

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 29, 2021 – 04:19 pm BST

PDB ID : 7A18	
Title : 50S Deinococcus radiodurans ribosome bounded with mycinam	nicin IV
Authors : Breiner, E.; Eyal, Z.; Matzov, D.; Halfon, Y.; Cimicata, G.; I	Rozenberg, H.;
Zimmerman, E.; Bashan, A.; Yonath, A.	
Deposited on : $2020-08-12$	
Resolution : $3.40 \text{ Å}(\text{reported})$	

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity		4 02b-467
Mon robity	•	1.020 101
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.40 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.



Motria	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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

Mol	Chain	Length		Quality of cha	in		
1	Х	2699	25%	45%		25%	5%
2	Y	122	8%	56%		18%	•
3	А	271	14%		41%		7%
4	В	206	4%		37%		14% •



Mol	Chain	Length	Q	uality of chain	
5	С	195	41%	49%	10%
6	D	176	43%	42%	15%
7	Е	171	20%	38%	12%
8	G	142	4% 50%	34%	15% •
9	Н	134	% 	47%	15%
10	Ι	137	15%	34%	9% •
11	J	134	7%	48%	10% •
12	K	115	36%	45%	17% •
13	L	104	17%	44%	6%
14	М	118	% 	47%	13% •
15	Ν	117	4%	38%	9%
16	0	98	<mark>6%</mark> 49%	35%	16%
17	Р	129	36%	52%	10% •
18	Q	93	<mark>6%</mark> 39%	41%	19% •
19	R	110	45%	35%	16% •
20	S	175	27%	44%	9%
21	Т	72	39%	46%	15%
22	U	74	16% 36%	47%	15% •
23	V	54	61%	31%	7%
24	W	55	42%	40%	18%
25	Z	57	33%	40%	25%
26	1	49	16%	31%	10% •
27	2	46	54%	39%	7%
28	3	63	32%	40%	29%

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	2	101	_	_	-	Х
30	MG	Х	2925	_	_	-	Х
30	MG	Х	2950	-	-	_	Х
30	MG	Х	2969	-	-	-	Х
30	MG	Х	2976	-	-	-	Х
30	MG	Х	2979	-	-	-	Х
30	MG	Х	3002	-	-	-	Х
30	MG	Х	3045	-	-	-	Х
30	MG	Х	3050	-	-	-	Х
30	MG	Х	3052	-	-	-	Х
30	MG	Х	3057	-	-	-	Х
30	MG	Х	3060	-	-	-	Х
30	MG	Х	3071	-	-	-	Х
30	MG	Х	3074	-	-	-	Х
30	MG	Х	3086	-	-	-	Х
30	MG	Х	3090	-	-	-	Х
30	MG	Х	3096	-	-	-	Х
30	MG	Х	3097	-	-	-	Х
30	MG	Х	3102	-	-	-	Х
30	MG	Х	3104	-	-	-	Х
30	MG	Х	3105	-	-	-	Х
30	MG	Х	3109	-	-	-	Х
30	MG	Х	3115	-	-	-	Х
30	MG	Х	3122	-	-	-	Х
30	MG	Х	3131	-	-	-	Х
30	MG	Х	3141	-	-	-	Х
30	MG	Х	3144	-	-	-	Х
30	MG	Х	3146	-	-	-	Х
30	MG	Х	3149	-	-	-	Х
30	MG	Х	3151	-	-	-	Х
30	MG	Х	3154	-	-	-	Х
30	MG	Х	3159	-	-	-	Х
30	MG	Х	3163	-	-	-	Х
30	MG	Y	202	-	-	-	Х
31	SPD	Х	3166	-	-	-	Х
31	SPD	Х	3167	-	-	Х	_



## 2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 84387 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a RNA chain called RNA (2699-MER).

Mol	Chain	Residues			Atoms	ZeroOcc	AltConf	Trace		
1	Х	2699	Total 57957	C 25853	N 10701	O 18704	Р 2699	0	1	0

• Molecule 2 is a RNA chain called RNA (122-MER).

Mol	Chain	Residues		At	toms		ZeroOcc	AltConf	Trace	
2	Y	122	Total 2598	C 1161	N 476	O 840	Р 121	0	0	0

• Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	Trace	
3	А	271	Total 2001	C 1246	N 390	O 362	${ m S} { m 3}$	0	0	0

• Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	В	206	Total 1544	C 968	N 296	0 272	S 8	0	0	0

• Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	С	195	Total 1467	C 912	N 280	0 273	${S \over 2}$	0	0	0

• Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	176	Total 1367	C 870	N 238	O 253	${ m S}{ m 6}$	0	0	0



• Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Е	171	Total 1286	C 812	N 237	O 236	S 1	0	0	0

• Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total 1107	C 698	N 208	0 198	${ m S} { m 3}$	0	0	0

• Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Н	134	Total 993	C 611	N 197	0 180	${ m S}{ m 5}$	0	0	0

• Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Ι	137	Total 982	C 603	N 194	0 184	S 1	0	0	0

• Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	134	Total 1042	C 668	N 188	0 179	${ m S} 7$	0	0	0

• Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	115	Total 897	$\begin{array}{c} \mathrm{C} \\ 552 \end{array}$	N 183	O 159	${ m S} { m 3}$	0	0	0

• Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
13	L	104	Total 751	C 457	N 154	O 140	0	0	0

• Molecule 14 is a protein called 50S ribosomal protein L19.



Mol

Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
		Total	С	Ν	0			

• Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	Ν	117	Total 962	$\begin{array}{c} \mathrm{C} \\ 599 \end{array}$	N 203	O 159	S 1	0	0	0

• Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	О	98	Total 734	C 459	N 135	O 139	S 1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	12	ALA	TYR	conflict	UNP Q9RY64

• Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
17	Р	129	Total 1020	C 643	N 199	0 176	${ m S} { m 2}$	0	0	0

• Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
18	Q	93	Total 718	C 452	N 134	0 130	${S \over 2}$	0	0	0

• Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
19	R	110	Total 793	C 492	N 149	0 151	S 1	0	0	0

• Molecule 20 is a protein called 50S ribosomal protein L25.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	S	175	Total 1290	C 811	N 224	O 251	${S \over 4}$	0	0	1

• Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
21	Т	72	Total 542	C 343	N 104	0 94	S 1	0	0	0

• Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		Ator	$\mathbf{ns}$		ZeroOcc	AltConf	Trace
22	U	74	Total 539	C 336	N 107	O 96	0	0	0

• Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
23	V	54	Total 438	C 270	N 89	0 78	S 1	0	0	0

• Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
24	W	55	Total 424	C 264	N 82	O 76	S 2	0	0	0

• Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
25	Z	57	Total 448	C 275	N 92	O 76	${ m S}{ m 5}$	0	0	0

• Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Aton	ıs		ZeroOcc	AltConf	Trace
26	1	49	Total 315	C 199	N 54	O 62	0	0	0

• Molecule 27 is a protein called 50S ribosomal protein L34.



Mol	Chain	Residues		Ato	ms			ZeroOcc	AltConf	Trace
27	2	46	Total	C 220	N 01	0 60	S 2	0	0	0

• Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
28	3	63	Total 470	C 295	N 97	O 75	${ m S} { m 3}$	0	0	0

• Molecule 29 is MYCINAMICIN IV (three-letter code: MIV) (formula:  $C_{37}H_{61}NO_{11}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf
29	Х	1	Total 49	C 37	N 1	0 11	0	0

• Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Х	264	Total Mg 264 264	0	0
30	Y	4	Total Mg 4 4	0	0
30	А	1	Total Mg 1 1	0	0
30	Ι	1	Total Mg 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Ν	1	Total Mg 1 1	0	0
30	Q	2	Total Mg 2 2	0	0
30	W	1	Total Mg 1 1	0	0
30	2	2	Total Mg 2 2	0	0
30	3	1	Total Mg 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	Х	1	Total         C         N           10         7         3	0	0
31	Х	1	Total         C         N           10         7         3	0	0
31	Х	1	Total         C         N           10         7         3	0	0
31	Х	1	Total         C         N           10         7         3	0	0
31	Х	1	Total         C         N           10         7         3	0	0
31	Х	1	Total         C         N           10         7         3	0	0



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Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
31	V	1	Total 10	${ m C} 7$	N 3	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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: RNA (2699-MER)



C700	U701	<mark>G704</mark>	C705	A / 06 U707		C711	6713 G713	-	U716	6717 4718	A719	A720	4 CEN	C/24 C725	G732	G733		G737 C737	G738	G739	0720	6742 8743		G746	A747	C749	C750	G751	G752 U753	G754	C755 C756	U757	G758	U760	G761	A762	A764	C765	A766	G767 11768	C769	0220	G773	A774	U775
G776	A777 G778		G781	0783 G783	U784		A/8/ G788	G7 89	A790	6791 11792	G793	A794	A795	A797 A797	G7 98	C799	0000	A801 A802	C803	C804	G805 4806	Aguo	<mark>C809</mark>	U810	6811 6812	4012 A813	G814	A815 11016	0816 A817	G818	C819	00200 A821	G822	0823 U824	C825	U826 C627	C828	C829	C830	(1831 1837	A833	A834	0835 G836	U837	A838
<mark>U839</mark>	U840 G841	A842	G843	6844 U845	A846	C847	A848 G849	<b>C850</b>	C851	0852 C853	G854	G855	A856	0858 G858	U859	U860	6861	A802 C863		G867	U868	C870	U871	G872	U873	40/4 G875	A876	G877	08/8 A879		C884	A886 A886	G887	0000 C889	068N	A891	A911 A912	A913	C914	C915 11016		0919	6920 A921	A922	A923
C924	0925 0926	C927	G928	A929 A930	G931	G932	G934 G934	<mark>C935</mark>	A936	0937 0938	C939	G940	0941	0942 11943	A944	G945	0946 0047	C94/ C948	G949	<b>G950</b>	(951 4052	A952 (953	<b>U954</b>	G955	A956	G958	C959	0960 0061	TOPD	A964	0965 1966	G967	C968	0303 A970	A971	C972	U974	C975		(1980) 7081	C982	G983	A984 G985	A986	G987
<b>G988</b>	6989 4990	A991	A992	6993 A994	A995	C996	C998	<b>A999</b>	G1000	A1001 C1002	C1003	A1004	U1005	01007 A1007	G1008	C1009	U1010	A1012 A1012	G1013	G1014	U1015	C1017		A1020	A1021	N1022	G1024	A1025	01026 C1027	G1028	C1029	C1031	A1032	01034 U1034	G1035	G1036	01038 01038	A1039	A1040	G1041	A1043	U1044	61045 U1046	G1047	U1048
C1049	G1050	C1052	G1053	C1054 A1055	U1056	A1057	41059	C1060	A1061	G1062 C1063	C1064	A1065	G1066	A1068	G1069	G1070	U1071	010/2 61073	G1074	C1075	U1076		G1079	A1080	A1081	C1083	A1084	G1085	C1087	A1088	C1089	C1091	U1092	C1094	A1095	A1096	G1098	A1099	G1100	U1101 C0112	C1103	G1104		A1107	
U1112	C1113 A1114	C1115	U1116	G1118 G1118	U1119	C1120	41121 A1122	G1123	U1124	C1127	G1128	A1129	U1130	G1132 C1132	G1133	C1134	C1135	41137 A1137	A1138	A1139	A1140	01141 G1142	A1143	U1144	C1145	07170	G1149	21 1 L O	C1152 A1153	A1154	G1155 114166	G1157	A1158	01159 C1160	U1161	A1162	C1164	G1165	A1166	A1167	A1171	U1172	G11/3 G1174	A1175	U1176
	A1179 A1180	C1181	U1182	G1183	G1191	A1192	01194	U1195	G1196	01197 C1198		G1201	U1202	G1204	G1205	G1206		G1210 G1211	U1212	U1213	C1214	G1216	U1217	C1218	C1219		G1223	A1224	61225 A1226	A1227	G1228	C1230	A1231	01232 A1233	C1234	C1235	A1238	A1239	G1240	G1241	7L7TH	G1245	G1246 U1247	G1248	G1249
A1250	G1251 C1252	C1253	G1254	A1255 C1256	U1257	G1258	A1259 A1260	G1261	U1262	G1263 C1264	G1265	G1266	A1267	01268 G1269	C1270	C1271	G1272	G1274 C1274	A1275	U1276	G1277	G1279	U1280	A1281	A1282	G1284	A1285	0000	A1266	G1291	A1292	G1294	U1295	06779	A1299	A1300 111201	C1302	U1303	U1304	C1305	U1307	C1308	G1309 C1310	C1311	G1312
U1313	A1314 A1315		C1319	A1320 A1321	G1322	100	01325 01326	C1327	C1 328	01329 61330	G1331	G1332	G1333	A1 335	G1336	G1337	G1338	01339 C1340	G1341	U1342	C1343	G1345	C1346	C1347	C1348	G1350	G1351	G1352	A1353 A1354	A1355	G1356	C1358	G1359 G1250	G1361		C1364	01.365	A1367	G1368	G1369	G1371	A1372	C1376	G1377	A1378
A1379	C1380 C1381	G1382	C1 383	G1385	A1386	00010	61390	A1391	U1392	61393	A1397	G1398	C1399	61401	G1402	U1403	C1404	A1405	G1407	A1408	U1409	01410 C1411	C1412		C1418	41419 A1420	U1421	C1422	A1423 U1424	G1425	U1426	G1428	A1429	01430 01431	G1432	A1433	01435 G1435	G1436	A1437	G1438	G1440	A1441	C1442 G1443	C1444	A1445
01446	01447 V1448		01454	1456 1456	<u> 1457</u>	A1458	1459	71461	C1462	A1463 V1464	1465	C1466	V1467	A1468	1470	31471	01472	V1474	1475	G1476	C1477	1479	1480	01481	01482 14483	1484	J1485	1 100	11490		31494 •	11496	C1497	41490 11499	71500	C1501	1503	1504	01505	C1506	11508	11509	11512	11513	01514
515 •	516	518	519	322	526	527	529 529	530	531 C	885	239	540	541	04.2 143	544	545		2000 1911	562	563	564	200	571 0	572 U	573 1	575 G	576 L	577 577	581 U	582	583		586	200 / 200 /	589		595 595	596	597 L	208	300 100	501	602 • 303 •	504	605 C
606 U1	607 A1.	609 C11	610 G1		617 U1	G1:	620 621 C1	622 U1	623 C1	624 625 415	626 U11	627 C11	628 620 610	629 630	631 A11	632 G1	633	635 A15	636 G11	637 U1	11 1	642 643 C15	644 G11	645 C1	646 G1	648 C1(	649 G1	650 G1	652 C1	653 A1	654 A1	656 A11	657 A1	659 A10	660 G1	661 744	663 A1	664 A1	665 A1	666 227 267	668 U16	010 U1	670 GT. 571 A16	672 A1	673 A1
5		61	A1	5	G1	2	5 5	G1	53	41 41	A1	C1	55	41 A	C1	A1	5	LA L	G1	U1	č	4 C	G1	U1	61	5 <mark>1</mark> 5	A1	A1	15 15	5	A1	55	TA TA	G1	5	5 E	3 13	61	5	5	G1	A	5 4	A1	5



C1674	C1675 U1676	C1677	G1678	01679 11680	A1681	A1682	G1683 G1684	A1685	A1686	C1687	01689 01689	U1690	G1691	C1692	A1693 A1694	U1695	C1696	0169/ C1698	A1699	C1700	C1701	C1703	G1704	U1705		U1709	U1710	C1711 G1712	G1713	A1714	A1715 G1716	A1717	A1718	G1720	G1721	C1706	C1727	A1728	C1729 G1730		G1735		G1739 C1740	G1741
G1742	C1743 G1744	C1745	A1746	G1/4/ 111748	G1749	A1750	A1/51 111752	A1753	G1754	G1755	G1760	G1761	C1762	G1763	A1/64 C1765	U1766	G1767	01769 U1769	01770	A1771	C1772	C1 / / 3 41 77 4	A1775	A1776	A1777 111 778	C1779	A1780	C1781 A1782	G1783	C1784	A1785 C1786	U1787	C1788	G1790	C1791	C1792 A1793	A1794		A1799 A1800	C1801	A1802	U1804	G1805 C1806	A1807
C1808	G1809 U1810	A1811	U1812	A1813 G1814	G1815	G1816	01817 G1818	U1819	G1820	A1821	01823 61823	C1824	C1825	U1826	17015	C1830	G1831	01833	G1834	C1835	C1836	G1837 C1838	A1839	A1840	C1 844	A1845	A1846	G1850		G1855	01856 G1857		C1865	A1867	1 200	G1871 A1872	A1873	G1874	C1877		G1880 111 881	G1882	A1883	C1885
G1886	C1887 C1888	G1889	G1890	C1891 C1908	U1909	A1910	A1911 61912	G1913		C1917	41918 A1919	A1920	A1921	U1922	01923 C1924	C1925	U1926	01927 G1928	U1929		G1932	G1933 111 934	A1935	A1936	G1937 111 038	01939 U1939	C1940	C1941 C1942		C1945	01946 G1947	C1948	A1949	G1951	A1952	A1953 A1954	G1955	G1956	C1957 G1958	U1959	A1960 A1961	C1962	G1963 A106A	11965 11965
C1966	01967 G1968		C1971	G1972 C1973	U1974	G1975 	C1977	U1978	C1979	A1980	A 1961 C 1982	G1983	A1984	G1985	G1987	A1988	C1989		G1992	G1993	U1994	61995 A1996	A1997	A1998	U1999 112000	G2001	A2002	A2003 112004	U2005	<b>G</b> 2006	G2007 C2008	U2009	G2010 112011	A2012	A2013	A2014 G2015	A2016	U2017	G2018 C2019	G2020	G2021 72022	C2023	COOD	C2027
C2028	G2029 U2030	A2031	G2032	C2033 A 2034	G2035	G2036	A2037 C2038	G2039	A2040	A2041	A 2043	G2044	A2045	C2046	C2048	C2049	G2050	G2052	G2053	A2054	G2055	02056	U2058	U2059	A2060	U2062	A2063	U2064 42065	G2066	U2067	C2068 112069	G2070	A 7072	C 1074	G2076	G2077	A2079	U2080	U2081 C2082	G2083	G2084	U2086		C2089
U2090	A2165 G2166	A2167	A2168	A2169	U2171	U2172	G2173	A2175	U2176	U2177 110178	02179 C2179	U2180	A2181	A2182	G2186	A2187	A2188	A2189 A2190	A2191	U2192	C2193	112196	U2197	U2198	C2199	A2204	C2205	112208	G2209	C2210	U2211 U2212	G2213	G2214	G2216 G2216	G2217	G2218 112219	A2220	G2221	U2222 U2223	U2224	G2225 A7776	C2227	U2228	62230 62230
G2231	G2233 C2233	G2234	G2235	02236	G2238		C2.242 C2.243	C2244	A2245	A2246	A2.241 A2.248	U2249	G2250	U2251	A2253 A2253	C2254	G2255	G2258	G2259	C2260	G2261	C2262	C2264	A2265	A2266	G2268	G2269	U2270	A2272	C2273	C2274 112275	C2276	A2277	G2279	A2280	C2281 C2281	G2283	U2284	02286	G2287		U2291	C2292 C2292	U2294
	U2298 A2299	G2300	A2301	G2302 C2303	G2304	C2305	A2306 A2307	A2308	G2309	G2310 117211	42312 A2312	G2313	A2314	A2315	02322	U2323	G2324	A2325 C2326	U2327	G2328	C2329	62330 42331	G2332	A2333	C2334	G2336	A2337	C2338 47339	C2340		C2343 G2344	A2345	G2346	A2348	G2349	G2350 C2351	A2352	G2353	G2354 A2355	A2356	A2357	U2359	C2360	G2362
G2363	C2364	A2367	G2368	02369 62370	A2371	A2372	C23/3 C2374	G2375	G2376	U2377	1271 0	C2383	G2384	U2385	u2387	G2388	G2389	A2390 A2391		G2394	C2395	C2396 47397	U2398	C2399	G2400	U2402	C2403	A2404 A2405	C2406	G2407	G2408 A7409	U2410	0110	A2414 A2414	G2415	U2416 112417	A2418	C2419	C2420 C2421	C2422	G2423 C2423	G2425	G2426	N2428 U2428
A2429	A2430 C2431	A2432	G2433	G2434 C2435	U2436	G2437	A2438 112439	C2440	U2441	C2442	C2444	C2445	C2446	G2447	62449 G2449	A2450	G2451	02453 C2453	C2454	A2455	U2456	A2457 112458	C2459	G2460	G2461	G2463	G2464	G2465 C2466	A2467	G2468	G2469 112470	U2471	U2472 C2473	G2474	C2475	A2476 C2477	C2478	U2479	C2480 G2481	A2482	U2483 C2484	U2485	C2486	uz 401 G2488
C2489	02490 C2491	G2492	U2493	C2494 G2495	C2496	A2497	0.24.98 C.24.99		U2507	G2508 A2500	A2510 A2510	G2511	A2512	A2513	G2515	U2516	C2517	21020	A2521	G2522	G2523	62524 112525	U2526	G2527	(2528 (2528	C2530	U2531	G2532 119533	U2534	C2535	G2536 C2537	C2538	C2539	U2541	U2542	A2543 A7544	A2545	G2546	C2547 G2548	G2549	C2550	C2552	G2553 C7554	62555
A2556	G25587 C2558	U2559	G2560	G2562	U2563	U2564	0.2565 A 7566	G2567	A2568	A2569	G2571	U2572	C2573		A2579	C2580		U2584	C2585	G2586	G2587	0.25.88 C25.89	U2590	C2591	U2592 A7593	U2594	C2595	C2596 C2597	C2598	U2599	A2600 C2601	G2602	G2603	C2605	G2606	C2607 ▲7608	G2609	G2610	A2611	G2619	G2620	G2622	A2623 67674	U2625
U2626	G2627 C2628	U2629	C2630	C2631 117632	A2633	G2634	47639	G2640	A2641	G2642	42644 A2644	C2645	C2646		42652 A2653	A2654	C2655	G2657	A2658	C2659	C2660	G2661 C2662	U2663	G2664	G2665 117666	02000 C2667	U2668	C2669 C2670	C2671	U2672	G2673 C2674	U2675	G2676 110677	C2678	G2679	U2680 ∆7681	C2682	C2683	A2684	G2688	C2689 A7600	C2691	A2692 117693	0209-0 G2694



















• Molecule 22: 50S ribosomal protein L28 16% Chain U: 47% 36% 15% 740 741 142 A64 N65 • Molecule 23: 50S ribosomal protein L29 11% Chain V: 61% 31% 7% • Molecule 24: 50S ribosomal protein L30 Chain W: 42% 40% 18% R26 K27 I28 D3( K4 L5 • Molecule 25: 50S ribosomal protein L32 Chain Z: 33% 40% 25% K3 H4 P5 V6 V6 K8 K8 K9 K10 • Molecule 26: 50S ribosomal protein L33 16% Chain 1: 57% 31% 10% P6 R7 • Molecule 27: 50S ribosomal protein L34 Chain 2: 54% 39% 7% • Molecule 28: 50S ribosomal protein L35 Chain 3: 32% 40% 29%



#### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	169.59Å 410.13Å 690.48Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Posolution} \left( \overset{\circ}{\mathbf{A}} \right)$	50.00 - 3.40	Depositor
Resolution (A)	50.07 - 3.30	EDS
% Data completeness	93.9 (50.00-3.40)	Depositor
(in resolution range)	91.9(50.07-3.30)	EDS
$R_{merge}$	0.29	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.76 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D D	0.284 , $0.318$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.284 , $0.318$	DCC
$R_{free}$ test set	16405  reflections  (4.98%)	wwPDB-VP
Wilson B-factor $(Å^2)$	79.6	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$  <  L  > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	84387	wwPDB-VP
Average B, all atoms $(Å^2)$	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: MIV, SPD, MG

