	119.61	121.90
33	2	1816	А	C4-C5-C6	5.72	119.86	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	50	А	C5-C6-N1	-5.72	114.84	117.70
33	2	283	А	C5-C6-N6	-5.72	119.12	123.70
33	2	293	А	C5-C6-N6	-5.72	119.12	123.70
33	2	404	А	C5-C6-N1	-5.72	114.84	117.70
33	2	540	С	O4'-C1'-N1	5.72	112.78	108.20
33	2	1297	А	C5-C6-N1	-5.72	114.84	117.70
33	2	1575	А	C5-C6-N1	-5.72	114.84	117.70
33	2	1803	А	C4-C5-C6	5.72	119.86	117.00
33	2	804	А	O4'-C1'-N9	5.72	112.78	108.20
33	2	459	А	C5-C6-N6	-5.72	119.12	123.70
33	2	992	А	C5-C6-N6	-5.72	119.12	123.70
33	2	1120	С	N3-C4-N4	5.72	122.00	118.00
33	2	1416	G	O4'-C1'-N9	5.72	112.78	108.20
33	2	1480	А	C5-C6-N6	-5.72	119.12	123.70
33	2	1601	G	N3-C2-N2	5.72	123.90	119.90
33	2	1734	С	N3-C4-N4	5.72	122.00	118.00
33	2	44	U	O4'-C1'-N1	5.72	112.77	108.20
33	2	423	А	C4-C5-C6	5.72	119.86	117.00
33	2	363	G	O4'-C1'-N9	5.71	112.77	108.20
33	2	915	А	O4'-C1'-N9	5.71	112.77	108.20
33	2	1557	С	N3-C4-N4	5.71	122.00	118.00
33	2	195	С	N3-C4-C5	-5.71	119.61	121.90
33	2	1144	А	C5-C6-N1	-5.71	114.84	117.70
33	2	1151	U	O4'-C1'-N1	5.71	112.77	108.20
33	2	1178	А	C5-C6-N1	-5.71	114.84	117.70
33	2	1158	С	N3-C4-C5	-5.71	119.62	121.90
33	2	1	U	O4'-C1'-N1	5.71	112.77	108.20
33	2	223	А	C5-C6-N6	-5.71	119.13	123.70
33	2	484	С	N3-C4-N4	5.71	122.00	118.00
33	2	899	А	C4-C5-C6	5.71	119.85	117.00
33	2	938	G	O4'-C1'-N9	5.71	112.77	108.20
33	2	1195	A	C4-C5-C6	5.71	119.85	117.00
33	2	1333	С	N3-C4-N4	5.71	122.00	118.00
33	2	85	А	C5-C6-N1	-5.71	114.85	117.70
33	2	175	A	C5-C6-N6	-5.71	119.14	123.70
33	2	1433	С	N3-C4-C5	-5.71	119.62	121.90
33	2	831	С	N3-C4-C5	-5.71	119.62	121.90
33	2	1826	A	C4-C5-C6	5.71	119.85	117.00
33	2	1114	C	N3-C4-N4	5.70	121.99	118.00
33	2	315	C	N3-C4-N4	5.70	121.99	118.00
33	2	912	А	C5-C6-N6	-5.70	119.14	123.70
33	2	214	A	C5-C6-N6	-5.70	119.14	123.70



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2	633	A	C4-C5-C6	5.70	119.85	117.00
33	2	960	A	O4'-C1'-N9	5.70	112.76	108.20
33	2	1004	A	C4-C5-C6	5.70	119.85	117.00
33	2	1025	G	O4'-C1'-N9	5.70	112.76	108.20
33	2	1533	С	N3-C4-C5	-5.70	119.62	121.90
33	2	85	A	C4-C5-C6	5.70	119.85	117.00
33	2	899	A	C5-C6-N1	-5.70	114.85	117.70
33	2	1245	С	N3-C4-N4	5.70	121.99	118.00
39	1	6	G	O4'-C1'-N9	5.70	112.76	108.20
33	2	860	A	C5-C6-N6	-5.70	119.14	123.70
33	2	969	С	N3-C4-C5	-5.70	119.62	121.90
33	2	1536	G	O4'-C1'-N9	5.70	112.76	108.20
33	2	1670	A	C5-C6-N6	-5.70	119.14	123.70
33	2	11	A	C5-C6-N6	-5.69	119.14	123.70
33	2	509	A	C4-C5-C6	5.69	119.85	117.00
33	2	825	С	N3-C4-N4	5.69	121.99	118.00
33	2	1026	A	C4-C5-C6	5.69	119.85	117.00
33	2	1632	A	C5-C6-N1	-5.69	114.85	117.70
33	2	849	С	N3-C4-N4	5.69	121.98	118.00
33	2	1270	G	O4'-C1'-N9	5.69	112.75	108.20
33	2	1433	С	N3-C4-N4	5.69	121.98	118.00
33	2	338	A	C5-C6-N6	-5.69	119.15	123.70
33	2	1206	G	O4'-C1'-N9	5.69	112.75	108.20
33	2	1640	С	N3-C4-N4	5.69	121.98	118.00
33	2	91	A	C5-C6-N1	-5.69	114.86	117.70
33	2	1384	A	C5-C6-N6	-5.69	119.15	123.70
33	2	290	A	C5-C6-N1	-5.69	114.86	117.70
33	2	535	A	C5-C6-N1	-5.69	114.86	117.70
33	2	805	A	C4-C5-C6	5.69	119.84	117.00
33	2	1644	U	O4'-C1'-N1	5.69	112.75	108.20
39	1	48	C	N3-C4-N4	5.69	121.98	118.00
33	2	42	A	C5-C6-N6	-5.69	119.15	123.70
33	2	140	U	P-O3'-C3'	5.68	126.52	119.70
33	2	1491	G	O4'-C1'-N9	5.68	112.75	108.20
33	2	1789	G	O4'-C1'-N9	5.68	112.75	108.20
33	2	1856	G	O4'-C1'-N9	5.68	112.75	108.20
33	2	537	G	P-O5'-C5'	5.68	129.99	120.90
33	2	1631	G	C4-N9-C1'	5.68	133.89	126.50
39	1	10	G	C4-N9-C1'	5.68	133.89	126.50
33	2	117	C	N3-C4-C5	-5.68	119.63	121.90
33	2	279	G	O4'-C1'-N9	5.68	112.74	108.20
33	2	822	A	C5-C6-N1	-5.68	114.86	117.70

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Mol	Chain	$\mathbf{Res}$	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
33	2	1205	А	C5-C6-N1	-5.68	114.86	117.70
33	2	1454	G	O4'-C1'-N9	5.68	112.74	108.20
33	2	1504	А	O4'-C1'-N9	5.68	112.74	108.20
33	2	7	G	O4'-C1'-N9	5.68	112.74	108.20
33	2	943	G	O4'-C1'-N9	5.68	112.74	108.20
33	2	502	А	C5-C6-N6	-5.68	119.16	123.70
33	2	583	С	N3-C4-N4	5.68	121.97	118.00
33	2	848	G	C5-C6-O6	-5.68	125.19	128.60
33	2	890	G	O4'-C1'-N9	5.68	112.74	108.20
33	2	1186	А	C5-C6-N1	-5.68	114.86	117.70
14	0	114	TYR	CB-CG-CD1	5.67	124.41	121.00
33	2	155	G	O4'-C1'-N9	5.67	112.74	108.20
33	2	533	С	N3-C4-C5	-5.67	119.63	121.90
33	2	566	А	C5-C6-N6	-5.67	119.16	123.70
33	2	820	С	N3-C4-N4	5.67	121.97	118.00
33	2	1602	А	O4'-C1'-N9	5.67	112.74	108.20
5	F	120	TYR	CB-CG-CD2	-5.67	117.60	121.00
33	2	958	А	C5-C6-N6	-5.67	119.16	123.70
33	2	1477	G	O4'-C1'-N9	5.67	112.74	108.20
33	2	114	G	O4'-C1'-N9	5.67	112.74	108.20
3	D	209	ASP	N-CA-CB	5.67	120.80	110.60
33	2	453	С	N3-C4-N4	5.67	121.97	118.00
33	2	540	С	N3-C4-C5	-5.67	119.63	121.90
33	2	1322	U	O4'-C1'-N1	5.67	112.73	108.20
33	2	1512	G	O4'-C1'-N9	5.67	112.73	108.20
33	2	90	G	O4'-C1'-N9	5.67	112.73	108.20
33	2	107	А	C5-C6-N1	-5.67	114.87	117.70
33	2	391	А	C4-C5-C6	5.67	119.83	117.00
33	2	405	А	C5-C6-N6	-5.67	119.17	123.70
33	2	968	А	C5-C6-N1	-5.67	114.87	117.70
33	2	61	А	C5-C6-N6	-5.66	119.17	123.70
33	2	1111	U	C6-N1-C1'	-5.66	113.27	121.20
33	2	1515	G	C8-N9-C1'	-5.66	119.64	127.00
33	2	1717	G	O4'-C1'-N9	5.66	112.73	108.20
39	1	5	А	O4'-C1'-N9	5.66	112.73	108.20
33	2	915	А	C5-C6-N1	-5.66	114.87	117.70
33	2	992	А	O4'-C1'-N9	5.66	112.73	108.20
33	2	1054	A	C5-C6-N6	-5.66	119.17	123.70
33	2	1475	G	O4'-C1'-N9	$5.6\overline{6}$	112.73	108.20
39	1	59	A	O4'-C1'-N9	5.66	112.73	108.20
39	1	75	С	N3-C4-N4	5.66	121.96	118.00
10	K	142	SER	C-N-CA	5.66	135.85	121.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	102	А	O4'-C1'-N9	5.66	112.73	108.20
33	2	1043	С	N3-C4-N4	5.66	121.96	118.00
33	2	1782	А	C5-C6-N1	-5.66	114.87	117.70
33	2	1280	А	C5-C6-N1	-5.66	114.87	117.70
33	2	1586	С	N3-C4-N4	5.66	121.96	118.00
33	2	2	А	O4'-C1'-N9	5.65	112.72	108.20
33	2	149	А	C4-C5-C6	5.65	119.83	117.00
33	2	466	А	C4-C5-C6	5.65	119.83	117.00
33	2	1273	С	N3-C4-C5	-5.65	119.64	121.90
33	2	1008	А	O4'-C1'-N9	5.65	112.72	108.20
33	2	1209	С	N3-C4-N4	5.65	121.96	118.00
33	2	158	А	C4-C5-C6	5.65	119.82	117.00
33	2	483	А	C4-C5-C6	5.65	119.82	117.00
33	2	490	А	C5-C6-N1	-5.65	114.88	117.70
33	2	492	С	N3-C4-N4	5.65	121.95	118.00
33	2	871	А	C4-C5-C6	5.65	119.82	117.00
33	2	909	А	C5-C6-N1	-5.65	114.88	117.70
33	2	350	А	C5-C6-N6	-5.65	119.18	123.70
33	2	589	А	O4'-C1'-N9	5.65	112.72	108.20
33	2	1410	А	O4'-C1'-N9	5.65	112.72	108.20
39	1	32	С	N3-C4-N4	5.65	121.95	118.00
33	2	1274	А	C5-C6-N1	-5.64	114.88	117.70
33	2	146	G	O4'-C1'-N9	5.64	112.71	108.20
33	2	221	А	C5-C6-N6	-5.64	119.19	123.70
33	2	399	С	N3-C4-N4	5.64	121.95	118.00
33	2	1412	С	N3-C4-N4	5.64	121.95	118.00
33	2	1499	С	N3-C4-N4	5.64	121.95	118.00
39	1	8	G	O4'-C1'-N9	5.64	112.71	108.20
33	2	1312	С	N3-C4-N4	5.64	121.95	118.00
33	2	1625	А	C4-C5-C6	5.64	119.82	117.00
34	3	68	А	C5-C6-N1	-5.64	114.88	117.70
33	2	4	С	N3-C4-N4	5.64	121.95	118.00
33	2	62	G	O4'-C1'-N9	5.64	112.71	108.20
33	2	1405	А	O4'-C1'-N9	5.64	112.71	108.20
33	2	77	А	C5-C6-N1	-5.63	114.88	117.70
33	2	833	А	C5-C6-N6	-5.63	119.19	123.70
33	2	1661	С	N3-C4-C5	-5.63	119.65	121.90
33	2	857	А	C5-C6-N6	-5.63	119.19	123.70
33	2	1558	G	O4'-C1'-N9	5.63	112.71	108.20
33	2	1666	G	N3-C2-N2	5.63	123.84	119.90
33	2	658	А	C4-C5-C6	5.63	119.82	117.00
33	2	1004	А	C5-C6-N6	-5.63	119 19	123 70



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1398	А	C5-C6-N6	-5.63	119.19	123.70
39	1	33	С	N3-C4-N4	5.63	121.94	118.00
33	2	655	G	O4'-C1'-N9	5.63	112.70	108.20
33	2	1639	С	N3-C4-N4	5.63	121.94	118.00
33	2	118	С	N3-C4-N4	5.63	121.94	118.00
33	2	13	С	N3-C4-C5	-5.62	119.65	121.90
33	2	196	U	O4'-C1'-N1	5.62	112.70	108.20
33	2	1200	А	O4'-C1'-N9	5.62	112.70	108.20
33	2	302	С	N3-C4-N4	5.62	121.94	118.00
33	2	1073	А	C5-C6-N6	-5.62	119.20	123.70
33	2	1483	А	O4'-C1'-N9	5.62	112.70	108.20
33	2	1504	А	C4-C5-C6	5.62	119.81	117.00
33	2	1514	U	O4'-C1'-N1	5.62	112.70	108.20
33	2	293	А	C5-C6-N1	-5.62	114.89	117.70
33	2	940	А	O4'-C1'-N9	5.62	112.70	108.20
33	2	983	А	C5-C6-N6	-5.62	119.20	123.70
33	2	1374	А	C5-C6-N6	-5.62	119.20	123.70
33	2	949	С	N3-C4-N4	5.62	121.93	118.00
33	2	1528	А	C4-C5-C6	5.62	119.81	117.00
39	1	15	А	C5-C6-N1	-5.62	114.89	117.70
33	2	958	А	O4'-C1'-N9	5.62	112.69	108.20
33	2	1248	С	N3-C4-N4	5.62	121.93	118.00
33	2	1655	С	N3-C4-C5	-5.62	119.65	121.90
33	2	438	А	C5-C6-N6	-5.62	119.21	123.70
33	2	1005	А	C4-C5-C6	5.62	119.81	117.00
33	2	473	С	N3-C4-C5	-5.61	119.65	121.90
33	2	573	А	C4-C5-C6	5.61	119.81	117.00
33	2	1121	С	N3-C4-N4	5.61	121.93	118.00
33	2	1186	А	O4'-C1'-N9	5.61	112.69	108.20
33	2	1204	А	C5-C6-N6	-5.61	119.21	123.70
33	2	354	А	C5-C6-N6	-5.61	119.21	123.70
39	1	56	С	N3-C4-N4	5.61	121.93	118.00
33	2	288	А	O4'-C1'-N9	5.61	112.69	108.20
33	2	947	С	N3-C4-N4	5.61	121.93	118.00
33	2	326	А	C4-C5-C6	5.61	119.81	117.00
33	2	437	A	C5-C6-N1	-5.61	114.90	117.70
33	2	1005	A	O4'-C1'-N9	5.61	112.69	108.20
33	2	1027	А	O4'-C1'-N9	5.61	112.69	108.20
33	2	1192	A	O4'-C1'-N9	5.61	112.69	108.20
33	2	1334	G	O4'-C1'-N9	5.61	112.69	108.20
33	2	1448	А	C5-C6-N1	-5.61	114.90	117.70
33	2	1118	A	O4'-C1'-N9	5.61	112.69	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	84	А	C5-C6-N1	-5.60	114.90	117.70
33	2	868	А	C5-C6-N1	-5.60	114.90	117.70
33	2	1205	А	C5-C6-N6	-5.60	119.22	123.70
33	2	127	С	N3-C4-N4	5.60	121.92	118.00
33	2	1538	U	P-O3'-C3'	5.60	126.42	119.70
33	2	1618	А	C5-C6-N1	-5.60	114.90	117.70
33	2	1703	С	N3-C4-N4	5.60	121.92	118.00
33	2	1744	G	O4'-C1'-N9	5.60	112.68	108.20
33	2	1816	А	C5-C6-N6	-5.60	119.22	123.70
33	2	46	А	C5-C6-N1	-5.60	114.90	117.70
33	2	873	С	N3-C4-N4	5.60	121.92	118.00
33	2	1019	А	C5-C6-N6	-5.60	119.22	123.70
33	2	1367	U	O4'-C1'-N1	5.60	112.68	108.20
33	2	1432	С	O4'-C1'-N1	5.60	112.68	108.20
33	2	1807	А	C5-C6-N6	-5.60	119.22	123.70
33	2	366	А	O4'-C1'-N9	5.60	112.68	108.20
33	2	609	А	O4'-C1'-N9	5.60	112.68	108.20
33	2	1256	А	C4-C5-C6	5.60	119.80	117.00
33	2	24	С	N3-C4-N4	5.60	121.92	118.00
33	2	234	С	O4'-C1'-N1	5.60	112.68	108.20
33	2	654	А	C4-C5-C6	5.60	119.80	117.00
33	2	1242	А	C5-C6-N6	-5.60	119.22	123.70
33	2	1659	А	C5-C6-N6	-5.60	119.22	123.70
33	2	234	С	N3-C4-C5	-5.59	119.66	121.90
33	2	866	А	O4'-C1'-N9	5.59	112.68	108.20
33	2	969	С	N3-C4-N4	5.59	121.92	118.00
33	2	1414	С	N3-C4-C5	-5.59	119.66	121.90
33	2	1716	U	O4'-C1'-N1	5.59	112.68	108.20
33	2	321	С	N3-C4-C5	-5.59	119.66	121.90
33	2	450	А	O4'-C1'-N9	5.59	112.67	108.20
33	2	1060	С	N3-C4-C5	-5.59	119.66	121.90
33	2	1795	А	C5-C6-N6	-5.59	119.23	123.70
33	2	1803	А	C5-C6-N6	-5.59	119.23	123.70
33	2	1479	А	C5-C6-N1	-5.59	114.91	117.70
33	2	519	А	C4-C5-C6	5.58	119.79	117.00
33	2	142	С	N3-C4-N4	5.58	121.91	118.00
33	2	1655	С	N3-C4-N4	5.58	121.91	118.00
33	2	449	С	N3-C4-N4	5.58	121.91	118.00
33	2	462	C	N3-C4-C5	-5.58	119.67	121.90
33	2	1036	G	O4'-C1'-N9	5.58	112.67	108.20
33	2	1526	A	C5-C6-N1	-5.58	114.91	117.70
33	2	45	А	C5-C6-N6	-5.58	119.24	123.70



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	Mol	Chain	$\operatorname{Res}$	Type	Atoms			
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	64	А	C5-C6-N1	-5.58	114.91	117.70
33	2	659	А	C5-C6-N6	-5.58	119.24	123.70
34	3	77	А	C5-C6-N6	-5.58	119.24	123.70
23	Ζ	41	PHE	CB-CG-CD2	-5.58	116.89	120.80
33	2	566	А	O4'-C1'-N9	5.58	112.66	108.20
33	2	918	А	C5-C6-N6	-5.58	119.24	123.70
33	2	940	А	C4-C5-C6	5.58	119.79	117.00
33	2	1845	А	C5-C6-N6	-5.58	119.24	123.70
39	1	21	А	C5-C6-N1	-5.58	114.91	117.70
33	2	631	А	C5-C6-N6	-5.58	119.24	123.70
33	2	1698	С	N3-C4-N4	5.58	121.90	118.00
8	Ι	145	PHE	CB-CG-CD2	-5.58	116.90	120.80
33	2	1004	А	O4'-C1'-N9	5.58	112.66	108.20
33	2	1166	А	C4-C5-C6	5.58	119.79	117.00
33	2	1243	С	N3-C4-C5	-5.58	119.67	121.90
33	2	1269	С	O4'-C1'-N1	5.58	112.66	108.20
33	2	78	С	C6-N1-C1'	-5.57	114.11	120.80
33	2	1056	А	C5-C6-N6	-5.57	119.24	123.70
33	2	1080	А	C5-C6-N6	-5.57	119.24	123.70
33	2	1726	А	O4'-C1'-N9	5.57	112.66	108.20
33	2	290	А	C4-C5-C6	5.57	119.79	117.00
33	2	473	С	N3-C4-N4	5.57	121.90	118.00
33	2	1307	С	N3-C4-N4	5.57	121.90	118.00
33	2	1115	А	C5-C6-N6	-5.57	119.24	123.70
33	2	812	A	C5-C6-N6	-5.57	119.25	123.70
33	2	1196	А	O4'-C1'-N9	5.57	112.65	108.20
33	2	1327	C	N3-C4-N4	5.57	121.90	118.00
33	2	1636	А	C5-C6-N1	-5.57	114.92	117.70
33	2	494	G	O4'-C1'-N9	5.57	112.65	108.20
33	2	949	C	N3-C4-C5	-5.57	119.67	121.90
33	2	1267	С	N3-C4-C5	-5.57	119.67	121.90
33	2	1673	A	C5-C6-N6	-5.57	119.25	123.70
33	2	1704	G	O4'-C1'-N9	5.57	112.65	108.20
33	2	1775	A	C4-C5-C6	5.57	119.78	117.00
33	2	340	С	N3-C4-C5	-5.56	119.67	121.90
33	2	1434	А	C5-C6-N6	-5.56	119.25	123.70
33	2	240	С	N3-C4-N4	5.56	121.89	118.00
33	2	512	А	C5-C6-N6	-5.56	119.25	123.70
33	2	1673	A	C5-C6-N1	-5.56	114.92	117.70
39	1	53	G	04'-C1'-N9	5.56	112.65	108.20
33	2	166	A	C5-C6-N6	-5.56	119.25	123.70
33	2	677	С	N3-C4-C5	-5.56	119.68	121.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1457	G	O4'-C1'-N9	5.56	112.65	108.20
33	2	805	А	C5-C6-N6	-5.56	119.25	123.70
33	2	521	А	C5-C6-N6	-5.56	119.25	123.70
33	2	618	А	C5-C6-N1	-5.56	114.92	117.70
33	2	1766	С	N3-C4-N4	5.56	121.89	118.00
33	2	606	A	C4-C5-C6	5.56	119.78	117.00
33	2	823	A	C5-C6-N1	-5.56	114.92	117.70
33	2	1295	А	O4'-C1'-N9	5.56	112.64	108.20
33	2	1691	С	N3-C4-C5	-5.56	119.68	121.90
33	2	1784	A	C4-C5-C6	5.56	119.78	117.00
33	2	1807	A	O4'-C1'-N9	5.56	112.64	108.20
33	2	85	A	C5-C6-N6	-5.55	119.26	123.70
33	2	118	С	N3-C4-C5	-5.55	119.68	121.90
33	2	823	А	C5-C6-N6	-5.55	119.26	123.70
33	2	918	A	C5-C6-N1	-5.55	114.92	117.70
33	2	1281	G	C5-C6-O6	-5.55	125.27	128.60
33	2	1345	G	O4'-C1'-N9	5.55	112.64	108.20
33	2	1522	С	N3-C4-N4	5.55	121.89	118.00
33	2	1849	G	O4'-C1'-N9	5.55	112.64	108.20
33	2	1857	A	C4-C5-C6	5.55	119.78	117.00
33	2	1502	A	C5-C6-N1	-5.55	114.92	117.70
33	2	1711	C	N3-C4-N4	5.55	121.89	118.00
33	2	643	A	C5-C6-N1	-5.55	114.92	117.70
33	2	1549	С	N3-C4-N4	5.55	121.89	118.00
33	2	72	С	N3-C4-C5	-5.55	119.68	121.90
33	2	275	С	N3-C4-C5	-5.55	119.68	121.90
33	2	1494	A	C5-C6-N1	-5.55	114.92	117.70
33	2	1739	G	N3-C2-N2	5.55	123.78	119.90
33	2	195	С	N3-C4-N4	5.55	121.88	118.00
33	2	174	С	N3-C4-N4	5.55	121.88	118.00
33	2	1086	С	N3-C4-N4	5.55	121.88	118.00
33	2	1435	A	C5-C6-N1	-5.55	114.93	117.70
34	3	66	С	N3-C4-C5	-5.55	119.68	121.90
33	2	376	С	N3-C4-N4	5.54	121.88	118.00
33	2	454	A	C5-C6-N6	-5.54	119.26	123.70
33	2	630	A	C5-C6-N1	-5.54	114.93	117.70
33	2	729	C	N3-C4-C5	-5.54	119.68	121.90
33	2	1087	C	N3-C4-C5	-5.54	119.68	121.90
33	2	142	C	C6-N1-C1'	-5.54	114.15	120.80
33	2	807	A	C5-C6-N6	-5.54	119.27	123.70
33	2	1045	A	C5-C6-N1	-5.54	114.93	117.70
- 33	2	1211	$\mathbf{C}$	N3-C4-C5	-5.54	119.68	121.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	1351	С	N3-C4-C5	-5.54	119.68	121.90
33	2	1770	G	O4'-C1'-N9	5.54	112.64	108.20
33	2	1845	A	O4'-C1'-N9	5.54	112.64	108.20
39	1	44	А	C4-C5-C6	5.54	119.77	117.00
33	2	1080	А	C5-C6-N1	-5.54	114.93	117.70
33	2	1452	G	O4'-C1'-N9	5.54	112.63	108.20
39	1	44	А	C5-C6-N6	-5.54	119.27	123.70
33	2	603	С	N3-C4-N4	5.54	121.88	118.00
33	2	631	A	C5-C6-N1	-5.54	114.93	117.70
33	2	865	A	C4-C5-C6	5.54	119.77	117.00
39	1	7	A	C5-C6-N1	-5.54	114.93	117.70
39	1	61	С	N3-C4-N4	5.54	121.88	118.00
33	2	22	А	C5-C6-N6	-5.54	119.27	123.70
33	2	596	G	O4'-C1'-N9	5.54	112.63	108.20
33	2	650	С	N3-C4-N4	5.54	121.88	118.00
33	2	871	A	C5-C6-N6	-5.54	119.27	123.70
33	2	994	A	O4'-C1'-N9	5.54	112.63	108.20
33	2	1267	С	N3-C4-N4	5.54	121.88	118.00
33	2	199	G	O4'-C1'-N9	5.54	112.63	108.20
33	2	329	A	C5-C6-N6	-5.54	119.27	123.70
33	2	1078	A	C5-C6-N6	-5.54	119.27	123.70
33	2	333	A	C5-C6-N6	-5.53	119.27	123.70
33	2	565	A	O4'-C1'-N9	5.53	112.63	108.20
34	3	77	A	C5-C6-N1	-5.53	114.93	117.70
33	2	1139	A	C5-C6-N6	-5.53	119.27	123.70
33	2	1824	U	O4'-C1'-N1	5.53	112.62	108.20
33	2	328	G	O4'-C1'-N9	5.53	112.62	108.20
33	2	491	С	N3-C4-C5	-5.53	119.69	121.90
33	2	908	C	N3-C4-N4	5.53	121.87	118.00
33	2	166	A	C5-C6-N1	-5.53	114.94	117.70
33	2	1483	A	C5-C6-N6	-5.53	119.28	123.70
33	2	1719	A	C5-C6-N6	-5.53	119.28	123.70
33	2	656	U	O4'-C1'-N1	5.53	112.62	108.20
33	2	675	A	C5-C6-N6	-5.53	119.28	123.70
33	2	1078	A	C5-C6-N1	-5.53	114.94	117.70
33	2	27	A	C5-C6-N1	-5.52	114.94	117.70
33	2	535	A	O4'-C1'-N9	5.52	112.62	108.20
33	2	576	G	O4'-C1'-N9	5.52	112.62	108.20
33	2	429	A	O4'-C1'-N9	5.52	112.62	108.20
33	2	958	A	C5-C6-N1	-5.52	114.94	117.70
39	1	56	C	N3-C4-C5	-5.52	119.69	121.90
33	2	72	С	N3-C4-N4	5.52	121.86	118.00

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	295	С	N3-C4-N4	5.52	121.86	118.00
33	2	595	А	C5-C6-N6	-5.52	119.28	123.70
33	2	1456	С	N3-C4-N4	5.52	121.86	118.00
33	2	1590	U	O4'-C1'-N1	5.52	112.61	108.20
33	2	58	С	O4'-C1'-N1	5.52	112.61	108.20
33	2	77	А	C5-C6-N6	-5.52	119.29	123.70
33	2	850	А	O4'-C1'-N9	5.52	112.61	108.20
33	2	1204	А	C5-C6-N1	-5.52	114.94	117.70
33	2	1694	A	C5-C6-N1	-5.52	114.94	117.70
33	2	1851	G	O4'-C1'-N9	5.52	112.61	108.20
33	2	290	А	O4'-C1'-N9	5.51	112.61	108.20
33	2	13	С	N3-C4-N4	5.51	121.86	118.00
33	2	27	А	C5-C6-N6	-5.51	119.29	123.70
33	2	390	С	N3-C4-N4	5.51	121.86	118.00
33	2	594	А	C5-C6-N1	-5.51	114.94	117.70
34	3	67	А	O4'-C1'-N9	5.51	112.61	108.20
33	2	574	А	C4-C5-C6	5.51	119.75	117.00
33	2	595	А	C5-C6-N1	-5.51	114.94	117.70
33	2	628	С	N3-C4-N4	5.51	121.86	118.00
33	2	1814	G	O4'-C1'-N9	5.51	112.61	108.20
10	K	177	SER	N-CA-CB	5.51	118.76	110.50
33	2	1074	С	N3-C4-N4	5.51	121.85	118.00
33	2	1101	G	O4'-C1'-N9	5.51	112.61	108.20
33	2	1450	А	O4'-C1'-N9	5.51	112.61	108.20
33	2	282	G	O4'-C1'-N9	5.50	112.60	108.20
39	1	20	А	C5-C6-N1	-5.50	114.95	117.70
39	1	21	А	C5-C6-N6	-5.50	119.30	123.70
33	2	993	А	C4-C5-C6	5.50	119.75	117.00
33	2	381	С	N3-C4-N4	5.50	121.85	118.00
33	2	860	А	C4-C5-C6	5.50	119.75	117.00
33	2	1826	А	C5-C6-N1	-5.50	114.95	117.70
34	3	66	С	N3-C4-N4	5.50	121.85	118.00
39	1	18	G	C4'-C3'-O3'	5.50	124.00	113.00
39	1	24	G	O4'-C1'-N9	5.50	112.60	108.20
33	2	448	А	O4'-C1'-N9	5.50	112.60	108.20
33	2	830	С	N3-C4-N4	5.50	121.85	118.00
33	2	907	С	N3-C4-C5	-5.50	119.70	121.90
33	2	511	А	C5-C6-N1	-5.50	114.95	117.70
33	2	645	A	C5-C6-N6	-5.50	119.30	123.70
33	2	302	С	O4'-C1'-N1	5.49	112.59	108.20
33	2	1179	A	C5-C6-N6	-5.49	119.31	123.70
33	2	1551	A	C5-C6-N6	-5.49	119.31	123.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
39	1	59	А	C5-C6-N6	-5.49	119.31	123.70
33	2	512	А	C5-C6-N1	-5.49	114.95	117.70
33	2	1604	С	N3-C4-C5	-5.49	119.70	121.90
33	2	555	G	O4'-C1'-N9	5.49	112.59	108.20
33	2	883	U	C2-N1-C1'	5.49	124.29	117.70
33	2	1176	С	N3-C4-N4	5.49	121.84	118.00
33	2	1449	С	N3-C4-N4	5.49	121.84	118.00
33	2	1794	А	C5-C6-N6	-5.49	119.31	123.70
33	2	1614	А	C5-C6-N1	-5.49	114.96	117.70
33	2	288	А	C5-C6-N1	-5.49	114.96	117.70
33	2	604	G	O4'-C1'-N9	5.49	112.59	108.20
33	2	1051	А	C5-C6-N6	-5.49	119.31	123.70
33	2	1114	С	N3-C4-C5	-5.49	119.71	121.90
33	2	1379	А	C5-C6-N1	-5.49	114.96	117.70
33	2	607	G	O4'-C1'-N9	5.48	112.59	108.20
33	2	39	А	O4'-C1'-N9	5.48	112.59	108.20
33	2	96	С	N3-C4-N4	5.48	121.84	118.00
33	2	226	А	O4'-C1'-N9	5.48	112.59	108.20
33	2	1250	С	N3-C4-C5	-5.48	119.71	121.90
33	2	66	G	O4'-C1'-N9	5.48	112.58	108.20
33	2	275	С	C6-N1-C1'	-5.48	114.22	120.80
33	2	1202	G	O4'-C1'-N9	5.48	112.58	108.20
33	2	1482	А	C5-C6-N6	-5.48	119.32	123.70
33	2	38	А	C4-C5-C6	5.48	119.74	117.00
33	2	172	U	O4'-C1'-N1	5.48	112.58	108.20
33	2	398	А	C5-C6-N6	-5.48	119.32	123.70
33	2	1693	С	N3-C4-N4	5.48	121.83	118.00
33	2	1738	G	N3-C2-N2	5.48	123.73	119.90
33	2	47	G	O4'-C1'-N9	5.47	112.58	108.20
33	2	292	А	C5-C6-N1	-5.47	114.96	117.70
33	2	1826	А	O4'-C1'-N9	5.47	112.58	108.20
33	2	496	G	O4'-C1'-N9	5.47	112.58	108.20
33	2	983	A	C5-C6-N1	-5.47	114.96	117.70
33	2	1064	G	N3-C2-N2	5.47	123.73	119.90
33	2	1787	А	C4-C5-C6	5.47	119.74	117.00
39	1	15	А	C4-C5-C6	5.47	119.74	117.00
39	1	42	А	C5-C6-N6	-5.47	119.32	123.70
33	2	1213	А	O4'-C1'-N9	5.47	112.58	108.20
33	2	1258	C	N3-C4-N4	5.47	121.83	118.00
33	2	1215	C	N3-C4-N4	5.47	121.83	118.00
33	2	1399	С	N3-C4-N4	5.47	121.83	118.00
33	2	1690	A	C5-C6-N6	-5.47	119.32	123.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1719	A	C5-C6-N1	-5.47	114.97	117.70
33	2	1793	G	N3-C2-N2	5.47	123.73	119.90
33	2	1710	А	C5-C6-N1	-5.47	114.97	117.70
34	3	77	А	O4'-C1'-N9	5.47	112.57	108.20
33	2	229	A	C5-C6-N1	-5.46	114.97	117.70
33	2	529	C	N3-C4-C5	-5.46	119.71	121.90
33	2	545	A	C5-C6-N1	-5.46	114.97	117.70
33	2	843	A	O4'-C1'-N9	5.46	112.57	108.20
33	2	1032	A	C5-C6-N1	-5.46	114.97	117.70
33	2	1083	A	C5-C6-N1	-5.46	114.97	117.70
33	2	3	С	N3-C4-N4	5.46	121.82	118.00
33	2	806	A	C5-C6-N6	-5.46	119.33	123.70
33	2	991	G	O4'-C1'-N9	5.46	112.57	108.20
33	2	159	А	C5-C6-N1	-5.46	114.97	117.70
33	2	490	A	C5-C6-N6	-5.46	119.33	123.70
39	1	73	A	C5-C6-N6	-5.46	119.33	123.70
33	2	117	С	N3-C4-N4	5.46	121.82	118.00
33	2	1242	A	C5-C6-N1	-5.46	114.97	117.70
33	2	1693	С	O4'-C1'-N1	5.46	112.57	108.20
33	2	609	A	C5-C6-N1	-5.46	114.97	117.70
33	2	826	A	O4'-C1'-N9	5.46	112.56	108.20
33	2	377	С	N3-C4-C5	-5.46	119.72	121.90
33	2	835	С	N3-C4-N4	5.46	121.82	118.00
33	2	1212	С	N3-C4-N4	5.46	121.82	118.00
33	2	1845	A	C5-C6-N1	-5.46	114.97	117.70
11	L	159	PHE	CB-CG-CD2	-5.45	116.98	120.80
33	2	336	С	N3-C4-C5	-5.45	119.72	121.90
33	2	951	A	O4'-C1'-N9	5.45	112.56	108.20
33	2	1031	A	O4'-C1'-N9	5.45	112.56	108.20
39	1	43	G	O4'-C1'-N9	5.45	112.56	108.20
33	2	455	A	C5-C6-N6	-5.45	119.34	123.70
33	2	661	A	C5-C6-N6	-5.45	119.34	123.70
33	2	835	С	C6-N1-C1'	-5.45	114.26	120.80
33	2	1085	G	O4'-C1'-N9	5.45	112.56	108.20
39	1	59	A	C5-C6-N1	-5.45	114.97	117.70
33	2	78	C	N3-C4-N4	5.45	121.82	118.00
33	2	223	A	C5-C6-N1	-5.45	114.97	117.70
33	2	364	G	O4'-C1'-N9	5.45	112.56	108.20
33	2	1549	C	N3-C4-C5	-5.45	119.72	121.90
33	2	1857	A	C5-C6-N6	-5.45	119.34	123.70
33	2	1419	C	N3-C4-N4	5.45	121.81	118.00
33	2	1050	G	O4'-C1'-N9	5.45	112.56	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal $(^{o})$
33	2	1424	G	O4'-C1'-N9	5.45	112.56	108.20
33	2	1502	А	C5-C6-N6	-5.45	119.34	123.70
33	2	84	А	C5-C6-N6	-5.45	119.34	123.70
33	2	835	С	N3-C4-C5	-5.45	119.72	121.90
33	2	1656	А	C5-C6-N6	-5.45	119.34	123.70
34	3	67	A	C5-C6-N1	-5.45	114.98	117.70
33	2	14	С	N3-C4-N4	5.44	121.81	118.00
33	2	347	С	N3-C4-N4	5.44	121.81	118.00
33	2	1649	G	O4'-C1'-N9	5.44	112.56	108.20
33	2	149	А	C5-C6-N6	-5.44	119.35	123.70
33	2	203	G	O4'-C1'-N9	5.44	112.55	108.20
33	2	454	А	C5-C6-N1	-5.44	114.98	117.70
33	2	1859	С	N3-C4-C5	-5.44	119.72	121.90
33	2	58	С	N3-C4-C5	-5.44	119.72	121.90
33	2	1105	С	N3-C4-C5	-5.44	119.72	121.90
33	2	418	U	C6-N1-C1'	-5.44	113.59	121.20
33	2	484	С	N3-C4-C5	-5.44	119.72	121.90
33	2	669	А	C4-C5-C6	5.44	119.72	117.00
33	2	675	А	O4'-C1'-N9	5.44	112.55	108.20
33	2	1375	А	C5-C6-N1	-5.44	114.98	117.70
33	2	1415	С	N3-C4-N4	5.44	121.81	118.00
33	2	1808	G	N3-C2-N2	5.44	123.71	119.90
33	2	1149	С	N3-C4-N4	5.44	121.81	118.00
33	2	42	A	O4'-C1'-N9	5.43	112.55	108.20
33	2	235	C	C5-C4-N4	-5.43	116.40	120.20
38	R	15	PHE	CB-CG-CD1	5.43	124.60	120.80
33	2	660	A	C5-C6-N6	-5.43	119.35	123.70
33	2	1134	С	N3-C4-C5	-5.43	119.73	121.90
39	1	5	A	C5-C6-N6	-5.43	119.35	123.70
33	2	497	G	O4'-C1'-N9	5.43	112.55	108.20
33	2	1250	С	N3-C4-N4	5.43	121.80	118.00
33	2	64	A	C5-C6-N6	-5.43	119.36	123.70
33	2	382	A	C5-C6-N1	-5.43	114.98	117.70
33	2	523	A	C4-C5-C6	5.43	119.72	117.00
33	2	1169	A	O4'-C1'-N9	5.43	112.54	108.20
33	2	1467	С	N3-C4-C5	-5.43	119.73	121.90
33	2	218	A	C5-C6-N6	-5.43	119.36	123.70
33	2	226	A	C4-C5-C6	5.43	119.71	117.00
33	2	$27\overline{5}$	C	N3-C4-N4	$5.4\overline{3}$	121.80	118.00
33	2	912	A	O4'-C1'-N9	5.43	112.54	108.20
33	2	$11\overline{95}$	A	C5-C6-N1	-5.43	114.99	117.70

С

33

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1698

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121.90

119.73



-5.43

N3-C4-C5

108.20

108.20

117.70

121.90

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	39	А	C5-C6-N6	-5.42	119.36	123.70
33	2	178	С	N3-C4-N4	5.42	121.80	118.00
33	2	847	С	N3-C4-N4	5.42	121.80	118.00
33	2	1054	А	C5-C6-N1	-5.42	114.99	117.70
33	2	809	A	O4'-C1'-N9	5.42	112.54	108.20
33	2	826	A	C5-C6-N1	-5.42	114.99	117.70
33	2	1503	G	O4'-C1'-N9	5.42	112.54	108.20
33	2	22	A	O4'-C1'-N9	5.42	112.54	108.20
33	2	833	A	O4'-C1'-N9	5.42	112.54	108.20
33	2	1076	A	C5-C6-N6	-5.42	119.36	123.70
33	2	1381	G	O4'-C1'-N9	5.42	112.54	108.20
33	2	1778	G	O4'-C1'-N9	5.42	112.54	108.20
34	3	68	A	C5-C6-N6	-5.42	119.36	123.70
33	2	180	G	O4'-C1'-N9	5.42	112.54	108.20
33	2	574	A	C5-C6-N1	-5.42	114.99	117.70
33	2	1216	A	C5-C6-N1	-5.42	114.99	117.70
33	2	379	A	O4'-C1'-N9	5.42	112.53	108.20
33	2	516	A	C4-C5-C6	5.42	119.71	117.00
33	2	594	A	O4'-C1'-N9	5.42	112.53	108.20
33	2	1427	G	O4'-C1'-N9	5.42	112.53	108.20
33	2	1641	С	N3-C4-N4	5.42	121.79	118.00
33	2	1750	С	N3-C4-C5	-5.42	119.73	121.90
39	1	44	A	C5-C6-N1	-5.42	114.99	117.70
33	2	405	A	C5-C6-N1	-5.42	114.99	117.70
33	2	493	С	N3-C4-C5	-5.42	119.73	121.90
39	1	74	С	O4'-C1'-N1	5.42	112.53	108.20
33	2	354	A	O4'-C1'-N9	5.42	112.53	108.20
33	2	359	C	N3-C4-C5	-5.42	119.73	121.90
33	2	1163	G	O4'-C1'-N9	5.42	112.53	108.20
33	2	1237	A	C5-C6-N6	-5.42	119.37	123.70
33	2	1646	A	C5-C6-N1	-5.42	114.99	117.70
33	2	46	A	O4'-C1'-N9	5.41	112.53	108.20
33	2	503	G	O4'-C1'-N9	5.41	112.53	108.20
33	2	544	A	C5-C6-N1	-5.41	114.99	117.70
33	2	1086	C	N3-C4-C5	-5.41	119.73	121.90
33	2	1230	C	N3-C4-C5	-5.41	119.73	121.90
33	2	1552	С	N3-C4-N4	5.41	121.79	118.00
33	2	592	G	O4'-C1'-N9	5.41	112.53	108.20