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

Mol Chair		Bo	ond lengths		Bond angles
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	Х	0.81	33/64897~(0.1%)	1.48	1063/101217~(1.1%)
2	Y	0.56	0/2904	1.27	26/4525~(0.6%)
3	А	0.37	0/2041	0.59	0/2765
4	В	0.59	0/1572	0.78	0/2112
5	С	0.44	0/1490	0.67	1/2021~(0.0%)
6	D	0.34	0/1385	0.58	0/1863
7	Е	0.34	0/1308	0.59	0/1771
8	G	0.46	0/1131	0.68	1/1531~(0.1%)
9	Н	0.71	1/1003~(0.1%)	0.85	0/1348
10	Ι	0.46	0/994	0.74	0/1338
11	J	0.50	0/1064	0.70	0/1425
12	Κ	0.71	0/905	0.92	1/1212~(0.1%)
13	L	0.31	0/755	0.65	0/1011
14	М	0.68	0/936	0.86	0/1257
15	Ν	0.53	0/978	0.75	1/1305~(0.1%)
16	0	0.43	0/741	0.66	0/992
17	Р	0.62	0/1033	0.79	1/1383~(0.1%)
18	Q	0.38	0/729	0.60	0/980
19	R	0.44	0/803	0.66	0/1087
20	S	0.36	0/1312	0.59	0/1791
21	Т	0.43	0/549	0.65	0/728
22	U	0.32	0/544	0.61	0/732
23	V	0.38	0/441	0.48	0/586
24	W	0.43	0/426	0.68	0/568
25	Ζ	0.69	0/460	0.87	2/618~(0.3%)
26	1	0.41	0/319	0.66	0/438
27	2	0.41	0/387	0.64	0/509
28	3	0.44	0/475	0.70	1/623 (0.2%)
All	All	0.73	34/91582~(0.0%)	1.33	1097/137736~(0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if



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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	В	0	5
5	С	0	1
8	G	0	1
10	Ι	0	2
11	J	0	2
12	Κ	0	1
14	М	0	2
16	0	0	1
19	R	0	2
20	S	0	1
25	Ζ	0	2
All	All	0	20

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	Ideal(Å)
1	Х	1278	А	N3-C4	-8.26	1.29	1.34
1	Х	1981	А	N3-C4	-7.72	1.30	1.34
9	Н	21	CYS	CB-SG	-7.46	1.69	1.82
1	Х	1278	А	N9-C4	-7.20	1.33	1.37
1	Х	2823	G	N7-C5	-6.66	1.35	1.39
1	Х	2796	А	N3-C4	-6.62	1.30	1.34
1	Х	1688	U	C2-N3	6.49	1.42	1.37
1	Х	1691	G	N7-C5	-6.45	1.35	1.39
1	Х	1686	А	N3-C4	-6.41	1.31	1.34
1	Х	1750	А	N7-C5	-6.35	1.35	1.39
1	Х	581	А	N3-C4	6.04	1.38	1.34
1	Х	1278	А	C6-N1	-5.98	1.31	1.35
1	Х	2823	G	N9-C8	-5.89	1.33	1.37
1	Х	484	G	N7-C5	-5.84	1.35	1.39
1	Х	1687	С	N3-C4	-5.83	1.29	1.33
1	Х	1976	U	N3-C4	-5.71	1.33	1.38
1	Х	994	А	C6-N1	-5.70	1.31	1.35
1	Х	2690	А	C5-C6	-5.62	1.35	1.41
1	Х	2848	А	N3-C4	-5.59	1.31	1.34
1	Х	2530	С	N3-C4	-5.53	1.30	1.33
1	Х	2804	G	N3-C4	-5.43	1.31	1.35
1	Х	1338	G	C2-N3	5.31	1.36	1.32
1	Х	970	А	N7-C5	-5.29	1.36	1.39
1	Х	2022	С	N3-C4	-5.28	1.30	1.33



Observed(Å)	Ideal(Å)	
1.43	1.38	

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Mol	Chain	$\operatorname{Res}$	Type	Atoms		Observed(A)	Ideal(A)
1	Х	1688	U	N3-C4	5.22	1.43	1.38
1	Х	1976	U	C4-O4	-5.22	1.19	1.23
1	Х	1981	A	C6-N1	-5.20	1.31	1.35
1	Х	2796	А	C5-C4	-5.18	1.35	1.38
1	Х	2488	G	C5-C4	-5.16	1.34	1.38
1	Х	1997	A	N7-C5	-5.12	1.36	1.39
1	Х	586	G	N7-C5	-5.11	1.36	1.39
1	Х	2435	С	N1-C6	-5.10	1.34	1.37
1	Х	1206	G	N9-C4	-5.10	1.33	1.38
1	Х	2817	A	N9-C4	-5.07	1.34	1.37

All (1097) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2489	С	C6-N1-C2	-19.63	112.45	120.30
1	Х	1675	С	O5'-P-OP1	-17.57	89.61	110.70
1	Х	2532	G	O5'-P-OP2	-13.57	93.48	105.70
1	Х	2489	С	N3-C4-C5	-13.52	116.49	121.90
1	Х	1973	С	C6-N1-C2	-12.59	115.27	120.30
1	Х	2491	С	C6-N1-C2	-12.17	115.43	120.30
1	Х	2800	С	C6-N1-C2	-11.79	115.58	120.30
1	Х	759	С	C6-N1-C2	-11.67	115.63	120.30
1	Х	2580	С	C6-N1-C2	-11.49	115.70	120.30
1	Х	2499	С	C6-N1-C2	-11.24	115.80	120.30
1	Х	1278	А	C2-N3-C4	-10.93	105.13	110.60
1	Х	1307	U	C5-C6-N1	10.92	128.16	122.70
1	Х	2692	А	O5'-P-OP2	-10.86	95.92	105.70
1	Х	527	С	C6-N1-C2	-10.81	115.98	120.30
1	Х	759	С	N3-C4-C5	-10.73	117.61	121.90
1	Х	2691	С	O4'-C1'-N1	10.66	116.73	108.20
1	Х	1973	С	C5-C6-N1	10.62	126.31	121.00
1	Х	2800	С	C5-C6-N1	10.57	126.28	121.00
1	Х	1685	А	O5'-P-OP1	-10.57	96.19	105.70
1	Х	1937	G	N3-C4-C5	-10.46	123.37	128.60
1	Х	1682	А	O5'-P-OP1	-10.44	96.30	105.70
1	Х	1466	С	N1-C2-O2	10.27	125.06	118.90
1	Х	169	С	N1-C2-O2	10.26	125.06	118.90
1	Х	2559	U	O5'-P-OP1	-10.13	96.58	105.70
1	Х	1288	А	O5'-P-OP2	-10.11	96.60	105.70
1	Х	1680	U	C5-C6-N1	-10.02	117.69	122.70
1	Х	1770	U	C5-C6-N1	-9.91	117.75	122.70
1	Х	1958	G	N9-C4-C5	-9.87	101.45	105.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1339	U	C5-C4-O4	-9.81	120.02	125.90
1	Х	1466	С	C2-N1-C1'	9.75	129.53	118.80
2	Y	39	С	N1-C2-O2	9.72	124.73	118.90
1	Х	1338	G	N3-C4-C5	-9.71	123.74	128.60
1	Х	1697	U	N3-C2-O2	-9.56	115.51	122.20
1	Х	1292	А	C8-N9-C4	9.40	109.56	105.80
1	Х	1291	G	C8-N9-C4	9.39	110.16	106.40
1	Х	1300	А	C2-N3-C4	9.38	115.29	110.60
2	Y	39	С	C2-N1-C1'	9.29	129.02	118.80
1	Х	2542	U	N3-C2-O2	-9.27	115.71	122.20
1	Х	2668	U	C2-N1-C1'	-9.25	106.60	117.70
1	Х	56	С	C2-N1-C1'	9.18	128.90	118.80
1	Х	2857	С	C6-N1-C2	-9.16	116.64	120.30
1	Х	2470	U	C2-N1-C1'	9.14	128.67	117.70
1	Х	1338	G	N3-C4-N9	9.14	131.48	126.00
1	Х	2675	U	N3-C2-O2	-9.11	115.82	122.20
1	Х	2551	А	C8-N9-C4	9.08	109.43	105.80
1	Х	2437	G	C8-N9-C4	-9.07	102.77	106.40
1	Х	583	С	C4-C5-C6	9.06	121.93	117.40
1	Х	1468	А	C8-N9-C4	-9.05	102.18	105.80
1	Х	2489	С	C5-C6-N1	9.05	125.52	121.00
1	Х	759	С	C5-C6-N1	9.04	125.52	121.00
1	Х	994	А	N1-C6-N6	-9.04	113.18	118.60
1	Х	2434	G	C8-N9-C4	-8.99	102.80	106.40
1	Х	1467	U	N1-C2-O2	8.87	129.01	122.80
1	Х	1995	G	N3-C4-N9	8.87	131.32	126.00
1	Х	1006	С	C6-N1-C2	-8.86	116.76	120.30
2	Υ	14	С	C6-N1-C2	-8.84	116.76	120.30
1	Х	343	А	O4'-C1'-N9	8.80	115.24	108.20
1	Х	1344	С	N1-C2-O2	8.80	124.18	118.90
1	X	2435	C	C6-N1-C2	8.77	123.81	120.30
1	X	2667	C	N3-C4-C5	8.74	125.40	121.90
1	X	2668	U	N1-C2-O2	-8.68	116.72	122.80
1	Х	2484	G	C4-C5-N7	8.68	114.27	110.80
1	X	2796	A	N1-C6-N6	-8.68	113.39	118.60
1	X	1467	U	N1-C2-N3	-8.68	109.69	114.90
1	X	484	G	C8-N9-C4	-8.67	102.93	106.40
1	X	2585	C	N1-C2-O2	8.61	124.06	118.90
1	X	1288	A	O5'-P-OP1	8.60	121.02	110.70
1	Х	1307	U	C5-C4-O4	-8.55	120.77	125.90
1	X	1697	U	N1-C2-O2	8.54	128.78	122.80
1	Х	2804	G	O5'-P-OP2	-8.54	98.02	105.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	559	С	C2-N1-C1'	8.53	128.19	118.80
1	Х	2681	А	C8-N9-C4	8.51	109.20	105.80
1	Х	689	А	N1-C6-N6	8.50	123.70	118.60
1	Х	1977	С	N1-C2-O2	8.50	124.00	118.90
1	Х	2040	А	C5-C6-N1	8.48	121.94	117.70
1	Х	540	G	C5-C6-O6	-8.45	123.53	128.60
1	Х	2499	С	C5-C6-N1	8.45	125.22	121.00
1	Х	1691	G	N3-C4-C5	-8.43	124.38	128.60
1	Х	2018	G	O4'-C1'-N9	8.43	114.94	108.20
1	Х	1265	G	N3-C4-C5	-8.39	124.40	128.60
1	Х	1675	С	O5'-P-OP2	8.39	120.76	110.70
1	Х	756	С	C6-N1-C2	-8.38	116.95	120.30
1	Х	1270	С	N3-C4-C5	-8.38	118.55	121.90
1	Х	2690	А	O5'-P-OP1	-8.35	98.19	105.70
1	Х	559	С	N1-C2-O2	8.33	123.90	118.90
1	Х	2828	С	C5-C6-N1	8.32	125.16	121.00
1	Х	1307	U	C4-C5-C6	-8.24	114.75	119.70
1	Х	219	G	P-O3'-C3'	8.23	129.57	119.70
1	Х	1466	С	C6-N1-C1'	-8.21	110.95	120.80
1	Х	1292	А	N7-C8-N9	-8.21	109.70	113.80
1	Х	1280	U	O5'-P-OP2	-8.19	98.33	105.70
1	Х	1308	С	C6-N1-C2	-8.18	117.03	120.30
1	Х	2434	G	C4-N9-C1'	8.18	137.13	126.50
1	Х	2470	U	N1-C2-O2	8.17	128.52	122.80
1	Х	2554	С	O5'-P-OP1	-8.12	98.39	105.70
1	Х	577	U	N3-C2-O2	-8.12	116.52	122.20
1	Х	56	С	N1-C2-O2	8.11	123.76	118.90
1	Х	2821	G	O5'-P-OP1	-8.08	98.43	105.70
1	Х	969	U	C5-C6-N1	-8.07	118.66	122.70
1	X	1172	U	C5-C6-N1	8.05	126.72	122.70
1	Х	2663	U	N1-C2-O2	-8.04	117.17	122.80
1	Х	592	G	C8-N9-C4	-8.02	103.19	106.40
1	Х	2551	А	N7-C8-N9	-8.01	109.79	113.80
1	Х	833	A	N1-C6-N6	7.99	123.39	118.60
1	Х	1717	А	N1-C6-N6	-7.98	113.81	118.60
1	X	2659	C	O5'-P-OP1	-7.97	98.52	105.70
1	X	2856	U	N1-C2-O2	-7.97	117.22	122.80
1	X	2484	G	C6-C5-N7	-7.97	125.62	130.40
1	Х	1468	A	N7-C8-N9	7.96	117.78	113.80
1	X	2543	A	N1-C6-N6	-7.95	113.83	118.60
1	X	2703	C	C6-N1-C2	-7.93	117.13	120.30
1	Х	1223	G	C4-N9-C1'	7.91	$1\overline{36.78}$	126.50



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	Х	583	С	C5-C6-N1	-7.89	117.05	121.00
1	Х	2531	U	C5-C4-O4	7.89	130.63	125.90
1	Х	1691	G	C8-N9-C4	-7.85	103.26	106.40
1	Х	1300	А	C5-C6-N1	7.84	121.62	117.70
1	Х	1684	G	C8-N9-C4	-7.82	103.27	106.40
1	Х	2470	U	C6-N1-C1'	-7.82	110.25	121.20
1	Х	1801	С	O5'-P-OP1	-7.82	98.66	105.70
1	Х	1338	G	C4-C5-C6	7.81	123.48	118.80
1	Х	2675	U	C6-N1-C2	-7.78	116.33	121.00
1	Х	1477	С	N3-C2-O2	-7.76	116.47	121.90
1	Х	2799	С	C6-N1-C2	-7.74	117.20	120.30
1	Х	1338	G	C4-N9-C1'	7.72	136.54	126.50
1	Х	1664	G	O5'-P-OP1	-7.71	98.76	105.70
1	Х	169	С	N3-C2-O2	-7.71	116.50	121.90
1	Х	884	С	N1-C2-O2	-7.70	114.28	118.90
1	Х	2533	U	N3-C4-C5	-7.68	110.00	114.60
1	Х	2796	А	N9-C4-C5	7.66	108.86	105.80
1	Х	1278	А	O4'-C1'-N9	7.65	114.32	108.20
1	Х	1697	U	C2-N1-C1'	7.64	126.87	117.70
1	Х	2040	А	C6-N1-C2	-7.63	114.02	118.60
1	Х	1972	G	C8-N9-C4	-7.62	103.35	106.40
1	Х	1696	С	N3-C2-O2	-7.59	116.58	121.90
1	Х	2847	G	C5-C6-O6	7.58	133.15	128.60
1	Х	1691	G	N3-C4-N9	7.57	130.54	126.00
1	Х	2531	U	C5-C6-N1	-7.57	118.92	122.70
1	Х	29	U	C5-C6-N1	7.57	126.48	122.70
1	Х	1989	С	C5-C6-N1	7.56	124.78	121.00
1	Х	2670	С	C6-N1-C2	-7.56	117.28	120.30
1	Х	1674	С	OP1-P-O3'	7.55	121.82	105.20
1	X	2797	G	N3-C4-N9	7.54	130.53	126.00
1	Х	958	G	O5'-P-OP1	-7.54	98.91	105.70
1	Х	1985	G	O5'-P-OP1	7.53	119.74	110.70
1	Х	1307	U	N3-C2-O2	7.53	127.47	122.20
1	X	1977	С	N3-C2-O2	-7.53	116.63	121.90
1	Х	527	С	C2-N1-C1'	7.53	127.08	118.80
1	X	577	U	C6-N1-C2	-7.52	116.49	121.00
1	X	1775	A	C8-N9-C4	7.51	108.81	105.80
1	X	2531	U	N1-C2-N3	7.50	119.40	114.90
1	Х	1750	А	O5'-P-OP1	-7.50	98.95	105.70
1	Х	538	A	C5-C6-N1	7.49	121.44	117.70
1	X	1691	G	C6-C5-N7	-7.49	125.91	130.40
1	Х	1656	U	C5-C6-N1	-7.48	118.96	122.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1743	С	N3-C4-C5	7.48	124.89	121.90
1	Х	1695	U	C2-N1-C1'	7.48	126.67	117.70
1	Х	1270	С	C6-N1-C2	-7.47	117.31	120.30
1	Х	2521	А	O5'-P-OP2	-7.47	98.98	105.70
1	Х	764	А	N1-C6-N6	-7.45	114.13	118.60
1	Х	1305	С	C6-N1-C2	7.44	123.28	120.30
1	Х	1786	С	C6-N1-C2	-7.44	117.32	120.30
1	Х	39	С	C5-C6-N1	7.42	124.71	121.00
1	Х	1223	G	C6-C5-N7	-7.42	125.95	130.40
1	Х	469	G	O4'-C1'-N9	7.42	114.14	108.20
1	Х	1249	G	C5-C6-O6	7.42	133.05	128.60
1	Х	39	С	C6-N1-C2	-7.41	117.33	120.30
1	Х	2674	С	N3-C4-C5	7.41	124.86	121.90
1	Х	2425	G	O5'-P-OP1	-7.40	99.04	105.70
1	Х	1683	G	N9-C4-C5	7.39	108.36	105.40
1	Х	994	А	C5-N7-C8	7.38	107.59	103.90
1	Х	504	G	C4-C5-N7	7.35	113.74	110.80
1	Х	2668	U	O5'-P-OP1	-7.33	99.10	105.70
1	Х	1937	G	N3-C4-N9	7.33	130.40	126.00
1	Х	1677	С	C6-N1-C2	7.32	123.23	120.30
1	Х	1636	G	N3-C4-C5	-7.31	124.94	128.60
1	Х	1467	U	C4-C5-C6	-7.30	115.32	119.70
1	Х	1037	U	N1-C2-O2	7.30	127.91	122.80
1	Х	1684	G	O5'-P-OP1	-7.28	99.14	105.70
1	Х	2847	G	N9-C4-C5	7.27	108.31	105.40
1	Х	1770	U	C4-C5-C6	7.26	124.06	119.70
1	Х	869	С	C6-N1-C2	-7.26	117.39	120.30
1	Х	1338	G	C6-C5-N7	-7.26	126.05	130.40
1	Х	2705	А	P-O3'-C3'	7.25	128.41	119.70
1	Х	2542	U	C5-C4-O4	7.24	130.25	125.90
1	Х	965	G	C8-N9-C4	-7.22	103.51	106.40
1	Х	1979	С	N3-C4-C5	7.22	124.79	121.90
1	X	2751	C	C6-N1-C2	7.22	123.19	120.30
1	Х	2704	U	N1-C2-N3	7.21	119.23	114.90
1	X	268	G	N9-C4-C5	-7.21	102.52	105.40
1	X	1339	U	N3-C4-O4	7.20	124.44	119.40
1	X	810	U	C5-C6-N1	7.20	126.30	122.70
1	Х	1279	G	O4'-C1'-N9	7.19	113.95	108.20
1	Х	2580	С	N3-C2-O2	-7.18	116.87	121.90
1	X	1574	A	04'-C1'-N9	7.17	113.94	108.20
1	X	2800	C	C2-N3-C4	7.17	123.48	119.90
1	Х	1974	U	C6-N1-C2	-7.17	116.70	121.00



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	Х	2681	А	N7-C8-N9	-7.16	110.22	113.80
1	Х	2031	А	C8-N9-C4	-7.16	102.94	105.80
1	Х	1691	G	C4-N9-C1'	7.16	135.80	126.50
2	Y	39	С	C6-N1-C1'	-7.14	112.23	120.80
1	Х	1984	А	O5'-P-OP1	-7.13	99.28	105.70
1	Х	1278	А	C5-C6-N1	-7.12	114.14	117.70
1	Х	994	А	C6-N1-C2	-7.12	114.33	118.60
1	Х	2484	G	N7-C8-N9	7.12	116.66	113.10
1	Х	2459	С	N1-C2-O2	-7.10	114.64	118.90
1	Х	2857	С	N3-C4-C5	-7.10	119.06	121.90
1	Х	18	U	N3-C2-O2	-7.09	117.23	122.20
1	Х	2484	G	C5-N7-C8	-7.09	100.75	104.30
1	Х	1497	С	C2-N3-C4	-7.09	116.36	119.90
1	Х	56	С	C6-N1-C1'	-7.08	112.31	120.80
1	Х	1696	С	N1-C2-O2	7.07	123.14	118.90
1	Х	2815	С	O5'-P-OP1	7.07	119.18	110.70
1	Х	994	А	C4-C5-N7	-7.06	107.17	110.70
1	Х	2043	А	OP2-P-O3'	7.06	120.73	105.20
1	Х	2492	G	O5'-P-OP2	-7.06	99.35	105.70
1	Х	959	С	C2-N1-C1'	7.05	126.55	118.80
1	Х	2815	С	O5'-P-OP2	-7.04	99.36	105.70
1	Х	2690	А	N1-C6-N6	7.04	122.83	118.60
1	Х	1680	U	C6-N1-C2	7.04	125.22	121.00
1	Х	1985	G	C4-C5-N7	7.04	113.61	110.80
1	Х	2668	U	C6-N1-C1'	7.04	131.05	121.20
1	Х	2838	U	N3-C2-O2	-7.03	117.28	122.20
1	Х	2672	U	O5'-P-OP1	-7.02	99.38	105.70
1	Х	2006	G	O5'-P-OP1	-7.01	99.39	105.70
1	Х	878	С	C6-N1-C2	-7.01	117.50	120.30
1	X	540	G	C4-C5-N7	7.00	113.60	110.80
1	Х	1278	A	N1-C2-N3	6.99	132.80	129.30
1	Х	1300	А	N1-C2-N3	-6.98	125.81	129.30
1	X	484	G	N7-C8-N9	6.96	116.58	113.10
1	Х	2821	G	C8-N9-C4	-6.95	103.62	106.40
1	Х	1765	С	N1-C2-O2	6.95	123.07	118.90
1	X	1301	U	N3-C4-C5	-6.91	110.45	114.60
1	X	2499	С	N3-C4-C5	-6.91	119.14	121.90
1	X	2550	С	C6-N1-C2	-6.91	117.54	120.30
1	Х	1663	С	N1-C2-O2	6.91	123.04	118.90
1	X	2472	U	C6-N1-C2	-6.90	116.86	121.00
1	Х	1750	A	C6-N1-C2	-6.89	114.47	118.60
1	Х	2019	С	N1-C2-O2	6.88	123.03	118.90