G

А

А

С

O4'-C1'-N9

O4'-C1'-N9

C5-C6-N1

N3-C4-C5

1040

1372

1726

507

33

33

33

33

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112.53

112.53

115.00

119.74



5.41

5.41

-5.41

-5.41

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	813	G	N3-C2-N2	5.41	123.69	119.90
33	2	1019	А	O4'-C1'-N9	5.41	112.53	108.20
33	2	1175	G	N3-C2-N2	5.41	123.69	119.90
33	2	1217	G	O4'-C1'-N9	5.41	112.53	108.20
33	2	1243	С	N3-C4-N4	5.41	121.79	118.00
33	2	1247	А	C5-C6-N1	-5.41	115.00	117.70
33	2	1656	А	C5-C6-N1	-5.41	115.00	117.70
33	2	141	А	C5-C6-N6	-5.41	119.37	123.70
33	2	181	А	C5-C6-N6	-5.41	119.37	123.70
33	2	861	А	C5-C6-N6	-5.41	119.37	123.70
33	2	980	С	N3-C4-N4	5.41	121.78	118.00
33	2	976	А	O4'-C1'-N9	5.41	112.53	108.20
33	2	1058	А	C5-C6-N1	-5.41	115.00	117.70
33	2	1219	А	C5-C6-N1	-5.41	115.00	117.70
33	2	1291	А	O4'-C1'-N9	5.41	112.53	108.20
33	2	1563	С	N3-C4-N4	5.41	121.78	118.00
33	2	1164	G	O4'-C1'-N9	5.40	112.52	108.20
33	2	1297	А	C5-C6-N6	-5.40	119.38	123.70
33	2	1485	А	C5-C6-N6	-5.40	119.38	123.70
33	2	1600	G	N3-C2-N2	5.40	123.68	119.90
33	2	45	А	C5-C6-N1	-5.40	115.00	117.70
33	2	353	А	C4-C5-C6	5.40	119.70	117.00
33	2	506	А	C5-C6-N6	-5.40	119.38	123.70
33	2	1045	А	C5-C6-N6	-5.40	119.38	123.70
33	2	1435	А	O4'-C1'-N9	5.40	112.52	108.20
33	2	1450	А	C5-C6-N1	-5.40	115.00	117.70
34	3	62	G	O4'-C1'-N9	5.40	112.52	108.20
33	2	667	G	N3-C2-N2	5.40	123.68	119.90
33	2	1137	G	O4'-C1'-N9	5.40	112.52	108.20
33	2	1278	A	C5-C6-N6	-5.40	119.38	123.70
39	1	60	А	C5-C6-N1	-5.40	115.00	117.70
33	2	294	С	N3-C4-N4	5.40	121.78	118.00
33	2	1260	С	N3-C4-C5	-5.40	119.74	121.90
33	2	1482	А	C5-C6-N1	-5.40	115.00	117.70
33	2	292	А	C5-C6-N6	-5.40	119.38	123.70
33	2	407	С	N3-C4-N4	5.40	121.78	118.00
33	2	1176	С	N3-C4-C5	-5.40	119.74	121.90
33	2	1212	С	N3-C4-C5	-5.40	119.74	121.90
33	2	283	А	C5-C6-N1	-5.39	115.00	117.70
33	2	1773	G	O4'-C1'-N9	5.39	112.52	108.20
33	2	1826	A	C5-C6-N6	-5.39	119.38	123.70
33	2	442	G	O4'-C1'-N9	5.39	112.51	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	464	G	O4'-C1'-N9	5.39	112.51	108.20
33	2	677	С	P-O3'-C3'	-5.39	113.23	119.70
39	1	20	А	C5-C6-N6	-5.39	119.39	123.70
33	2	850	А	C5-C6-N6	-5.39	119.39	123.70
33	2	1365	А	C5-C6-N6	-5.39	119.39	123.70
33	2	435	А	O4'-C1'-N9	5.39	112.51	108.20
33	2	510	А	C5-C6-N1	-5.39	115.01	117.70
33	2	843	А	C5-C6-N6	-5.39	119.39	123.70
33	2	1361	G	O4'-C1'-N9	5.39	112.51	108.20
33	2	141	А	C5-C6-N1	-5.38	115.01	117.70
33	2	353	А	C5-C6-N1	-5.38	115.01	117.70
33	2	1224	А	O4'-C1'-N9	5.38	112.51	108.20
33	2	1303	U	O4'-C1'-N1	5.38	112.51	108.20
33	2	1465	А	O4'-C1'-N9	5.38	112.51	108.20
33	2	182	С	N3-C4-C5	-5.38	119.75	121.90
33	2	466	А	O4'-C1'-N9	5.38	112.51	108.20
33	2	993	А	C5-C6-N1	-5.38	115.01	117.70
33	2	162	С	N3-C4-C5	-5.38	119.75	121.90
33	2	351	U	OP2-P-O3'	5.38	117.04	105.20
33	2	369	С	N3-C4-C5	-5.38	119.75	121.90
33	2	1583	А	C5-C6-N6	-5.38	119.39	123.70
33	2	1793	G	O4'-C1'-N9	5.38	112.50	108.20
33	2	1287	А	O4'-C1'-N9	5.38	112.50	108.20
33	2	371	С	N3-C4-N4	5.38	121.76	118.00
33	2	650	С	N3-C4-C5	-5.38	119.75	121.90
33	2	805	А	O4'-C1'-N9	5.38	112.50	108.20
39	1	75	С	N3-C4-C5	-5.38	119.75	121.90
33	2	238	G	O4'-C1'-N9	5.37	112.50	108.20
33	2	1383	G	O4'-C1'-N9	5.37	112.50	108.20
33	2	1567	С	N3-C4-N4	5.37	121.76	118.00
33	2	25	А	C5-C6-N1	-5.37	115.02	117.70
33	2	290	А	C5-C6-N6	-5.37	119.40	123.70
33	2	1708	С	N3-C4-C5	-5.37	119.75	121.90
33	2	1248	С	N3-C4-C5	-5.37	119.75	121.90
33	2	1291	А	C5-C6-N6	-5.37	119.41	123.70
33	2	491	С	N3-C4-N4	5.37	121.76	118.00
33	2	159	A	C5-C6-N6	-5.37	119.41	123.70
33	2	645	А	O4'-C1'-N9	5.37	112.49	108.20
35	A	57	ARG	C-N-CA	5.37	135.12	121.70
33	2	448	A	C5-C6-N1	-5.36	115.02	117.70
33	2	1024	A	C5-C6-N6	-5.36	119.41	123.70
33	2	1448	A	C4-C5-C6	5.36	119.68	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
39	1	27	С	N3-C4-C5	-5.36	119.75	121.90
39	1	32	С	N3-C4-C5	-5.36	119.75	121.90
33	2	1564	А	C5-C6-N1	-5.36	115.02	117.70
33	2	1414	С	N3-C4-N4	5.36	121.75	118.00
33	2	102	A	C5-C6-N1	-5.36	115.02	117.70
33	2	493	С	N3-C4-N4	5.36	121.75	118.00
33	2	1145	А	O4'-C1'-N9	5.36	112.48	108.20
33	2	296	U	O4'-C1'-N1	5.35	112.48	108.20
33	2	1696	С	N3-C4-C5	-5.35	119.76	121.90
33	2	408	A	C5-C6-N6	-5.35	119.42	123.70
33	2	1565	G	O4'-C1'-N9	5.35	112.48	108.20
3	D	82	ARG	N-CA-CB	5.35	120.23	110.60
33	2	901	C	N3-C4-N4	5.35	121.75	118.00
33	2	79	A	O4'-C1'-N9	5.35	112.48	108.20
33	2	537	G	N3-C2-N2	5.35	123.64	119.90
33	2	804	A	C5-C6-N6	-5.35	119.42	123.70
33	2	429	A	C5-C6-N1	-5.35	115.03	117.70
33	2	564	A	C5-C6-N1	-5.35	115.03	117.70
33	2	896	С	N3-C4-N4	5.35	121.74	118.00
33	2	968	A	C5-C6-N6	-5.35	119.42	123.70
33	2	1442	А	C5-C6-N1	-5.35	115.03	117.70
33	2	1693	С	N3-C4-C5	-5.35	119.76	121.90
33	2	284	С	N3-C4-N4	5.35	121.74	118.00
33	2	476	A	C5-C6-N1	-5.35	115.03	117.70
33	2	1444	А	C5-C6-N6	-5.35	119.42	123.70
33	2	516	A	C5-C6-N1	-5.34	115.03	117.70
33	2	857	А	O4'-C1'-N9	5.34	112.48	108.20
33	2	1576	С	N3-C4-N4	5.34	121.74	118.00
33	2	78	С	N3-C4-C5	-5.34	119.76	121.90
33	2	1133	U	O4'-C1'-N1	5.34	112.47	108.20
33	2	1468	С	N3-C4-C5	-5.34	119.76	121.90
33	2	1561	G	O4'-C1'-N9	5.34	112.47	108.20
33	2	381	С	N3-C4-C5	-5.34	119.76	121.90
33	2	1694	A	C5-C6-N6	-5.34	119.43	123.70
33	2	52	G	O4'-C1'-N9	5.34	112.47	108.20
36	В	276	ASP	C-N-CA	5.34	135.04	121.70
33	2	842	G	O4'-C1'-N9	5.34	112.47	108.20
33	2	1448	A	C5-C6-N6	-5.34	119.43	123.70
33	2	1167	G	O4'-C1'-N9	5.33	112.47	108.20
33	2	1190	A	C4-C5-C6	5.33	119.67	117.00
33	2	323	G	04'-C1'-N9	5.33	112.47	108.20
- 33	2	515	A	C4-C5-C6	5.33	119.67	117.00

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	619	А	C5-C6-N1	-5.33	115.03	117.70
33	2	928	G	O4'-C1'-N9	5.33	112.46	108.20
33	2	977	A	O4'-C1'-N9	5.33	112.47	108.20
33	2	1004	А	C5-C6-N1	-5.33	115.03	117.70
33	2	1786	G	O4'-C1'-N9	5.33	112.47	108.20
33	2	1837	G	O4'-C1'-N9	5.33	112.47	108.20
33	2	1664	G	O4'-C1'-N9	5.33	112.46	108.20
33	2	37	C	N3-C4-N4	5.33	121.73	118.00
33	2	450	A	C4-C5-C6	5.33	119.66	117.00
33	2	632	U	O4'-C1'-N1	5.33	112.46	108.20
33	2	1245	С	N3-C4-C5	-5.33	119.77	121.90
33	2	1278	А	C5-C6-N1	-5.33	115.03	117.70
33	2	1712	С	N3-C4-C5	-5.33	119.77	121.90
33	2	1730	A	C5-C6-N1	-5.33	115.04	117.70
33	2	1831	G	C5-C6-O6	-5.33	125.40	128.60
33	2	1432	С	N3-C4-C5	-5.33	119.77	121.90
33	2	99	А	O4'-C1'-N9	5.33	112.46	108.20
33	2	185	С	N3-C4-C5	-5.33	119.77	121.90
33	2	457	G	O4'-C1'-N9	5.32	112.46	108.20
33	2	1073	А	C5-C6-N1	-5.32	115.04	117.70
33	2	1249	А	O4'-C1'-N9	5.32	112.46	108.20
33	2	104	А	C5-C6-N1	-5.32	115.04	117.70
33	2	523	А	C5-C6-N6	-5.32	119.44	123.70
33	2	1674	А	C5-C6-N1	-5.32	115.04	117.70
33	2	16	G	O4'-C1'-N9	5.32	112.46	108.20
33	2	185	С	N3-C4-N4	5.32	121.72	118.00
33	2	509	А	O4'-C1'-N9	5.32	112.46	108.20
33	2	609	А	C5-C6-N6	-5.32	119.44	123.70
33	2	1378	А	C5-C6-N1	-5.32	115.04	117.70
33	2	316	С	N3-C4-C5	-5.32	119.77	121.90
33	2	479	A	C5-C6-N1	-5.32	115.04	117.70
33	2	594	А	C5-C6-N6	-5.32	119.45	123.70
33	2	633	А	C5-C6-N1	-5.32	115.04	117.70
33	2	970	C	N3-C4-C5	-5.32	119.77	121.90
33	2	351	U	O4'-C1'-N1	5.32	112.45	108.20
33	2	370	G	O4'-C1'-N9	5.32	112.45	108.20
33	2	390	С	N3-C4-C5	-5.31	119.77	121.90
33	2	1358	U	O4'-C1'-N1	5.31	112.45	108.20
33	2	1401	A	C5-C6-N6	-5.31	119.45	123.70
33	2	1424	G	C5'-C4'-C3'	5.31	124.50	116.00
33	2	1642	A	C5-C6-N1	-5.31	115.04	117.70
33	2	511	A	C5-C6-N6	-5.31	119.45	123.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	1149	С	N3-C4-C5	-5.31	119.78	121.90
33	2	435	А	C5-C6-N1	-5.31	115.04	117.70
33	2	1450	А	C5-C6-N6	-5.31	119.45	123.70
33	2	1461	А	C5-C6-N6	-5.31	119.45	123.70
33	2	1299	С	N3-C4-N4	5.31	121.72	118.00
33	2	1541	G	O4'-C1'-N9	5.31	112.45	108.20
33	2	1815	U	P-O3'-C3'	5.31	126.07	119.70
33	2	1844	A	C4-C5-C6	5.31	119.66	117.00
33	2	521	A	O4'-C1'-N9	5.31	112.45	108.20
33	2	1024	А	O4'-C1'-N9	5.31	112.45	108.20
33	2	1487	G	O4'-C1'-N9	5.31	112.45	108.20
33	2	1519	G	O4'-C1'-N9	5.31	112.45	108.20
33	2	99	А	C5-C6-N1	-5.30	115.05	117.70
33	2	179	С	N3-C4-N4	5.30	121.71	118.00
33	2	476	А	C5-C6-N6	-5.30	119.46	123.70
33	2	1166	А	O4'-C1'-N9	5.30	112.44	108.20
33	2	1650	С	N3-C4-C5	-5.30	119.78	121.90
33	2	1237	А	C5-C6-N1	-5.30	115.05	117.70
34	3	67	A	C5-C6-N6	-5.30	119.46	123.70
33	2	613	G	O4'-C1'-N9	5.30	112.44	108.20
33	2	846	С	N3-C4-N4	5.30	121.71	118.00
33	2	955	G	N3-C2-N2	5.30	123.61	119.90
33	2	984	С	N3-C4-C5	-5.30	119.78	121.90
33	2	1423	С	N3-C4-C5	-5.30	119.78	121.90
33	2	391	А	O4'-C1'-N9	5.30	112.44	108.20
33	2	440	С	N3-C4-C5	-5.30	119.78	121.90
33	2	1220	G	O4'-C1'-N9	5.30	112.44	108.20
33	2	1451	А	O4'-C1'-N9	5.30	112.44	108.20
33	2	329	А	C5-C6-N1	-5.30	115.05	117.70
33	2	873	С	C6-N1-C1'	-5.30	114.44	120.80
33	2	1485	A	C5-C6-N1	-5.30	115.05	117.70
33	2	1540	А	O4'-C1'-N9	5.30	112.44	108.20
33	2	1631	G	O4'-C1'-N9	5.30	112.44	108.20
33	2	388	А	C5-C6-N1	-5.29	115.05	117.70
33	2	1397	А	C5-C6-N6	-5.29	119.46	123.70
33	2	1557	С	N3-C4-C5	-5.29	119.78	121.90
39	1	17	С	O4'-C1'-N1	5.29	112.44	108.20
33	2	924	G	O4'-C1'-N9	5.29	112.44	108.20
33	2	1430	C	N3-C4-C5	-5.29	119.78	121.90
33	2	1544	U	O4'-C1'-N1	5.29	112.44	108.20
33	2	189	G	N3-C2-N2	5.29	123.60	119.90
33	2	218	A	C5-C6-N1	-5.29	115.05	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	605	С	N3-C4-N4	5.29	121.70	118.00
39	1	16	G	O3'-P-O5'	-5.29	93.95	104.00
33	2	354	А	C5-C6-N1	-5.29	115.06	117.70
33	2	486	С	N3-C4-C5	-5.29	119.78	121.90
33	2	1146	А	C5-C6-N6	-5.29	119.47	123.70
33	2	1200	А	C5-C6-N1	-5.29	115.06	117.70
33	2	1859	С	N3-C4-N4	5.29	121.70	118.00
39	1	40	С	N3-C4-C5	-5.29	119.78	121.90
8	Ι	7	PHE	CB-CG-CD1	5.29	124.50	120.80
33	2	102	А	C5-C6-N6	-5.29	119.47	123.70
33	2	517	С	N3-C4-C5	-5.29	119.79	121.90
39	1	63	А	O4'-C1'-N9	5.29	112.43	108.20
33	2	483	А	O4'-C1'-N9	5.28	112.43	108.20
33	2	1829	А	C5-C6-N1	-5.28	115.06	117.70
33	2	873	С	O4'-C1'-N1	5.28	112.43	108.20
33	2	435	А	C5-C6-N6	-5.28	119.47	123.70
33	2	538	С	N3-C4-C5	-5.28	119.79	121.90
33	2	899	А	C5-C6-N6	-5.28	119.47	123.70
33	2	1218	G	O3'-P-O5'	-5.28	93.97	104.00
33	2	1327	С	N3-C4-C5	-5.28	119.79	121.90
33	2	1178	А	O4'-C1'-N9	5.28	112.42	108.20
33	2	1451	А	C5-C6-N6	-5.28	119.48	123.70
33	2	68	А	C5-C6-N1	-5.28	115.06	117.70
33	2	1016	А	C5-C6-N1	-5.28	115.06	117.70
33	2	1692	А	C5-C6-N1	-5.28	115.06	117.70
33	2	912	А	C5-C6-N1	-5.27	115.06	117.70
33	2	1096	А	C5-C6-N6	-5.27	119.48	123.70
33	2	1613	С	N3-C4-C5	-5.27	119.79	121.90
33	2	19	А	C5-C6-N1	-5.27	115.06	117.70
33	2	125	С	N3-C4-C5	-5.27	119.79	121.90
33	2	270	G	O4'-C1'-N9	5.27	112.42	108.20
33	2	455	А	C5-C6-N1	-5.27	115.06	117.70
33	2	1180	G	O4'-C1'-N9	5.27	112.42	108.20
33	2	1634	G	O4'-C1'-N9	5.27	112.42	108.20
33	2	226	А	C5-C6-N6	-5.27	119.48	123.70
33	2	502	А	C5-C6-N1	-5.27	115.06	117.70
33	2	1105	С	N3-C4-N4	5.27	121.69	118.00
33	2	1128	C	N3-C4-C5	-5.27	119.79	121.90
33	2	1214	C	N3-C4-C5	-5.27	119.79	121.90
33	2	1614	A	C5-C6-N6	-5.27	119.48	123.70
33	2	536	G	O4'-C1'-N9	5.27	112.41	108.20
33	2	871	A	C5-C6-N1	-5.27	115.07	117.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	901	С	N3-C4-C5	-5.27	119.79	121.90
33	2	1129	A	C5-C6-N1	-5.27	115.07	117.70
33	2	1372	А	C5-C6-N1	-5.27	115.07	117.70
33	2	1599	G	O4'-C1'-N9	5.27	112.42	108.20
33	2	513	А	C5-C6-N1	-5.27	115.07	117.70
33	2	820	С	N3-C4-C5	-5.27	119.79	121.90
39	1	57	G	O4'-C1'-N9	5.27	112.41	108.20
33	2	142	С	N3-C4-C5	-5.26	119.79	121.90
33	2	438	A	O4'-C1'-N9	5.26	112.41	108.20
33	2	836	С	N3-C4-C5	-5.26	119.79	121.90
8	Ι	145	PHE	CB-CG-CD1	5.26	124.48	120.80
34	3	61	С	N3-C4-C5	-5.26	119.80	121.90
33	2	452	С	N3-C4-C5	-5.26	119.80	121.90
33	2	55	U	O4'-C1'-N1	5.26	112.41	108.20
33	2	1326	G	O4'-C1'-N9	5.26	112.41	108.20
33	2	1816	A	O4'-C1'-N9	5.26	112.41	108.20
33	2	1397	А	C5-C6-N1	-5.26	115.07	117.70
33	2	1394	G	O4'-C1'-N9	5.26	112.41	108.20
33	2	798	A	O5'-C5'-C4'	5.25	121.69	111.70
33	2	980	С	N3-C4-C5	-5.25	119.80	121.90
33	2	331	С	N3-C4-C5	-5.25	119.80	121.90
33	2	110	U	O4'-C1'-N1	5.25	112.40	108.20
33	2	591	G	O4'-C1'-N9	5.25	112.40	108.20
33	2	873	С	N3-C4-C5	-5.25	119.80	121.90
33	2	905	G	O4'-C1'-N9	5.25	112.40	108.20
33	2	920	G	O4'-C1'-N9	5.25	112.40	108.20
33	2	1439	С	N3-C4-N4	5.25	121.67	118.00
33	2	1658	А	C4-C5-C6	5.25	119.62	117.00
34	3	61	С	N3-C4-N4	5.25	121.67	118.00
33	2	371	С	N3-C4-C5	-5.25	119.80	121.90
33	2	440	С	N3-C4-N4	5.25	121.67	118.00
33	2	551	А	C5-C6-N1	-5.25	115.08	117.70
33	2	1075	С	N3-C4-N4	5.25	121.67	118.00
33	2	1126	G	O4'-C1'-N9	5.25	112.40	108.20
33	2	953	A	C5-C6-N1	-5.25	115.08	117.70
33	2	1596	А	C5-C6-N1	-5.25	115.08	117.70
33	2	994	А	C5-C6-N6	-5.25	119.50	123.70
33	2	1112	С	N3-C4-C5	-5.25	119.80	121.90
33	2	1641	С	N3-C4-C5	-5.25	119.80	121.90
33	2	1816	A	C5-C6-N1	-5.25	115.08	117.70
33	2	79	A	C4-C5-C6	5.24	119.62	117.00
33	2	330	С	N3-C4-C5	-5.24	119.80	121.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	1809	A	C5-C6-N1	-5.24	115.08	117.70
33	2	393	G	O4'-C1'-N9	5.24	112.39	108.20
33	2	471	С	N3-C4-C5	-5.24	119.80	121.90
33	2	1333	С	N3-C4-C5	-5.24	119.80	121.90
33	2	240	С	O4'-C1'-N1	5.24	112.39	108.20
33	2	798	A	O4'-C1'-N9	5.24	112.39	108.20
33	2	1283	А	C5-C6-N1	-5.24	115.08	117.70
33	2	806	А	C5-C6-N1	-5.24	115.08	117.70
39	1	48	С	P-O3'-C3'	5.24	125.98	119.70
33	2	221	А	C5-C6-N1	-5.24	115.08	117.70
33	2	1053	С	N3-C4-C5	-5.24	119.81	121.90
33	2	1309	А	O4'-C1'-N9	5.24	112.39	108.20
33	2	1429	С	N3-C4-C5	-5.24	119.81	121.90
33	2	1690	А	C5-C6-N1	-5.24	115.08	117.70
39	1	76	А	C5-C6-N1	-5.24	115.08	117.70
33	2	95	G	O4'-C1'-N9	5.23	112.39	108.20
33	2	1825	А	C5-C6-N1	-5.23	115.08	117.70
33	2	624	А	O4'-C1'-N9	5.23	112.39	108.20
33	2	1038	А	C5-C6-N1	-5.23	115.08	117.70
33	2	1730	А	C5-C6-N6	-5.23	119.51	123.70
35	А	82	TYR	CB-CG-CD2	-5.23	117.86	121.00
33	2	38	А	C5-C6-N1	-5.23	115.08	117.70
33	2	67	С	N3-C4-C5	-5.23	119.81	121.90
33	2	959	А	C5-C6-N1	-5.23	115.08	117.70
33	2	1682	С	N3-C4-C5	-5.23	119.81	121.90
33	2	83	A	C5-C6-N1	-5.23	115.09	117.70
33	2	1179	А	C5-C6-N1	-5.23	115.09	117.70
39	1	23	С	N3-C4-C5	-5.23	119.81	121.90
25	b	62	TYR	CB-CG-CD2	-5.22	117.87	121.00
33	2	1360	U	C6-N1-C1'	-5.22	113.89	121.20
33	2	1457	G	N3-C2-N2	5.22	123.56	119.90
33	2	1551	А	C5-C6-N1	-5.22	115.09	117.70
33	2	1784	А	C5-C6-N6	-5.22	119.52	123.70
39	1	42	А	C5-C6-N1	-5.22	115.09	117.70
33	2	817	G	O4'-C1'-N9	5.22	112.38	108.20
33	2	1705	С	N3-C4-C5	-5.22	119.81	121.90
33	2	193	С	N3-C4-C5	-5.22	119.81	121.90
33	2	407	С	N3-C4-C5	-5.22	119.81	121.90
33	2	628	С	N3-C4-C5	-5.22	119.81	121.90
33	2	677	С	O4'-C1'-N1	5.22	112.37	108.20
33	2	833	A	C5-C6-N1	-5.22	115.09	117.70
33	2	1478	С	N3-C4-C5	-5.22	119.81	121.90
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	908	С	O4'-C1'-N1	5.22	112.37	108.20
33	2	1199	G	O4'-C1'-N9	5.22	112.37	108.20
33	2	1569	С	N3-C4-C5	-5.22	119.81	121.90
33	2	1583	А	C5-C6-N1	-5.22	115.09	117.70
33	2	1614	А	O4'-C1'-N9	5.22	112.37	108.20
33	2	1812	А	C5-C6-N1	-5.22	115.09	117.70
33	2	35	С	N3-C4-C5	-5.21	119.81	121.90
33	2	645	A	C5-C6-N1	-5.21	115.09	117.70
33	2	654	А	C5-C6-N6	-5.21	119.53	123.70
33	2	1020	А	O4'-C1'-N9	5.21	112.37	108.20
33	2	1563	С	N3-C4-C5	-5.21	119.81	121.90
33	2	909	А	C5-C6-N6	-5.21	119.53	123.70
33	2	1412	С	N3-C4-C5	-5.21	119.81	121.90
33	2	1734	С	N3-C4-C5	-5.21	119.81	121.90
33	2	315	С	N3-C4-C5	-5.21	119.81	121.90
33	2	605	С	N3-C4-C5	-5.21	119.81	121.90
39	1	61	С	N3-C4-C5	-5.21	119.82	121.90
33	2	986	А	C5-C6-N1	-5.21	115.09	117.70
33	2	1113	С	N3-C4-C5	-5.21	119.82	121.90
33	2	1398	А	C4-C5-C6	5.21	119.61	117.00
33	2	345	G	O4'-C1'-N9	5.21	112.37	108.20
33	2	1087	С	N3-C4-N4	5.21	121.65	118.00
33	2	618	А	C5-C6-N6	-5.21	119.53	123.70
33	2	1379	А	O4'-C1'-N9	5.21	112.36	108.20
33	2	293	А	O4'-C1'-N9	5.21	112.36	108.20
33	2	319	G	O4'-C1'-N9	5.21	112.36	108.20
33	2	1836	C	N3-C4-C5	-5.20	119.82	121.90
33	2	2	А	C5-C6-N1	-5.20	115.10	117.70
33	2	812	А	C5-C6-N1	-5.20	115.10	117.70
33	2	1026	А	C5-C6-N1	-5.20	115.10	117.70
33	2	1405	A	C5-C6-N1	-5.20	115.10	117.70
33	2	398	А	O4'-C1'-N9	5.20	112.36	108.20
33	2	934	A	C5-C6-N6	-5.20	119.54	123.70
33	2	1578	С	N3-C4-C5	-5.20	119.82	121.90
33	2	427	G	O4'-C1'-N9	5.20	112.36	108.20
33	2	550	А	C4-C5-C6	5.20	119.60	117.00
33	2	917	G	O4'-C1'-N9	5.20	112.36	108.20
33	2	921	G	O4'-C1'-N9	5.20	112.36	108.20
33	2	526	A	C5-C6-N6	-5.20	119.54	123.70
33	2	1195	A	C5-C6-N6	-5.20	119.54	123.70
33	2	1612	G	N3-C2-N2	5.20	123.54	119.90
33	2	17	С	C2-N1-C1'	5.20	124.52	118.80



Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	608	С	N3-C4-C5	-5.20	119.82	121.90
33	2	631	А	O4'-C1'-N9	5.20	112.36	108.20
33	2	916	А	C5-N7-C8	5.20	106.50	103.90
33	2	1401	А	O4'-C1'-N9	5.20	112.36	108.20
33	2	1442	А	C5-C6-N6	-5.20	119.54	123.70
33	2	1740	А	C5-C6-N1	-5.20	115.10	117.70
39	1	49	G	O4'-C1'-N9	5.20	112.36	108.20
33	2	550	А	C5-C6-N1	-5.19	115.10	117.70
33	2	1261	А	C5-C6-N1	-5.19	115.10	117.70
33	2	1494	А	C5-C6-N6	-5.19	119.55	123.70
33	2	1524	С	N3-C4-C5	-5.19	119.82	121.90
33	2	440	С	O4'-C1'-N1	5.19	112.35	108.20
33	2	459	А	C5-C6-N1	-5.19	115.11	117.70
33	2	1805	С	N3-C4-C5	-5.19	119.82	121.90
24	a	86	GLU	N-CA-CB	5.19	119.94	110.60
33	2	1341	G	O4'-C1'-N9	5.19	112.35	108.20
33	2	1521	G	O4'-C1'-N9	5.19	112.35	108.20
33	2	1628	А	C5-C6-N1	-5.19	115.11	117.70
33	2	1733	С	N3-C4-C5	-5.19	119.83	121.90
33	2	659	А	C5-C6-N1	-5.19	115.11	117.70
33	2	822	А	O4'-C1'-N9	5.19	112.35	108.20
33	2	1729	G	N3-C2-N2	5.19	123.53	119.90
33	2	42	А	C5-C6-N1	-5.18	115.11	117.70
33	2	232	А	C5-C6-N1	-5.18	115.11	117.70
33	2	1430	С	N3-C4-N4	5.18	121.63	118.00
33	2	39	А	C5-C6-N1	-5.18	115.11	117.70
33	2	566	А	C5-C6-N1	-5.18	115.11	117.70
33	2	676	U	P-O3'-C3'	-5.18	113.48	119.70
33	2	1290	G	O4'-C1'-N9	5.18	112.35	108.20
39	1	47	U	C2-N1-C1'	5.18	123.92	117.70
33	2	303	G	P-O3'-C3'	5.18	125.91	119.70
33	2	1056	А	C5-C6-N1	-5.18	115.11	117.70
33	2	1179	А	O4'-C1'-N9	5.18	112.34	108.20
33	2	1257	С	N3-C4-C5	-5.18	119.83	121.90
33	2	1696	С	O4'-C1'-N1	5.18	112.34	108.20
33	2	1076	А	C5-C6-N1	-5.17	115.11	117.70
33	2	1215	С	N3-C4-C5	-5.17	119.83	121.90
39	1	2	A	O4'-C1'-N9	5.17	112.34	108.20
33	2	856	G	04'-C1'-N9	5.17	112.34	108.20
33	2	1483	A	C5-C6-N1	-5.17	115.11	117.70
33	2	1523	G	O4'-C1'-N9	5.17	112.34	108.20
33	2	1835	С	N3-C4-C5	-5.17	119.83	121.90



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G

А

N3-C4-C5

P-O3'-C3'

C5-C6-N6

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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
39	1	45	G	O4'-C1'-N9	5.17	112.34	108.20
33	2	49	С	N3-C4-N4	5.17	121.62	118.00
33	2	1272	А	O4'-C1'-N9	5.17	112.33	108.20
33	2	1476	А	C5-C6-N1	-5.17	115.12	117.70
33	2	208	G	P-O3'-C3'	5.17	125.90	119.70
33	2	1589	А	C5-C6-N1	-5.17	115.12	117.70
39	1	26	G	O4'-C1'-N9	5.17	112.33	108.20
33	2	181	А	C5-C6-N1	-5.16	115.12	117.70
33	2	1670	А	C5-C6-N1	-5.16	115.12	117.70
33	2	527	С	N3-C4-C5	-5.16	119.84	121.90
33	2	619	А	C5-C6-N6	-5.16	119.57	123.70
33	2	1043	С	N3-C4-C5	-5.16	119.84	121.90
33	2	425	А	C5-C6-N1	-5.16	115.12	117.70
33	2	1807	А	C5-C6-N1	-5.16	115.12	117.70
34	3	76	А	O4'-C1'-N9	5.16	112.33	108.20
39	1	35	А	C5-C6-N6	-5.16	119.57	123.70
33	2	1353	А	C5-C6-N6	-5.16	119.57	123.70
33	2	60	А	C5-C6-N1	-5.16	115.12	117.70
33	2	1284	U	O4'-C1'-N1	5.16	112.33	108.20
33	2	408	А	C5-C6-N1	-5.15	115.12	117.70
33	2	646	G	O4'-C1'-N9	5.15	112.32	108.20
33	2	988	А	C5-C6-N1	-5.15	115.12	117.70
33	2	1008	А	C5-C6-N1	-5.15	115.12	117.70
33	2	40	А	C5-C6-N1	-5.15	115.12	117.70
33	2	852	С	N3-C4-C5	-5.15	119.84	121.90
33	2	212	G	O4'-C1'-N9	5.15	112.32	108.20
33	2	569	С	N3-C4-C5	-5.15	119.84	121.90
33	2	658	А	C5-C6-N6	-5.15	119.58	123.70
33	2	1066	A	C5-C6-N6	-5.15	119.58	123.70
33	2	1374	A	C5-C6-N1	-5.15	115.13	117.70
8	Ι	7	PHE	CB-CG-CD2	-5.15	117.20	120.80
33	2	338	A	C5-C6-N1	-5.15	115.13	117.70
33	2	861	A	C5-C6-N1	-5.15	115.13	117.70
33	2	438	А	C5-C6-N1	-5.14	115.13	117.70
33	2	519	A	C5-C6-N1	-5.14	115.13	117.70
33	2	1075	C	N3-C4-C5	-5.14	119.84	121.90
33	2	601	G	O4'-C1'-N9	5.14	112.31	108.20
33	2	1010	G	O4'-C1'-N9	5.14	112.31	108.20
33	2	1201	C	N3-C4-C5	-5.14	119.84	121.90