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	Х	972	С	N3-C2-O2	-6.88	117.09	121.90
1	Х	268	G	N3-C4-N9	6.87	130.12	126.00
1	Х	1391	А	P-O3'-C3'	6.87	127.95	119.70
1	Х	2537	С	C6-N1-C2	-6.86	117.56	120.30
1	Х	2010	G	O5'-P-OP2	-6.85	99.53	105.70
1	Х	1958	G	C4-C5-N7	6.85	113.54	110.80
1	Х	1497	С	N1-C2-O2	-6.83	114.80	118.90
1	Х	2847	G	C4-C5-N7	-6.82	108.07	110.80
1	Х	956	А	C8-N9-C4	-6.81	103.08	105.80
1	Х	1407	G	C4-N9-C1'	6.81	135.35	126.50
2	Y	69	G	O5'-P-OP2	-6.80	99.58	105.70
1	Х	2585	С	N3-C2-O2	-6.80	117.14	121.90
1	Х	2019	С	N3-C2-O2	-6.80	117.14	121.90
1	Х	1681	А	O4'-C1'-N9	-6.79	102.77	108.20
1	Х	1665	С	C6-N1-C2	6.77	123.01	120.30
1	Х	507	А	N1-C6-N6	-6.75	114.55	118.60
1	Х	2434	G	N3-C4-C5	-6.75	125.22	128.60
1	Х	489	А	N1-C6-N6	-6.75	114.55	118.60
1	Х	1973	С	N1-C2-O2	6.75	122.95	118.90
1	Х	2036	G	C8-N9-C4	-6.74	103.70	106.40
1	Х	1265	G	N3-C4-N9	6.72	130.03	126.00
1	Х	484	G	N3-C4-C5	-6.71	125.25	128.60
1	Х	1335	А	C8-N9-C4	6.71	108.48	105.80
1	Х	2800	С	N1-C2-O2	6.71	122.92	118.90
2	Y	14	С	C5-C6-N1	6.71	124.35	121.00
1	Х	2658	А	OP2-P-O3'	6.69	119.92	105.20
1	Х	1671	А	OP2-P-O3'	6.68	119.89	105.20
1	Х	1997	А	C4-C5-C6	6.68	120.34	117.00
1	Х	587	А	C4-C5-N7	-6.67	107.36	110.70
1	Х	1688	U	N3-C4-O4	6.66	124.06	119.40
1	Х	595	А	O5'-P-OP1	-6.66	99.70	105.70
1	Х	975	С	C6-N1-C2	-6.66	117.64	120.30
1	Х	1855	G	C6-C5-N7	-6.65	126.41	130.40
1	Х	2523	G	C8-N9-C4	-6.64	103.74	106.40
1	Х	2558	С	OP1-P-O3'	6.64	119.82	105.20
1	Х	1338	G	C8-N9-C1'	-6.64	118.37	127.00
1	X	2542	U	C6-N1-C2	-6.63	117.02	121.00
1	X	2557	G	OP1-P-O3'	6.63	119.78	105.20
1	Х	2822	U	N3-C4-O4	6.63	124.04	119.40
1	X	776	G	C8-N9-C4	-6.62	103.75	106.40
1	Х	2034	А	C5-N7-C8	-6.62	100.59	103.90
28	3	60	LEU	CA-CB-CG	6.61	130.50	115.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1855	G	N3-C4-N9	6.61	129.97	126.00
1	Х	1345	G	C8-N9-C4	-6.60	103.76	106.40
1	Х	1994	U	C5-C4-O4	-6.59	121.94	125.90
1	Х	1213	U	C5-C6-N1	6.58	125.99	122.70
1	Х	2531	U	C2-N1-C1'	-6.58	109.81	117.70
1	Х	1670	G	C8-N9-C4	6.58	109.03	106.40
1	Х	1223	G	C8-N9-C1'	-6.57	118.46	127.00
1	Х	1265	G	C4-N9-C1'	6.57	135.03	126.50
1	Х	1684	G	N3-C4-N9	-6.57	122.06	126.00
1	Х	2466	G	C6-C5-N7	-6.56	126.47	130.40
1	Х	1683	G	N3-C4-N9	-6.56	122.07	126.00
1	Х	2005	U	C5-C6-N1	-6.55	119.42	122.70
1	Х	2419	С	N1-C2-O2	6.55	122.83	118.90
1	Х	591	G	C8-N9-C4	6.54	109.02	106.40
1	Х	2235	G	N1-C6-O6	6.54	123.83	119.90
1	Х	940	G	C4-N9-C1'	-6.54	118.00	126.50
1	Х	2255	G	C4-C5-N7	-6.54	108.18	110.80
1	Х	1326	U	C2-N1-C1'	6.54	125.54	117.70
1	Х	343	А	C4-C5-C6	6.53	120.27	117.00
1	Х	1819	U	N3-C2-O2	-6.53	117.63	122.20
1	Х	1475	U	C2-N1-C1'	6.53	125.53	117.70
1	Х	1984	А	O5'-P-OP2	6.53	118.53	110.70
1	Х	2699	G	N3-C2-N2	-6.53	115.33	119.90
1	Х	559	С	OP1-P-O3'	6.52	119.55	105.20
1	Х	2489	С	N1-C2-N3	6.52	123.77	119.20
1	Х	2042	А	C8-N9-C4	6.52	108.41	105.80
1	Х	2624	G	C8-N9-C4	-6.51	103.79	106.40
1	Х	1686	А	N1-C2-N3	6.50	132.55	129.30
1	Х	2667	С	C2-N3-C4	-6.50	116.65	119.90
1	Х	219	G	OP2-P-O3'	6.49	119.49	105.20
1	Х	499	G	N3-C4-C5	-6.49	125.35	128.60
1	Х	1958	G	C8-N9-C4	6.49	109.00	106.40
1	Х	2543	А	N9-C4-C5	6.49	108.40	105.80
1	Х	1668	G	C6-C5-N7	-6.49	126.51	130.40
1	Х	1291	G	N7-C8-N9	-6.49	109.86	113.10
1	X	$13\overline{45}$	G	N7-C8-N9	6.49	116.34	113.10
1	Х	1006	C	N3-C2-O2	-6.48	117.36	121.90
1	Х	1333	G	C8-N9-C4	-6.48	103.81	106.40
1	X	2010	G	N1-C6-O6	-6.48	116.01	119.90
1	Х	2015	G	C4-N9-C1	-6.48	118.08	126.50
1	Х	2043	A	C2-N3-C4	6.48	113.84	110.60
1	Х	2702	G	N3-C4-N9	6.47	129.88	126.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2808	U	O5'-P-OP1	-6.47	99.88	105.70
1	Х	803	С	O5'-P-OP1	-6.47	99.88	105.70
1	Х	1918	G	C8-N9-C4	-6.46	103.81	106.40
1	Х	2408	G	C8-N9-C4	-6.45	103.82	106.40
1	Х	1958	G	N1-C6-O6	6.45	123.77	119.90
1	Х	1428	G	N3-C2-N2	-6.45	115.38	119.90
1	Х	617	U	N3-C2-O2	-6.45	117.69	122.20
1	Х	1973	С	N3-C2-O2	-6.45	117.39	121.90
1	Х	2598	С	N1-C2-O2	-6.45	115.03	118.90
1	Х	2443	С	C6-N1-C2	-6.44	117.72	120.30
1	Х	1278	А	C5-C6-N6	6.44	128.85	123.70
2	Y	39	С	N3-C2-O2	-6.44	117.39	121.90
1	Х	69	G	N3-C4-N9	6.43	129.86	126.00
1	Х	2488	G	C2-N3-C4	6.43	115.11	111.90
1	Х	756	С	N3-C4-C5	-6.43	119.33	121.90
1	Х	761	G	O4'-C1'-N9	6.42	113.34	108.20
1	Х	2298	U	N1-C2-O2	6.42	127.30	122.80
1	Х	1035	G	C8-N9-C4	-6.42	103.83	106.40
1	Х	1206	G	N3-C4-C5	6.42	131.81	128.60
2	Y	69	G	N3-C4-N9	6.42	129.85	126.00
1	Х	1685	А	N1-C6-N6	-6.41	114.75	118.60
1	Х	1340	С	N1-C2-O2	-6.40	115.06	118.90
1	Х	1224	А	C8-N9-C4	6.39	108.36	105.80
1	Х	1770	U	O4'-C1'-N1	6.39	113.31	108.20
1	Х	1407	G	C6-C5-N7	-6.38	126.57	130.40
1	Х	2799	С	N1-C2-N3	6.38	123.67	119.20
1	Х	1687	С	C5-C6-N1	-6.38	117.81	121.00
1	Х	2671	С	C6-N1-C2	-6.38	117.75	120.30
1	Х	2848	A	C4-C5-C6	6.38	120.19	117.00
1	Х	1684	G	N7-C8-N9	6.38	116.29	113.10
1	Х	1786	С	C5-C6-N1	6.38	124.19	121.00
1	Х	1995	G	N9-C4-C5	-6.38	102.85	105.40
1	Х	940	G	C6-C5-N7	6.37	134.22	130.40
1	Х	2589	С	O5'-P-OP1	-6.37	99.97	105.70
1	Х	527	С	C5-C6-N1	6.37	124.18	121.00
1	X	2848	A	OP1-P-O3'	6.37	119.21	105.20
1	X	583	С	N1-C2-O2	-6.35	115.09	118.90
1	X	1475	U	P-O3'-C3'	6.35	127.31	119.70
1	X	2015	G	C4-C5-C6	-6.34	114.99	118.80
1	Х	487	G	N9-C4-C5	6.33	107.93	105.40
1	X	2026	C	C6-N1-C2	-6.32	117.77	120.30
1	Х	559	С	C6-N1-C1'	-6.31	113.23	120.80

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1660	G	C4-C5-N7	-6.31	108.28	110.80
1	Х	519	С	C5-C6-N1	6.29	124.15	121.00
1	Х	699	G	N3-C4-C5	6.29	131.75	128.60
1	Х	1279	G	N3-C2-N2	6.29	124.31	119.90
1	Х	1475	U	C5-C6-N1	6.29	125.84	122.70
1	Х	992	А	O5'-P-OP2	-6.28	100.05	105.70
1	Х	1681	А	C8-N9-C4	-6.28	103.29	105.80
1	Х	1688	U	C5-C6-N1	6.28	125.84	122.70
1	Х	2841	U	N3-C2-O2	-6.27	117.81	122.20
1	Х	2531	U	N3-C4-O4	-6.27	115.01	119.40
1	Х	1687	С	C5-C4-N4	6.27	124.59	120.20
1	Х	1346	С	N3-C2-O2	-6.26	117.51	121.90
1	Х	2255	G	OP1-P-O3'	6.26	118.98	105.20
1	Х	1249	G	N1-C6-O6	-6.26	116.15	119.90
1	Х	1974	U	N1-C2-N3	6.26	118.65	114.90
1	Х	56	С	C5-C6-N1	6.25	124.12	121.00
1	Х	1830	С	P-O3'-C3'	6.25	127.20	119.70
1	Х	2818	G	C8-N9-C4	-6.25	103.90	106.40
1	Х	981	С	C2-N1-C1'	6.25	125.67	118.80
1	Х	559	С	N3-C2-O2	-6.24	117.53	121.90
1	Х	1293	А	C5-C6-N1	6.24	120.82	117.70
1	Х	2694	G	OP2-P-O3'	6.24	118.93	105.20
1	Х	2694	G	O5'-P-OP2	6.23	118.18	110.70
1	Х	2674	С	C6-N1-C2	6.23	122.79	120.30
1	Х	1636	G	N3-C4-N9	6.22	129.73	126.00
1	Х	2530	С	C6-N1-C2	-6.21	117.81	120.30
2	Y	55	С	N1-C2-O2	6.21	122.62	118.90
1	Х	2402	U	N3-C2-O2	-6.20	117.86	122.20
1	Х	2867	G	C5-N7-C8	-6.19	101.21	104.30
1	Х	2820	С	OP2-P-O3'	6.18	118.81	105.20
1	Х	574	С	C5-C6-N1	6.18	124.09	121.00
1	Х	2691	С	OP2-P-O3'	6.18	118.80	105.20
1	Х	1015	U	N3-C2-O2	-6.18	117.88	122.20
1	Х	69	G	C4-N9-C1'	6.17	134.53	126.50
1	Х	2847	G	OP1-P-OP2	6.17	128.86	119.60
1	Х	1670	G	N7-C8-N9	-6.17	110.01	113.10
1	Х	486	U	C2-N1-C1'	6.17	125.10	117.70
1	Х	2445	С	N3-C4-C5	-6.17	119.43	121.90
1	Х	2469	G	C8-N9-C4	-6.17	103.93	106.40
1	Х	1467	U	C6-N1-C1'	-6.16	112.57	121.20
1	Х	1679	U	O5'-P-OP1	6.16	118.10	110.70
1	Х	1635	G	C2-N3-C4	6.16	114.98	111.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2664	G	C2-N3-C4	6.16	114.98	111.90
1	Х	787	А	C2-N3-C4	-6.15	107.52	110.60
1	Х	1258	G	C8-N9-C4	-6.15	103.94	106.40
1	Х	1986	G	N1-C6-O6	-6.15	116.21	119.90
1	Х	586	G	C4-N9-C1'	6.14	134.49	126.50
1	Х	841	G	C2-N3-C4	-6.14	108.83	111.90
1	Х	69	G	N3-C4-C5	-6.14	125.53	128.60
1	Х	1668	G	N1-C6-O6	6.14	123.58	119.90
1	Х	2564	U	C2-N1-C1'	6.14	125.06	117.70
1	Х	1327	С	C2-N1-C1'	6.13	125.54	118.80
1	Х	2627	G	N1-C6-O6	6.13	123.58	119.90
1	Х	1309	G	N3-C4-C5	-6.13	125.53	128.60
1	Х	1630	А	C4-C5-C6	6.13	120.06	117.00
12	Κ	28	LEU	CA-CB-CG	6.13	129.40	115.30
1	Х	1958	G	C6-C5-N7	-6.12	126.72	130.40
1	Х	972	С	O5'-P-OP1	-6.12	100.19	105.70
1	Х	1660	G	N9-C4-C5	6.12	107.85	105.40
1	Х	19	С	C6-N1-C2	-6.11	117.86	120.30
1	Х	504	G	C5-N7-C8	-6.11	101.24	104.30
1	Х	1643	А	N9-C4-C5	-6.11	103.35	105.80
1	Х	1328	С	C6-N1-C2	-6.10	117.86	120.30
1	Х	689	А	C6-C5-N7	-6.09	128.04	132.30
1	Х	35	G	O5'-P-OP2	-6.09	100.22	105.70
1	Х	2857	С	N3-C2-O2	-6.08	117.64	121.90
1	Х	2554	С	O5'-P-OP2	6.08	117.99	110.70
1	Х	1673	С	C5-C6-N1	6.07	124.04	121.00
1	Х	2463	G	C2-N3-C4	6.07	114.94	111.90
1	Х	1240	G	C6-C5-N7	-6.07	126.76	130.40
1	Х	587	A	N9-C4-C5	6.06	108.22	105.80
1	Х	29	U	N3-C4-O4	6.06	123.64	119.40
1	Х	940	G	C8-N9-C1'	6.06	134.87	127.00
1	Х	1855	G	C8-N9-C1'	-6.06	119.12	127.00
1	X	1963	G	N9-C4-C5	6.06	107.82	105.40
1	X	1958	G	N3-C4-N9	6.05	129.63	126.00
1	X	2463	G	N3-C4-C5	-6.05	125.58	128.60
1	Х	1644	G	N9-C4-C5	-6.05	102.98	105.40
1	Х	2827	G	N3-C4-C5	-6.05	125.58	128.60
1	X	526	С	OP1-P-O3'	6.05	118.51	105.20
1	Х	1958	G	C8-N9-C1'	-6.04	119.14	127.00
1	X	2029	G	N1-C6-O6	6.04	123.53	119.90
1	X	1660	G	N3-C4-C5	-6.04	125.58	128.60
1	Х	1673	С	C4-C5-C6	-6.04	114.38	117.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Y	14	С	OP2-P-O3'	6.03	118.48	105.20
2	Y	58	G	C4-N9-C1'	6.03	134.34	126.50
1	Х	29	U	C5-C4-O4	-6.03	122.28	125.90
1	Х	35	G	O4'-C1'-N9	6.03	113.03	108.20
1	Х	852	U	C5-C6-N1	-6.03	119.69	122.70
1	Х	1998	А	N1-C2-N3	6.03	132.31	129.30
1	Х	2232	G	C4-N9-C1'	6.03	134.33	126.50
1	Х	264	U	C2-N1-C1'	6.02	124.93	117.70
1	Х	343	А	C4-N9-C1'	6.02	137.14	126.30
1	Х	1765	С	N3-C2-O2	-6.02	117.68	121.90
1	Х	1217	U	N3-C2-O2	-6.02	117.98	122.20
1	Х	2668	U	N3-C4-O4	-6.01	115.19	119.40
1	Х	2695	С	OP2-P-O3'	6.01	118.43	105.20
1	Х	268	G	C4-C5-N7	6.01	113.20	110.80
1	Х	2034	А	C4-C5-N7	6.01	113.71	110.70
1	Х	927	С	C5-C6-N1	6.01	124.00	121.00
1	Х	1981	А	N1-C2-N3	6.01	132.30	129.30
1	Х	2531	U	C6-N1-C1'	6.01	129.61	121.20
1	Х	994	А	N9-C4-C5	5.99	108.20	105.80
1	Х	812	G	C8-N9-C4	-5.99	104.00	106.40
1	Х	1755	G	O5'-P-OP2	-5.99	100.31	105.70
1	Х	1760	G	C4-C5-N7	5.99	113.20	110.80
1	Х	1721	G	N3-C4-N9	-5.99	122.41	126.00
1	Х	2848	А	N9-C4-C5	5.99	108.19	105.80
1	Х	1974	U	N3-C2-O2	-5.99	118.01	122.20
1	Х	1855	G	C4-N9-C1'	5.98	134.28	126.50
1	Х	1310	С	O5'-P-OP1	-5.98	100.32	105.70
1	Х	1467	U	O5'-P-OP1	-5.98	100.32	105.70
1	Х	381	С	C2-N1-C1'	5.98	125.38	118.80
1	Х	523	А	C8-N9-C4	5.98	108.19	105.80
1	X	1655	C	C6-N1-C2	5.97	122.69	120.30
1	X	1770	U	C2-N1-C1'	-5.97	110.54	117.70
1	X	1664	G	O5'-P-OP2	5.97	117.86	110.70
1	X	$2\overline{255}$	G	N1-C6-O6	-5.96	116.32	119.90
1	X	2673	G	C8-N9-C4	-5.96	104.02	106.40
1	X	749	C	C6-N1-C2	-5.96	117.92	120.30
1	X	2848	A	C8-N9-C4	-5.96	103.42	105.80
1	X	1309	G	C5-C6-N1	5.96	114.48	111.50
1	X	530	G	O5'-P-OP1	-5.95	100.35	105.70
1	Х	1683	G	C5-C6-O6	5.95	132.17	128.60
1	X	587	A	N1-C6-N6	-5.94	115.04	118.60
1	Х	2624	G	N7-C8-N9	5.94	116.07	113.10


Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1750	А	C4-C5-C6	5.94	119.97	117.00
1	Х	2671	С	N3-C2-O2	-5.94	117.74	121.90
1	Х	2788	С	OP1-P-O3'	5.94	118.26	105.20
1	Х	1627	С	C6-N1-C2	-5.93	117.93	120.30
1	Х	458	G	O4'-C1'-N9	5.93	112.95	108.20
1	Х	1691	G	C5-C6-N1	5.93	114.47	111.50
2	Y	14	С	P-O3'-C3'	5.93	126.81	119.70
1	Х	1217	U	N1-C2-N3	5.93	118.46	114.90
1	Х	1644	G	C5-C6-O6	-5.92	125.05	128.60
1	Х	587	А	C5-N7-C8	5.92	106.86	103.90
1	Х	1284	G	O5'-P-OP1	5.91	117.80	110.70
1	Х	836	G	N9-C4-C5	5.91	107.76	105.40
1	Х	1681	А	OP2-P-O3'	5.91	118.20	105.20
1	Х	2593	А	C2-N3-C4	5.91	113.55	110.60
1	Х	1718	А	O5'-P-OP1	-5.91	100.39	105.70
1	Х	2690	А	C4-C5-N7	5.90	113.65	110.70
1	Х	930	А	N1-C6-N6	-5.90	115.06	118.60
1	Х	1354	А	N1-C6-N6	5.90	122.14	118.60
1	Х	959	С	C6-N1-C2	-5.89	117.94	120.30
1	Х	2539	С	C5-C6-N1	5.89	123.95	121.00
1	Х	1656	U	C6-N1-C2	5.89	124.53	121.00
1	Х	1691	G	C4-C5-N7	5.89	113.16	110.80
1	Х	2606	G	C8-N9-C4	-5.89	104.05	106.40
1	Х	1265	G	C8-N9-C4	-5.88	104.05	106.40
1	Х	2666	U	N3-C4-C5	-5.88	111.07	114.60
1	Х	2822	U	C5-C4-O4	-5.88	122.37	125.90
1	Х	678	G	O5'-P-OP1	-5.88	100.41	105.70
1	Х	2542	U	N3-C4-C5	-5.88	111.07	114.60
1	Х	1977	С	O5'-P-OP1	-5.88	100.41	105.70
1	Х	1676	U	N1-C2-O2	-5.87	118.69	122.80
1	X	1217	U	C2-N3-C4	-5.87	123.48	127.00
1	Х	2232	G	C6-C5-N7	-5.87	126.88	130.40
1	Х	576	А	N1-C6-N6	-5.86	115.08	118.60
1	Х	2580	C	N3-C4-C5	-5.86	119.56	121.90
1	Х	343	A	N1-C2-N3	5.86	132.23	129.30
1	X	860	U	C2-N1-C1	5.86	124.73	117.70
1	Х	1037	U	N3-C2-O2	-5.86	118.10	122.20
1	Х	2530	С	N3-C4-C5	-5.85	119.56	121.90
1	X	2408	G	N3-C4-C5	-5.85	125.67	128.60
1	Х	1404	С	C6-N1-C2	5.85	122.64	120.30
1	Х	1010	U	N3-C2-O2	-5.84	118.11	122.20
1	Х	1249	G	C4-C5-N7	-5.84	108.46	110.80



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2021	G	O5'-P-OP1	-5.84	100.44	105.70
1	Х	2434	G	C8-N9-C1'	-5.84	119.41	127.00
8	G	166	LEU	CA-CB-CG	5.84	128.72	115.30
1	Х	1339	U	C2-N1-C1'	5.83	124.70	117.70
1	Х	1206	G	N3-C4-N9	-5.83	122.50	126.00
1	Х	2445	С	C2-N1-C1'	5.83	125.21	118.80
1	Х	699	G	C5-N7-C8	-5.83	101.39	104.30
1	Х	527	С	N3-C2-O2	-5.82	117.83	121.90
1	Х	1155	G	C8-N9-C4	5.82	108.73	106.40
1	Х	1681	А	N7-C8-N9	5.82	116.71	113.80
1	Х	1466	С	N3-C2-O2	-5.81	117.83	121.90
1	Х	1020	А	N1-C6-N6	-5.81	115.11	118.60
1	Х	2598	С	OP1-P-O3'	5.81	117.98	105.20
1	Х	2702	G	N3-C4-C5	-5.81	125.70	128.60
1	Х	1976	U	N3-C4-C5	5.81	118.08	114.60
1	Х	460	U	C6-N1-C2	-5.80	117.52	121.00
1	Х	1935	А	C8-N9-C4	-5.80	103.48	105.80
1	Х	2041	А	N9-C4-C5	-5.80	103.48	105.80
2	Y	93	G	N9-C4-C5	-5.80	103.08	105.40
1	Х	277	G	N3-C4-N9	5.80	129.48	126.00
1	Х	2622	G	N3-C4-N9	5.80	129.48	126.00
1	Х	2482	А	O5'-P-OP2	5.80	117.66	110.70
1	Х	2557	G	N9-C4-C5	5.79	107.72	105.40
1	Х	484	G	C6-C5-N7	-5.79	126.93	130.40
1	Х	1709	U	N3-C2-O2	-5.79	118.15	122.20
1	Х	2030	U	N1-C2-O2	-5.79	118.75	122.80
1	Х	837	U	C5-C6-N1	-5.79	119.81	122.70
1	Х	2235	G	C4-C5-N7	5.78	113.11	110.80
1	Х	2263	С	N1-C2-O2	5.78	122.37	118.90
1	Х	1258	G	N9-C4-C5	5.78	107.71	105.40
1	Х	1668	G	C5-C6-N1	-5.78	108.61	111.50
1	Х	967	G	O5'-P-OP2	-5.78	100.50	105.70
1	Х	1167	А	C2-N3-C4	5.78	113.49	110.60
1	Х	2611	A	C8-N9-C4	5.78	108.11	105.80
1	Х	2434	G	N7-C8-N9	5.77	115.99	113.10
1	X	1278	A	N3-C4-N9	-5.77	122.79	127.40
1	Х	1669	A	C2-N3-C4	-5.77	107.72	110.60
1	Х	2702	G	C8-N9-C1'	-5.77	119.50	127.00
1	X	2430	A	N1-C2-N3	5.77	132.18	129.30
1	Х	1671	A	C8-N9-C4	5.76	108.11	105.80
2	Y	17	A	O4'-C1'-N9	5.76	112.81	108.20
1	Х	2828	С	C2-N3-C4	5.76	122.78	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2460	G	P-O3'-C3'	5.76	126.61	119.70
1	Х	2856	U	N3-C2-O2	5.76	126.23	122.20
1	Х	967	G	C8-N9-C4	-5.76	104.10	106.40
1	Х	495	С	N3-C4-C5	5.75	124.20	121.90
1	Х	2041	А	O4'-C1'-N9	-5.75	103.60	108.20
1	Х	1989	С	C2-N1-C1'	5.75	125.12	118.80
1	Х	2015	G	N3-C4-C5	5.75	131.47	128.60
1	Х	2698	G	OP1-P-O3'	5.75	117.84	105.20
1	Х	800	U	O5'-P-OP2	-5.74	100.53	105.70
1	Х	1937	G	C4-N9-C1'	5.74	133.96	126.50
1	Х	2702	G	N3-C2-N2	5.73	123.91	119.90
1	Х	1407	G	C8-N9-C1'	-5.73	119.55	127.00
1	Х	818	G	C4-C5-N7	5.73	113.09	110.80
1	Х	2232	G	N7-C8-N9	5.73	115.97	113.10
1	Х	24	G	OP1-P-O3'	5.73	117.80	105.20
1	Х	2627	G	C6-C5-N7	-5.73	126.96	130.40
1	Х	2004	U	C6-N1-C2	5.72	124.44	121.00
2	Y	69	G	N3-C4-C5	-5.72	125.74	128.60
1	Х	2564	U	C6-N1-C2	-5.72	117.57	121.00
1	Х	2822	U	C2-N1-C1'	5.72	124.56	117.70
1	Х	763	А	O5'-P-OP2	5.71	117.56	110.70
1	Х	1709	U	N1-C2-O2	5.71	126.80	122.80
1	Х	797	А	O5'-P-OP2	-5.71	100.56	105.70
1	Х	2409	А	C4-C5-N7	5.71	113.56	110.70
1	Х	1161	U	C2-N1-C1'	5.71	124.55	117.70
1	Х	2402	U	N1-C2-O2	5.71	126.79	122.80
1	Х	2430	А	C2-N3-C4	-5.71	107.75	110.60
1	Х	2702	G	C5-C6-N1	5.70	114.35	111.50
1	Х	2830	U	C5-C6-N1	5.70	125.55	122.70
1	X	2541	U	N3-C2-O2	-5.70	118.21	122.20
1	Х	559	С	P-O3'-C3'	5.70	126.53	119.70
1	Х	2573	С	C6-N1-C2	-5.70	118.02	120.30
1	X	878	C	C5-C6-N1	5.69	123.85	121.00
1	Х	1935	A	N9-C4-C5	5.69	108.08	105.80
1	Х	1750	А	N1-C2-N3	5.69	132.15	129.30
1	X	818	G	N9-C4-C5	-5.69	103.12	105.40
1	X	921	A	C2-N3-C4	5.68	113.44	110.60
1	X	1333	G	C5-N7-C8	-5.68	101.46	104.30
1	Х	932	G	C8-N9-C4	5.68	108.67	106.40
1	X	1217	U	C5-C6-N1	-5.68	119.86	122.70
1	X	2564	U	N3-C2-O2	-5.68	118.22	122.20
1	Х	1680	U	C2-N1-C1'	-5.67	110.89	117.70



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	Х	302	U	C2-N1-C1'	5.67	124.51	117.70
1	Х	679	С	C6-N1-C2	-5.67	118.03	120.30
1	Х	1958	G	C5-C6-O6	-5.67	125.20	128.60
1	Х	2543	А	C8-N9-C4	-5.67	103.53	105.80
1	Х	1685	А	OP1-P-OP2	5.66	128.09	119.60
1	Х	679	С	N3-C2-O2	-5.66	117.94	121.90
1	Х	1691	G	N7-C8-N9	5.66	115.93	113.10
1	Х	1036	G	N1-C6-O6	-5.66	116.50	119.90
1	Х	2830	U	C5-C4-O4	-5.66	122.51	125.90
1	Х	343	A	P-O3'-C3'	5.65	126.48	119.70
1	Х	343	A	C6-C5-N7	-5.65	128.34	132.30
1	Х	1704	G	C8-N9-C4	-5.65	104.14	106.40
1	Х	2701	A	N9-C4-C5	5.65	108.06	105.80
1	Х	2797	G	N1-C2-N2	-5.65	111.11	116.20
1	Х	1473	U	P-O3'-C3'	5.65	126.48	119.70
1	Х	2011	U	C6-N1-C2	-5.64	117.62	121.00
1	Х	1687	C	N3-C4-N4	-5.63	114.06	118.00
1	Х	2855	C	C4-C5-C6	-5.63	114.58	117.40
1	Х	2867	G	N7-C8-N9	5.63	115.92	113.10
1	Х	533	C	N1-C2-O2	5.63	122.28	118.90
1	Х	2673	G	N9-C4-C5	5.63	107.65	105.40
1	Х	2432	A	C8-N9-C4	-5.63	103.55	105.80
1	Х	2561	G	N3-C4-N9	5.62	129.37	126.00
1	Х	759	C	C2-N3-C4	5.62	122.71	119.90
1	Х	931	G	N3-C4-N9	5.62	129.37	126.00
1	Х	1985	G	C5-N7-C8	-5.62	101.49	104.30
1	Х	2691	С	C2-N1-C1'	-5.62	112.62	118.80
1	Х	2832	G	C8-N9-C1'	5.62	134.30	127.00
1	Х	2854	G	C4-C5-N7	5.62	113.05	110.80
1	Х	268	G	C5-C6-O6	-5.62	125.23	128.60
1	Х	2534	U	C5-C6-N1	5.62	125.51	122.70
1	Х	2001	G	N9-C4-C5	-5.61	103.15	105.40
1	Х	2708	U	O5'-P-OP1	-5.61	100.65	105.70
1	Х	1937	G	C2-N3-C4	5.61	114.70	111.90
1	Х	2423	G	OP2-P-O3'	5.61	117.54	105.20
1	X	460	U	N3-C4-C5	-5.61	111.24	114.60
1	X	2814	G	C4-C5-N7	-5.61	108.56	110.80
1	X	540	G	N9-C4-C5	-5.60	103.16	105.40
1	Х	1333	G	N7-C8-N9	5.60	115.90	113.10
1	X	2041	A	C8-N9-C1'	-5.60	117.62	127.70
1	X	100	G	P-O3'-C3'	$5.\overline{60}$	126.42	119.70
1	Х	1226	A	N1-C6-N6	5.60	121.96	118.60



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2042	А	C5-C6-N1	-5.60	114.90	117.70
1	Х	2564	U	C5-C6-N1	5.60	125.50	122.70
1	Х	362	С	N1-C2-O2	5.59	122.26	118.90
1	Х	937	С	C6-N1-C2	-5.59	118.06	120.30
1	Х	2015	G	C8-N9-C1'	5.59	134.27	127.00
1	Х	2692	А	N1-C6-N6	5.59	121.96	118.60
1	Х	699	G	N3-C4-N9	-5.59	122.64	126.00
1	Х	1937	G	C8-N9-C4	-5.58	104.17	106.40
1	Х	1307	U	N1-C2-N3	-5.58	111.55	114.90
1	Х	13	А	N9-C4-C5	5.58	108.03	105.80
1	Х	1681	А	O5'-P-OP1	-5.58	100.68	105.70
1	Х	484	G	N3-C4-N9	5.57	129.34	126.00
1	Х	1223	G	C4-C5-C6	5.57	122.14	118.80
1	Х	833	А	C6-C5-N7	-5.57	128.40	132.30
1	Х	2037	А	N1-C6-N6	-5.57	115.26	118.60
1	Х	495	С	C4-C5-C6	-5.57	114.62	117.40
1	Х	1708	С	C6-N1-C2	5.57	122.53	120.30
1	Х	1684	G	C5-N7-C8	-5.56	101.52	104.30
1	Х	2042	А	N9-C4-C5	-5.56	103.58	105.80
1	Х	2797	G	C6-C5-N7	-5.56	127.07	130.40
1	Х	2843	А	OP2-P-O3'	5.56	117.43	105.20
1	Х	1778	U	N3-C2-O2	-5.55	118.31	122.20
1	Х	2466	G	C4-N9-C1'	5.55	133.72	126.50
1	Х	1242	А	C8-N9-C4	5.55	108.02	105.80
1	Х	2027	С	C6-N1-C2	-5.55	118.08	120.30
1	Х	2871	U	C5-C6-N1	5.54	125.47	122.70
1	Х	1230	С	O5'-P-OP1	-5.54	100.71	105.70
1	Х	1269	G	O5'-P-OP1	-5.54	100.71	105.70
1	Х	1981	А	C4-C5-C6	5.54	119.77	117.00
1	Х	1407	G	N7-C8-N9	5.54	115.87	113.10
1	X	2036	G	OP1-P-OP2	-5.54	111.29	119.60
1	X	1253	C	C6-N1-C2	-5.54	118.08	120.30
1	X	1995	G	N3-C4-C5	-5.54	125.83	128.60
1	X	689	A	C4-C5-C6	5.54	119.77	117.00
1	X	2845	C	OP2-P-O3'	5.54	117.38	105.20
1	X	15	G	$C4-\overline{N9-C1}$	-5.53	119.31	126.50
1	X	2867	G	C4-C5-N7	5.53	113.01	110.80
1	Х	1235	C	C6-N1-C2	5.53	122.51	120.30
1	Х	2702	G	N1-C2-N2	-5.53	111.22	116.20
1	X	544	U	N3-C2-O2	-5.53	118.33	122.20
1	X	1288	A	N1-C6-N6	5.53	121.92	118.60
25	Ζ	49	CYS	CA-CB-SG	5.53	123.95	114.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	27	G	O4'-C1'-N9	5.52	112.62	108.20
1	Х	1773	С	N1-C2-O2	5.52	122.21	118.90
1	Х	1271	С	N3-C4-C5	-5.52	119.69	121.90
1	Х	2691	С	C5-C6-N1	-5.52	118.24	121.00
1	Х	485	G	N3-C4-C5	-5.51	125.84	128.60
1	Х	2557	G	N3-C2-N2	-5.51	116.04	119.90
1	Х	1995	G	N1-C2-N2	-5.51	111.24	116.20
1	Х	684	С	C4-C5-C6	5.50	120.15	117.40
1	Х	1855	G	N9-C4-C5	-5.50	103.20	105.40
1	Х	2675	U	N1-C2-O2	5.50	126.65	122.80
1	Х	1995	G	C6-C5-N7	-5.49	127.10	130.40
1	Х	1775	А	OP1-P-O3'	5.49	117.28	105.20
1	Х	1002	С	C5-C6-N1	5.49	123.75	121.00
1	Х	683	А	O4'-C1'-N9	-5.49	103.81	108.20
1	Х	2587	G	O5'-P-OP1	-5.49	100.76	105.70
1	Х	1143	А	C8-N9-C4	-5.49	103.61	105.80
1	Х	2850	U	O5'-P-OP1	-5.48	100.76	105.70
1	Х	2593	А	N1-C2-N3	-5.48	126.56	129.30
1	Х	1644	G	C4-C5-N7	5.48	112.99	110.80
1	Х	1941	С	O5'-P-OP1	-5.48	100.77	105.70
1	Х	2480	С	N3-C4-C5	5.48	124.09	121.90
1	Х	21	А	C8-N9-C4	-5.48	103.61	105.80
1	Х	2243	С	C6-N1-C2	-5.48	118.11	120.30
1	Х	2553	G	C8-N9-C4	-5.48	104.21	106.40
1	Х	2012	А	C2-N3-C4	5.47	113.34	110.60
1	Х	2537	С	O5'-P-OP2	5.47	117.27	110.70
1	Х	2026	С	N3-C2-O2	-5.47	118.07	121.90
1	Х	2606	G	N7-C8-N9	5.47	115.83	113.10
1	Х	2030	U	OP1-P-O3'	5.46	117.22	105.20
1	Х	1010	U	C2-N1-C1'	5.46	124.25	117.70
1	Х	2836	U	C5-C4-O4	-5.46	122.62	125.90
1	Х	2466	G	N3-C4-N9	5.46	129.28	126.00
1	X	2434	G	C4-C5-C6	5.46	122.08	118.80
1	Х	2838	U	N1-C2-O2	5.46	126.62	122.80
1	X	970	A	N9-C4-C5	-5.46	103.62	105.80
1	X	1690	U	C6-N1-C2	5.46	124.27	121.00
1	Х	2702	G	C4-N9-C1'	5.46	133.59	126.50
1	Х	1235	С	C5-C6-N1	-5.45	118.27	121.00
1	Х	381	С	C6-N1-C1'	-5.45	114.26	120.80
1	X	524	A	C5-C6-N1	5.45	120.42	117.70
1	X	1683	G	C4-C5-N7	-5.45	108.62	110.80
1	Х	840	U	N1-C2-N3	5.45	118.17	114.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2830	U	C2-N1-C1'	5.45	124.23	117.70
1	Х	924	С	N1-C2-O2	5.44	122.17	118.90
1	Х	761	G	N3-C4-C5	-5.44	125.88	128.60
1	Х	1679	U	N3-C2-O2	-5.44	118.39	122.20
1	Х	2794	G	OP2-P-O3'	5.44	117.18	105.20
1	Х	754	G	N3-C4-N9	5.44	129.26	126.00
1	Х	2532	G	C8-N9-C4	5.44	108.58	106.40
1	Х	10	А	C8-N9-C4	-5.44	103.62	105.80
1	Х	1981	А	C5-C6-N6	5.44	128.05	123.70
1	Х	1746	А	N9-C4-C5	5.43	107.97	105.80
1	Х	689	А	O4'-C1'-N9	5.43	112.55	108.20
1	Х	1989	С	O5'-P-OP2	5.43	117.22	110.70
1	Х	540	G	P-O3'-C3'	5.43	126.22	119.70
1	Х	763	А	O5'-P-OP1	-5.43	100.81	105.70
1	Х	884	С	N3-C2-O2	5.43	125.70	121.90
1	Х	1986	G	N9-C4-C5	5.43	107.57	105.40
1	Х	2036	G	N7-C8-N9	5.43	115.81	113.10
1	Х	995	А	C5-C6-N1	-5.42	114.99	117.70
1	Х	1398	G	C4-N9-C1'	-5.42	119.45	126.50
1	Х	1855	G	C4-C5-N7	5.42	112.97	110.80
1	Х	579	G	C5-C6-O6	5.42	131.85	128.60
1	Х	591	G	N7-C8-N9	-5.42	110.39	113.10
1	Х	2408	G	O5'-P-OP1	-5.42	100.82	105.70
1	Х	2429	А	OP1-P-OP2	-5.42	111.47	119.60
1	Х	2854	G	C5-N7-C8	-5.42	101.59	104.30
1	Х	1684	G	N3-C4-C5	5.42	131.31	128.60
1	Х	543	G	O5'-P-OP1	-5.41	100.83	105.70
1	Х	586	G	C6-C5-N7	-5.41	127.15	130.40
1	Х	1480	G	N3-C4-N9	-5.41	122.75	126.00
1	Х	1163	С	N3-C4-C5	-5.41	119.74	121.90
1	Х	519	С	C6-N1-C2	-5.41	118.14	120.30
1	Х	2049	C	N1-C2-O2	-5.40	115.66	118.90
1	X	2523	G	N3-C4-C5	-5.40	125.90	128.60
1	Х	69	G	C8-N9-C1'	-5.40	119.98	127.00
1	X	673	G	C8-N9-C4	5.40	108.56	106.40
1	X	2602	G	N3-C4-C5	-5.40	125.90	128.60
1	Х	2491	С	C5-C6-N1	5.40	123.70	121.00
2	Y	53	G	C4-N9-C1'	5.40	133.52	126.50
2	Y	79	U	N1-C2-O2	5.39	126.57	122.80
1	X	1663	C	O5'-P-OP2	5.39	117.16	110.70
1	X	1636	G	C5-C6-N1	5.38	114.19	111.50
1	Х	112	U	C2-N1-C1'	5.38	124.16	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1982	С	OP2-P-O3'	5.38	117.04	105.20
1	Х	2420	С	C6-N1-C2	-5.38	118.15	120.30
1	Х	2844	G	OP2-P-O3'	5.38	117.04	105.20
1	Х	1166	А	C8-N9-C4	5.38	107.95	105.80
1	Х	804	С	N1-C2-O2	5.38	122.12	118.90
1	Х	1000	G	N3-C4-N9	-5.38	122.78	126.00
1	Х	1963	G	C8-N9-C4	-5.37	104.25	106.40
1	Х	2403	С	N1-C2-O2	5.37	122.12	118.90
1	Х	2560	G	C8-N9-C4	-5.37	104.25	106.40
1	Х	1292	А	C5-N7-C8	5.37	106.58	103.90
1	Х	2668	U	N3-C2-O2	5.37	125.96	122.20
1	Х	2432	А	N7-C8-N9	5.37	116.48	113.80
1	Х	2533	U	C2-N3-C4	5.37	130.22	127.00
1	Х	2800	С	OP2-P-O3'	5.37	117.00	105.20
1	Х	1668	G	N3-C2-N2	-5.36	116.15	119.90
1	Х	2709	С	N1-C2-O2	-5.36	115.68	118.90
1	Х	2861	А	N7-C8-N9	5.36	116.48	113.80
1	Х	324	С	C6-N1-C2	-5.36	118.16	120.30
1	Х	586	G	C8-N9-C1'	-5.36	120.03	127.00
1	Х	1979	С	C4-C5-C6	-5.36	114.72	117.40
1	Х	2863	U	N1-C2-N3	5.36	118.12	114.90
2	Y	33	С	C5-C6-N1	5.36	123.68	121.00
1	Х	852	U	C5-C4-O4	5.36	129.12	125.90
1	Х	2042	А	N1-C6-N6	5.36	121.81	118.60
1	Х	842	А	O4'-C1'-N9	-5.36	103.92	108.20
1	Х	2532	G	O5'-P-OP1	5.36	117.13	110.70
1	Х	2599	U	C6-N1-C2	-5.36	117.79	121.00
1	Х	1293	А	C8-N9-C4	-5.36	103.66	105.80
1	Х	2034	А	N7-C8-N9	5.36	116.48	113.80
1	Х	2845	С	N1-C2-O2	5.36	122.11	118.90
1	Х	508	G	N3-C2-N2	5.35	123.65	119.90
1	Х	2470	U	N3-C2-O2	-5.35	118.46	122.20
1	Х	994	А	N3-C4-C5	-5.34	123.06	126.80
1	Х	527	С	N1-C2-O2	5.34	122.11	118.90
1	X	1260	A	C8-N9-C4	5.34	107.94	105.80
1	Х	2699	G	N1-C6-O6	5.34	123.11	119.90
1	Х	1981	А	N9-C4-C5	5.34	107.94	105.80
1	Х	1819	U	C5-C4-O4	5.34	129.10	125.90
1	X	1288	A	C6-C5-N7	-5.34	128.56	132.30
1	Х	2409	А	C6-C5-N7	-5.33	128.57	132.30
1	X	2334	С	C2-N1-C1'	5.33	124.67	118.80
1	Х	1223	G	N3-C4-N9	5.33	129.20	126.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1671	А	N9-C4-C5	-5.33	103.67	105.80
1	Х	787	А	N3-C4-C5	5.33	130.53	126.80
1	Х	973	U	C5-C6-N1	5.32	125.36	122.70
2	Y	39	С	C5-C6-N1	5.32	123.66	121.00
1	Х	381	С	N1-C2-O2	5.32	122.09	118.90
1	Х	810	U	C6-N1-C2	-5.32	117.81	121.00
1	Х	1570	С	N1-C2-O2	5.32	122.09	118.90
1	Х	1751	А	C8-N9-C4	5.32	107.93	105.80
1	Х	2571	G	C8-N9-C4	-5.32	104.27	106.40
1	Х	2701	А	N1-C2-N3	5.32	131.96	129.30
1	Х	1633	С	C6-N1-C2	5.32	122.43	120.30
1	Х	2482	А	C4-C5-C6	5.32	119.66	117.00
1	Х	2854	G	C5-C6-O6	-5.31	125.41	128.60
1	Х	2557	G	C4-C5-N7	-5.31	108.67	110.80
1	Х	1775	А	N9-C4-C5	-5.31	103.68	105.80
1	Х	689	А	C4-N9-C1'	5.31	135.85	126.30
1	Х	937	С	C5-C6-N1	5.31	123.65	121.00
1	Х	927	С	N1-C2-O2	5.30	122.08	118.90
1	Х	1335	А	N7-C8-N9	-5.30	111.15	113.80
1	Х	1191	G	N3-C4-N9	5.30	129.18	126.00
1	Х	2242	С	C6-N1-C2	-5.30	118.18	120.30
1	Х	2409	А	C5-N7-C8	-5.30	101.25	103.90
1	Х	2028	С	C6-N1-C2	5.30	122.42	120.30
1	Х	2799	С	C5-C4-N4	5.30	123.91	120.20
1	Х	1775	А	N7-C8-N9	-5.29	111.15	113.80
1	Х	1979	С	C6-N1-C2	5.29	122.42	120.30
1	Х	993	С	C6-N1-C2	-5.29	118.18	120.30
1	Х	2704	U	C6-N1-C2	-5.29	117.83	121.00
1	Х	600	G	P-O3'-C3'	5.29	126.05	119.70
1	Х	579	G	N9-C4-C5	5.29	107.52	105.40
1	Х	2042	А	C2-N3-C4	-5.29	107.96	110.60
1	X	1167	A	N1-C2-N3	-5.29	126.66	129.30
1	Х	2805	G	C4-C5-N7	-5.29	108.69	110.80
1	Х	2011	U	N1-C2-N3	5.28	118.07	114.90
1	Х	503	G	N3-C2-N2	5.28	123.60	119.90
1	Х	1948	С	C6-N1-C2	-5.28	118.19	120.30
1	X	2028	С	OP1-P-O3'	5.28	116.82	105.20
1	X	2524	G	C5-C6-N1	5.28	114.14	111.50
1	Х	2663	U	N3-C2-O2	5.28	125.89	122.20
1	X	536	A	C5-C6-N1	5.28	120.34	117.70
1	X	803	C	O5'-P-OP2	5.28	117.03	110.70
2	Y	55	С	N3-C2-O2	-5.28	118.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	863	С	C6-N1-C2	-5.27	118.19	120.30
1	Х	2797	G	N3-C4-C5	-5.27	125.96	128.60
1	Х	2472	U	N3-C4-O4	5.27	123.09	119.40
1	Х	933	G	C6-C5-N7	-5.27	127.24	130.40
1	Х	2857	С	N1-C2-O2	5.27	122.06	118.90
5	С	150	LEU	CA-CB-CG	5.26	127.40	115.30
1	Х	2518	С	N1-C2-O2	-5.26	115.74	118.90
1	Х	2796	А	C5-C6-N6	5.26	127.91	123.70
1	Х	855	G	N9-C4-C5	-5.26	103.30	105.40
1	Х	2561	G	N3-C4-C5	-5.26	125.97	128.60
1	Х	1239	А	C8-N9-C4	-5.26	103.70	105.80
1	Х	2010	G	N3-C4-C5	-5.26	125.97	128.60
1	Х	993	С	C5-C6-N1	5.25	123.63	121.00
1	Х	2029	G	C6-C5-N7	-5.25	127.25	130.40
1	Х	2327	U	O5'-P-OP1	-5.25	100.97	105.70
1	Х	2745	А	N1-C6-N6	5.25	121.75	118.60
1	Х	941	U	O5'-P-OP1	-5.25	100.97	105.70
1	Х	9	U	N3-C2-O2	-5.25	118.53	122.20
1	Х	13	А	N1-C6-N6	-5.25	115.45	118.60
1	Х	1398	G	C8-N9-C1'	5.25	133.82	127.00
1	Х	1466	С	C5-C6-N1	5.25	123.62	121.00
1	Х	2489	С	N3-C4-N4	5.25	121.67	118.00
1	Х	2797	G	N3-C2-N2	5.25	123.57	119.90
1	Х	2594	U	N3-C4-O4	5.25	123.07	119.40
1	Х	1663	С	C2-N1-C1'	5.24	124.57	118.80
2	Y	32	С	C6-N1-C2	-5.24	118.20	120.30
15	Ν	61	TRP	CA-CB-CG	5.24	123.66	113.70
1	Х	2823	G	C5-C6-O6	5.24	131.74	128.60
1	Х	1036	G	C6-C5-N7	5.24	133.54	130.40
1	Х	1663	С	OP1-P-O3'	5.24	116.72	105.20
1	Х	2466	G	C8-N9-C1'	-5.24	120.19	127.00
1	Х	1308	C	N3-C4-C5	-5.23	119.81	121.90
1	Х	15	G	C8-N9-C1'	5.23	133.80	127.00
1	Х	500	G	N1-C6-O6	5.23	123.04	119.90
1	Х	2708	U	N3-C2-O2	-5.23	118.54	122.20
1	Х	1687	С	C4-C5-C6	5.23	120.01	117.40
1	X	2817	A	O5'-P-OP1	5.23	116.97	110.70
1	X	2626	U	OP2-P-O3'	5.23	116.70	105.20
1	X	2702	G	N1-C6-O6	-5.23	116.76	119.90
1	Х	124	A	C8-N9-C4	-5.22	103.71	105.80
1	Х	487	G	N3-C2-N2	-5.22	116.24	119.90
1	Х	2537	С	O5'-P-OP1	-5.22	101.00	105.70