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121.90

119.70

123.70

119.84

125.87

119.59



-5.14

5.14

-5.14

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	139	С	N3-C4-N4	5.14	121.60	118.00
33	2	361	А	O4'-C1'-N9	5.14	112.31	108.20
33	2	416	А	C5-C6-N1	-5.14	115.13	117.70
33	2	944	С	N3-C4-C5	-5.14	119.84	121.90
33	2	1839	А	O4'-C1'-N9	5.14	112.31	108.20
33	2	1371	G	O4'-C1'-N9	5.14	112.31	108.20
33	2	1602	A	C5-C6-N1	-5.14	115.13	117.70
33	2	4	C	N3-C4-C5	-5.14	119.85	121.90
33	2	866	А	C5-C6-N1	-5.14	115.13	117.70
33	2	824	G	O4'-C1'-N9	5.13	112.31	108.20
33	2	1185	А	C5-C6-N1	-5.13	115.13	117.70
33	2	622	С	N3-C4-C5	-5.13	119.85	121.90
33	2	652	G	N1-C6-O6	5.13	122.98	119.90
33	2	1256	A	C5-C6-N1	-5.13	115.13	117.70
33	2	1461	А	C5-C6-N1	-5.13	115.13	117.70
33	2	1497	С	N3-C4-C5	-5.13	119.85	121.90
33	2	1537	С	N3-C4-C5	-5.13	119.85	121.90
33	2	1540	А	C5-C6-N6	-5.13	119.59	123.70
33	2	1795	А	C5-C6-N1	-5.13	115.14	117.70
33	2	11	А	C5-C6-N1	-5.13	115.14	117.70
33	2	240	С	N3-C4-C5	-5.13	119.85	121.90
33	2	73	С	N3-C4-C5	-5.13	119.85	121.90
33	2	951	А	C4-C5-C6	5.13	119.56	117.00
36	В	251	TYR	CB-CG-CD1	5.13	124.08	121.00
34	3	63	U	C6-N1-C1'	-5.12	114.03	121.20
33	2	985	С	N3-C4-N4	5.12	121.59	118.00
33	2	1159	С	N3-C4-C5	-5.12	119.85	121.90
33	2	1254	A	C5-C6-N1	-5.12	115.14	117.70
33	2	49	С	N3-C4-C5	-5.12	119.85	121.90
33	2	845	A	O4'-C1'-N9	5.12	112.30	108.20
33	2	919	G	O4'-C1'-N9	5.12	112.30	108.20
33	2	1058	А	C5-C6-N6	-5.12	119.60	123.70
33	2	1258	С	N3-C4-C5	-5.12	119.85	121.90
33	2	1472	А	C5-C6-N6	-5.12	119.60	123.70
4	Е	175	SER	N-CA-CB	5.12	118.18	110.50
33	2	225	С	N3-C4-C5	-5.12	119.85	121.90
33	2	559	A	O4'-C1'-N9	5.12	112.29	108.20
33	2	654	A	C5-C6-N1	-5.12	115.14	117.70
33	2	1387	С	N3-C4-C5	-5.12	119.85	121.90
33	2	372	C	N3-C4-N4	5.12	121.58	118.00
33	2	398	A	C5-C6-N1	-5.12	115.14	117.70
33	2	1229	G	O4'-C1'-N9	5.12	112.29	108.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1569	С	N3-C4-N4	5.12	121.58	118.00
33	2	564	A	C5-C6-N6	-5.12	119.61	123.70
33	2	666	С	N3-C4-C5	-5.12	119.85	121.90
33	2	1787	A	C5-C6-N6	-5.12	119.61	123.70
33	2	333	А	O4'-C1'-N9	5.11	112.29	108.20
33	2	502	A	O4'-C1'-N9	5.11	112.29	108.20
33	2	1389	G	O4'-C1'-N9	5.11	112.29	108.20
33	2	295	С	N3-C4-C5	-5.11	119.86	121.90
33	2	615	G	N3-C2-N2	5.11	123.48	119.90
33	2	1288	С	N3-C4-C5	-5.11	119.86	121.90
33	2	329	А	O4'-C1'-N9	5.11	112.29	108.20
33	2	1030	А	C5-C6-N1	-5.11	115.15	117.70
33	2	611	С	N3-C4-C5	-5.11	119.86	121.90
33	2	1049	С	N3-C4-C5	-5.11	119.86	121.90
33	2	1254	А	P-O3'-C3'	5.11	125.83	119.70
33	2	1337	С	N3-C4-C5	-5.11	119.86	121.90
33	2	1392	А	O4'-C1'-N9	5.11	112.29	108.20
33	2	1278	А	O4'-C1'-N9	5.11	112.28	108.20
33	2	1548	С	P-O3'-C3'	5.11	125.83	119.70
33	2	1742	С	N3-C4-C5	-5.11	119.86	121.90
11	L	159	PHE	CB-CG-CD1	5.10	124.37	120.80
33	2	142	С	O4'-C1'-N1	5.10	112.28	108.20
33	2	159	А	O4'-C1'-N9	5.10	112.28	108.20
33	2	376	С	N3-C4-C5	-5.10	119.86	121.90
33	2	812	А	O4'-C1'-N9	5.10	112.28	108.20
33	2	1526	А	C4-C5-C6	5.10	119.55	117.00
39	1	50	A	C5-C6-N1	-5.10	115.15	117.70
33	2	959	A	O4'-C1'-N9	5.10	112.28	108.20
33	2	1247	A	O4'-C1'-N9	5.10	112.28	108.20
4	Ε	221	PHE	CB-CG-CD1	5.10	124.37	120.80
33	2	809	A	C5-C6-N1	-5.10	115.15	117.70
33	2	821	A	C5-C6-N1	-5.10	115.15	117.70
33	2	858	A	C5-C6-N1	-5.10	115.15	117.70
33	2	1028	C	N3-C4-C5	-5.10	119.86	121.90
33	2	1366	A	C5-C6-N1	-5.10	115.15	117.70
33	2	1583	A	O4'-C1'-N9	5.10	112.28	108.20
33	2	624	A	C5-C6-N1	-5.10	115.15	117.70
33	2	860	A	C5-C6-N1	-5.10	115.15	117.70
33	2	1181	C	N3-C4-C5	-5.10	119.86	121.90
33	2	1494	A	O4'-C1'-N9	5.10	112.28	108.20
33	2	1623	C	N3-C4-C5	-5.10	119.86	121.90
33	2	1659	A	C5-C6-N1	-5.10	115.15	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$ $ Ideal( $^{o}$ )
33	2	472	G	N3-C2-N2	5.10	123.47	119.90
33	2	648	U	O4'-C1'-N1	5.10	112.28	108.20
33	2	997	А	C5-C6-N1	-5.10	115.15	117.70
33	2	1035	С	N3-C4-C5	-5.10	119.86	121.90
33	2	1177	А	C5-C6-N1	-5.09	115.15	117.70
33	2	1348	G	O4'-C1'-N9	5.09	112.28	108.20
33	2	918	А	O4'-C1'-N9	5.09	112.27	108.20
33	2	1113	С	N3-C4-N4	5.09	121.56	118.00
39	1	74	С	N3-C4-C5	-5.09	119.86	121.90
33	2	1528	А	C5-C6-N6	-5.09	119.63	123.70
33	2	1785	A	O4'-C1'-N9	5.09	112.27	108.20
33	2	1809	А	C5-C6-N6	-5.09	119.63	123.70
33	2	453	С	N3-C4-C5	-5.09	119.86	121.90
33	2	1139	A	O4'-C1'-N9	5.09	112.27	108.20
33	2	1365	А	C5-C6-N1	-5.09	115.16	117.70
33	2	29	G	O4'-C1'-N9	5.09	112.27	108.20
33	2	985	С	O4'-C1'-N1	5.09	112.27	108.20
33	2	1635	А	C5-C6-N1	-5.09	115.16	117.70
33	2	1737	С	N3-C4-C5	-5.09	119.86	121.90
33	2	516	А	C5-C6-N6	-5.09	119.63	123.70
33	2	600	G	O4'-C1'-N9	5.09	112.27	108.20
33	2	623	С	N3-C4-C5	-5.09	119.86	121.90
33	2	1120	С	N3-C4-C5	-5.09	119.87	121.90
33	2	414	С	N3-C4-C5	-5.08	119.87	121.90
33	2	79	А	P-O3'-C3'	5.08	125.80	119.70
33	2	583	С	N3-C4-C5	-5.08	119.87	121.90
33	2	1271	G	O4'-C1'-N9	5.08	112.27	108.20
33	2	6	G	O4'-C1'-N9	5.08	112.26	108.20
33	2	297	C	N3-C4-C5	-5.08	119.87	121.90
33	2	492	C	N3-C4-C5	-5.08	119.87	121.90
33	2	559	А	C5-C6-N1	-5.08	115.16	117.70
33	2	847	C	N3-C4-C5	-5.08	119.87	121.90
33	2	1604	С	N3-C4-N4	5.08	121.55	118.00
39	1	2	А	C5-C6-N1	-5.08	115.16	117.70
33	2	389	С	N3-C4-N4	5.08	121.55	118.00
33	2	1275	С	N3-C4-C5	-5.08	119.87	121.90
33	2	1498	С	N3-C4-C5	-5.08	119.87	121.90
33	2	1572	G	O4'-C1'-N9	5.08	112.26	108.20
33	2	1307	С	N3-C4-C5	-5.07	119.87	121.90
33	2	1491	G	C5-C6-O6	-5.07	125.56	128.60
33	2	168	С	N3-C4-C5	-5.07	119.87	121.90
33	2	597	U	C6-N1-C1'	-5.07	114.10	121.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	1426	С	N3-C4-C5	-5.07	119.87	121.90
33	2	1566	G	O4'-C1'-N9	5.07	112.26	108.20
33	2	1831	G	N3-C2-N2	5.07	123.45	119.90
33	2	880	С	N3-C4-N4	5.07	121.55	118.00
33	2	1186	А	C5-C6-N6	-5.07	119.64	123.70
33	2	150	А	O4'-C1'-N9	5.07	112.25	108.20
33	2	178	С	N3-C4-C5	-5.07	119.87	121.90
33	2	231	С	N3-C4-C5	-5.07	119.87	121.90
33	2	533	С	N3-C4-N4	5.07	121.55	118.00
33	2	560	С	N3-C4-C5	-5.07	119.87	121.90
33	2	819	U	C2-N1-C1'	5.07	123.78	117.70
33	2	1658	А	O4'-C1'-N9	5.07	112.25	108.20
33	2	174	С	N3-C4-C5	-5.07	119.87	121.90
33	2	554	А	C5-C6-N1	-5.07	115.17	117.70
33	2	1262	С	N3-C4-C5	-5.07	119.87	121.90
33	2	1619	U	C6-N1-C1'	-5.07	114.11	121.20
33	2	1413	С	O4'-C1'-N1	5.06	112.25	108.20
33	2	982	G	O4'-C1'-N9	5.06	112.25	108.20
33	2	1051	А	C5-C6-N1	-5.06	115.17	117.70
34	3	74	G	O4'-C1'-N9	5.06	112.25	108.20
33	2	880	С	N3-C4-C5	-5.06	119.88	121.90
33	2	954	G	C4-N9-C1'	5.06	133.08	126.50
33	2	644	А	O4'-C1'-N9	5.06	112.25	108.20
33	2	551	А	C5-C6-N6	-5.06	119.65	123.70
33	2	1155	G	O4'-C1'-N9	5.06	112.25	108.20
33	2	1447	G	O4'-C1'-N9	5.06	112.25	108.20
34	3	52	А	C5-C6-N1	-5.06	115.17	117.70
33	2	904	А	O4'-C1'-N9	5.05	112.24	108.20
33	2	1032	А	O4'-C1'-N9	5.05	112.24	108.20
33	2	1102	С	N3-C4-C5	-5.05	119.88	121.90
33	2	1328	А	O4'-C1'-N9	5.05	112.24	108.20
33	2	663	G	O4'-C1'-N9	5.05	112.24	108.20
33	2	171	А	C5-C6-N1	-5.05	115.18	117.70
33	2	213	С	N3-C4-C5	-5.05	119.88	121.90
33	2	1678	С	N3-C4-N4	5.05	121.53	118.00
33	2	1153	G	O4'-C1'-N9	5.05	112.24	108.20
33	2	482	С	N3-C4-N4	5.05	121.53	118.00
33	2	1411	С	N3-C4-N4	5.05	121.53	118.00
33	2	1705	С	N3-C4-N4	5.04	121.53	118.00
33	2	83	A	C5-C6-N6	-5.04	119.67	123.70
33	2	448	A	C5-C6-N6	-5.04	119.67	123.70
33	2	593	С	N3-C4-N4	5.04	121.53	118.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	830	С	N3-C4-C5	-5.04	119.88	121.90
15	Р	65	PHE	CB-CG-CD1	5.04	124.33	120.80
33	2	69	С	N3-C4-C5	-5.04	119.88	121.90
33	2	1209	С	N3-C4-C5	-5.04	119.88	121.90
39	1	4	С	N3-C4-C5	-5.04	119.88	121.90
33	2	18	С	N3-C4-C5	-5.04	119.88	121.90
33	2	1385	С	N3-C4-C5	-5.04	119.88	121.90
33	2	1628	А	C5-C6-N6	-5.04	119.67	123.70
33	2	1777	С	N3-C4-C5	-5.04	119.88	121.90
33	2	1382	А	O4'-C1'-N9	5.04	112.23	108.20
33	2	1170	U	C6-N1-C1'	-5.04	114.15	121.20
33	2	1419	С	N3-C4-C5	-5.04	119.89	121.90
33	2	1635	А	C5-C6-N6	-5.04	119.67	123.70
33	2	1694	А	O4'-C1'-N9	5.04	112.23	108.20
33	2	107	А	C5-C6-N6	-5.03	119.67	123.70
33	2	932	G	O4'-C1'-N9	5.03	112.23	108.20
33	2	1554	С	N3-C4-C5	-5.03	119.89	121.90
39	1	54	А	O4'-C1'-N9	5.03	112.23	108.20
4	Е	221	PHE	CB-CG-CD2	-5.03	117.28	120.80
33	2	1079	А	C5-C6-N1	-5.03	115.19	117.70
33	2	1118	А	C5-C6-N1	-5.03	115.19	117.70
33	2	339	А	C5-C6-N1	-5.03	115.19	117.70
33	2	1461	А	O4'-C1'-N9	5.03	112.22	108.20
33	2	11	A	O4'-C1'-N9	5.03	112.22	108.20
33	2	547	U	O4'-C1'-N1	5.03	112.22	108.20
33	2	1026	A	O4'-C1'-N9	5.03	112.22	108.20
33	2	1593	G	O4'-C1'-N9	5.03	112.22	108.20
33	2	311	C	O4'-C1'-N1	5.03	112.22	108.20
33	2	431	С	N3-C4-N4	5.03	121.52	118.00
33	2	537	G	O4'-C1'-N9	5.03	112.22	108.20
33	2	1078	A	O4'-C1'-N9	5.03	112.22	108.20
33	2	1328	А	C5-C6-N1	-5.03	115.19	117.70
33	2	1472	A	O4'-C1'-N9	5.03	112.22	108.20
33	2	167	G	O4'-C1'-N9	5.02	112.22	108.20
33	2	1413	С	N3-C4-C5	-5.02	119.89	121.90
33	2	61	A	C5-C6-N1	-5.02	115.19	117.70
33	2	1399	C	N3-C4-C5	-5.02	119.89	121.90
33	2	1556	A	C5-C6-N1	-5.02	115.19	117.70
33	2	1123	C	N3-C4-C5	-5.02	119.89	121.90
33	2	204	G	O4'-C1'-N9	5.02	112.22	108.20
33	2	526	A	C4-C5-C6	5.02	119.51	117.00
33	2	1542	С	N3-C4-C5	-5.02	119.89	121.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	2	379	А	C5-C6-N1	-5.02	115.19	117.70
39	1	38	A	C5-C6-N1	-5.02	115.19	117.70
39	1	54	А	C5-C6-N1	-5.02	115.19	117.70
33	2	462	С	N3-C4-N4	5.01	121.51	118.00
33	2	629	С	N3-C4-C5	-5.01	119.89	121.90
33	2	1629	А	C5-C6-N6	-5.01	119.69	123.70
39	1	46	G	O4'-C1'-N9	5.01	112.21	108.20
33	2	1011	U	C2-N1-C1'	5.01	123.72	117.70
33	2	1516	С	N3-C4-C5	-5.01	119.89	121.90
10	K	143	LYS	N-CA-CB	5.01	119.62	110.60
33	2	350	А	C5-C6-N1	-5.01	115.19	117.70
33	2	546	U	O4'-C1'-N1	5.01	112.21	108.20
33	2	933	С	N3-C4-C5	-5.01	119.89	121.90
15	Р	65	PHE	CB-CG-CD2	-5.01	117.29	120.80
33	2	934	А	O4'-C1'-N9	5.01	112.21	108.20
33	2	1589	А	O4'-C1'-N9	5.01	112.21	108.20
33	2	1018	U	C2-N1-C1'	5.01	123.71	117.70
33	2	1382	А	C5-C6-N1	-5.01	115.20	117.70
33	2	846	С	N3-C4-C5	-5.01	119.90	121.90
33	2	1066	А	C5-C6-N1	-5.01	115.20	117.70
33	2	385	G	O4'-C1'-N9	5.00	112.20	108.20
33	2	1288	С	O4'-C1'-N1	5.00	112.20	108.20
33	2	1796	С	N3-C4-C5	-5.00	119.90	121.90
39	1	73	А	O4'-C1'-N9	5.00	112.20	108.20
33	2	400	G	O4'-C1'-N9	5.00	112.20	108.20
33	2	560	С	N3-C4-N4	5.00	121.50	118.00
33	2	1242	A	O4'-C1'-N9	5.00	112.20	108.20

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All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	2	1244	C4J	C4'
34	3	65	G	C3'
39	1	17	С	C2',C3'
39	1	18	G	C3'

All (113) planarity outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Group
39	1	18	G	Sidechain
39	1	48	С	Sidechain
39	1	69	U	Sidechain



Mol	Chain	Res	Type	Group
33	2	112	U	Sidechain
33	2	1125	G	Sidechain
33	2	1139	А	Sidechain
33	2	1170	U	Sidechain
33	2	1171	G	Sidechain
33	2	1192	А	Sidechain
33	2	1251	G	Sidechain
33	2	1259	U	Sidechain
33	2	1285	U	Sidechain
33	2	1288	С	Sidechain
33	2	1289	А	Sidechain
33	2	1383	G	Sidechain
33	2	1416	G	Sidechain
33	2	1423	С	Sidechain
33	2	145	G	Sidechain
33	2	1452	G	Sidechain
33	2	146	G	Sidechain
33	2	1511	G	Sidechain
33	2	1515	G	Sidechain
33	2	1545	G	Sidechain
33	2	1547	G	Sidechain
33	2	1595	G	Sidechain
33	2	1598	G	Sidechain
33	2	1599	G	Sidechain
33	2	1607	G	Sidechain
33	2	1611	U	Sidechain
33	2	167	G	Sidechain
33	2	170	А	Sidechain
33	2	1702	U	Sidechain
33	2	1783	G	Sidechain
33	2	1784	А	Sidechain
33	2	1808	G	Sidechain
33	2	188	U	Sidechain
33	2	190	A	Sidechain
33	2	196	U	Sidechain
33	2	228	A	Sidechain
33	2	318	U	Sidechain
33	2	319	G	Sidechain
33	2	321	С	Sidechain
33	2	361	A	Sidechain
33	2	39	A	Sidechain
33	2	41	G	Sidechain

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Mol	Chain	Res	Type	Group
33	2	421	G	Sidechain
33	2	435	A	Sidechain
33	2	44	U	Sidechain
33	2	452	С	Sidechain
33	2	519	A	Sidechain
33	2	525	G	Sidechain
33	2	528	U	Sidechain
33	2	574	A	Sidechain
33	2	576	G	Sidechain
33	2	581	U	Sidechain
33	2	649	G	Sidechain
33	2	652	G	Sidechain
33	2	657	U	Sidechain
33	2	66	G	Sidechain
33	2	82	G	Sidechain
33	2	869	G	Sidechain
33	2	874	G	Sidechain
33	2	877	G	Sidechain
33	2	88	G	Sidechain
33	2	903	G	Sidechain
33	2	92	А	Sidechain
33	2	955	G	Sidechain
35	А	184	LEU	Peptide
35	А	185	THR	Peptide
35	А	186	PRO	Peptide
35	А	187	GLN	Peptide
35	А	200	TYR	Sidechain
35	А	54	ARG	Mainchain
35	А	55	ARG	Sidechain
35	А	57	ARG	Peptide
36	В	133	THR	Peptide
36	В	280	PRO	Peptide
36	В	282	CYS	Peptide
36	В	284	VAL	Peptide
36	В	285	ASP	Peptide
36	В	286	ASP	Peptide
36	В	287	LEU	Peptide
36	В	288	LYS	Peptide
36	В	289	GLY	Peptide
36	В	322	LEU	Peptide
36	В	373	ALA	Peptide
2	С	193	HIS	Peptide

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Mol	Chain	Res	Type	Group
3	D	208	HIS	Peptide
5	F	107	TYR	Sidechain
5	F	167	TYR	Sidechain
8	Ι	68	LEU	Peptide
8	Ι	69	THR	Peptide
9	J	105	THR	Peptide
9	J	66	VAL	Peptide
11	L	147	PHE	Peptide
11	L	54	ARG	Sidechain
12	М	1	MET	Peptide
12	М	34	GLU	Peptide
12	М	35	LEU	Peptide
12	М	43	LEU	Peptide
12	М	82	TYR	Sidechain
17	S	42	ILE	Peptide
17	S	43	GLU	Peptide
37	U	89	ASP	Peptide
37	U	94	LYS	Peptide
37	U	99	LEU	Peptide
26	с	81	ARG	Peptide
28	е	28	HIS	Peptide
28	е	49	ASP	Peptide
29	f	90	LYS	Peptide
31	h	109	TYR	Sidechain
32	i	120	VAL	Peptide
32	i	126	LYS	Peptide

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## 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	1	240	0	289	0	0
2	С	1643	0	1646	1	0
3	D	1742	0	1815	0	0
4	Е	1743	0	1836	0	0
5	F	1765	0	1863	23	0
6	G	2083	0	2189	0	0
7	Н	1509	0	1563	8	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
8	Ι	1924	0	2086	12	0	
9	J	1530	0	1623	27	0	
10	K	1680	0	1762	1	0	
11	L	1499	0	1608	0	0	
12	М	828	0	854	0	0	
13	N	1296	0	1374	0	0	
14	0	958	0	993	0	0	
15	Р	1208	0	1294	1	0	
16	Q	1016	0	1039	0	0	
17	S	1123	0	1193	2	0	
18	Т	1020	0	1075	0	0	
19	V	1113	0	1149	5	0	
20	W	822	0	887	1	0	
21	Х	620	0	622	0	0	
22	Y	1034	0	1080	0	0	
23	Z	1107	0	1179	2	0	
24	a	1022	0	1084	0	0	
25	b	790	0	839	0	0	
26	с	659	0	683	0	0	
27	d	507	0	536	0	0	
28	е	445	0	442	0	0	
29	f	582	0	599	0	0	
30	g	2437	0	2393	0	0	
31	h	599	0	655	0	0	
32	i	473	0	524	0	0	
33	2	37202	0	18777	310	0	
34	3	774	0	390	81	0	
35	А	2147	0	2187	26	0	
36	В	3214	0	3354	0	0	
37	U	1172	0	1226	50	0	
38	R	1111	0	1166	58	0	
39	1	1614	0	824	60	0	
All	All	84251	0	66698	517	0	

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (517) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:U:147:GLY:CA	38:R:131:PRO:HG3	1.22	1.68


	juo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
37:U:147:GLY:HA3	38:R:131:PRO:CG	1.34	1.55
39:1:16:G:O3'	39:1:17:C:P	1.14	1.52
33:2:1817:A:C2'	33:2:1818:A:H5'	1.47	1.42
5:F:117:ARG:HH12	34:3:67:A:N6	1.14	1.41
35:A:183:ARG:NE	39:1:18:G:O6	1.59	1.33
8:I:230:LYS:NZ	33:2:747:G:OP2	1.57	1.33
5:F:117:ARG:NH1	34:3:67:A:N6	1.79	1.29
8:I:236:SER:O	8:I:237:LEU:HG	1.21	1.29
33:2:1817:A:O2'	33:2:1818:A:H5'	1.19	1.29
33:2:1518:C:OP1	37:U:143:GLY:HA2	1.17	1.25
33:2:1517:A:C2	38:R:128:HIS:CE1	2.26	1.24
33:2:1518:C:OP1	37:U:143:GLY:CA	1.86	1.23
33:2:1696:C:H5'	34:3:54:G:O6	1.38	1.23
5:F:117:ARG:NH2	34:3:65:G:H2'	1.50	1.23
33:2:740:G:H21	33:2:794:G:C1'	1.50	1.23
39:1:16:G:C8	39:1:17:C:C6	2.27	1.23
39:1:16:G:HO3'	39:1:17:C:P	1.07	1.22
39:1:16:G:C2'	39:1:17:C:H5"	1.71	1.21
39:1:17:C:O3'	39:1:18:G:P	1.99	1.21
8:I:230:LYS:NZ	33:2:747:G:P	2.17	1.18
39:1:16:G:C8	39:1:17:C:H6	1.61	1.18
33:2:1817:A:H2'	33:2:1818:A:H5'	1.30	1.13
9:J:108:SER:HA	33:2:740:G:O3'	1.47	1.12
9:J:108:SER:HA	33:2:740:G:C3'	1.65	1.12
33:2:740:G:N2	33:2:794:G:H1'	1.62	1.12
35:A:183:ARG:NE	39:1:18:G:C6	2.19	1.11
9:J:107:LYS:HE3	33:2:738:U:C4'	1.81	1.09
34:3:57:U:H5'	34:3:58:G:OP2	1.51	1.09
5:F:116:ARG:HE	5:F:150:MET:CE	1.65	1.09
39:1:16:G:H2'	39:1:17:C:H5"	1.28	1.08
7:H:130:ARG:CD	34:3:47:U:H4'	1.83	1.08
38:R:128:HIS:HB3	38:R:129:GLY:HA3	1.28	1.08
7:H:130:ARG:HD3	34:3:47:U:C4'	1.84	1.07
39:1:19:G:O3'	39:1:20:A:P	2.13	1.06
33:2:1817:A:C2'	33:2:1818:A:C5'	2.31	1.06
39:1:16:G:C3'	39:1:17:C:H5"	1.84	1.06
5:F:117:ARG:NH1	34:3:67:A:H61	1.42	1.03
39:1:16:G:C3'	39:1:17:C:P	2.46	1.03
9:J:106:ARG:HG3	33:2:794:G:N7	1.68	1.02
33:2:1817:A:H2'	33:2:1818:A:C5'	1.87	1.02
7:H:132:GLY:O	35:A:55:ARG:NH2	1.91	1.02



	Jus page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
37:U:147:GLY:HA2	38:R:131:PRO:HG3	1.37	1.01
33:2:742:C:C2'	33:2:743:U:H5'	1.91	1.01
9:J:107:LYS:HE3	33:2:738:U:H4'	1.38	1.01
34:3:57:U:C5'	34:3:58:G:OP2	2.08	1.01
8:I:236:SER:O	8:I:237:LEU:CG	2.09	1.00
33:2:1817:A:O2'	33:2:1818:A:C5'	2.09	1.00
37:U:143:GLY:O	37:U:144:ARG:NH1	1.93	1.00
33:2:737:C:H3'	33:2:738:U:H5"	1.42	1.00
33:2:683:G:N2	33:2:731:C:N3	2.10	1.00
33:2:1518:C:O2'	37:U:146:VAL:CG1	2.08	0.99
5:F:116:ARG:HE	5:F:150:MET:HE2	1.26	0.99
33:2:749:C:H3'	33:2:750:G:H5"	1.43	0.99
33:2:740:G:H21	33:2:794:G:H1'	0.81	0.97
33:2:684:A:C2	33:2:731:C:N3	2.32	0.97
8:I:237:LEU:HB2	33:2:784:G:H4'	1.42	0.97
9:J:107:LYS:HE2	33:2:737:C:H2'	1.46	0.97
5:F:117:ARG:HH22	34:3:65:G:H2'	1.16	0.97
34:3:51:C:H4'	39:1:37:T6A:ODB	1.64	0.97
23:Z:61:GLN:HG3	33:2:1818:A:OP1	1.64	0.96
33:2:1518:C:O2'	37:U:146:VAL:HG13	1.64	0.96
35:A:183:ARG:CZ	39:1:18:G:H1	1.80	0.95
33:2:740:G:N2	33:2:794:G:C1'	2.21	0.95
39:1:16:G:H8	39:1:17:C:H6	1.04	0.94
37:U:147:GLY:HA3	38:R:131:PRO:CB	1.96	0.94
33:2:745:U:H2'	33:2:746:C:C6	2.01	0.94
34:3:42:G:H2'	34:3:43:G:N7	1.83	0.94
35:A:183:ARG:CZ	39:1:18:G:O6	2.16	0.94
33:2:1818:A:O2'	33:2:1819:A:H5"	1.67	0.93
33:2:680:G:H1	33:2:734:C:H42	1.00	0.93
33:2:742:C:O2'	33:2:743:U:H5'	1.68	0.93
33:2:738:U:O2'	33:2:740:G:OP2	1.86	0.93
39:1:16:G:C8	39:1:17:C:C5	2.56	0.92
33:2:742:C:H2'	33:2:743:U:H5'	1.49	0.92
39:1:16:G:H2'	39:1:17:C:C5'	1.98	0.92
33:2:683:G:H1	33:2:731:C:H42	1.18	0.92
9:J:107:LYS:CE	33:2:738:U:C4'	2.38	0.91
9:J:106:ARG:CG	33:2:794:G:N7	2.23	0.91
5:F:117:ARG:HH22	34:3:65:G:C2'	1.82	0.91
33:2:733:G:N7	33:2:738:U:O4	2.04	0.90
33:2:1696:C:C5'	34:3:54:G:O6	2.19	0.90
33:2:680:G:H1	33:2:734:C:N4	1.68	0.90



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
39:1:16:G:H8	39:1:17:C:C6	1.75	0.90
38:R:136:THR:O	38:R:138:SER:N	2.05	0.90
39:1:16:G:O3'	39:1:17:C:OP2	1.90	0.90
33:2:734:C:H2'	33:2:735:C:H5"	1.53	0.90
33:2:787:C:H2'	33:2:788:C:C6	2.06	0.89
33:2:739:U:O2'	33:2:740:G:OP1	1.88	0.89
35:A:183:ARG:CZ	39:1:18:G:N1	2.36	0.89
8:I:235:SER:O	8:I:237:LEU:N	2.07	0.88
33:2:949:C:C3'	33:2:950:U:P	2.62	0.88
9:J:107:LYS:HD2	33:2:740:G:P	2.13	0.88
33:2:751:C:O2'	33:2:752:C:H5'	1.74	0.87
35:A:183:ARG:CZ	39:1:18:G:C6	2.57	0.87
5:F:117:ARG:NH1	34:3:67:A:H62	1.69	0.87
33:2:746:C:H2'	33:2:747:G:C8	2.10	0.87
7:H:130:ARG:HD3	34:3:47:U:H4'	0.92	0.87
8:I:230:LYS:HZ2	33:2:747:G:P	1.91	0.87
33:2:742:C:O2'	33:2:743:U:C5'	2.23	0.87
33:2:685:G:N2	33:2:730:C:N3	2.22	0.87
37:U:147:GLY:CA	38:R:131:PRO:CG	2.13	0.85
33:2:740:G:N1	33:2:793:C:C2	2.44	0.85
33:2:684:A:H2'	33:2:685:G:C8	2.12	0.85
33:2:732:C:H2'	33:2:733:G:O4'	1.76	0.85
33:2:1244:C4J:C3	33:2:1244:C4J:O36	2.23	0.84
33:2:740:G:N1	33:2:793:C:O2	2.09	0.84
33:2:731:C:H2'	33:2:732:C:H5"	1.57	0.84
9:J:107:LYS:HG2	33:2:737:C:O2'	1.77	0.83
37:U:91:LYS:HA	38:R:18:ARG:H	1.42	0.82
39:1:16:G:H2'	39:1:17:C:O4'	1.80	0.81
39:1:11:G:H1	39:1:25:U:H3	1.27	0.81
39:1:16:G:C2'	39:1:17:C:C5'	2.56	0.81
9:J:108:SER:CA	33:2:740:G:C3'	2.54	0.81
37:U:147:GLY:HA3	38:R:131:PRO:CD	2.11	0.81
33:2:1518:C:OP1	37:U:143:GLY:N	2.12	0.80
33:2:1518:C:O2'	37:U:146:VAL:HG11	1.81	0.80
33:2:1518:C:C5'	33:2:1518:C:H6	1.95	0.80
33:2:1518:C:H6	33:2:1518:C:H5"	1.47	0.79
33:2:743:U:H1'	33:2:744:C:C1'	2.12	0.79
33:2:1264:C:C4'	38:R:100:LYS:HE3	2.13	0.79
5:F:116:ARG:NE	5:F:150:MET:HE2	1.98	0.79
33:2:743:U:O2'	33:2:744:C:O4'	2.00	0.79
39:1:17:C:H2'	39:1:18:G:H5'	1.63	0.79



	las puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
33:2:748:G:O2'	33:2:749:C:O5'	2.01	0.79
34:3:51:C:C4'	39:1:37:T6A:ODB	2.30	0.79
33:2:1510:G:C3'	33:2:1510:G:C5'	2.61	0.78
38:R:128:HIS:HB3	38:R:129:GLY:CA	2.13	0.78
33:2:734:C:C2'	33:2:735:C:H5"	2.13	0.78
33:2:1517:A:H2	38:R:128:HIS:CE1	2.01	0.78
39:1:18:G:O4'	39:1:61:C:H5'	1.84	0.78
5:F:117:ARG:HH21	34:3:65:G:H2'	1.45	0.77
39:1:16:G:O3'	39:1:17:C:O5'	2.01	0.77
34:3:47:U:P	34:3:47:U:H6	2.07	0.77
33:2:743:U:O4	33:2:791:A:N1	2.18	0.77
23:Z:61:GLN:CG	33:2:1818:A:OP1	2.33	0.76
5:F:116:ARG:HE	5:F:150:MET:HE1	1.48	0.76
33:2:749:C:H2'	33:2:750:G:O4'	1.86	0.76
33:2:1696:C:C4'	34:3:54:G:C6	2.68	0.76
9:J:106:ARG:N	33:2:794:G:N7	2.34	0.75
35:A:183:ARG:CD	39:1:18:G:C6	2.69	0.75
5:F:116:ARG:NE	5:F:150:MET:CE	2.48	0.75
34:3:59:G:H5"	34:3:59:G:N3	2.02	0.74
35:A:183:ARG:NH2	39:1:18:G:H1	1.84	0.74
33:2:1817:A:C8	33:2:1817:A:OP2	2.41	0.74
35:A:107:THR:HG22	39:1:18:G:C6	2.23	0.74
37:U:147:GLY:HA3	38:R:131:PRO:HG3	0.76	0.74
33:2:1232:G:H5'	38:R:134:GLY:O	1.88	0.74
33:2:797:U:H2'	33:2:798:A:O4'	1.88	0.73
33:2:748:G:C2	33:2:749:C:C2	2.77	0.73
34:3:42:G:H2'	34:3:43:G:C8	2.23	0.73
8:I:236:SER:C	8:I:237:LEU:HG	2.09	0.72
33:2:684:A:C2	33:2:731:C:C4	2.78	0.72
33:2:749:C:C3'	33:2:750:G:H5"	2.18	0.72
33:2:683:G:H1	33:2:731:C:N4	1.87	0.72
9:J:107:LYS:HA	33:2:740:G:O5'	1.89	0.71
34:3:58:G:O2'	34:3:59:G:O5'	2.06	0.71
9:J:107:LYS:CE	33:2:737:C:H2'	2.18	0.71
33:2:68:A:H61	33:2:81:U:H3	1.38	0.71
33:2:733:G:C5	33:2:738:U:O4	2.44	0.71
33:2:748:G:N2	33:2:749:C:O2	2.23	0.71
34:3:56:C:H1'	34:3:57:U:OP1	1.89	0.71
33:2:683:G:H2'	33:2:684:A:C8	2.24	0.71
9:J:107:LYS:CG	33:2:737:C:O2'	2.37	0.71
33:2:745:U:H2'	33:2:746:C:C5	2.25	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
39:1:19:G:O3'	39:1:20:A:OP1	2.08	0.70
39:1:18:G:O4'	39:1:61:C:C5'	2.39	0.70
33:2:740:G:N2	33:2:794:G:O4'	2.23	0.70
34:3:51:C:H1'	39:1:37:T6A:O14	1.92	0.70
33:2:1236:A:N1	38:R:99:GLY:HA3	2.06	0.69
33:2:737:C:C3'	33:2:738:U:H5"	2.22	0.69
37:U:143:GLY:C	37:U:144:ARG:HG3	2.13	0.68
33:2:793:C:O2'	33:2:794:G:H4'	1.93	0.68
34:3:49:A:H2'	34:3:50:C:H5'	1.75	0.68
5:F:117:ARG:HH12	34:3:67:A:H61	0.68	0.68
39:1:16:G:C3'	39:1:17:C:C5'	2.70	0.68
33:2:685:G:N2	33:2:730:C:C2	2.62	0.68
33:2:795:U:OP2	33:2:795:U:H4'	1.93	0.68
34:3:59:G:N3	34:3:59:G:H3'	2.08	0.67
5:F:117:ARG:NH2	34:3:65:G:C2'	2.39	0.67
33:2:740:G:O6	33:2:793:C:N3	2.27	0.67
37:U:147:GLY:C	38:R:131:PRO:HG3	2.09	0.67
35:A:179:ASN:OD1	35:A:183:ARG:NH2	2.28	0.67
33:2:526:A:H62	33:2:537:G:H21	1.42	0.66
34:3:55:U:H5	34:3:56:C:C5	2.13	0.66
39:1:16:G:O3'	39:1:17:C:C5'	2.43	0.66
8:I:237:LEU:HB2	33:2:784:G:C4'	2.20	0.66
33:2:1608:G:H5"	38:R:42:ARG:HH22	1.60	0.66
33:2:1859:C:H4'	33:2:1860:A:OP2	1.95	0.66
33:2:1510:G:C5'	33:2:1510:G:O4'	2.44	0.66
9:J:109:ARG:HB2	33:2:740:G:H2'	1.77	0.65
33:2:1232:G:H4'	38:R:135:ALA:HB2	1.79	0.65
33:2:739:U:H4'	33:2:740:G:OP2	1.96	0.65
33:2:785:G:N2	33:2:786:C:O2	2.30	0.65
33:2:1232:G:C4'	38:R:135:ALA:HB2	2.27	0.64
33:2:743:U:H1'	33:2:744:C:H1'	1.78	0.64
33:2:1518:C:P	37:U:143:GLY:HA2	2.35	0.64
33:2:1696:C:O4'	34:3:54:G:C6	2.50	0.64
33:2:683:G:C6	33:2:684:A:C6	2.86	0.64
33:2:1518:C:H5"	33:2:1518:C:C6	2.31	0.64
34:3:46:A:O5'	34:3:46:A:H8	1.81	0.64
37:U:91:LYS:H	38:R:18:ARG:HG2	1.62	0.64
8:I:235:SER:C	8:I:237:LEU:H	2.02	0.63
39:1:16:G:C2'	39:1:17:C:O4'	2.44	0.63
19:V:38:LYS:CG	37:U:39:ARG:NH1	2.61	0.63
38:R:129:GLY:O	38:R:130:ARG:HB2	1.99	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
33:2:743:U:H1'	33:2:744:C:O4'	1.99	0.63
33:2:784:G:H2'	33:2:785:G:H5'	1.79	0.63
33:2:790:A:O5'	33:2:790:A:H8	1.81	0.63
39:1:16:G:H2'	39:1:17:C:C4'	2.28	0.63
33:2:740:G:C6	33:2:793:C:N3	2.67	0.62
9:J:106:ARG:CA	33:2:794:G:N7	2.46	0.62
33:2:685:G:H1	33:2:730:C:H42	1.47	0.62
33:2:688:U:H6	33:2:688:U:O5'	1.83	0.62
33:2:740:G:C2	33:2:793:C:O2	2.52	0.62
37:U:91:LYS:HG2	38:R:17:TYR:HA	1.82	0.62
33:2:746:C:H2'	33:2:747:G:N7	2.14	0.62
7:H:130:ARG:HH11	34:3:47:U:H5'	1.64	0.62
19:V:38:LYS:HG2	37:U:39:ARG:NH1	2.15	0.62
38:R:133:ILE:O	38:R:133:ILE:HG22	2.01	0.61
33:2:745:U:O2'	33:2:746:C:O4'	2.18	0.61
33:2:1696:C:H4'	34:3:54:G:C5	2.35	0.61
33:2:682:G:C2	33:2:683:G:N7	2.69	0.61
33:2:733:G:N7	33:2:738:U:C4	2.69	0.61
33:2:751:C:H2'	33:2:752:C:C6	2.35	0.61
33:2:1618:A:C5'	37:U:133:GLY:HA3	2.30	0.61
39:1:19:G:N1	39:1:56:C:N3	2.49	0.61
33:2:734:C:C3'	33:2:735:C:H5"	2.31	0.61
33:2:790:A:C6	33:2:791:A:N6	2.69	0.61
33:2:1618:A:H5"	37:U:133:GLY:CA	2.31	0.60
33:2:793:C:C2'	33:2:794:G:H4'	2.31	0.60
34:3:56:C:H1'	34:3:57:U:P	2.41	0.60
33:2:744:C:C4	33:2:745:U:O4	2.55	0.60
5:F:117:ARG:NH2	34:3:65:G:C8	2.70	0.60
19:V:45:LEU:HD11	37:U:38:ARG:NH2	2.17	0.59
35:A:107:THR:HG22	39:1:18:G:O6	2.01	0.59
33:2:686:G:O5'	33:2:686:G:H8	1.84	0.59
33:2:790:A:H2'	33:2:791:A:C8	2.37	0.59
33:2:682:G:C2	33:2:683:G:C5	2.91	0.59
33:2:743:U:C6	33:2:744:C:C2	2.91	0.59
33:2:1264:C:H4'	38:R:100:LYS:HE3	1.85	0.59
38:R:128:HIS:CB	38:R:129:GLY:HA3	2.15	0.58
33:2:683:G:N1	33:2:684:A:C6	2.71	0.58
33:2:682:G:H2'	33:2:683:G:H8	1.68	0.58
33:2:743:U:HO2'	33:2:744:C:C1'	2.16	0.58
33:2:784:G:C5	33:2:785:G:N7	2.71	0.58
33:2:1517:A:C2	38:R:128:HIS:NE2	2.71	0.58



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
33:2:793:C:H4'	33:2:793:C:OP1	2.03	0.58
33:2:743:U:H3	33:2:791:A:H2	1.51	0.58
9:J:107:LYS:HD2	33:2:740:G:O5'	2.03	0.57
33:2:683:G:O2'	33:2:684:A:H5'	2.04	0.57
33:2:784:G:C2'	33:2:785:G:H5'	2.33	0.57
38:R:135:ALA:O	38:R:136:THR:HB	2.04	0.57
33:2:1170:U:H2'	33:2:1171:G:C8	2.38	0.57
33:2:746:C:C2'	33:2:747:G:C8	2.86	0.57
33:2:787:C:H2'	33:2:788:C:C5	2.38	0.57
33:2:750:G:C6	33:2:751:C:N4	2.73	0.57
33:2:683:G:C6	33:2:684:A:N6	2.73	0.57
34:3:49:A:H2	34:3:49:A:OP1	1.88	0.57
19:V:38:LYS:HG3	37:U:39:ARG:NH1	2.20	0.57
33:2:740:G:H2'	33:2:741:C:H5"	1.87	0.57
35:A:64:ARG:HE	35:A:67:ARG:HG3	1.70	0.56
37:U:147:GLY:HA3	38:R:131:PRO:HB3	1.85	0.56
33:2:1244:C4J:O2	33:2:1244:C4J:C31	2.53	0.56
35:A:183:ARG:NH2	39:1:18:G:N1	2.51	0.56
33:2:1618:A:H5"	37:U:133:GLY:N	2.20	0.56
9:J:107:LYS:CA	33:2:740:G:O5'	2.54	0.56
33:2:745:U:C2	33:2:746:C:C4	2.94	0.56
33:2:1817:A:HO2'	33:2:1818:A:H5'	1.60	0.56
33:2:1618:A:H5"	37:U:133:GLY:HA3	1.87	0.56
33:2:734:C:C5	33:2:737:C:N4	2.73	0.56
34:3:56:C:C1'	34:3:57:U:P	2.94	0.56
34:3:54:G:O2'	34:3:55:U:OP1	2.18	0.55
33:2:848:G:H3'	33:2:849:C:H5"	1.88	0.55
34:3:54:G:O5'	34:3:54:G:H8	1.89	0.55
7:H:131:ALA:O	34:3:49:A:OP2	2.23	0.55
33:2:1862:U:O2	33:2:1862:U:H2'	2.06	0.55
33:2:681:U:H2'	33:2:681:U:O2	2.07	0.55
34:3:51:C:H1'	39:1:37:T6A:HO4	1.70	0.55
34:3:49:A:H2'	34:3:50:C:C5'	2.36	0.55
34:3:49:A:C5'	34:3:49:A:N3	2.70	0.55
39:1:18:G:C1'	39:1:61:C:H5'	2.36	0.55
9:J:75:ILE:HG23	9:J:76:GLN:H	1.72	0.55
33:2:687:G:H2'	33:2:688:U:H5'	1.89	0.55
33:2:739:U:O2	33:2:739:U:H2'	2.06	0.55
33:2:1232:G:C2	33:2:1518:C:N4	2.75	0.55
33:2:1696:C:H4'	34:3:54:G:C6	2.40	0.55
33:2:787:C:N3	33:2:788:C:N4	2.55	0.54



	juo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
35:A:64:ARG:HD3	35:A:64:ARG:N	2.23	0.54
33:2:684:A:O5'	33:2:684:A:H8	1.91	0.54
33:2:1330:G:H22	33:2:1492:U:H3	1.55	0.54
33:2:1518:C:C5'	33:2:1518:C:C6	2.85	0.54
9:J:108:SER:CA	33:2:740:G:O3'	2.38	0.54
35:A:64:ARG:HD3	35:A:64:ARG:H	1.73	0.54
34:3:42:G:H2'	34:3:43:G:C5	2.41	0.54
37:U:88:LYS:CG	38:R:37:TYR:CD2	2.91	0.54
33:2:786:C:H6	33:2:786:C:O5'	1.91	0.54
33:2:683:G:N2	33:2:731:C:C2	2.66	0.53
10:K:142:SER:H	10:K:143:LYS:HB2	1.73	0.53
5:F:117:ARG:CZ	34:3:67:A:H62	2.22	0.53
33:2:1407:G:H3'	33:2:1408:C:H5"	1.90	0.53
5:F:5:ILE:HD13	5:F:5:ILE:H	1.73	0.53
33:2:1518:C:C1'	37:U:146:VAL:HG13	2.38	0.53
37:U:91:LYS:HZ3	38:R:17:TYR:HD1	1.52	0.53
33:2:1294:G:P	38:R:77:LYS:HE2	2.49	0.53
33:2:682:G:N3	33:2:683:G:C8	2.76	0.53
33:2:744:C:C5	33:2:745:U:O4	2.62	0.53
34:3:54:G:H4'	34:3:55:U:OP1	2.07	0.53
33:2:687:G:C5	33:2:729:C:N4	2.77	0.53
33:2:685:G:H1	33:2:730:C:N4	2.06	0.52
34:3:50:C:H2'	34:3:51:C:H5'	1.92	0.52
5:F:117:ARG:CZ	34:3:67:A:N6	2.67	0.52
5:F:99:ILE:HD12	5:F:99:ILE:H	1.74	0.52
33:2:683:G:C2	33:2:684:A:C4	2.97	0.52
33:2:682:G:O5'	33:2:682:G:H8	1.92	0.52
34:3:54:G:O2'	34:3:55:U:H5"	2.09	0.52
33:2:745:U:H3'	33:2:745:U:H6	1.75	0.52
33:2:794:G:O2'	33:2:795:U:OP1	2.20	0.52
9:J:100:ILE:CD1	33:2:736:C:O2	2.58	0.51
33:2:734:C:C3'	33:2:735:C:C5'	2.88	0.51
33:2:747:G:O5'	33:2:747:G:H8	1.91	0.51
33:2:1294:G:OP1	38:R:77:LYS:HE2	2.10	0.51
7:H:130:ARG:HD3	34:3:47:U:C5'	2.40	0.51
34:3:51:C:O2'	39:1:37:T6A:ODB	2.14	0.51
39:1:16:G:C8	39:1:17:C:H5	2.26	0.51
20:W:20:ILE:HG21	20:W:98:VAL:HG21	1.93	0.51
33:2:687:G:C6	33:2:729:C:N4	2.78	0.51
33:2:790:A:C5	33:2:791:A:N6	2.78	0.51
33:2:1817:A:H2'	33:2:1818:A:O5'	2.10	0.51