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	528	G	C8-N9-C4	-5.22	104.31	106.40
1	Х	773	G	C8-N9-C4	-5.22	104.31	106.40
1	Х	1660	G	N1-C6-O6	-5.22	116.77	119.90
1	Х	2027	С	OP1-P-O3'	5.22	116.68	105.20
1	Х	2847	G	O5'-P-OP1	-5.22	101.00	105.70
1	Х	1238	А	C8-N9-C4	5.21	107.89	105.80
1	Х	1356	G	C4-N9-C1'	5.21	133.28	126.50
1	Х	586	G	C4-C5-C6	5.21	121.93	118.80
1	Х	343	А	C8-N9-C1'	-5.21	118.32	127.70
1	Х	1709	U	C2-N1-C1'	5.21	123.95	117.70
17	Р	90	LEU	CA-CB-CG	5.21	127.29	115.30
1	Х	2018	G	O5'-P-OP2	-5.21	101.01	105.70
1	Х	2037	А	C4-C5-C6	-5.21	114.39	117.00
1	Х	2489	С	N1-C2-O2	-5.21	115.77	118.90
1	Х	2712	G	N3-C4-N9	5.21	129.13	126.00
1	Х	2822	U	C6-N1-C1'	-5.21	113.91	121.20
1	Х	2036	G	C5-N7-C8	-5.21	101.70	104.30
1	Х	2530	С	C4-C5-C6	5.21	120.00	117.40
1	Х	1954	А	C2-N3-C4	-5.20	108.00	110.60
1	Х	1694	А	N1-C6-N6	5.20	121.72	118.60
1	Х	2453	С	N1-C2-O2	5.20	122.02	118.90
1	Х	2826	С	N3-C4-N4	-5.20	114.36	118.00
1	Х	689	А	N7-C8-N9	5.20	116.40	113.80
1	Х	931	G	C8-N9-C1'	-5.20	120.24	127.00
1	Х	23	G	N3-C4-C5	-5.20	126.00	128.60
1	Х	1344	С	N3-C2-O2	-5.20	118.26	121.90
1	Х	1300	А	C4-C5-C6	-5.19	114.40	117.00
1	Х	998	С	C6-N1-C2	-5.19	118.22	120.30
1	Х	2591	С	C2-N1-C1'	5.19	124.51	118.80
1	Х	2701	А	C8-N9-C4	-5.19	103.72	105.80
1	Х	485	G	OP2-P-O3'	5.19	116.61	105.20
1	Х	970	А	N1-C6-N6	5.19	121.71	118.60
1	Х	2480	С	O4'-C1'-N1	5.19	112.35	108.20
1	Х	975	С	N3-C4-C5	-5.18	119.83	121.90
1	Х	1284	G	C6-C5-N7	-5.18	127.29	130.40
1	Х	302	U	C5-C4-O4	-5.18	122.79	125.90
1	X	759	C	P-O3'-C3'	5.18	125.92	119.70
1	Х	2795	А	P-O3'-C3'	5.18	125.92	119.70
1	Х	1887	G	C8-N9-C4	-5.18	104.33	106.40
1	X	2489	С	C2-N3-C4	5.18	122.49	119.90
1	Х	1309	G	C6-N1-C2	-5.18	121.99	125.10
1	Х	2474	G	C5-C6-N1	5.18	114.09	111.50



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	Х	1692	С	N3-C4-C5	-5.18	119.83	121.90
1	Х	2023	С	C2-N1-C1'	5.18	124.49	118.80
2	Y	93	G	C4-C5-N7	5.17	112.87	110.80
1	Х	1284	G	C4-C5-C6	5.17	121.90	118.80
1	Х	1279	G	C5-C6-N1	5.17	114.08	111.50
1	Х	1775	А	O5'-P-OP1	-5.17	101.05	105.70
1	Х	649	G	N3-C2-N2	-5.16	116.29	119.90
1	Х	2751	С	N1-C2-O2	5.16	122.00	118.90
1	Х	2844	G	OP1-P-OP2	-5.16	111.86	119.60
1	Х	2038	С	OP2-P-O3'	5.16	116.55	105.20
1	Х	1717	А	N9-C4-C5	5.16	107.86	105.80
1	Х	2422	С	C6-N1-C2	-5.15	118.24	120.30
1	Х	2486	С	N3-C4-N4	-5.15	114.39	118.00
1	Х	2553	G	N9-C4-C5	5.15	107.46	105.40
1	Х	1662	G	C8-N9-C4	5.15	108.46	106.40
1	Х	2662	С	C5-C6-N1	5.15	123.58	121.00
1	Х	2700	U	N3-C4-C5	-5.15	111.51	114.60
2	Y	77	G	N1-C6-O6	-5.15	116.81	119.90
1	Х	956	А	N7-C8-N9	5.15	116.37	113.80
1	Х	2817	А	C5-N7-C8	-5.15	101.33	103.90
1	Х	1643	А	C8-N9-C4	5.14	107.86	105.80
1	Х	1685	А	C4-C5-N7	-5.14	108.13	110.70
1	Х	1743	С	O5'-P-OP2	-5.14	101.07	105.70
1	Х	1855	G	C5-C6-O6	-5.14	125.52	128.60
1	Х	776	G	N7-C8-N9	5.14	115.67	113.10
1	Х	836	G	C8-N9-C4	-5.14	104.34	106.40
1	Х	1674	С	N3-C4-C5	5.14	123.95	121.90
1	Х	2832	G	N3-C4-N9	-5.14	122.92	126.00
1	Х	1468	А	C2-N3-C4	5.13	113.17	110.60
1	Х	863	С	C5-C6-N1	5.13	123.57	121.00
1	Х	1313	U	N1-C2-O2	-5.13	119.21	122.80
1	Х	2513	А	OP1-P-O3'	5.13	116.49	105.20
2	Y	58	G	N3-C4-C5	-5.13	126.03	128.60
1	Х	1790	G	P-O3'-C3'	5.13	125.86	119.70
1	X	2818	G	N3-C4-C5	-5.13	126.04	128.60
1	Х	1035	G	N7-C8-N9	5.13	115.66	113.10
1	X	2699	G	O5'-P-OP2	5.13	116.85	110.70
1	X	2551	A	C5-N7-C8	5.12	106.46	103.90
1	Х	940	G	C4-C5-N7	-5.12	108.75	110.80
1	X	2030	U	C2-N1-C1'	-5.12	111.56	117.70
1	X	1933	G	C8-N9-C4	$-5.1\overline{2}$	104.35	106.40
1	Х	1975	G	C5-C6-N1	5.12	114.06	111.50



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2751	С	C6-N1-C1'	-5.12	114.66	120.80
1	Х	1670	G	C4-N9-C1'	-5.12	119.85	126.50
1	Х	1819	U	N1-C2-O2	5.12	126.38	122.80
1	Х	1038	U	C6-N1-C2	-5.11	117.93	121.00
1	Х	1664	G	C8-N9-C4	5.11	108.44	106.40
1	Х	2461	G	N1-C6-O6	5.11	122.97	119.90
1	Х	343	А	N9-C1'-C2'	5.11	120.64	114.00
1	Х	1277	G	N1-C6-O6	-5.11	116.83	119.90
1	Х	1206	G	C4-N9-C1'	-5.11	119.86	126.50
1	Х	1234	С	C2-N1-C1'	5.11	124.42	118.80
1	Х	268	G	C6-C5-N7	-5.11	127.34	130.40
1	Х	1288	А	N7-C8-N9	5.11	116.35	113.80
1	Х	39	С	N3-C4-C5	-5.10	119.86	121.90
1	Х	1480	G	N3-C4-C5	5.10	131.15	128.60
1	Х	1527	G	N3-C2-N2	-5.10	116.33	119.90
1	Х	2580	С	C2-N1-C1'	5.10	124.41	118.80
1	Х	2705	А	OP1-P-O3'	5.10	116.42	105.20
1	Х	834	А	C2-N3-C4	-5.10	108.05	110.60
1	Х	2409	А	N1-C6-N6	5.10	121.66	118.60
1	Х	2817	А	C4-C5-N7	5.10	113.25	110.70
1	Х	1972	G	N7-C8-N9	5.09	115.65	113.10
1	Х	2542	U	N1-C2-N3	5.09	117.96	114.90
1	Х	1786	С	C2-N1-C1'	5.09	124.40	118.80
1	Х	777	А	O4'-C1'-N9	5.09	112.27	108.20
1	Х	2402	U	C2-N1-C1'	5.09	123.81	117.70
1	Х	2437	G	N7-C8-N9	5.09	115.65	113.10
1	Х	2469	G	O5'-P-OP2	-5.09	101.12	105.70
1	Х	2832	G	C4-N9-C1'	-5.09	119.88	126.50
1	Х	2846	G	N9-C4-C5	5.09	107.44	105.40
1	X	699	G	C4-C5-N7	5.09	112.84	110.80
1	X	969	U	<u>C6-N1-C2</u>	5.09	124.05	121.00
1	X	2604	G	C8-N9-C4	-5.09	104.36	106.40
1	Х	2658	А	N9-C4-C5	-5.09	103.77	105.80
1	Х	2043	A	N1-C2-N3	-5.08	126.76	129.30
1	Х	2857	С	C5-C6-N1	5.08	123.54	121.00
1	X	2828	C	C6-N1-C2	-5.08	118.27	120.30
1	X	763	A	OP2-P-O3'	5.08	116.38	105.20
1	X	1006	C	N3-C4-C5	-5.08	119.87	121.90
1	Х	949	G	C4-C5-N7	-5.08	108.77	110.80
1	X	1269	G	C4-C5-N7	5.08	112.83	110.80
1	X	1704	G	C4-N9-C1'	5.07	133.09	126.50
1	Х	$2\overline{437}$	G	OP1-P-O3'	5.07	116.36	105.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Х	955	G	C4-N9-C1'	5.07	133.09	126.50
1	Х	1745	С	C2-N1-C1'	-5.07	113.22	118.80
1	Х	523	А	N7-C8-N9	-5.07	111.27	113.80
1	Х	2260	С	C6-N1-C2	-5.07	118.27	120.30
25	Ζ	46	CYS	CA-CB-SG	5.07	123.12	114.00
1	Х	1309	G	C2-N3-C4	5.07	114.43	111.90
1	Х	1994	U	N3-C2-O2	5.07	125.75	122.20
1	Х	2655	С	N3-C2-O2	-5.07	118.36	121.90
1	Х	2808	U	C6-N1-C2	5.07	124.04	121.00
1	Х	2408	G	N7-C8-N9	5.06	115.63	113.10
1	Х	1679	U	C5-C6-N1	-5.06	120.17	122.70
1	Х	1745	С	C6-N1-C1'	5.06	126.88	120.80
1	Х	2459	С	C2-N3-C4	-5.06	117.37	119.90
1	Х	1336	G	C4-C5-N7	5.06	112.83	110.80
1	Х	1980	А	C2-N3-C4	-5.06	108.07	110.60
1	Х	1036	G	C5-C6-O6	5.06	131.63	128.60
1	Х	1830	С	C2-N1-C1'	5.06	124.36	118.80
1	Х	2472	U	C2-N1-C1'	5.06	123.77	117.70
1	Х	2693	U	O4'-C1'-N1	-5.06	104.15	108.20
1	Х	2759	U	C2-N1-C1'	5.06	123.77	117.70
1	Х	1668	G	C4-N9-C1'	5.06	133.08	126.50
1	Х	592	G	C4-C5-N7	5.06	112.82	110.80
1	Х	1242	А	N7-C8-N9	-5.05	111.28	113.80
1	Х	2258	G	C5-C6-N1	5.05	114.03	111.50
1	Х	2370	G	O4'-C1'-N9	5.05	112.24	108.20
1	Х	1658	А	C8-N9-C4	5.05	107.82	105.80
1	Х	2459	С	C5-C4-N4	-5.05	116.67	120.20
1	Х	2711	G	N1-C6-O6	-5.04	116.87	119.90
1	Х	1223	G	N3-C4-C5	-5.04	126.08	128.60
1	Х	560	G	O5'-P-OP1	-5.04	101.16	105.70
1	X	2444	C	N3-C4-C5	-5.04	119.88	121.90
1	X	787	A	N3-C4-N9	-5.04	123.37	127.40
1	Х	2491	С	C2-N1-C1'	5.04	124.34	118.80
1	Х	2594	U	C2-N1-C1'	5.04	123.74	117.70
1	Х	2601	С	C6-N1-C2	-5.04	118.29	120.30
1	Х	2668	U	C2-N3-C4	-5.04	123.98	127.00
1	Х	1142	G	N9-C4-C5	-5.03	103.39	105.40
1	X	1697	U	O4'-C1'-N1	5.03	112.23	108.20
1	Х	1686	А	C6-N1-C2	-5.03	115.58	118.60
1	X	1974	U	C2-N1-C1'	5.03	123.74	117.70
1	Х	2542	U	N1-C2-O2	5.03	126.32	122.80
1	Х	1660	G	C2-N3-C4	5.03	114.41	111.90



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	Х	2528	G	N3-C4-C5	-5.03	126.08	128.60
2	Y	97	С	N1-C2-O2	5.03	121.92	118.90
1	Х	1636	G	C6-N1-C2	-5.03	122.08	125.10
1	Х	2499	С	C2-N3-C4	5.03	122.41	119.90
1	Х	2545	А	C6-N1-C2	-5.03	115.58	118.60
1	Х	2836	U	C5-C6-N1	5.03	125.21	122.70
1	Х	2662	С	C2-N3-C4	5.02	122.41	119.90
1	Х	2857	С	N3-C4-N4	5.02	121.52	118.00
2	Y	58	G	C8-N9-C1'	-5.02	120.47	127.00
1	Х	1240	G	C4-C5-N7	5.02	112.81	110.80
1	Х	1691	G	C6-N1-C2	-5.02	122.09	125.10
1	Х	2492	G	N3-C4-C5	-5.02	126.09	128.60
1	Х	981	С	N3-C4-N4	5.02	121.51	118.00
1	Х	493	А	C8-N9-C4	5.01	107.81	105.80
1	Х	1676	U	OP1-P-OP2	5.01	127.12	119.60
1	Х	1746	А	N1-C6-N6	-5.01	115.59	118.60
1	Х	1037	U	C5-C6-N1	5.01	125.20	122.70
1	Х	1748	U	C5-C4-O4	-5.01	122.90	125.90
1	Х	2322	U	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	В	130	GLY	Peptide
4	В	131	SER	Peptide
4	В	135	HIS	Peptide
4	В	146	THR	Peptide
4	В	149	ARG	Peptide
5	С	49	ALA	Peptide
8	G	114	THR	Peptide
10	Ι	48	PHE	Peptide
10	Ι	57	ILE	Peptide
11	J	11	ARG	Peptide
11	J	12	LYS	Peptide
12	Κ	8	ARG	Peptide
14	М	27	PHE	Peptide
14	М	28	ARG	Peptide
16	0	78	VAL	Peptide
19	R	57	ASN	Peptide
19	R	68	GLY	Peptide
20	S	32	PHE	Peptide



Continued from previous page...

Mol	Chain	$\mathbf{Res}$	Type	Group
25	Ζ	37	HIS	Peptide
25	Ζ	53	ASP	Peptide

## 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Х	57957	0	29205	1932	0
2	Y	2598	0	1328	88	0
3	А	2001	0	1994	121	0
4	В	1544	0	1605	107	0
5	С	1467	0	1472	100	0
6	D	1367	0	1423	81	0
7	Е	1286	0	1336	61	0
8	G	1107	0	1124	66	0
9	Н	993	0	1035	84	0
10	Ι	982	0	973	49	0
11	J	1042	0	1059	64	0
12	K	897	0	955	68	0
13	L	751	0	770	40	0
14	М	923	0	942	76	0
15	N	962	0	987	65	0
16	0	734	0	736	35	0
17	Р	1020	0	1096	72	0
18	Q	718	0	731	48	0
19	R	793	0	804	68	0
20	S	1290	0	1268	56	0
21	Т	542	0	566	39	0
22	U	539	0	556	37	0
23	V	438	0	456	18	0
24	W	424	0	470	18	0
25	Ζ	448	0	446	41	0
26	1	315	0	252	16	0
27	2	383	0	414	19	0
28	3	470	0	512	48	0
29	Х	49	0	61	8	0
30	2	2	0	0	0	0
30	3	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	А	1	0	0	0	0
30	Ι	1	0	0	0	0
30	Ν	1	0	0	0	0
30	Q	2	0	0	0	0
30	W	1	0	0	0	0
30	Х	264	0	0	0	0
30	Y	4	0	0	0	0
31	V	10	0	19	0	0
31	Х	60	0	104	15	0
All	All	84387	0	54699	3132	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 23.

All (3132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
13:L:30:SER:O	13:L:40:ALA:HA	1.55	1.03
15:N:66:ASN:HB3	15:N:76:TYR:HB2	1.40	1.03
1:X:1673:C:H5"	4:B:136:ARG:HB3	1.39	1.02
8:G:119:LEU:HD12	8:G:126:VAL:HG23	1.41	1.01
1:X:2796:A:H2'	1:X:2797:G:H8	1.24	1.01
17:P:21:ARG:HH11	17:P:21:ARG:HA	1.29	0.98
14:M:69:ARG:NH1	14:M:78:GLU:OE2	2.00	0.95
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.47	0.92
1:X:226:C:OP2	1:X:2373:C:O2'	1.88	0.91
28:3:61:MET:N	28:3:61:MET:SD	2.40	0.91
25:Z:32:GLU:HG3	25:Z:39:LYS:HD3	1.54	0.90
8:G:70:PHE:HB2	8:G:76:GLN:HE22	1.37	0.90
1:X:2542:U:H5'	9:H:37:GLY:HA2	1.53	0.90
6:D:124:GLY:HA3	6:D:163:ASP:HA	1.54	0.89
2:Y:67:C:H2'	2:Y:111:C:H41	1.36	0.89
12:K:33:ARG:HG3	12:K:114:GLU:HB3	1.52	0.89
9:H:110:VAL:HG23	9:H:129:LEU:HB2	1.55	0.88
1:X:2551:A:H5"	1:X:2553:G:H4'	1.56	0.88
1:X:2796:A:H2'	1:X:2797:G:C8	2.09	0.87
14:M:14:ARG:HH11	14:M:15:GLY:HA2	1.37	0.87
1:X:1277:G:OP1	25:Z:19:ARG:NH2	2.06	0.87
4:B:174:GLU:HB3	4:B:183:LEU:HD22	1.56	0.87
8:G:100:TYR:HB2	8:G:115:ALA:H	1.39	0.87
1:X:479:G:N7	27:2:39:ARG:NH2	2.21	0.87



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:X:693:A:H2'	1:X:694:G:C8	2.09	0.87	
3:A:55:GLY:HA3	3:A:218:LYS:HG2	1.55	0.87	
11:J:18:MET:SD	11:J:19:THR:N	2.48	0.87	
13:L:91:ARG:NH1	13:L:94:TYR:O	2.06	0.87	
27:2:22:MET:O	27:2:28:ARG:NH2	2.08	0.87	
1:X:338:G:H5'	19:R:9:HIS:CE1	2.10	0.86	
1:X:492:G:O2'	1:X:516:G:N2	2.09	0.86	
1:X:494:A:O2'	19:R:58:VAL:HG13	1.74	0.86	
22:U:74:PRO:HB3	22:U:78:ILE:HA	1.58	0.85	
1:X:1936:A:H61	31:X:3167:SPD:HN11	1.25	0.85	
3:A:223:GLY:HA2	3:A:226:MET:HG3	1.59	0.85	
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.59	0.85	
3:A:17:THR:HB	3:A:205:VAL:H	1.41	0.85	
1:X:1283:C:H5"	1:X:1284:G:H5'	1.59	0.84	
1:X:1542:G:H22	1:X:1562:G:H1	1.24	0.84	
1:X:1570:C:N4	1:X:1651:U:O4	2.10	0.84	
1:X:2307:A:H2'	1:X:2308:A:C8	2.12	0.84	
1:X:337:G:O2'	19:R:9:HIS:ND1	2.09	0.84	
1:X:683:A:OP1	10:I:40:ARG:NE	2.10	0.84	
1:X:2186:G:H2'	1:X:2187:A:H8	1.43	0.84	
2:Y:82:U:H3	2:Y:99:G:H1	1.26	0.84	
1:X:2399:C:N4	28:3:31:HIS:O	2.10	0.83	
5:C:56:ARG:NH2	5:C:57:LYS:O	2.11	0.83	
9:H:62:GLY:O	9:H:65:LYS:NZ	2.12	0.83	
14:M:33:VAL:HG22	14:M:51:GLU:HB2	1.61	0.83	
1:X:938:G:O2'	1:X:940:G:N7	2.11	0.82	
1:X:38:G:H2'	1:X:39:C:C6	2.15	0.82	
1:X:320:A:N6	1:X:1223:G:O2'	2.13	0.82	
1:X:2020:G:H2'	1:X:2021:G:C8	2.15	0.82	
1:X:517:A:H5"	1:X:518:A:H5'	1.60	0.82	
1:X:2605:C:H2'	1:X:2606:G:H8	1.45	0.82	
1:X:474:G:N2	1:X:477:A:OP2	2.13	0.81	
10:I:89:ASP:OD1	10:I:89:ASP:N	2.12	0.81	
8:G:35:LYS:HD3	8:G:35:LYS:H	1.45	0.81	
1:X:1793:A:H2'	1:X:1794:A:C8	2.15	0.81	
1:X:2609:G:H2'	1:X:2610:G:H8	1.45	0.81	
4:B:194:GLY:HA2	14:M:2:GLN:HA	1.61	0.81	
1:X:1165:G:OP2	15:N:58:ARG:NH2	2.12	0.81	
1:X:1662:G:H5"	1:X:1663:C:H5'	1.63	0.81	
1:X:546:A:H2'	1:X:547:U:C6	2.15	0.81	
1:X:1882:G:H21	1:X:1885:C:H41	1.29	0.81	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:1481:U:HO2'	1:X:1562:G:HO2'	1.21	0.81
1:X:2306:A:H2'	1:X:2307:A:C8	2.15	0.81
1:X:2432:A:H2'	1:X:2433:G:H8	1.45	0.81
1:X:1582:A:OP1	3:A:211:ARG:NH1	2.14	0.80
20:S:91:PRO:HD2	20:S:92:VAL:HG23	1.63	0.80
1:X:219:G:HO2'	1:X:231:G:H1	1.29	0.80
1:X:1850:G:O2'	1:X:1866:G:N2	2.15	0.80
2:Y:32:C:H1'	2:Y:59:A:H61	1.44	0.80
15:N:24:PHE:O	15:N:29:SER:OG	2.00	0.80
1:X:1919:A:H2	1:X:1926:U:H3	1.29	0.80
1:X:2261:G:H21	1:X:2369:U:H3	1.30	0.80
15:N:47:TYR:O	15:N:51:ARG:NH1	2.15	0.80
1:X:1345:G:N7	1:X:1625:A:O2'	2.14	0.80
1:X:2662:C:H2'	1:X:2663:U:H6	1.47	0.79
24:W:1:MET:HB3	24:W:34:VAL:HG12	1.64	0.79
1:X:2659:C:H5'	4:B:189:PRO:HA	1.64	0.79
6:D:128:TYR:HB3	6:D:156:ILE:HD12	1.64	0.79
1:X:1154:A:N7	8:G:53:ARG:NH2	2.30	0.79
1:X:2246:A:H5"	1:X:2247:A:H5"	1.65	0.79
1:X:2516:U:H2'	1:X:2517:C:C6	2.16	0.79
1:X:2795:A:OP1	12:K:2:ARG:NH1	2.15	0.79
1:X:704:G:OP1	3:A:218:LYS:NZ	2.15	0.79
16:O:66:GLY:O	16:O:87:ARG:NH1	2.16	0.79
5:C:47:THR:H	5:C:51:VAL:HB	1.46	0.79
25:Z:15:LYS:HA	25:Z:18:MET:HG3	1.65	0.78
1:X:1014:G:O2'	1:X:1021:A:N1	2.16	0.78
1:X:1996:A:H2	17:P:109:ARG:HH22	1.31	0.78
1:X:1075:C:O2	1:X:1085:G:N2	2.17	0.78
10:I:55:ARG:H	10:I:55:ARG:CZ	1.97	0.78
1:X:2518:C:HO2'	1:X:2721:A:HO2'	1.29	0.78
1:X:2533:U:H2'	1:X:2534:U:C6	2.19	0.78
15:N:48:ARG:O	15:N:52:ASN:ND2	2.15	0.78
1:X:2186:G:H2'	1:X:2187:A:C8	2.18	0.77
1:X:2266:A:H62	1:X:2323:U:H3	1.31	0.77
1:X:2567:G:C6	1:X:2586:G:C2	2.72	0.77
16:O:50:ASP:HA	16:O:53:LYS:HD3	1.67	0.77
27:2:3:ARG:O	27:2:6:GLN:NE2	2.17	0.77
1:X:224:G:H4'	1:X:399:G:C5	2.19	0.77
4:B:48:GLN:HB2	4:B:80:GLU:HG2	1.66	0.77
1:X:2640:G:H2'	1:X:2641:A:C8	2.20	0.77
12:K:35:GLN:HB2	12:K:112:LEU:HD23	1.66	0.77