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:64:ARG:N	35:A:64:ARG:CD	2.74	0.51
33:2:682:G:C4	33:2:683:G:N7	2.79	0.51
34:3:57:U:C4'	34:3:58:G:OP2	2.59	0.51
34:3:59:G:N3	34:3:59:G:C3'	2.73	0.51
33:2:687:G:C2'	33:2:688:U:H5'	2.41	0.51
33:2:749:C:H3'	33:2:750:G:C5'	2.29	0.51
34:3:50:C:C2'	34:3:51:C:H5'	2.41	0.50
33:2:787:C:O5'	33:2:787:C:H6	1.94	0.50
34:3:55:U:C5	34:3:56:C:C5	2.98	0.50
19:V:38:LYS:HG2	37:U:39:ARG:CZ	2.42	0.50
34:3:46:A:O3'	34:3:47:U:H6	1.95	0.50
33:2:1264:C:O2'	38:R:100:LYS:HG3	2.12	0.50
34:3:55:U:H3'	34:3:56:C:H5"	1.94	0.50
34:3:58:G:HO2'	34:3:59:G:C5'	2.22	0.50
39:1:19:G:C3'	39:1:20:A:OP1	2.59	0.50
7:H:131:ALA:C	34:3:49:A:OP2	2.50	0.50
39:1:16:G:C3'	39:1:17:C:OP2	2.53	0.50
33:2:679:U:H2'	33:2:680:G:C8	2.47	0.49
33:2:683:G:C2	33:2:684:A:C5	3.00	0.49
33:2:745:U:N3	33:2:746:C:N4	2.60	0.49
33:2:741:C:N3	33:2:792:G:O6	2.46	0.49
33:2:743:U:O4	33:2:791:A:C2	2.65	0.49
34:3:47:U:P	34:3:47:U:C6	2.97	0.49
39:1:16:G:O2'	39:1:17:C:O4'	2.28	0.49
8:I:236:SER:O	8:I:237:LEU:CB	2.60	0.49
33:2:225:C:H3'	33:2:226:A:C5'	2.42	0.49
33:2:740:G:C3'	33:2:741:C:H5"	2.43	0.49
34:3:49:A:OP1	34:3:49:A:C2	2.66	0.49
33:2:740:G:H3'	33:2:741:C:H5"	1.95	0.48
34:3:49:A:N3	34:3:49:A:O5'	2.46	0.48
34:3:58:G:N3	34:3:58:G:H2'	2.28	0.48
33:2:784:G:C6	33:2:785:G:C5	3.01	0.48
33:2:1264:C:O4'	38:R:100:LYS:HE3	2.13	0.48
33:2:745:U:C2	33:2:746:C:N4	2.81	0.48
39:1:19:G:N2	39:1:56:C:C2	2.81	0.48
33:2:1264:C:H4'	38:R:100:LYS:HG2	1.96	0.47
33:2:1517:A:C2	38:R:128:HIS:HE1	2.16	0.47
5:F:116:ARG:NE	5:F:150:MET:HE1	2.18	0.47
33:2:743:U:O2'	33:2:744:C:O5'	2.32	0.47
33:2:1264:C:O4'	38:R:100:LYS:NZ	2.46	0.47
33:2:1294:G:OP2	38:R:77:LYS:NZ	2.46	0.47



	Jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
33:2:1105:C:H3'	33:2:1106:G:H5"	1.97	0.47
33:2:742:C:O2'	33:2:743:U:H5"	2.09	0.47
33:2:1244:C4J:C4	39:1:34:C:H5'	2.44	0.47
35:A:179:ASN:HB3	35:A:183:ARG:NH1	2.30	0.47
37:U:146:VAL:HG12	37:U:147:GLY:H	1.79	0.47
33:2:784:G:H8	33:2:784:G:P	2.38	0.47
33:2:784:G:C4	33:2:785:G:C8	3.02	0.47
33:2:1860:A:O2'	33:2:1861:U:H5'	2.15	0.47
35:A:182:ARG:HB3	39:1:53:G:H21	1.80	0.47
37:U:147:GLY:CA	38:R:131:PRO:CB	2.76	0.47
33:2:741:C:H3'	33:2:741:C:H6	1.80	0.47
34:3:43:G:H2'	34:3:44:U:C5	2.50	0.47
33:2:684:A:H2'	33:2:685:G:H8	1.73	0.47
33:2:731:C:C2'	33:2:732:C:H5"	2.37	0.47
33:2:749:C:C3'	33:2:750:G:C5'	2.89	0.47
33:2:682:G:C2	33:2:683:G:C8	3.03	0.46
33:2:742:C:H3'	33:2:742:C:H6	1.80	0.46
33:2:793:C:H2'	33:2:794:G:H4'	1.97	0.46
33:2:685:G:H8	33:2:685:G:O5'	1.98	0.46
34:3:55:U:C5	34:3:56:C:C6	3.03	0.46
39:1:16:G:H3'	39:1:17:C:OP2	2.15	0.46
33:2:676:U:O2	33:2:913:U:C2	2.68	0.46
33:2:745:U:C2'	33:2:746:C:C6	2.89	0.46
39:1:19:G:H3'	39:1:20:A:OP1	2.15	0.46
33:2:1547:G:OP2	33:2:1547:G:C8	2.68	0.46
34:3:55:U:H3'	34:3:56:C:C5'	2.45	0.46
35:A:55:ARG:HD3	35:A:55:ARG:HA	1.64	0.46
33:2:748:G:N2	33:2:749:C:C2	2.84	0.46
33:2:1517:A:N3	38:R:128:HIS:NE2	2.64	0.46
39:1:17:C:H2'	39:1:18:G:C5'	2.41	0.46
17:S:145:TYR:O	17:S:146:ARG:HB3	2.16	0.46
33:2:741:C:H2'	33:2:742:C:O4'	2.15	0.46
33:2:751:C:C2'	33:2:752:C:H5'	2.44	0.46
33:2:1518:C:C2'	37:U:146:VAL:HG13	2.44	0.46
33:2:679:U:H3'	33:2:679:U:H6	1.81	0.46
33:2:1517:A:N3	38:R:128:HIS:CE1	2.78	0.46
33:2:1236:A:C4	38:R:100:LYS:HE2	2.16	0.45
33:2:1294:G:C5'	38:R:77:LYS:HB2	$2.\overline{47}$	0.45
35:A:183:ARG:NH1	39:1:18:G:O6	2.49	0.45
37:U:91:LYS:HA	38:R:18:ARG:N	2.22	0.45
33:2:785:G:C2	33:2:786:C:C2	3.04	0.45



	Jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
33:2:684:A:H2	33:2:731:C:N3	2.09	0.45
33:2:740:G:C2'	33:2:741:C:H5"	2.46	0.45
33:2:1518:C:H1'	37:U:146:VAL:HG13	1.99	0.45
37:U:139:THR:HG22	37:U:140:GLY:N	2.30	0.45
38:R:84:ILE:HD12	38:R:84:ILE:H	1.81	0.45
38:R:136:THR:O	38:R:136:THR:HG23	2.16	0.45
34:3:45:C:H3'	34:3:45:C:O2	2.17	0.45
5:F:198:ILE:HD12	5:F:198:ILE:H	1.82	0.44
17:S:39:LEU:H	17:S:39:LEU:HD23	1.81	0.44
33:2:743:U:OP2	33:2:743:U:H2'	2.17	0.44
33:2:743:U:C5	33:2:744:C:N3	2.85	0.44
35:A:24:VAL:HA	35:A:34:VAL:HG12	1.98	0.44
37:U:143:GLY:C	37:U:144:ARG:CG	2.85	0.44
8:I:237:LEU:OXT	33:2:784:G:O3'	2.35	0.44
33:2:684:A:C6	33:2:685:G:O6	2.70	0.44
33:2:1407:G:H3'	33:2:1408:C:C5'	2.46	0.44
33:2:1429:C:C5	33:2:1430:C:C5	3.06	0.44
33:2:792:G:H8	33:2:792:G:P	2.40	0.44
33:2:1236:A:H1'	38:R:100:LYS:HE2	1.99	0.44
35:A:57:ARG:O	35:A:57:ARG:HG2	2.17	0.44
34:3:58:G:HO2'	34:3:59:G:P	2.36	0.44
35:A:64:ARG:NE	35:A:67:ARG:HG3	2.30	0.44
39:1:17:C:H2'	39:1:18:G:P	2.58	0.44
33:2:784:G:C5	33:2:785:G:C5	3.04	0.44
33:2:682:G:H2'	33:2:683:G:C8	2.52	0.44
33:2:735:C:H3'	33:2:736:C:H5"	2.00	0.44
33:2:737:C:H3'	33:2:738:U:C5'	2.30	0.44
33:2:787:C:O5'	33:2:787:C:C6	2.70	0.44
34:3:47:U:C6	34:3:47:U:OP2	2.70	0.44
37:U:88:LYS:HG3	38:R:37:TYR:CD2	2.52	0.44
33:2:1518:C:C6	33:2:1518:C:C4'	3.01	0.43
33:2:682:G:N3	33:2:683:G:N7	2.66	0.43
33:2:745:U:C2	33:2:746:C:N3	2.86	0.43
33:2:785:G:C2	33:2:786:C:O2	2.70	0.43
33:2:1232:G:O4'	38:R:135:ALA:HB2	2.18	0.43
9:J:107:LYS:HG3	33:2:737:C:O2'	2.17	0.43
33:2:201:G:H3'	33:2:202:U:H5"	2.00	0.43
33:2:683:G:H2'	33:2:684:A:H8	1.78	0.43
33:2:1818:A:HO2'	33:2:1819:A:H5"	1.77	0.43
37:U:147:GLY:C	38:R:131:PRO:CG	2.77	0.43
9:J:100:ILE:HG13	33:2:736:C:O2	2.18	0.43



	Jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
33:2:746:C:H5"	33:2:747:G:OP2	2.19	0.43
35:A:183:ARG:HD2	39:1:18:G:C6	2.49	0.43
38:R:128:HIS:CB	38:R:129:GLY:CA	2.85	0.43
9:J:100:ILE:HD12	33:2:736:C:O2	2.19	0.43
15:P:26:LEU:H	15:P:26:LEU:HD12	1.83	0.43
33:2:790:A:H8	33:2:790:A:P	2.42	0.43
33:2:734:C:H5	33:2:737:C:N4	2.17	0.43
34:3:46:A:O3'	34:3:47:U:C6	2.70	0.43
33:2:682:G:N1	33:2:683:G:C5	2.87	0.43
33:2:684:A:H2'	33:2:685:G:N7	2.32	0.43
33:2:734:C:H3'	33:2:735:C:C5'	2.49	0.43
33:2:790:A:N6	33:2:791:A:N6	2.67	0.43
34:3:59:G:N3	34:3:59:G:C5'	2.78	0.43
33:2:1172:G:C6	33:2:1173:U:C4	3.07	0.42
9:J:109:ARG:N	33:2:741:C:OP1	2.52	0.42
33:2:737:C:H5'	33:2:738:U:OP2	2.19	0.42
33:2:791:A:C8	33:2:791:A:O5'	2.72	0.42
34:3:47:U:O2'	34:3:48:A:P	2.77	0.42
39:1:16:G:C2'	39:1:17:C:C4'	2.93	0.42
33:2:786:C:O5'	33:2:786:C:C6	2.71	0.42
37:U:141:ARG:HD2	37:U:141:ARG:HA	1.78	0.42
33:2:791:A:O5'	33:2:791:A:H8	2.03	0.42
33:2:1618:A:C5'	37:U:133:GLY:H	2.33	0.42
33:2:1828:A:H2	33:2:1831:G:H1	1.66	0.42
34:3:57:U:H3'	34:3:57:U:O2	2.20	0.42
33:2:1276:G:H1	33:2:1313:U:H3	1.66	0.42
33:2:1408:C:H2'	33:2:1409:G:C8	2.54	0.42
37:U:90:VAL:HG13	38:R:18:ARG:HH11	1.85	0.42
33:2:519:A:N6	33:2:545:A:H61	2.17	0.41
33:2:737:C:C3'	33:2:738:U:C5'	2.97	0.41
33:2:1264:C:C5'	38:R:100:LYS:HE3	2.49	0.41
34:3:46:A:C3'	34:3:47:U:C6	3.03	0.41
33:2:1696:C:C5'	34:3:54:G:C6	2.94	0.41
34:3:44:U:O2'	34:3:45:C:OP2	2.34	0.41
37:U:146:VAL:HG12	37:U:147:GLY:N	2.35	0.41
33:2:745:U:C4	33:2:746:C:N4	2.88	0.41
35:A:56:ILE:O	35:A:58:SER:N	2.52	0.41
2:C:5:LEU:HD22	2:C:5:LEU:H	1.85	0.41
37:U:90:VAL:HG22	38:R:18:ARG:HD3	2.01	0.41
37:U:91:LYS:NZ	38:R:17:TYR:HD1	2.19	0.41
33:2:741:C:C6	33:2:741:C:C3'	3.03	0.41



	P "J official and the second s	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
33:2:790:A:H2'	33:2:791:A:H8	1.83	0.41	
9:J:107:LYS:HD2	33:2:740:G:OP2	2.20	0.41	
37:U:116:LYS:HG2	38:R:110:GLU:OE2	2.20	0.41	
39:1:18:G:H1'	39:1:61:C:H5'	2.01	0.41	
33:2:686:G:O5'	33:2:686:G:C8	2.70	0.41	
33:2:746:C:C3'	33:2:747:G:C8	3.03	0.41	
33:2:924:G:H1	33:2:1009:U:H3	1.67	0.41	
33:2:546:U:H3'	33:2:547:U:H5"	2.03	0.41	
33:2:552:U:H2'	33:2:553:G:C8	2.56	0.41	
33:2:742:C:C3'	33:2:742:C:C6	3.04	0.41	
33:2:874:G:H22	33:2:904:A:H2	1.68	0.41	
34:3:51:C:C2'	34:3:52:A:OP2	2.68	0.41	
33:2:124:U:H3	33:2:330:C:H42	1.68	0.41	
33:2:734:C:H41	33:2:737:C:N4	2.19	0.41	
33:2:745:U:C3'	33:2:745:U:C6	3.03	0.41	
33:2:1264:C:O4'	38:R:100:LYS:CE	2.68	0.41	
33:2:1618:A:H5"	37:U:133:GLY:H	1.84	0.41	
34:3:43:G:O2'	34:3:44:U:C6	2.70	0.41	
33:2:987:G:C6	33:2:1130:G:H4'	2.56	0.40	
33:2:516:A:N6	33:2:578:G:H22	2.20	0.40	
33:2:744:C:OP1	33:2:744:C:H4'	2.21	0.40	
34:3:42:G:C2'	34:3:43:G:C5	3.04	0.40	
5:F:70:THR:HG22	5:F:86:LEU:HD13	2.03	0.40	
33:2:745:U:H3'	33:2:745:U:C6	2.56	0.40	

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	Percer	ntiles
1	1	23/25~(92%)	23~(100%)	0	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	С	206/208~(99%)	176 (85%)	21 (10%)	9~(4%)	2	20
3	D	213/215~(99%)	185 (87%)	19 (9%)	9~(4%)	3	22
4	Ε	224/226~(99%)	203~(91%)	16 (7%)	5(2%)	6	35
5	F	225/227~(99%)	205 (91%)	13~(6%)	7~(3%)	4	28
6	G	261/263~(99%)	229~(88%)	26 (10%)	6(2%)	6	34
7	Н	189/191~(99%)	165 (87%)	16 (8%)	8 (4%)	3	22
8	Ι	233/237~(98%)	206 (88%)	20 (9%)	7 (3%)	4	28
9	J	188/190~(99%)	162 (86%)	18 (10%)	8 (4%)	2	21
10	К	204/206~(99%)	180 (88%)	18 (9%)	6 (3%)	4	29
11	L	180/182~(99%)	167 (93%)	6 (3%)	7~(4%)	3	23
12	М	96/98~(98%)	78 (81%)	12 (12%)	6~(6%)	1	13
13	Ν	156/158~(99%)	130 (83%)	19 (12%)	7~(4%)	2	20
14	Ο	122/124~(98%)	103 (84%)	15 (12%)	4 (3%)	4	27
15	Р	148/150~(99%)	143 (97%)	5 (3%)	0	100	100
16	Q	134/136~(98%)	116 (87%)	11 (8%)	7~(5%)	2	16
17	S	139/141~(99%)	123 (88%)	12 (9%)	4(3%)	4	29
18	Т	124/126~(98%)	114 (92%)	8 (6%)	2(2%)	9	41
19	V	139/141~(99%)	124 (89%)	10 (7%)	5(4%)	3	25
20	W	102/104~(98%)	95~(93%)	4 (4%)	3~(3%)	4	29
21	Х	80/82~(98%)	66 (82%)	13 (16%)	1 (1%)	12	45
22	Y	127/129~(98%)	119 (94%)	6 (5%)	2(2%)	9	41
23	Z	140/142~(99%)	127 (91%)	11 (8%)	2(1%)	11	43
24	a	122/126~(97%)	106 (87%)	12 (10%)	4(3%)	4	27
25	b	97/99~(98%)	81 (84%)	13 (13%)	3~(3%)	4	28
26	с	82/84~(98%)	72 (88%)	8 (10%)	2(2%)	6	33
27	d	62/64~(97%)	54 (87%)	5 (8%)	3~(5%)	2	18
28	е	51/53~(96%)	39(76%)	8 (16%)	4 (8%)	1	9
29	f	69/71~(97%)	56 (81%)	6(9%)	7 (10%)	0	6
30	g	$\overline{311/313}\ (99\%)$	273 (88%)	31 (10%)	7(2%)	6	34
31	h	$\overline{73/75}\ (97\%)$	70 (96%)	2(3%)	1 (1%)	11	43
32	i	$57/\overline{59}\ (97\%)$	45 (79%)	7 (12%)	5(9%)	1	7



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Per	centiles
35	А	264/266~(99%)	225~(85%)	29 (11%)	10 (4%)	3	24
36	В	420/422 (100%)	350~(83%)	48 (11%)	22~(5%)	2	16
37	U	140/142~(99%)	121 (86%)	14 (10%)	5(4%)	3	25
38	R	133/135~(98%)	105 (79%)	18 (14%)	10 (8%)	1	9
All	All	5534/5610~(99%)	4836 (87%)	500~(9%)	198 (4%)	6	25

All (198) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	209	ASP
3	D	221	PRO
5	F	193	ASP
5	F	219	PRO
6	G	2	ALA
6	G	17	HIS
8	Ι	46	LYS
8	Ι	104	ALA
8	Ι	155	GLN
8	Ι	236	SER
9	J	67	PRO
9	J	88	SER
10	K	158	ILE
10	Κ	177	SER
11	L	63	LEU
11	L	148	ILE
11	L	155	LYS
12	М	89	ILE
13	Ν	66	VAL
14	0	99	LYS
19	V	143	LYS
22	Y	3	ARG
24	a	86	GLU
29	f	91	ASN
29	f	95	ARG
35	А	58	SER
35	А	186	PRO
35	А	187	GLN
36	В	194	LYS
37	U	90	VAL
38	R	126	VAL
38	R	137	HIS



Mol	Chain	Res	Type
2	С	6	ASP
3	D	149	GLN
5	F	142	LEU
5	F	215	ASP
5	F	216	GLU
6	G	153	LEU
7	Н	79	HIS
7	Н	164	ARG
8	Ι	41	LEU
9	J	106	ARG
9	J	190	PRO
11	L	21	GLU
12	М	2	LEU
12	М	42	ASN
13	N	81	LYS
14	0	103	VAL
16	Q	99	ALA
16	Q	140	THR
17	S	29	ASN
17	S	44	PRO
19	V	34	VAL
19	V	40	ALA
21	Х	10	ASP
27	d	67	ARG
28	е	8	TRP
29	f	122	PRO
30	g	107	ASP
32	i	131	ALA
35	А	218	CYS
35	А	221	GLU
36	В	65	HIS
36	В	283	GLU
36	В	285	ASP
36	В	462	LYS
37	U	145	THR
38	R	12	PHE
38	R	136	THR
2	С	155	ARG
3	D	82	ARG
4	Е	156	GLY
4	E	159	ILE
4	Е	260	LYS



Mol	Chain	Res	Type
5	F	199	GLY
6	G	240	ARG
7	Н	22	LYS
7	Н	41	VAL
7	Н	50	PRO
7	Н	58	ALA
7	Н	62	ARG
8	Ι	83	CYS
10	K	11	ARG
10	K	142	SER
10	K	144	LYS
11	L	187	ALA
13	Ν	42	LEU
13	Ν	119	ASP
13	Ν	148	ALA
14	0	75	ASN
14	0	81	ASP
16	Q	66	ARG
16	Q	138	ASP
18	Т	84	TYR
18	Т	90	ALA
20	W	72	GLU
23	Ζ	126	ALA
25	b	11	ALA
26	С	83	GLN
28	е	24	CYS
29	f	123	SER
30	g	13	GLY
30	g	48	ASP
31	h	111	ARG
32	i	84	GLY
35	А	242	LEU
35	A	244	ARG
36	В	131	PRO
36	В	174	GLY
36	B	177	SER
36	В	224	VAL
36	В	277	VAL
37	U	144	ARG
38	R	10	ARG
38	R	83	MET
38	R	128	HIS