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:212:SER:HA	3:A:215:LEU:HD12	1.67	0.77
18:Q:33:ALA:O	18:Q:76:LYS:NZ	2.14	0.77
14:M:90:GLN:OE1	14:M:91:VAL:N	2.18	0.77
1:X:1993:G:OP2	17:P:62:ARG:NH1	2.18	0.76
4:B:14:ILE:HG22	4:B:21:ILE:HG13	1.66	0.76
6:D:108:LEU:HD22	6:D:110:ARG:H	1.48	0.76
1:X:1212:U:H2'	1:X:1213:U:C6	2.20	0.76
4:B:55:ALA:HB3	4:B:58:LYS:HD3	1.66	0.76
1:X:2727:G:OP1	7:E:74:ASN:ND2	2.18	0.76
14:M:29:PRO:HB3	14:M:104:LEU:HD11	1.67	0.76
9:H:33:GLY:HA3	9:H:102:GLN:HE21	1.50	0.76
1:X:335:A:N6	1:X:349:G:O2'	2.19	0.76
1:X:2264:C:OP2	26:1:30:ASN:ND2	2.17	0.76
4:B:179:GLU:HB3	4:B:181:LEU:HD23	1.68	0.76
12:K:87:TYR:HD1	12:K:90:ARG:HD2	1.51	0.76
19:R:95:ARG:HA	19:R:104:VAL:HG12	1.68	0.76
1:X:168:A:H2'	1:X:169:C:H6	1.50	0.76
1:X:1938:U:O4	1:X:2535:C:N4	2.17	0.76
18:Q:7:LEU:O	23:V:29:ARG:NH1	2.19	0.76
1:X:2225:G:H2'	1:X:2226:A:H8	1.49	0.76
16:O:4:ILE:HA	16:O:11:GLN:HB3	1.66	0.76
6:D:111:ILE:HG21	6:D:137:ILE:HG22	1.68	0.75
12:K:103:ARG:NH2	12:K:106:ASP:OD2	2.18	0.75
1:X:2053:G:H2'	1:X:2054:A:C8	2.22	0.75
19:R:14:LEU:HD12	19:R:41:PRO:HB3	1.68	0.75
1:X:596:C:OP2	10:I:21:ARG:NH1	2.19	0.75
1:X:763:A:OP1	1:X:1631:C:N4	2.20	0.75
1:X:870:C:H4'	21:T:23:VAL:HG21	1.69	0.75
1:X:224:G:H4'	1:X:399:G:C6	2.21	0.75
1:X:758:G:O2'	1:X:763:A:N6	2.20	0.75
1:X:1436:G:N2	1:X:1514:C:O2	2.19	0.75
1:X:2811:G:H2'	1:X:2812:A:C8	2.22	0.75
11:J:32:ASP:N	11:J:107:VAL:O	2.19	0.75
11:J:46:ASN:OD1	11:J:46:ASN:N	2.16	0.75
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.20	0.75
1:X:2372:A:H62	1:X:2401:A:H61	1.34	0.75
6:D:170:LEU:HB2	6:D:175:LEU:HB2	1.69	0.74
20:S:90:GLU:HB3	20:S:125:PRO:HA	1.68	0.74
1:X:2048:C:H1'	1:X:2428:U:H3	1.52	0.74
14:M:31:ASP:N	14:M:31:ASP:OD1	2.17	0.74
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.68	0.74



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:1348:C:H2'	1:X:1349:A:C8	2.23	0.74
1:X:1762:C:H2'	1:X:1763:G:C8	2.21	0.74
16:O:38:LEU:HD23	16:O:47:PHE:HB3	1.69	0.74
1:X:71:A:O2'	1:X:72:A:OP1	2.05	0.74
1:X:219:G:O2'	1:X:220:U:OP2	2.05	0.74
1:X:1444:C:H2'	1:X:1445:A:C8	2.22	0.74
1:X:2283:G:H22	1:X:2291:U:H3	1.36	0.74
11:J:32:ASP:HB2	11:J:108:ALA:HA	1.70	0.74
14:M:27:PHE:HZ	14:M:96:ARG:HA	1.53	0.74
1:X:689:A:H8	1:X:2052:G:H21	1.32	0.74
1:X:1022:A:H2'	1:X:1024:G:H5"	1.69	0.74
1:X:640:C:H4'	1:X:660:G:H21	1.51	0.74
1:X:1355:A:O2'	1:X:1357:U:OP2	2.05	0.74
1:X:1997:A:H2'	1:X:1998:A:C8	2.22	0.74
1:X:2191:A:OP1	1:X:2193:C:N4	2.19	0.74
9:H:16:ALA:HA	9:H:58:ALA:HA	1.69	0.74
1:X:2225:G:H2'	1:X:2226:A:C8	2.23	0.74
1:X:1727:C:H2'	1:X:1728:A:C8	2.23	0.73
19:R:84:VAL:HG12	19:R:88:THR:HA	1.70	0.73
1:X:2867:G:OP2	1:X:2867:G:H8	1.70	0.73
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.21	0.73
1:X:313:U:H2'	1:X:314:G:H8	1.53	0.73
1:X:1081:A:N7	1:X:1107:A:O2'	2.21	0.73
1:X:1684:G:O2'	1:X:1974:U:O4	2.06	0.73
5:C:171:PRO:HB2	5:C:172:VAL:HG23	1.69	0.73
1:X:222:G:O6	28:3:7:HIS:NE2	2.21	0.73
1:X:339:U:H3	1:X:343:A:H2	1.35	0.73
1:X:1179:A:H2'	1:X:1180:A:C8	2.22	0.73
19:R:23:ILE:HG23	19:R:81:VAL:HB	1.70	0.73
1:X:37:C:H2'	1:X:38:G:H8	1.51	0.73
1:X:2402:U:O2'	1:X:2404:A:H2'	1.88	0.73
16:O:78:VAL:HG13	16:O:80:TYR:HB3	1.70	0.73
1:X:38:G:H2'	1:X:39:C:H6	1.54	0.73
15:N:94:VAL:HG13	15:N:95:LEU:HD22	1.68	0.73
3:A:34:THR:HG22	3:A:63:ARG:HB3	1.71	0.73
5:C:111:ARG:HB3	5:C:116:LYS:HB3	1.71	0.73
1:X:2567:G:O6	1:X:2586:G:C6	2.42	0.72
4:B:135:HIS:HB2	4:B:136:ARG:HG2	1.70	0.72
1:X:2873:G:H2'	1:X:2874:A:H8	1.54	0.72
3:A:203:ASN:OD1	3:A:203:ASN:N	2.21	0.72
1:X:5:A:H2'	1:X:6:A:C8	2.23	0.72



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:2400:G:N7	28:3:32:GLN:NE2	2.37	0.72
1:X:2284:U:H1'	6:D:151:GLY:HA3	1.70	0.72
9:H:11:ALA:N	9:H:96:ALA:O	2.21	0.72
1:X:2605:C:H2'	1:X:2606:G:C8	2.24	0.72
7:E:7:GLN:H	7:E:8:PRO:HD2	1.54	0.72
1:X:2011:U:H2'	1:X:2012:A:C8	2.24	0.72
1:X:115:G:OP2	1:X:117:A:O2'	2.08	0.72
11:J:133:VAL:HB	20:S:76:ARG:HH21	1.55	0.72
17:P:30:TYR:H	17:P:123:HIS:CE1	2.08	0.72
1:X:705:C:H2'	1:X:706:A:H8	1.53	0.71
1:X:2800:C:H3'	1:X:2801:A:H8	1.54	0.71
3:A:36:ALA:HB1	3:A:61:LEU:HD22	1.72	0.71
1:X:1352:G:OP2	18:Q:77:LYS:NZ	2.23	0.71
21:T:21:LEU:HD11	21:T:41:ARG:HE	1.54	0.71
1:X:1466:C:H2'	1:X:1467:U:H1'	1.72	0.71
12:K:2:ARG:O	12:K:4:GLY:N	2.23	0.71
1:X:1587:A:H2'	1:X:1588:A:C8	2.26	0.71
6:D:36:VAL:HG22	6:D:154:ILE:HG12	1.72	0.71
20:S:104:SER:HA	20:S:139:THR:HA	1.72	0.71
1:X:1573:G:H3'	1:X:1574:A:H5"	1.72	0.71
1:X:1996:A:N3	17:P:109:ARG:NH1	2.34	0.71
4:B:176:ARG:HE	14:M:16:ILE:HG22	1.55	0.71
1:X:37:C:H2'	1:X:38:G:C8	2.26	0.71
4:B:188:ILE:HG22	4:B:189:PRO:HD2	1.72	0.71
21:T:22:GLY:H	21:T:39:ARG:HB2	1.56	0.71
9:H:105:PRO:HG3	9:H:126:ILE:HG12	1.73	0.71
20:S:69:VAL:HG22	20:S:81:VAL:HG12	1.73	0.71
1:X:1419:G:H2'	1:X:1420:A:H8	1.56	0.70
1:X:1448:A:H61	1:X:1574:A:H61	1.39	0.70
1:X:2434:G:H2'	1:X:2435:C:C6	2.26	0.70
21:T:27:GLY:HA2	21:T:67:VAL:HG13	1.73	0.70
1:X:489:A:H2'	1:X:490:A:H5"	1.73	0.70
17:P:102:THR:HG21	17:P:118:LYS:HG3	1.71	0.70
26:1:13:GLU:H	26:1:54:LYS:HG2	1.56	0.70
1:X:1727:C:H2'	1:X:1728:A:H8	1.56	0.70
11:J:136:GLU:OE2	20:S:44:ARG:NH1	2.24	0.70
1:X:1418:C:H2'	1:X:1419:G:C8	2.27	0.70
1:X:1446:U:H3	1:X:1577:G:H1	1.37	0.70
1:X:2772:U:H2'	1:X:2773:G:C8	2.26	0.70
1:X:1465:G:H2'	1:X:1466:C:C6	2.25	0.70
1:X:2226:A:H2'	1:X:2227:C:C6	2.27	0.70



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:1030:U:H2'	1:X:1032:A:C2	2.27	0.70
1:X:2609:G:H2'	1:X:2610:G:C8	2.26	0.70
1:X:1348:C:H2'	1:X:1349:A:H8	1.54	0.70
1:X:1440:G:N7	3:A:31:LYS:NZ	2.30	0.70
2:Y:6:C:H2'	2:Y:7:C:H6	1.55	0.70
1:X:1674:C:H2'	1:X:1675:C:H6	1.56	0.70
1:X:2621:G:H5'	8:G:106:TYR:CD2	2.27	0.70
2:Y:51:G:H2'	2:Y:52:G:H8	1.55	0.69
14:M:41:GLU:OE2	14:M:46:ARG:NE	2.22	0.69
18:Q:11:VAL:HG23	18:Q:27:PHE:HA	1.73	0.69
1:X:612:G:O2'	1:X:614:G:O2'	2.08	0.69
1:X:969:U:O2	2:Y:92:G:H4'	1.92	0.69
1:X:1212:U:H2'	1:X:1213:U:H6	1.54	0.69
1:X:577:U:OP1	10:I:35:LYS:NZ	2.20	0.69
1:X:1697:U:N3	1:X:1755:G:OP2	2.22	0.69
26:1:36:GLU:HB2	26:1:52:GLU:HB2	1.75	0.69
1:X:1856:U:OP1	1:X:2389:G:O2'	2.05	0.69
1:X:2078:G:N2	1:X:2178:U:H3	1.91	0.69
1:X:1762:C:H2'	1:X:1763:G:H8	1.58	0.69
1:X:2231:G:H2'	1:X:2232:G:H8	1.58	0.69
2:Y:26:G:N3	2:Y:29:C:N4	2.40	0.69
21:T:64:ASP:OD1	21:T:64:ASP:N	2.22	0.69
28:3:5:LYS:H	28:3:5:LYS:NZ	1.91	0.69
1:X:341:A:H2	1:X:1223:G:H2'	1.57	0.69
1:X:356:A:HO2'	1:X:357:A:H8	1.38	0.69
1:X:1283:C:H5"	1:X:1284:G:C5'	2.22	0.69
1:X:1465:G:H2'	1:X:1466:C:H6	1.55	0.69
3:A:29:PRO:O	3:A:104:TYR:OH	2.09	0.69
17:P:94:GLU:HB2	17:P:127:ILE:HB	1.75	0.69
22:U:47:HIS:CD2	22:U:63:SER:HA	2.27	0.69
11:J:6:LYS:HD2	11:J:45:SER:HB2	1.75	0.69
9:H:13:ASN:OD1	9:H:108:THR:N	2.26	0.68
1:X:932:G:H2'	1:X:933:G:C8	2.28	0.68
13:L:75:LEU:HD12	13:L:78:ALA:HB3	1.74	0.68
1:X:463:C:N4	1:X:466:A:OP2	2.26	0.68
7:E:9:ILE:HG13	7:E:50:LEU:H	1.57	0.68
10:I:82:ASP:O	10:I:86:THR:OG1	2.11	0.68
1:X:1329:U:H2'	1:X:1330:G:H8	1.59	0.68
7:E:108:GLY:O	7:E:152:ARG:NH1	2.26	0.68
21:T:38:VAL:HG21	21:T:45:PHE:CD2	2.28	0.68
1:X:1785:A:H2'	1:X:1786:C:C6	2.28	0.68



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
5:C:123:PHE:HB3	5:C:125:ILE:HG12	1.74	0.68
21:T:23:VAL:HA	21:T:38:VAL:HG23	1.75	0.68
4:B:60:ASN:HB3	4:B:62:PRO:HD2	1.73	0.68
1:X:859:U:O2'	1:X:860:U:O5'	2.09	0.68
1:X:862:A:H2'	1:X:863:C:C6	2.29	0.68
1:X:1693:A:H2	1:X:1976:U:H5'	1.58	0.68
3:A:142:VAL:HG12	3:A:193:ILE:HA	1.75	0.68
1:X:1422:C:H2'	1:X:1423:A:H8	1.59	0.68
1:X:1462:C:O2'	1:X:1560:A:N3	2.27	0.68
7:E:52:VAL:O	7:E:65:HIS:NE2	2.23	0.68
8:G:70:PHE:HB2	8:G:76:GLN:NE2	2.08	0.68
1:X:797:A:C5	3:A:229:VAL:HG21	2.29	0.68
1:X:1039:A:N6	1:X:1136:G:H2'	2.09	0.68
1:X:1419:G:H2'	1:X:1420:A:C8	2.29	0.68
1:X:1428:G:N2	1:X:1602:G:H5'	2.08	0.68
1:X:1674:C:H2'	1:X:1675:C:C6	2.29	0.68
6:D:150:ARG:H	6:D:150:ARG:HD3	1.58	0.68
1:X:1142:G:H21	8:G:101:THR:HG22	1.58	0.68
1:X:2653:A:O2'	9:H:41:ASN:OD1	2.11	0.68
8:G:67:ARG:O	8:G:69:ASP:N	2.27	0.68
15:N:58:ARG:HA	15:N:61:TRP:CD1	2.29	0.68
1:X:1279:G:O2'	1:X:1995:G:O6	2.07	0.67
1:X:1422:C:H2'	1:X:1423:A:C8	2.28	0.67
1:X:1693:A:C2	1:X:1976:U:H5'	2.29	0.67
1:X:494:A:H4'	19:R:57:ASN:HA	1.76	0.67
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.75	0.67
9:H:76:ARG:O	9:H:94:ASN:HA	1.94	0.67
1:X:652:C:O2'	1:X:2329:C:OP1	2.11	0.67
5:C:95:LEU:HD23	5:C:96:PRO:HD2	1.76	0.67
19:R:58:VAL:HG12	19:R:68:GLY:N	2.09	0.67
1:X:585:U:H2'	1:X:586:G:C8	2.30	0.67
11:J:28:VAL:H	11:J:138:TYR:HE2	1.40	0.67
1:X:242:A:N6	1:X:440:U:O2'	2.27	0.67
1:X:1656:U:H2'	1:X:1657:A:H5"	1.76	0.67
1:X:2692:A:H5'	1:X:2693:U:OP2	1.94	0.67
5:C:170:LEU:HD12	5:C:171:PRO:HD2	1.76	0.67
10:I:58:ALA:HA	28:3:11:LYS:HD3	1.76	0.67
13:L:54:ALA:HB2	13:L:75:LEU:HD13	1.77	0.67
15:N:60:LEU:HD22	15:N:64:ARG:HH11	1.59	0.67
19:R:58:VAL:HB	19:R:67:GLY:N	2.10	0.67
1:X:705:C:H2'	1:X:706:A:C8	2.29	0.67



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:2002:A:H61	1:X:2018:G:H1	1.43	0.67
4:B:132:LYS:HA	4:B:134:TRP:CD1	2.29	0.67
8:G:56:THR:HG22	8:G:134:MET:SD	2.34	0.67
8:G:118:ALA:O	8:G:121:LYS:HB3	1.94	0.67
1:X:833:A:N3	1:X:954:U:O2'	2.26	0.67
1:X:1329:U:H2'	1:X:1330:G:C8	2.30	0.67
1:X:2307:A:H2'	1:X:2308:A:H8	1.58	0.67
15:N:88:ILE:HG21	16:O:49:GLU:HB2	1.76	0.67
1:X:82:G:H22	1:X:100:G:H1'	1.60	0.67
1:X:719:A:H3'	1:X:720:A:H8	1.60	0.67
1:X:868:U:H2'	1:X:869:C:C6	2.30	0.67
1:X:2824:C:OP1	14:M:100:ARG:NH1	2.27	0.67
21:T:42:GLY:HA2	21:T:57:HIS:ND1	2.10	0.67
25:Z:58:LEU:H	25:Z:58:LEU:HD13	1.58	0.67
14:M:27:PHE:CZ	14:M:96:ARG:HA	2.29	0.67
21:T:32:LYS:N	21:T:35:ASN:OD1	2.28	0.67
25:Z:36:CYS:SG	25:Z:49:CYS:HB3	2.35	0.67
1:X:2191:A:H5"	1:X:2192:U:H5	1.59	0.66
1:X:2662:C:H2'	1:X:2663:U:C6	2.29	0.66
9:H:7:ARG:HH21	9:H:7:ARG:HG2	1.60	0.66
14:M:38:LYS:NZ	14:M:46:ARG:HD2	2.10	0.66
1:X:114:C:O2'	1:X:124:A:N3	2.25	0.66
1:X:556:A:OP1	1:X:1233:A:O2'	2.13	0.66
1:X:2040:A:H2'	1:X:2041:A:C8	2.31	0.66
3:A:223:GLY:HA3	3:A:231:HIS:CD2	2.30	0.66
5:C:189:ASP:O	5:C:191:ALA:N	2.24	0.66
11:J:6:LYS:HB2	11:J:45:SER:HB2	1.77	0.66
12:K:28:LEU:HD11	12:K:115:LEU:HD21	1.77	0.66
1:X:2567:G:O6	1:X:2586:G:N1	2.28	0.66
1:X:2594:U:C2	25:Z:7:PRO:HA	2.29	0.66
1:X:2700:U:H2'	1:X:2701:A:H8	1.59	0.66
13:L:32:TYR:O	13:L:34:SER:N	2.29	0.66
17:P:68:VAL:HG22	17:P:124:ILE:HG21	1.76	0.66
24:W:46:THR:HG22	24:W:47:VAL:HG13	1.75	0.66
20:S:1:MET:N	20:S:2:GLU:OE1	2.29	0.66
7:E:48:ASP:OD2	7:E:49:GLN:NE2	2.28	0.66
20:S:117:VAL:HG23	20:S:168:VAL:HA	1.78	0.66
4:B:112:GLY:O	4:B:159:HIS:HA	1.95	0.66
14:M:41:GLU:HG2	14:M:44:ARG:HH22	1.60	0.66
15:N:15:LYS:HB2	15:N:15:LYS:NZ	2.09	0.66
1:X:1583:A:H3'	3:A:86:PRO:HG3	1.78	0.66



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:2085:G:H2'	1:X:2086:U:C6	2.31	0.66
1:X:2332:G:O2'	21:T:33:ALA:O	2.12	0.66
14:M:50:PHE:HD2	14:M:79:ARG:HH11	1.43	0.66
1:X:17:G:H2'	1:X:18:U:C6	2.30	0.65
1:X:249:A:N6	1:X:278:G:O2'	2.29	0.65
1:X:2847:G:OP1	31:X:3168:SPD:H32	1.96	0.65
5:C:190:ALA:HA	5:C:194:GLU:HG3	1.76	0.65
19:R:29:HIS:HE2	19:R:51:VAL:HA	1.60	0.65
1:X:2000:U:O2'	25:Z:10:LYS:N	2.27	0.65
1:X:2270:U:OP1	1:X:2359:U:O2'	2.14	0.65
2:Y:78:A:H4'	20:S:20:ALA:HB1	1.78	0.65
5:C:152:THR:O	5:C:158:ARG:NH2	2.30	0.65
12:K:60:LEU:HG	12:K:64:ARG:HD2	1.79	0.65
28:3:12:ARG:O	28:3:14:ILE:N	2.28	0.65
1:X:693:A:H2'	1:X:694:G:H8	1.58	0.65
1:X:1444:C:H2'	1:X:1445:A:H8	1.62	0.65
21:T:15:ASP:OD1	21:T:16:SER:N	2.26	0.65
1:X:927:C:OP2	21:T:74:LYS:NZ	2.29	0.65
1:X:1012:A:H62	1:X:1165:G:H21	1.45	0.65
1:X:1326:U:H4'	1:X:1345:G:H4'	1.78	0.65
9:H:83:ARG:HH12	9:H:134:LEU:HD21	1.61	0.65
17:P:114:ALA:O	17:P:115:ASN:ND2	2.30	0.65
1:X:2077:G:O6	1:X:2078:G:N2	2.28	0.65
1:X:2801:A:H5"	1:X:2802:C:OP2	1.97	0.65
10:I:66:ASN:N	10:I:98:LEU:O	2.25	0.65
1:X:2688:G:N7	31:X:3171:SPD:N1	2.44	0.65
15:N:83:LEU:HD21	15:N:109:LEU:HD23	1.77	0.65
1:X:621:U:H2'	1:X:622:U:C6	2.31	0.65
5:C:5:ASN:HB3	5:C:120:VAL:HG23	1.77	0.65
1:X:341:A:C2	1:X:1223:G:H2'	2.31	0.65
1:X:572:G:N3	15:N:37:GLN:NE2	2.45	0.65
1:X:1264:C:OP1	15:N:13:ARG:NH1	2.29	0.65
1:X:2293:G:H2'	1:X:2294:U:C6	2.32	0.65
4:B:115:GLY:O	4:B:119:ARG:HB2	1.97	0.65
12:K:8:ARG:HD3	12:K:10:LEU:HD21	1.78	0.65
17:P:59:PHE:HD2	25:Z:41:LEU:HD22	1.62	0.65
1:X:1991:C:H2'	1:X:1992:G:H8	1.62	0.65
12:K:52:ILE:HD11	12:K:94:TYR:CG	2.32	0.65
1:X:1017:C:H1'	8:G:134:MET:SD	2.37	0.64
1:X:1265:G:N2	15:N:37:GLN:OE1	2.28	0.64
1:X:2567:G:C6	1:X:2586:G:N1	2.65	0.64



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
16:O:20:ILE:HD12	16:O:21:ARG:H	1.62	0.64
17:P:34:SER:HB3	17:P:37:LYS:HD2	1.78	0.64
8:G:115:ALA:HB3	8:G:116:ARG:HG3	1.80	0.64
22:U:24:ALA:HB3	22:U:36:GLY:H	1.61	0.64
1:X:759:C:O2'	1:X:760:U:OP2	2.13	0.64
1:X:2447:G:HO2'	1:X:2448:A:H8	1.44	0.64
3:A:210:GLY:O	3:A:213:ARG:N	2.30	0.64
5:C:154:ASP:OD1	5:C:157:THR:OG1	2.14	0.64
1:X:320:A:N3	1:X:340:G:O2'	2.29	0.64
1:X:605:G:H2'	1:X:606:A:H8	1.63	0.64
1:X:2039:G:C2	1:X:2040:A:C8	2.86	0.64
1:X:2873:G:H2'	1:X:2874:A:C8	2.32	0.64
1:X:116:A:OP2	1:X:117:A:H8	1.80	0.64
1:X:2357:A:H4'	13:L:26:ARG:CZ	2.28	0.64
7:E:9:ILE:HD11	7:E:49:GLN:HB3	1.79	0.64
8:G:114:THR:OG1	8:G:119:LEU:HD23	1.97	0.64
17:P:97:VAL:HG22	17:P:124:ILE:HG23	1.80	0.64
1:X:2069:U:H2'	1:X:2070:G:C8	2.32	0.64
5:C:153:ASP:HA	5:C:158:ARG:HH22	1.60	0.64
1:X:1467:U:H3'	1:X:1468:A:O4'	1.97	0.64
1:X:2363:G:OP2	21:T:55:ARG:NH2	2.31	0.64
1:X:2490:U:O3'	4:B:123:ALA:HB3	1.97	0.64
1:X:72:A:H5"	23:V:47:ARG:HH21	1.61	0.64
1:X:992:A:N1	1:X:2010:G:O2'	2.26	0.64
1:X:1687:C:H42	1:X:1691:G:H5'	1.61	0.64
3:A:252:LYS:NZ	3:A:253:PRO:HD2	2.13	0.64
11:J:28:VAL:HA	11:J:68:ARG:HH22	1.63	0.64
12:K:87:TYR:CD1	12:K:90:ARG:HD2	2.32	0.64
17:P:44:VAL:O	17:P:48:LYS:NZ	2.31	0.64
18:Q:64:ARG:HB2	18:Q:69:ILE:HG13	1.80	0.64
1:X:994:A:N6	1:X:995:A:N1	2.46	0.63
2:Y:14:C:H4'	2:Y:17:A:H62	1.63	0.63
2:Y:26:G:N7	2:Y:58:G:H2'	2.12	0.63
6:D:166:ALA:O	6:D:169:LEU:HG	1.97	0.63
1:X:1153:A:O2'	1:X:1154:A:O5'	2.16	0.63
1:X:1117:G:N2	1:X:1118:G:N7	2.45	0.63
1:X:1464:A:H2'	1:X:1465:G:C8	2.33	0.63
1:X:1584:G:H5"	3:A:61:LEU:HG	1.80	0.63
1:X:2795:A:O2'	12:K:3:HIS:HD2	1.79	0.63
1:X:310:A:N3	1:X:330:C:O2'	2.31	0.63
1:X:712:A:H2'	1:X:713:G:O4'	1.99	0.63



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:1123:G:H2'	1:X:1124:U:O4'	1.99	0.63
1:X:1872:A:N3	1:X:2069:U:O2'	2.31	0.63
1:X:2220:A:H2'	1:X:2221:G:C8	2.34	0.63
1:X:2814:G:N2	12:K:91:PRO:O	2.30	0.63
1:X:1402:G:H2'	1:X:1403:U:C6	2.33	0.63
1:X:1987:G:C5	1:X:1988:A:C8	2.86	0.63
11:J:19:THR:HG22	11:J:99:LYS:HD3	1.81	0.63
12:K:98:LEU:HD22	12:K:98:LEU:H	1.64	0.63
13:L:28:ARG:NH1	13:L:90:ASP:OD2	2.28	0.63
1:X:544:U:H2'	1:X:545:C:C6	2.34	0.63
1:X:759:C:H3'	1:X:759:C:H6	1.63	0.63
1:X:2871:U:H2'	1:X:2872:U:C6	2.33	0.63
2:Y:62:C:H2'	2:Y:63:A:H8	1.63	0.63
7:E:86:ASN:OD1	7:E:86:ASN:N	2.31	0.63
22:U:47:HIS:CG	22:U:48:LYS:H	2.16	0.63
1:X:1300:A:H2'	1:X:1300:A:N3	2.14	0.63
4:B:110:GLY:O	12:K:3:HIS:NE2	2.32	0.63
20:S:24:TYR:HB3	20:S:29:ASN:OD1	1.99	0.63
22:U:20:ARG:HE	22:U:41:VAL:HG22	1.63	0.63
19:R:105:ARG:HH11	19:R:112:LYS:HG2	1.64	0.63
20:S:122:ILE:HG22	20:S:160:LEU:HA	1.81	0.63
25:Z:36:CYS:HB2	25:Z:49:CYS:SG	2.38	0.63
1:X:171:G:H2'	1:X:172:A:O4'	1.99	0.62
1:X:2311:U:OP1	21:T:46:LYS:NZ	2.32	0.62
6:D:123:ASP:OD1	6:D:125:ARG:NE	2.31	0.62
1:X:1105:U:H2'	1:X:1106:A:H5"	1.81	0.62
1:X:1800:A:H4'	1:X:1801:C:OP1	2.00	0.62
1:X:2672:U:H2'	1:X:2673:G:H8	1.63	0.62
1:X:2711:G:OP1	4:B:169:ASN:ND2	2.29	0.62
11:J:15:ARG:HG2	11:J:74:PRO:HD2	1.80	0.62
13:L:69:ALA:HB2	13:L:102:ALA:HB1	1.81	0.62
7:E:9:ILE:H	7:E:9:ILE:HD13	1.65	0.62
26:1:30:ASN:N	26:1:30:ASN:OD1	2.31	0.62
1:X:38:G:H21	5:C:42:THR:HG21	1.64	0.62
1:X:546:A:H2'	1:X:547:U:H6	1.62	0.62
1:X:936:A:H2'	1:X:937:C:H6	1.65	0.62
1:X:2189:A:H3'	1:X:2190:A:H5"	1.81	0.62
12:K:92:GLY:HA2	12:K:94:TYR:CE2	2.35	0.62
1:X:995:A:H5"	1:X:996:C:H5	1.64	0.62
1:X:1985:G:OP1	12:K:9:LYS:HE2	1.99	0.62
18:Q:48:VAL:HG21	18:Q:82:LEU:HD13	1.81	0.62



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:19:C:OP1	15:N:30:LYS:NZ	2.24	0.62
1:X:957:G:H2'	1:X:958:G:H8	1.64	0.62
1:X:967:G:H5"	11:J:78:LYS:HD3	1.82	0.62
1:X:2417:U:O2'	1:X:2419:C:OP1	2.14	0.62
1:X:2674:C:H2'	1:X:2675:U:C6	2.35	0.62
3:A:164:GLN:HB3	3:A:176:ARG:HB3	1.81	0.62
1:X:70:A:H5'	1:X:71:A:H2'	1.81	0.62
1:X:1890:G:H2'	1:X:1890:G:N3	2.15	0.62
1:X:1995:G:O3'	17:P:117:ILE:HD11	1.99	0.62
1:X:2191:A:H5"	1:X:2192:U:C5	2.33	0.62
6:D:61:THR:HA	6:D:99:PHE:CZ	2.35	0.62
17:P:24:GLY:O	17:P:127:ILE:HA	2.00	0.62
1:X:1785:A:H2'	1:X:1786:C:H6	1.65	0.62
4:B:5:LEU:HD21	4:B:79:ARG:HG3	1.81	0.62
1:X:590:C:C2	1:X:591:G:C8	2.87	0.62
1:X:1055:A:O2'	1:X:1058:G:O2'	2.16	0.62
1:X:1562:G:H8	1:X:1562:G:OP2	1.82	0.62
1:X:1675:C:OP1	4:B:134:TRP:CD1	2.53	0.62
10:I:51:GLY:O	10:I:53:ARG:NH1	2.28	0.62
1:X:946:U:H2'	1:X:947:C:C6	2.34	0.61
1:X:1264:C:H5"	15:N:13:ARG:HH12	1.65	0.61
1:X:1370:U:H3'	1:X:1371:G:C8	2.35	0.61
1:X:967:G:O3'	11:J:78:LYS:HE2	2.00	0.61
1:X:1275:A:OP2	17:P:120:ARG:NH1	2.33	0.61
1:X:1687:C:N4	1:X:1691:G:H5'	2.14	0.61
1:X:1982:C:OP1	1:X:2704:U:H5'	2.00	0.61
5:C:27:LEU:HG	5:C:181:LEU:HD21	1.82	0.61
6:D:162:THR:HB	6:D:165:GLU:HG3	1.82	0.61
2:Y:37:C:H2'	2:Y:38:C:O4'	2.00	0.61
3:A:29:PRO:HB2	3:A:34:THR:HG21	1.83	0.61
6:D:104:ILE:HG13	6:D:174:GLY:HA3	1.82	0.61
1:X:1099:A:H5'	1:X:1100:G:H5'	1.82	0.61
1:X:1105:U:HO2'	1:X:1106:A:H8	1.49	0.61
1:X:1937:G:O2'	1:X:1939:U:O4	2.10	0.61
2:Y:50:U:H2'	2:Y:51:G:C8	2.36	0.61
1:X:1425:G:H2'	1:X:1426:U:C6	2.36	0.61
5:C:82:VAL:HG12	5:C:83:ALA:O	2.00	0.61
1:X:205:A:H2'	1:X:206:U:H5'	1.82	0.61
1:X:833:A:OP2	1:X:984:A:N6	2.33	0.61
1:X:1225:G:H1'	1:X:1250:A:N6	2.16	0.61
1:X:1686:A:H5'	31:X:3167:SPD:H22	1.83	0.61



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:2020:G:H2'	1:X:2021:G:H8	1.63	0.61
9:H:99:ILE:HD12	9:H:103:GLY:HA2	1.81	0.61
17:P:57:LEU:HD13	17:P:69:ALA:HA	1.82	0.61
20:S:23:ALA:H	20:S:30:VAL:HG22	1.64	0.61
1:X:580:A:H4'	1:X:581:A:OP1	1.99	0.61
1:X:826:U:H2'	1:X:827:C:C6	2.35	0.61
1:X:2212:U:H2'	1:X:2213:G:C8	2.36	0.61
1:X:2344:G:H4'	21:T:60:PHE:CE1	2.36	0.61
1:X:2441:U:H2'	1:X:2442:C:C6	2.36	0.61
2:Y:59:A:H3'	2:Y:60:A:H8	1.66	0.61
12:K:98:LEU:HD23	12:K:112:LEU:HB2	1.83	0.61
14:M:14:ARG:NH1	14:M:15:GLY:HA2	2.12	0.61
1:X:1427:G:O2'	1:X:1604:A:N6	2.32	0.61
1:X:2795:A:H61	14:M:2:GLN:HE22	1.48	0.61
2:Y:51:G:H2'	2:Y:52:G:C8	2.35	0.61
20:S:75:LYS:O	20:S:77:ALA:N	2.34	0.61
1:X:1882:G:H21	1:X:1885:C:N4	1.96	0.61
1:X:2440:C:C2	1:X:2441:U:C5	2.89	0.61
5:C:9:GLN:HG3	5:C:120:VAL:HG21	1.81	0.61
28:3:5:LYS:H	28:3:5:LYS:HZ2	1.47	0.61
1:X:13:A:O2'	1:X:15:G:N7	2.34	0.61
1:X:809:C:H2'	1:X:810:U:C6	2.36	0.61
1:X:1264:C:H5"	15:N:13:ARG:NH1	2.16	0.61
1:X:1386:A:H5"	1:X:2191:A:N6	2.16	0.61
1:X:1484:G:H2'	1:X:1485:U:C6	2.36	0.61
1:X:2053:G:H2'	1:X:2054:A:H8	1.63	0.61
1:X:2705:A:H2'	1:X:2706:U:H2'	1.81	0.61
19:R:77:HIS:O	19:R:79:SER:N	2.27	0.61
1:X:2432:A:H2'	1:X:2433:G:C8	2.31	0.60
4:B:54:LYS:HE2	4:B:58:LYS:HB3	1.81	0.60
1:X:840:U:H4'	1:X:841:G:N2	2.16	0.60
1:X:1278:A:N6	1:X:1996:A:H5"	2.16	0.60
1:X:1979:C:OP1	9:H:43:ARG:NH1	2.33	0.60
1:X:2229:G:H5"	1:X:2229:G:N3	2.16	0.60
1:X:2674:C:H2'	1:X:2675:U:H6	1.66	0.60
5:C:153:ASP:HA	5:C:158:ARG:NH2	2.16	0.60
3:A:145:LEU:HB3	3:A:155:LEU:HB2	1.82	0.60
3:A:246:PRO:HD2	3:A:250:TRP:H	1.66	0.60
1:X:874:A:H2'	1:X:875:G:O4'	2.01	0.60
1:X:923:A:C5	11:J:12:LYS:HE3	2.36	0.60
1:X:1163:C:HO2'	15:N:76:TYR:HE1	1.50	0.60



Atom-1	Atom-2	Interatomic	Clash
1 V 1109 () H0		distance (A)	overlap (A)
1:Л:1195:G:П2 1.V.1549.C.N9	1:A:1194:U:H0	1.07	0.00
1:A:1042:G:N2	1:A:1502:G:П1 1 У 5257 Ц СС	1.90	0.00
1:A:2320:U:H2	1:A:2327:U:U0	2.37	0.00
1:X:2824:C:P	14:M:100:ARG:HH11	2.24	0.60
2:Y:14:C:H4 <sup>7</sup>	2:Y:17:A:N6	2.17	0.60
3:A:17:THR:O	3:A:211:ARG:NH2	2.34	0.60
11:J:20:GLY:C	11:J:99:LYS:HE2	2.21	0.60
1:X:15:G:H5'	25:Z:21:SER:HA	1.83	0.60
1:X:313:U:H2'	1:X:314:G:C8	2.36	0.60
3:A:69:ARG:NH2	3:A:192:THR:OG1	2.34	0.60
4:B:55:ALA:H	4:B:58:LYS:HZ3	1.49	0.60
6:D:170:LEU:HD11	6:D:177:PHE:HD2	1.67	0.60
9:H:121:ARG:HH21	9:H:121:ARG:HB3	1.65	0.60
1:X:16:G:H2'	1:X:17:G:H8	1.65	0.60
1:X:2796:A:OP2	12:K:3:HIS:NE2	2.33	0.60
5:C:22:VAL:O	5:C:24:SER:N	2.35	0.60
1:X:650:U:H2'	1:X:651:C:C6	2.37	0.60
1:X:687:G:H1'	5:C:68:ARG:HD2	1.82	0.60
1:X:1454:U:H2'	1:X:1455:C:C6	2.37	0.60
1:X:2595:C:H2'	1:X:2596:C:H6	1.67	0.60
1:X:936:A:H2'	1:X:937:C:C6	2.37	0.60
1:X:1377:G:N7	22:U:6:TYR:N	2.48	0.60
3:A:16:MET:HG2	3:A:206:LEU:O	2.02	0.60
28:3:53:ALA:O	28:3:57:ARG:HG2	2.01	0.60
1:X:63:A:H1'	18:Q:65:VAL:HG13	1.84	0.60
1:X:1805:G:N3	3:A:50:THR:HG21	2.17	0.60
1:X:2516:U:H2'	1:X:2517:C:H6	1.62	0.60
3:A:85:ASP:HB2	3:A:92:ILE:HD12	1.84	0.60
9:H:23:ARG:HG2	9:H:23:ARG:HH21	1.67	0.60
9:H:125:LYS:CE	9:H:125:LYS:H	2.14	0.60
1:X:520:C:H2'	1:X:521:U:O4'	2.02	0.60
1:X:1030:U:OP1	1:X:1046:U:O2'	2.20	0.60
10:I:54:SER:O	28:3:12:ARG:NE	2.35	0.60
16:O:24:SER:O	16:O:24:SER:OG	2.20	0.60
21:T:24:LYS:N	21:T:37:LEU:O	2.34	0.60
1:X:276:A:H2'	1:X:277:G:C8	2.36	0.59
1:X:1769:U:H2'	1:X:1775:A:N6	2.17	0.59
1:X:1981:A:OP2	4:B:136:ARG:NH1	2.26	0.59
6:D:146:VAL:HA	6:D:148:LYS:HE3	1.83	0.59
14:M:54:VAL:HG22	14:M:68:VAL:HG12	1.84	0.59
1:X:585:U:H2'	1:X:586:G:H8	1.67	0.59



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:697:G:N2	1:X:801:A:OP2	2.34	0.59
1:X:1478:U:H2'	1:X:1479:G:C8	2.37	0.59
1:X:2266:A:N6	1:X:2323:U:H3	1.99	0.59
31:X:3167:SPD:H21	9:H:5:GLN:NE2	2.17	0.59
8:G:49:VAL:HG11	8:G:54:LEU:HB2	1.84	0.59
17:P:35:PRO:HB2	17:P:39:ARG:NH2	2.17	0.59
1:X:689:A:H8	1:X:2052:G:N2	2.00	0.59
1:X:1295:U:H2'	1:X:1296:G:O4'	2.03	0.59
1:X:2546:G:H2'	1:X:2547:C:C6	2.37	0.59
8:G:99:VAL:HA	8:G:115:ALA:HA	1.83	0.59
9:H:125:LYS:H	9:H:125:LYS:HE2	1.67	0.59
10:I:83:LEU:HD13	10:I:115:SER:HA	1.84	0.59
19:R:53:VAL:HG11	19:R:74:LEU:HD23	1.84	0.59
1:X:70:A:H4'	1:X:71:A:H5"	1.84	0.59
1:X:252:G:H2'	1:X:253:A:O4'	2.03	0.59
1:X:706:A:O2'	1:X:1366:A:N3	2.31	0.59
1:X:2278:A:H2'	1:X:2279:G:H8	1.67	0.59
5:C:28:HIS:HA	10:I:6:LEU:HD22	1.83	0.59
5:C:57:LYS:HA	5:C:70:GLY:O	2.03	0.59
19:R:29:HIS:NE2	19:R:51:VAL:HA	2.17	0.59
1:X:220:U:OP1	28:3:5:LYS:HE3	2.03	0.59
1:X:1225:G:H1'	1:X:1250:A:H61	1.65	0.59
1:X:2691:C:O2'	1:X:2692:A:H5"	2.03	0.59
18:Q:14:GLU:O	18:Q:18:SER:OG	2.20	0.59
1:X:699:G:H21	27:2:7:PRO:HA	1.65	0.59
7:E:58:ALA:HB3	7:E:61:HIS:HB2	1.84	0.59
8:G:116:ARG:NH2	8:G:118:ALA:HB3	2.18	0.59
1:X:413:G:N7	22:U:68:ARG:NH1	2.45	0.59
1:X:2172:U:H2'	1:X:2173:G:O4'	2.02	0.59
1:X:2223:U:H1'	1:X:2413:A:C4	2.36	0.59
1:X:627:A:H2'	1:X:628:A:C8	2.37	0.59
1:X:691:C:H2'	1:X:692:C:C6	2.38	0.59
1:X:2345:A:H3'	1:X:2346:G:H8	1.68	0.59
19:R:23:ILE:O	19:R:81:VAL:N	2.36	0.59
1:X:76:C:O2'	23:V:59:GLU:OE2	2.19	0.59
1:X:304:A:N6	1:X:356:A:N7	2.51	0.59
1:X:994:A:N7	1:X:995:A:C6	2.71	0.59
1:X:1325:U:H4'	1:X:1326:U:O5'	2.03	0.59
7:E:130:ARG:NH1	7:E:132:ASP:OD2	2.36	0.59
8:G:44:VAL:HG22	8:G:166:LEU:HD11	1.84	0.59
11:J:36:ILE:HD11	11:J:101:GLY:HA2	1.83	0.59



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
13:L:9:ARG:HD3	13:L:9:ARG:H	1.68	0.59
1:X:1300:A:H3'	1:X:1301:U:H6	1.68	0.59
1:X:1478:U:H2'	1:X:1479:G:H8	1.67	0.59
1:X:2264:C:P	26:1:30:ASN:HD22	2.25	0.59
8:G:68:PRO:HB2	8:G:70:PHE:CE1	2.38	0.59
1:X:1779:C:H2'	1:X:1780:A:C8	2.38	0.58
1:X:2441:U:H2'	1:X:2442:C:H6	1.67	0.58
2:Y:66:G:H2'	2:Y:67:C:O4'	2.03	0.58
3:A:146:GLU:HB2	3:A:189:CYS:HB3	1.85	0.58
12:K:9:LYS:HA	12:K:17:ARG:HD3	1.85	0.58
1:X:82:G:N2	1:X:101:A:OP2	2.34	0.58
1:X:2030:U:H2'	1:X:2031:A:C8	2.38	0.58
1:X:2355:A:N6	13:L:91:ARG:HD3	2.17	0.58
2:Y:6:C:H2'	2:Y:7:C:C6	2.35	0.58
3:A:63:ARG:H	3:A:63:ARG:HE	1.51	0.58
1:X:1370:U:H3'	1:X:1371:G:H8	1.67	0.58
1:X:2370:G:H2'	1:X:2403:C:H41	1.68	0.58
2:Y:109:G:OP1	20:S:26:LYS:NZ	2.33	0.58
12:K:12:ARG:O	12:K:17:ARG:NH1	2.36	0.58
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.86	0.58
1:X:652:C:H42	1:X:657:A:H61	1.51	0.58
1:X:1223:G:H4'	1:X:1224:A:H5'	1.86	0.58
6:D:2:GLN:HA	6:D:5:LYS:HZ3	1.69	0.58
1:X:2691:C:H2'	1:X:2694:G:H5"	1.85	0.58
5:C:54:THR:HG21	5:C:73:SER:HB3	1.85	0.58
7:E:97:LYS:NZ	7:E:98:LEU:H	2.02	0.58
1:X:640:C:C4'	1:X:660:G:H21	2.16	0.58
1:X:1012:A:N6	1:X:1165:G:H21	2.02	0.58
1:X:1631:C:C5	1:X:1633:C:C2	2.91	0.58
1:X:1807:A:H5'	1:X:1809:G:H1'	1.85	0.58
1:X:2001:G:OP1	25:Z:9:LYS:NZ	2.29	0.58
4:B:119:ARG:HG3	4:B:160:MET:HB2	1.84	0.58
5:C:22:VAL:HG11	5:C:26:VAL:HG23	1.84	0.58
1:X:1033:G:OP2	8:G:93:LYS:NZ	2.21	0.58
1:X:2696:A:C2'	1:X:2697:G:H5'	2.33	0.58
4:B:32:PRO:HD2	4:B:50:GLY:O	2.02	0.58
1:X:661:C:H2'	1:X:662:G:C8	2.39	0.58
1:X:1503:G:H2'	1:X:1504:G:C8	2.39	0.58
1:X:2344:G:H4'	21:T:60:PHE:CZ	2.39	0.58
1:X:2555:G:H21	1:X:2555:G:P	2.27	0.58
1:X:2658:A:O2'	4:B:189:PRO:HB3	2.04	0.58