Mol	Chain	Res	Type
38	R	130	ARG
2	С	113	GLN
2	С	149	ASN
3	D	20	LYS
3	D	77	ASP
5	F	194	PRO
6	G	30	ARG
6	G	83	PRO
7	Н	42	LYS
9	J	6	ALA
9	J	12	ASN
9	J	16	PRO
9	J	45	ILE
11	L	185	ALA
12	М	38	LYS
12	М	94	LEU
17	S	138	ARG
19	V	90	SER
24	a	52	PRO
25	b	8	ASN
27	d	37	ASP
30	g	163	PRO
30	g	190	GLY
30	g	223	GLU
32	i	85	LYS
35	А	143	LYS
35	А	161	SER
35	А	224	PRO
36	В	64	ALA
36	В	196	LYS
36	В	205	ILE
36	В	257	PRO
36	В	321	LYS
36	В	461	GLU
37	U	89	ASP
37	U	95	TYR
2	С	72	ALA
2	С	104	THR
2	С	110	ASN
2	С	191	ARG
3	D	117	TRP
3	D	129	THR



7 6 1		<u> </u>	
Mol	Chain	Res	Type
3	D	207	LEU
4	Ε	45	TRP
4	Е	161	LYS
8	Ι	70	HIS
12	М	41	PRO
13	Ν	31	GLU
19	V	28	LEU
20	W	70	CYS
20	W	107	GLU
22	Y	58	ALA
24	a	34	THR
24	a	96	LEU
25	b	62	TYR
27	d	66	ARG
29	f	125	GLU
30	g	104	HIS
32	i	83	VAL
32	i	86	VAL
36	В	85	GLU
36	В	260	PRO
38	R	38	SER
38	R	74	GLU
10	Κ	156	ALA
13	Ν	6	THR
16	Q	64	ALA
16	Q	129	ILE
16	Q	134	PRO
23	Ζ	127	ASN
26	с	78	SER
36	В	135	GLY
36	В	154	LEU
2	С	126	ASP
28	е	50	ILE
29	f	102	VAL
29	f	88	PRO
36	В	368	GLY
11	L	163	SER
17	S	100	VAL
28	е	51	GLY
36	В	450	VAL



### 5.3.2 Protein sidechains (i)

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	1	24/24~(100%)	21~(88%)	3~(12%)	4	21
2	С	174/174~(100%)	171~(98%)	3~(2%)	60	82
3	D	196/196~(100%)	192~(98%)	4 (2%)	55	79
4	Ε	187/187~(100%)	183~(98%)	4 (2%)	53	78
5	F	190/190~(100%)	182 (96%)	8 (4%)	30	61
6	G	225/225~(100%)	223~(99%)	2 (1%)	78	91
7	Н	161/161~(100%)	159~(99%)	2 (1%)	71	87
8	Ι	207/207~(100%)	205~(99%)	2 (1%)	76	89
9	J	170/170~(100%)	164 (96%)	6 (4%)	36	66
10	K	177/177~(100%)	174 (98%)	3 (2%)	60	82
11	L	157/157~(100%)	156 (99%)	1 (1%)	86	94
12	М	89/89~(100%)	86~(97%)	3 (3%)	37	67
13	Ν	142/142~(100%)	135~(95%)	7 (5%)	25	57
14	О	104/104~(100%)	103 (99%)	1 (1%)	76	89
15	Р	130/130~(100%)	129~(99%)	1 (1%)	81	92
16	Q	106/106~(100%)	103~(97%)	3(3%)	43	72
17	S	117/117~(100%)	112 (96%)	5 (4%)	29	61
18	Т	114/114~(100%)	113 (99%)	1 (1%)	78	91
19	V	113/113~(100%)	113 (100%)	0	100	100
20	W	94/94~(100%)	92~(98%)	2(2%)	53	78
21	Х	67/67~(100%)	66~(98%)	1 (2%)	65	84
22	Y	112/112~(100%)	111 (99%)	1 (1%)	78	91
23	Ζ	114/114~(100%)	112 (98%)	2 (2%)	59	81
24	a	108/108~(100%)	107 (99%)	1 (1%)	78	91
25	b	87/87~(100%)	86~(99%)	1 (1%)	73	88
26	с	76/76~(100%)	73 (96%)	3 (4%)	32	63



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
27	d	57/57~(100%)	55~(96%)	2(4%)	36	66
28	е	47/47~(100%)	46 (98%)	1 (2%)	53	78
29	f	64/64~(100%)	58 (91%)	6 (9%)	8	33
30	g	272/272~(100%)	267~(98%)	5 (2%)	59	81
31	h	66/66~(100%)	66 (100%)	0	100	100
32	i	49/49~(100%)	48 (98%)	1 (2%)	55	79
35	А	238/238~(100%)	230~(97%)	8(3%)	37	67
36	В	354/354~(100%)	350~(99%)	4 (1%)	73	88
37	U	122/122~(100%)	118 (97%)	4 (3%)	38	68
38	R	121/121 (100%)	114 (94%)	7 (6%)	20	52
All	All	4831/4831 (100%)	4723 (98%)	108 (2%)	54	77

All (108) residues with a non-rotameric side chain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	1	2	ARG
1	1	5	TRP
1	1	23	ARG
2	С	85	ARG
2	С	140	VAL
2	С	201	LEU
3	D	49	VAL
3	D	212	VAL
3	D	220	LYS
3	D	228	LEU
4	Е	39	LYS
4	Е	43	LYS
4	Е	122	VAL
4	Е	239	ASP
5	F	5	ILE
5	F	76	ARG
5	F	108	LYS
5	F	117	ARG
5	F	124	ARG
5	F	148	LYS
5	F	150	MET
5	F	174	HIS
6	G	156	MET



Mol	Chain	Res	Type
6	G	176	ASP
7	Н	29	GLN
7	Н	201	LYS
8	Ι	164	LYS
8	Ι	167	LYS
9	J	32	MET
9	J	35	ASP
9	J	76	GLN
9	J	78	ARG
9	J	85	LYS
9	J	126	HIS
10	K	10	LYS
10	K	22	HIS
10	K	166	PHE
11	L	116	LYS
12	М	16	PHE
12	М	58	VAL
12	М	94	LEU
13	N	1	MET
13	N	4	ILE
13	N	31	GLU
13	Ν	39	ASN
13	N	119	ASP
13	N	124	ASP
13	N	157	LYS
14	0	45	ARG
15	Р	39	LYS
16	Q	34	PHE
16	Q	39	ASP
16	Q	150	ARG
17	S	41	MET
17	S	49	TYR
17	S	51	LEU
17	S	73	LYS
17	S	131	LYS
18	Т	106	LEU
20	W	75	LYS
20	W	79	ARG
21	Х	40	ASP
22	Y	9	ASP
23	Ζ	32	LEU
23	Ζ	105	PHE



Mol	Chain	Res	Type
24	a	29	HIS
25	b	33	ASP
26	с	17	ARG
26	с	34	ASP
26	с	83	GLN
27	d	60	GLU
27	d	67	ARG
28	е	39	CYS
29	f	99	LYS
29	f	104	LYS
29	f	109	ASP
29	f	118	ARG
29	f	119	ARG
29	f	125	GLU
30	g	49	GLU
30	g	51	ASN
30	g	113	PHE
30	g	206	LEU
30	g	246	TYR
32	i	82	ARG
35	А	9	TYR
35	А	55	ARG
35	А	57	ARG
35	А	64	ARG
35	А	126	GLN
35	А	221	GLU
35	А	244	ARG
35	А	246	GLU
36	В	137	PHE
36	В	155	MET
36	В	203	ASN
36	В	392	ARG
37	U	13	LEU
37	U	94	LYS
37	U	141	ARG
37	U	144	ARG
38	R	10	ARG
38	R	51	ARG
38	R	72	LYS
38	R	100	LYS
38	R	127	LYS
38	R	130	ARG



Continued from previous page...

Mol	Chain	Res	Type
38	R	137	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	207	HIS
6	G	50	ASN
13	N	5	GLN
15	Р	105	ASN
16	Q	32	HIS
17	S	48	GLN
23	Ζ	16	HIS
24	a	29	HIS
25	b	17	HIS
30	g	14	HIS
30	g	188	HIS
31	h	89	GLN
31	h	103	HIS
36	В	65	HIS
36	В	160	ASN
36	В	180	GLN
36	В	203	ASN
36	В	305	GLN

### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	2	1732/1863~(92%)	263~(15%)	11 (0%)
34	3	35/36~(97%)	20~(57%)	5 (14%)
39	1	74/75~(98%)	15 (20%)	5~(6%)
All	All	1841/1974~(93%)	298 (16%)	21 (1%)

All (298) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
33	2	4	С
33	2	33	G
33	2	41	G
33	2	42	А
33	2	44	U



Mol	Chain	Res	Type
33	2	46	А
33	2	55	U
33	2	56	G
33	2	59	U
33	2	60	А
33	2	67	С
33	2	68	А
33	2	73	С
33	2	74	G
33	2	75	G
33	2	76	U
33	2	79	А
33	2	80	G
33	2	94	G
33	2	113	G
33	2	126	G
33	2	143	U
33	2	147	А
33	2	148	U
33	2	178	С
33	2	179	С
33	2	181	А
33	2	182	С
33	2	183	G
33	2	184	G
33	2	191	С
33	2	197	U
33	2	202	U
33	2	223	А
33	2	224	U
33	2	225	С
33	2	226	A
33	2	271	G
33	2	274	G
33	2	277	U
33	2	278	U
33	2	285	U
33	2	296	U
33	2	299	G
33	2	300	G
33	2	309	A
33	2	310	G



Mol	Chain	Res	Type
33	2	311	С
33	2	315	С
33	2	316	С
33	2	317	G
33	2	322	G
33	2	337	G
33	2	347	С
33	2	352	С
33	2	354	А
33	2	358	U
33	2	375	G
33	2	376	С
33	2	397	G
33	2	398	A
33	2	399	С
33	2	418	U
33	2	438	A
33	2	439	A
33	2	440	С
33	2	442	G
33	2	457	G
33	2	462	С
33	2	463	А
33	2	464	G
33	2	472	G
33	2	477	U
33	2	483	A
33	2	492	С
33	2	513	А
33	2	515	A
33	2	522	С
33	2	542	G
33	2	543	U
33	2	546	U
33	2	547	U
33	2	554	A
33	2	558	С
33	2	579	G
33	2	580	A
33	2	581	U
33	2	582	С
33	2	583	С



Mol	Chain	Res	Type
33	2	584	А
33	2	596	G
33	2	597	U
33	2	598	С
33	2	604	G
33	2	618	А
33	2	633	А
33	2	658	А
33	2	659	А
33	2	661	А
33	2	662	А
33	2	678	U
33	2	679	U
33	2	680	G
33	2	681	U
33	2	682	G
33	2	729	С
33	2	732	С
33	2	733	G
33	2	734	С
33	2	735	С
33	2	736	С
33	2	737	С
33	2	738	U
33	2	739	U
33	2	740	G
33	2	741	С
33	2	742	С
33	2	743	U
33	2	744	С
33	2	746	С
33	2	747	G
33	2	748	G
33	2	749	С
33	2	750	G
33	2	751	С
33	2	785	G
33	2	786	C
33	2	787	С
33	2	788	С
33	2	789	G
33	2	790	A



Mol	Chain	Res	Type
33	2	791	А
33	2	793	С
33	2	794	G
33	2	795	U
33	2	807	А
33	2	817	G
33	2	818	U
33	2	819	U
33	2	820	С
33	2	833	А
33	2	835	С
33	2	843	А
33	2	849	С
33	2	865	A
33	2	867	U
33	2	868	А
33	2	869	G
33	2	870	G
33	2	874	G
33	2	883	U
33	2	884	U
33	2	906	G
33	2	907	С
33	2	909	А
33	2	915	A
33	2	916	А
33	2	918	А
33	2	929	G
33	2	951	A
33	2	966	G
33	2	967	G
33	2	986	A
33	2	988	A
33	2	1004	A
33	2	1012	U
33	2	1013	U
33	2	1019	A
33	2	1041	U
33	2	1045	A
33	2	1057	U
33	2	1058	A
33	2	1081	С



Mol	Chain	Res	Type
33	2	1082	G
33	2	1106	G
33	2	1112	С
33	2	1113	С
33	2	1144	А
33	2	1145	А
33	2	1153	G
33	2	1154	G
33	2	1203	G
33	2	1211	С
33	2	1217	G
33	2	1238	U
33	2	1246	А
33	2	1247	А
33	2	1253	G
33	2	1255	A
33	2	1270	G
33	2	1271	G
33	2	1280	А
33	2	1298	G
33	2	1299	С
33	2	1340	A
33	2	1367	U
33	2	1368	U
33	2	1374	A
33	2	1382	A
33	2	1391	С
33	2	1399	С
33	2	1406	С
33	2	1408	С
33	2	1413	С
33	2	1414	С
33	2	1415	С
33	2	1427	G
33	2	1431	С
33	2	1432	С
33	2	1450	A
33	2	1470	A
33	2	1471	G
33	2	1472	A
33	2	1473	U
33	2	1474	U



Mol	Chain	Res	Type
33	2	1485	А
33	2	1486	G
33	2	1506	G
33	2	1507	U
33	2	1516	С
33	2	1517	А
33	2	1518	С
33	2	1539	С
33	2	1547	G
33	2	1548	С
33	2	1549	С
33	2	1550	U
33	2	1575	А
33	2	1580	U
33	2	1583	А
33	2	1596	А
33	2	1616	U
33	2	1618	А
33	2	1632	А
33	2	1643	G
33	2	1659	А
33	2	1660	G
33	2	1666	G
33	2	1675	G
33	2	1683	С
33	2	1716	U
33	2	1717	G
33	2	1743	G
33	2	1747	С
33	2	1748	G
33	2	1777	С
33	2	1778	G
33	2	1817	A
33	2	1819	А
33	2	1820	G
33	2	1823	G
33	2	1825	А
33	2	1829	А
33	2	1843	G
33	2	1846	С
33	2	1855	G
33	2	1856	G



Mol	Chain	Res	Type
33	2	1857	А
33	2	1858	U
33	2	1859	С
33	2	1860	А
33	2	1862	U
33	2	1863	А
34	3	43	G
34	3	44	U
34	3	45	С
34	3	46	A
34	3	47	U
34	3	48	А
34	3	50	С
34	3	54	G
34	3	55	U
34	3	56	С
34	3	57	U
34	3	58	G
34	3	59	G
34	3	60	А
34	3	61	С
34	3	65	G
34	3	66	С
34	3	69	G
34	3	72	U
34	3	75	U
39	1	9	U
39	1	11	G
39	1	15	A
39	1	16	G
39	1	17	C
39	1	18	G
39	1	19	G
39	1	21	A
39	1	43	G
39	1	45	G
39	1	47	U
39	1	56	С
39	1	61	С
39	1	74	С
39	1	76	A

All (21) RNA pucker outliers are listed below:



Mol	Chain	Res	Type
33	2	224	U
33	2	397	G
33	2	739	U
33	2	817	G
33	2	866	А
33	2	1012	U
33	2	1057	U
33	2	1153	G
33	2	1549	С
33	2	1616	U
33	2	1818	А
34	3	54	G
34	3	56	С
34	3	57	U
34	3	58	G
34	3	65	G
39	1	8	G
39	1	16	G
39	1	17	С
39	1	18	G
39	1	74	С

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

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

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

Mol Type	Chain	Chain	Chain	Chain	Chain	Chain	Chain	hain Res	Dog Link	Bo	Bond lengths			Bond angles		
INIOI	туре	Unam	nes	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2						
33	C4J	2	1244	33	24,29,30	0.79	1 (4%)	29,42,45	1.03	1 (3%)						
39	T6A	1	37	39	27,34,35	1.04	2 (7%)	29,49,52	2.64	9 (31%)						

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	C4J	2	1244	33	1/1/7/7	9/16/34/35	0/2/2/2
39	T6A	1	37	39	-	6/19/41/42	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
39	1	37	T6A	C5-C4	2.51	1.47	1.40
39	1	37	T6A	O4'-C1'	2.21	1.44	1.41
33	2	1244	C4J	C1'-C5	-2.07	1.45	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
39	1	37	T6A	C12-N11-C10	8.56	136.20	121.94
39	1	37	T6A	C2-N1-C6	7.01	122.61	116.59
39	1	37	T6A	C14-C12-C13	3.68	116.47	110.19
39	1	37	T6A	N3-C2-N1	-3.57	123.09	128.68
33	2	1244	C4J	C4-N3-C2	-3.41	121.15	125.46
39	1	37	T6A	N6-C6-N1	3.04	122.79	118.72
39	1	37	T6A	O10-C10-N6	-2.97	118.60	123.62
39	1	37	T6A	C4-C5-N7	-2.77	106.51	109.40
39	1	37	T6A	C14-C12-N11	2.70	118.63	111.72
39	1	37	T6A	N6-C10-N11	2.10	116.70	113.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	2	1244	C4J	C4'

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	2	1244	C4J	C31-C3-N3-C2
33	2	1244	C4J	C31-C3-N3-C4
33	2	1244	C4J	C3-C31-C32-C34
33	2	1244	C4J	C3-C31-C32-N33
33	2	1244	C4J	N33-C32-C34-O36
39	1	37	T6A	C14-C12-N11-C10
33	2	1244	C4J	N33-C32-C34-O35
39	1	37	T6A	N11-C12-C13-ODA
39	1	37	T6A	N11-C12-C13-ODB
39	1	37	T6A	C13-C12-C14-C15



Mol	Chain	Res	Type	Atoms
33	2	1244	C4J	N3-C3-C31-C32
39	1	37	T6A	O4'-C4'-C5'-O5'
33	2	1244	C4J	C31-C32-C34-O35
33	2	1244	C4J	C31-C32-C34-O36
39	1	37	T6A	C13-C12-N11-C10

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	2	1244	C4J	3	0
39	1	37	T6A	5	0

## 5.5 Carbohydrates (i)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	2	6
39	1	5
8	Ι	1
24	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	Р	8.58



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ι	217:MET	С	218:LYS	Ν	3.94
1	a	9:THR	С	10:ARG	Ν	3.27
1	1	19:G	O3'	20:A	Р	2.13
1	1	17:C	O3'	18:G	Р	1.99
1	1	18:G	O3'	19:G	Р	1.87
1	2	350:A	O3'	351:U	Р	1.86
1	2	675:A	O3'	676:U	Р	1.84
1	2	676:U	O3'	677:C	Р	1.38
1	2	1172:G	O3'	1173:U	Р	1.37
1	1	36:U	O3'	37:T6A	Р	1.28
1	2	1815:U	O3'	1816:A	Р	1.26
1	1	16:G	O3'	17:C	Р	1.14

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#### 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10762. 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.

#### Orthogonal projections (i) 6.1

#### Primary map 6.1.1



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

#### 6.2Central slices (i)

#### 6.2.1Primary map



X Index: 192


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

#### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map



X Index: 208

Y Index: 160

Z Index: 199

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

#### 6.4 Orthogonal surface views (i)

#### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation (i)

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



# 7 Map analysis (i)

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

## 7.1 Map-value distribution (i)



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



#### 7.2 Volume estimate (i)



The volume at the recommended contour level is 753  $\rm nm^3;$  this corresponds to an approximate mass of 680 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 (i)



\*Reported resolution corresponds to spatial frequency of 0.287  $\mathrm{\AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

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-10762 and PDB model 6YAN. Per-residue inclusion information can be found in section 3 on page 11.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



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



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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0109).



#### 9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

#### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7631	0.3510
1	0.5062	0.1520
2	0.8838	0.4010
3	0.3269	0.1390
А	0.1818	0.0510
В	0.0079	-0.0120
С	0.8302	0.4210
D	0.7890	0.4010
Е	0.8249	0.4440
F	0.7364	0.3530
G	0.8137	0.4160
Н	0.7841	0.3830
Ι	0.7258	0.2980
J	0.6342	0.2810
K	0.7708	0.3630
L	0.8230	0.4160
М	0.7419	0.3150
Ν	0.7486	0.3830
0	0.4364	0.1240
Р	0.8055	0.3960
Q	0.8065	0.4090
R	0.7001	0.3020
S	0.8142	0.4180
Т	0.7288	0.3300
U	0.7693	0.3430
V	0.7773	0.3790
W	0.7503	0.3450
Х	0.7921	0.3780
Y	0.8683	0.4780
Z	0.8509	0.4510
a	0.7968	0.3730
b	0.8331	0.4320
с	0.7403	0.3230
d	0.7536	0.3660
е	0.8103	0.3800

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Chain	Atom inclusion	Q-score
f	0.4427	0.0750
g	0.7391	0.3250
h	0.7055	0.3110
i	0.6228	0.2840
l	0.7671	0.3910