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
6:D:5:LYS:HG2	6:D:6:THR:N	2.18	0.58
19:R:47:VAL:HG22	19:R:75:ALA:HB2	1.85	0.58
28:3:8:LYS:O	28:3:12:ARG:HB2	2.04	0.58
1:X:14:A:C6	1:X:536:A:C2	2.92	0.58
1:X:247:A:N1	1:X:382:U:H4'	2.19	0.58
20:S:70:GLN:O	20:S:79:ILE:HB	2.03	0.58
1:X:28:A:H1'	1:X:523:A:C2	2.39	0.58
1:X:2406:C:H5"	1:X:2408:G:OP1	2.04	0.58
6:D:100:LEU:O	6:D:104:ILE:HG22	2.03	0.58
9:H:89:ILE:HD12	9:H:134:LEU:HD22	1.86	0.58
11:J:15:ARG:CG	11:J:74:PRO:HD2	2.34	0.58
13:L:26:ARG:HG2	13:L:86:GLN:HB3	1.86	0.58
1:X:3:U:H2'	1:X:4:C:C6	2.39	0.57
1:X:1300:A:O5'	12:K:103:ARG:HD2	2.04	0.57
1:X:1685:A:H5"	9:H:5:GLN:HG2	1.84	0.57
4:B:48:GLN:HA	4:B:79:ARG:O	2.04	0.57
20:S:89:GLY:H	20:S:127:PRO:HG3	1.69	0.57
1:X:536:A:N6	1:X:2605:C:H4'	2.19	0.57
1:X:588:G:C2	1:X:1275:A:C5	2.92	0.57
1:X:876:A:H2'	1:X:877:G:H8	1.68	0.57
1:X:1006:C:O2	8:G:31:THR:OG1	2.23	0.57
1:X:1332:G:C2	1:X:1333:G:C2	2.92	0.57
1:X:1941:C:H2'	1:X:1942:G:H8	1.69	0.57
1:X:2058:U:H2'	1:X:2217:G:N2	2.18	0.57
1:X:2245:A:H4'	1:X:2246:A:N3	2.18	0.57
14:M:14:ARG:NH1	14:M:18:GLN:OE1	2.36	0.57
21:T:46:LYS:NZ	21:T:75:GLY:O	2.21	0.57
24:W:8:SER:HB2	24:W:10:ILE:HG13	1.85	0.57
1:X:29:U:O5'	1:X:29:U:H6	1.87	0.57
1:X:168:A:H2'	1:X:169:C:C6	2.35	0.57
1:X:1050:G:H21	1:X:1127:C:H42	1.51	0.57
1:X:2054:A:H2'	1:X:2055:G:H8	1.69	0.57
1:X:2370:G:H2'	1:X:2403:C:N4	2.19	0.57
3:A:223:GLY:O	3:A:233:HIS:HB2	2.05	0.57
6:D:147:ASP:OD1	6:D:147:ASP:N	2.37	0.57
8:G:35:LYS:HD3	8:G:35:LYS:N	2.19	0.57
8:G:42:VAL:HB	8:G:166:LEU:HD12	1.86	0.57
19:R:98:ILE:HG13	19:R:99:VAL:H	1.67	0.57
20:S:17:SER:H	20:S:36:ARG:CB	2.16	0.57
1:X:605:G:H2'	1:X:606:A:C8	2.39	0.57
1:X:1070:G:H5"	1:X:1071:U:H2'	1.85	0.57



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:X:1835:C:H2'	1:X:1836:C:C6	2.40	0.57
1:X:2457:A:C8	1:X:2508:G:C6	2.93	0.57
1:X:2543:A:C6	1:X:2544:A:N1	2.71	0.57
1:X:2552:C:H5"	1:X:2553:G:H5"	1.86	0.57
5:C:149:LEU:HD23	5:C:180:ILE:HG22	1.85	0.57
11:J:76:THR:HB	11:J:91:VAL:HA	1.84	0.57
19:R:81:VAL:HG11	19:R:89:GLY:HA2	1.87	0.57
1:X:767:G:H2'	1:X:768:U:C6	2.39	0.57
1:X:912:A:H3'	1:X:913:A:H8	1.68	0.57
1:X:1024:G:H2'	1:X:1025:A:H8	1.68	0.57
1:X:1256:C:H2'	1:X:1257:U:C6	2.40	0.57
1:X:1818:G:OP1	3:A:233:HIS:ND1	2.32	0.57
1:X:2801:A:H2'	1:X:2801:A:N3	2.19	0.57
2:Y:68:A:N6	2:Y:111:C:OP2	2.37	0.57
8:G:111:LYS:O	8:G:113:GLU:HG3	2.04	0.57
14:M:32:THR:O	14:M:51:GLU:HA	2.05	0.57
22:U:47:HIS:CG	22:U:48:LYS:N	2.72	0.57
1:X:255:A:N6	1:X:265:U:O4	2.37	0.57
1:X:765:C:C4	29:X:2901:MIV:H36	2.39	0.57
1:X:773:G:H2'	1:X:774[A]:A:O4'	2.05	0.57
1:X:2007:G:C2	1:X:2023:C:C2	2.92	0.57
12:K:98:LEU:CD2	12:K:112:LEU:HB2	2.35	0.57
28:3:32:GLN:NE2	28:3:32:GLN:HA	2.19	0.57
1:X:940:G:O2'	1:X:941:U:O5'	2.18	0.57
1:X:1658:A:H2'	1:X:1659:G:O4'	2.05	0.57
1:X:1919:A:N6	1:X:1946:U:H3	2.02	0.57
1:X:2226:A:H2'	1:X:2227:C:H6	1.69	0.57
1:X:2526:U:H2'	1:X:2527:G:C8	2.39	0.57
2:Y:59:A:H1'	6:D:27:ALA:HB2	1.87	0.57
27:2:10:ARG:O	27:2:14:LYS:HB2	2.05	0.57
1:X:151:G:H2'	1:X:152:G:H8	1.69	0.57
1:X:227:G:H2'	1:X:228:A:C8	2.40	0.57
1:X:554:U:H5"	1:X:556:A:C2	2.39	0.57
1:X:691:C:H2'	1:X:692:C:H6	1.70	0.57
1:X:1141:U:N3	1:X:2008:C:H5"	2.19	0.57
1:X:1835:C:O2'	3:A:254:THR:HB	2.04	0.57
1:X:2067:U:H2'	1:X:2068:C:C6	2.40	0.57
1:X:2336:G:N2	1:X:2339:A:OP2	2.38	0.57
1:X:2337:A:C2	1:X:2338:C:H1'	2.40	0.57
5:C:158:ARG:NH2	5:C:171:PRO:HA	2.20	0.57
17:P:31:VAL:O	17:P:122:SER:N	2.37	0.57



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
19:R:100:ASP:HB2	19:R:102:LYS:HG3	1.85	0.57
1:X:2408:G:H5	1:X:2409:A:P	2.45	0.57
2:Y:77:G:H2'	2:Y:78:A:O4'	2.04	0.57
3:A:183:ARG:HG3	3:A:267:ASP:HB3	1.87	0.57
7:E:58:ALA:O	7:E:62:ARG:N	2.37	0.57
7:E:136:ILE:HG13	7:E:137:ASP:H	1.69	0.57
9:H:125:LYS:H	9:H:125:LYS:CD	2.18	0.57
28:3:39:ASP:HB3	28:3:42:ARG:HH22	1.69	0.57
1:X:174:A:H62	1:X:2409:A:H2'	1.69	0.57
1:X:487:G:H22	1:X:490:A:H5'	1.70	0.57
1:X:494:A:H4'	19:R:58:VAL:H	1.70	0.57
1:X:764:A:H4'	29:X:2901:MIV:H342	1.87	0.57
1:X:1004:A:OP1	15:N:50:ARG:NH1	2.38	0.57
1:X:1300:A:H3'	1:X:1301:U:C6	2.40	0.57
1:X:1607:A:H2'	1:X:1608:U:C6	2.39	0.57
1:X:2477:C:O2'	1:X:2478:C:H5'	2.04	0.57
10:I:100:ARG:HA	10:I:117:ALA:O	2.05	0.57
12:K:22:ARG:HD3	12:K:69:ASP:HA	1.87	0.57
1:X:2371:A:C5	1:X:2372:A:C8	2.93	0.56
2:Y:68:A:H4'	2:Y:69:G:OP2	2.03	0.56
1:X:573:C:H2'	1:X:574:C:C6	2.41	0.56
1:X:859:U:HO2'	1:X:860:U:P	2.28	0.56
2:Y:50:U:H2'	2:Y:51:G:H8	1.70	0.56
7:E:7:GLN:HB3	7:E:51:LEU:HD11	1.86	0.56
7:E:156:ALA:HB1	7:E:172:LYS:HG3	1.87	0.56
8:G:68:PRO:O	8:G:70:PHE:N	2.38	0.56
14:M:38:LYS:HA	14:M:87:LEU:HD13	1.87	0.56
21:T:40:GLN:OE1	21:T:45:PHE:N	2.34	0.56
1:X:18:U:O2'	1:X:563:U:OP1	2.19	0.56
1:X:242:A:N6	1:X:440:U:HO2'	2.03	0.56
1:X:276:A:H2'	1:X:277:G:H8	1.69	0.56
1:X:530:G:H2'	1:X:531:G:H8	1.70	0.56
1:X:588:G:O2'	1:X:2002:A:OP1	2.20	0.56
1:X:597:U:H1'	5:C:84:PHE:CD1	2.40	0.56
1:X:876:A:H2'	1:X:877:G:C8	2.41	0.56
1:X:1367:A:H2'	1:X:1368:G:O4'	2.05	0.56
1:X:1701:C:H2'	1:X:1702:C:C6	2.40	0.56
1:X:1702:C:C2	1:X:1721:G:N2	2.73	0.56
1:X:1729:C:H2'	1:X:1730:G:H8	1.70	0.56
1:X:1975:G:N2	1:X:1979:C:O2'	2.39	0.56
1:X:2700:U:H2'	1:X:2701:A:C8	2.39	0.56


Atom 1	Atom-2	Interatomic	Clash
Atom-1		distance $(\text{\AA})$	overlap (Å)
1:X:2859:U:OP2	25:Z:43:HIS:NE2	2.36	0.56
17:P:13:GLN:O	17:P:17:GLN:HG2	2.05	0.56
18:Q:35:LYS:HE3	18:Q:55:THR:HG22	1.87	0.56
19:R:58:VAL:HG12	19:R:68:GLY:CA	2.35	0.56
19:R:106:VAL:O	19:R:112:LYS:HA	2.05	0.56
20:S:146:HIS:ND1	20:S:170:SER:OG	2.34	0.56
21:T:56:ASP:OD1	21:T:58:THR:HG22	2.05	0.56
1:X:661:C:H2'	1:X:662:G:H8	1.69	0.56
1:X:1310:C:C2	1:X:1311:C:C5	2.93	0.56
1:X:1320:A:H2'	1:X:1321:A:O4'	2.06	0.56
1:X:1742:G:H2'	1:X:1743:C:C6	2.41	0.56
1:X:1812:U:N3	3:A:199:ALA:O	2.30	0.56
1:X:2437:G:H2'	1:X:2469:G:O6	2.05	0.56
1:X:2646:C:N3	7:E:110:SER:OG	2.34	0.56
1:X:2790:C:H2'	1:X:2791:C:H6	1.71	0.56
1:X:2824:C:H4'	1:X:2825:A:H5'	1.87	0.56
5:C:178:TYR:O	5:C:182:ARG:HB2	2.05	0.56
18:Q:88:ILE:HG23	18:Q:89:GLU:O	2.06	0.56
1:X:409:G:OP1	22:U:14:VAL:HG11	2.06	0.56
1:X:1630:A:N1	17:P:114:ALA:HB2	2.20	0.56
4:B:53:PRO:HA	4:B:75:THR:HA	1.86	0.56
6:D:10:ASP:O	6:D:14:PRO:HD2	2.05	0.56
6:D:125:ARG:HA	6:D:160:ALA:HB3	1.87	0.56
14:M:59:GLY:HA3	14:M:64:LYS:HA	1.88	0.56
17:P:54:GLU:OE2	17:P:76:LYS:NZ	2.32	0.56
19:R:58:VAL:HA	19:R:67:GLY:HA3	1.86	0.56
1:X:529:U:H2'	1:X:530:G:H8	1.71	0.56
1:X:919:U:OP1	11:J:25:GLY:HA2	2.05	0.56
1:X:2030:U:H2'	1:X:2031:A:H8	1.71	0.56
1:X:2661:G:H4'	14:M:63:ARG:HD3	1.87	0.56
16:O:35:LEU:HA	16:O:55:THR:HG22	1.88	0.56
1:X:14:A:H2'	1:X:15:G:O4'	2.06	0.56
1:X:453:U:H2'	1:X:454:G:C8	2.40	0.56
1:X:491:A:H5'	1:X:492:G:O5'	2.05	0.56
1:X:1045:G:H2'	1:X:1046:U:C6	2.40	0.56
1:X:1398:G:O2'	1:X:1399:C:O5'	2.24	0.56
1:X:2251:U:H5"	1:X:2252:A:OP1	2.05	0.56
2:Y:45:C:H4'	6:D:95:ARG:HH22	1.71	0.56
4:B:152:LYS:HG2	8:G:106:TYR:CE1	2.40	0.56
5:C:45:THR:O	5:C:87:LYS:NZ	2.38	0.56
8:G:38:GLU:HG3	8:G:67:ARG:HH12	1.70	0.56



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
8:G:51:LEU:HD12	8:G:88:VAL:HG21	1.88	0.56
9:H:11:ALA:O	9:H:111:PHE:N	2.38	0.56
1:X:200:A:N1	1:X:420:C:O2'	2.28	0.56
1:X:661:C:H5"	28:3:18:GLY:HA2	1.86	0.56
1:X:946:U:H2'	1:X:947:C:H6	1.71	0.56
1:X:1283:C:H2'	1:X:1665:C:H5"	1.87	0.56
1:X:1729:C:H2'	1:X:1730:G:C8	2.41	0.56
15:N:72:HIS:CE1	15:N:107:LYS:HD3	2.41	0.56
20:S:49:THR:OG1	20:S:49:THR:O	2.24	0.56
27:2:17:GLY:O	27:2:21:ARG:HG2	2.06	0.56
1:X:453:U:O2'	5:C:40:ARG:NH1	2.39	0.56
1:X:1211:G:C2	1:X:1212:U:C5	2.94	0.56
3:A:246:PRO:HD3	3:A:252:LYS:HG3	1.88	0.56
10:I:114:ILE:HG23	10:I:134:GLU:HB2	1.87	0.56
1:X:136:A:H2'	1:X:137:A:C8	2.41	0.56
1:X:932:G:H2'	1:X:933:G:H8	1.70	0.56
1:X:1061:A:N6	1:X:2731:G:O6	2.39	0.56
1:X:1261:G:OP1	5:C:86:PRO:HG3	2.06	0.56
1:X:2043:A:H1'	1:X:2481:G:C1'	2.36	0.56
1:X:2673:G:H2'	1:X:2674:C:H6	1.71	0.56
3:A:258:LYS:NZ	3:A:264:LYS:HG2	2.20	0.56
8:G:101:THR:HG23	8:G:111:LYS:HA	1.87	0.56
9:H:11:ALA:HB3	9:H:97:VAL:HB	1.87	0.56
12:K:92:GLY:HA2	12:K:94:TYR:CZ	2.41	0.56
1:X:1104:G:H2'	1:X:1105:U:H5	1.71	0.55
1:X:1155:G:H5"	1:X:1156:U:OP2	2.06	0.55
3:A:71:ASP:OD1	3:A:71:ASP:N	2.36	0.55
7:E:27:LYS:HA	7:E:31:GLY:HA2	1.88	0.55
9:H:49:ASP:OD1	9:H:121:ARG:NH1	2.39	0.55
10:I:53:ARG:NH2	28:3:12:ARG:HD3	2.21	0.55
11:J:27:TYR:HB2	11:J:138:TYR:CD2	2.41	0.55
16:O:40:VAL:HG12	16:O:43:GLU:HA	1.88	0.55
18:Q:89:GLU:O	18:Q:91:LEU:N	2.34	0.55
1:X:16:G:H2'	1:X:17:G:C8	2.41	0.55
1:X:796:A:H4'	1:X:2567:G:H4'	1.88	0.55
1:X:1469:U:O2	12:K:63:ARG:HD3	2.06	0.55
1:X:2468:G:H2'	1:X:2469:G:O4'	2.06	0.55
1:X:2867:G:OP2	1:X:2867:G:C8	2.55	0.55
7:E:17:VAL:HG22	7:E:26:VAL:HG22	1.89	0.55
1:X:24:G:H2'	1:X:25:U:H6	1.71	0.55
1:X:331:U:H4'	1:X:333:A:N7	2.20	0.55



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:X:578:U:H5"	1:X:579:G:OP2	2.06	0.55
1:X:806:A:OP2	1:X:806:A:H8	1.89	0.55
1:X:914:C:H2'	1:X:915:C:C6	2.42	0.55
1:X:1071:U:H3	1:X:1099:A:H8	1.54	0.55
1:X:1314:A:H2	1:X:1642:G:N3	2.04	0.55
1:X:2040:A:H2'	1:X:2041:A:H8	1.72	0.55
2:Y:11:G:P	13:L:28:ARG:HH22	2.29	0.55
5:C:123:PHE:CD2	5:C:157:THR:HG21	2.41	0.55
17:P:89:ARG:HA	17:P:89:ARG:HE	1.71	0.55
17:P:130:GLU:C	17:P:132:GLY:H	2.08	0.55
1:X:542:A:OP1	1:X:570:G:N2	2.37	0.55
1:X:746:G:H2'	1:X:747:A:H5"	1.88	0.55
1:X:789:G:C6	1:X:806:A:C5	2.94	0.55
1:X:1976:U:C4	1:X:1977:C:C5	2.93	0.55
1:X:2269:G:H2'	1:X:2270:U:O4'	2.06	0.55
1:X:2368:G:H5"	1:X:2369:U:H5'	1.88	0.55
3:A:63:ARG:H	3:A:63:ARG:NE	2.03	0.55
5:C:172:VAL:HG12	5:C:173:ALA:H	1.72	0.55
1:X:501:G:H3'	1:X:502:A:H8	1.72	0.55
1:X:759:C:OP1	1:X:761:G:H4'	2.07	0.55
1:X:877:G:H2'	1:X:878:C:C6	2.41	0.55
1:X:2398:U:O4	28:3:31:HIS:NE2	2.39	0.55
4:B:132:LYS:O	4:B:132:LYS:HG2	2.06	0.55
5:C:6:VAL:HG22	5:C:120:VAL:H	1.71	0.55
5:C:17:LEU:HD21	5:C:112:GLN:HG2	1.88	0.55
15:N:101:ARG:HD3	15:N:102:GLU:HG3	1.89	0.55
1:X:544:U:O2'	15:N:49:ASP:OD2	2.15	0.55
1:X:654:A:N1	1:X:2348:A:O2'	2.37	0.55
1:X:670:U:H2'	1:X:671:A:C8	2.41	0.55
1:X:1457:A:H2'	1:X:1458:A:C8	2.41	0.55
1:X:1608:U:H2'	1:X:1609:G:C8	2.42	0.55
1:X:2556:A:O2'	25:Z:3:LYS:HA	2.06	0.55
1:X:2721:A:H8	1:X:2721:A:O5'	1.90	0.55
12:K:90:ARG:HB2	12:K:94:TYR:HE1	1.72	0.55
16:O:20:ILE:O	16:O:90:PHE:HB2	2.06	0.55
17:P:31:VAL:HG23	17:P:122:SER:O	2.07	0.55
1:X:790:A:H2'	1:X:791:G:C8	2.42	0.55
1:X:836:G:H2'	1:X:837:U:H6	1.72	0.55
1:X:841:G:H2'	1:X:842:A:C8	2.41	0.55
1:X:1171:A:H2'	1:X:1172:U:C6	2.42	0.55
1:X:1654:A:H4'	1:X:2690:A:O2'	2.06	0.55



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:1845:A:H2'	1:X:1846:A:C8	2.42	0.55
1:X:2511:G:N2	1:X:2642:G:O2'	2.40	0.55
4:B:38:THR:O	4:B:42:ASP:N	2.39	0.55
19:R:64:ASN:ND2	19:R:67:GLY:HA2	2.22	0.55
20:S:88:TYR:HA	20:S:127:PRO:CB	2.37	0.55
1:X:980:G:O3'	24:W:11:GLY:HA2	2.07	0.55
1:X:1040:A:C8	1:X:1041:G:C8	2.94	0.55
1:X:2371:A:H2	1:X:2403:C:H42	1.55	0.55
1:X:2630:C:H2'	1:X:2631:C:H6	1.72	0.55
2:Y:22:U:H2'	2:Y:23:G:C8	2.41	0.55
3:A:171:ASP:O	3:A:187:SER:HB2	2.07	0.55
16:O:11:GLN:O	16:O:36:LYS:HA	2.07	0.55
1:X:336:A:H2'	1:X:337:G:C8	2.42	0.55
1:X:757:U:H2'	1:X:758:G:O4'	2.07	0.55
1:X:2270:U:H2'	1:X:2271:C:C6	2.41	0.55
1:X:2273:C:OP2	13:L:15:ARG:NH2	2.39	0.55
1:X:2673:G:H2'	1:X:2674:C:C6	2.41	0.55
1:X:2799:C:H2'	1:X:2800:C:O4'	2.07	0.55
17:P:40:LEU:HD13	25:Z:25:LEU:HD11	1.89	0.55
18:Q:20:MET:HG3	18:Q:25:TYR:CE1	2.42	0.55
1:X:500:G:C2	1:X:501:G:H1'	2.42	0.55
1:X:1834:G:H2'	1:X:1835:C:C6	2.42	0.55
1:X:1888:C:H5"	1:X:1889:G:H5'	1.89	0.55
1:X:1992:G:H2'	1:X:1993:G:H5'	1.88	0.55
14:M:17:GLU:HG3	14:M:62:SER:HB3	1.89	0.55
1:X:1608:U:H2'	1:X:1609:G:H8	1.72	0.54
1:X:1908:C:O2'	1:X:1909:U:H5"	2.07	0.54
1:X:1987:G:C2	1:X:1988:A:H1'	2.43	0.54
1:X:2292:C:H5'	6:D:68:THR:HG21	1.89	0.54
6:D:40:LEU:HD11	6:D:53:ALA:HB3	1.89	0.54
16:O:86:HIS:NE2	16:O:88:GLN:HG2	2.22	0.54
24:W:36:ASP:OD1	24:W:41:ARG:NH1	2.40	0.54
1:X:654:A:H2'	1:X:655:A:H5'	1.89	0.54
1:X:1256:C:H2'	1:X:1257:U:H6	1.71	0.54
1:X:2567:G:C5	1:X:2586:G:C2	2.95	0.54
1:X:2665:G:C2	1:X:2704:U:O2	2.60	0.54
3:A:141:VAL:HG23	3:A:194:GLY:HA2	1.89	0.54
4:B:77:ILE:HD12	4:B:195:LEU:HD22	1.88	0.54
8:G:71:THR:HG22	8:G:73:ASN:H	1.72	0.54
11:J:15:ARG:HG3	11:J:73:LYS:HG3	1.89	0.54
11:J:42:TRP:CE3	11:J:95:VAL:HG21	2.42	0.54



Atom 1	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
14:M:110:LEU:HB3	14:M:115:ALA:CB	2.38	0.54
1:X:1215:A:H2'	1:X:1216:G:C8	2.42	0.54
1:X:1269:G:N2	5:C:76:THR:O	2.41	0.54
1:X:1674:C:C2	1:X:1675:C:C5	2.95	0.54
1:X:1919:A:H2	1:X:1926:U:N3	2.01	0.54
1:X:2208:U:H2'	1:X:2209:G:H8	1.71	0.54
1:X:2495:G:O2'	1:X:2496:C:H5'	2.07	0.54
1:X:2571:G:H1	1:X:2580:C:H41	1.53	0.54
2:Y:7:C:H2'	2:Y:8:C:H6	1.72	0.54
1:X:1956:G:H2'	1:X:1957:C:H6	1.72	0.54
1:X:2839:G:H2'	1:X:2840:U:C6	2.42	0.54
5:C:47:THR:HB	5:C:51:VAL:H	1.72	0.54
19:R:25:LEU:HG	19:R:81:VAL:HG23	1.88	0.54
1:X:2370:G:O2'	1:X:2408:G:N2	2.41	0.54
1:X:2440:C:H2'	1:X:2441:U:C6	2.43	0.54
1:X:2543:A:C2	1:X:2626:U:H4'	2.42	0.54
1:X:2567:G:C5	1:X:2586:G:N2	2.75	0.54
1:X:2705:A:O2'	1:X:2706:U:C6	2.60	0.54
3:A:131:LEU:O	3:A:190:TYR:HA	2.08	0.54
1:X:47:G:N2	1:X:154:U:OP2	2.39	0.54
1:X:456:C:OP2	15:N:2:PRO:HD3	2.06	0.54
1:X:1398:G:O2'	1:X:1399:C:O4'	2.25	0.54
1:X:1538:A:H2'	1:X:1539:U:O4'	2.07	0.54
1:X:1928:G:H2'	1:X:1929:U:C6	2.42	0.54
1:X:2214:G:H2'	1:X:2215:C:H6	1.73	0.54
3:A:134:ARG:HB2	3:A:187:SER:OG	2.08	0.54
4:B:25:VAL:HG12	4:B:181:LEU:HD12	1.88	0.54
17:P:107:ILE:O	17:P:107:ILE:HG12	2.07	0.54
1:X:1484:G:H2'	1:X:1485:U:H6	1.71	0.54
1:X:1561:A:H3'	1:X:1562:G:C8	2.42	0.54
6:D:5:LYS:HD2	6:D:97:TYR:HB3	1.90	0.54
1:X:125:A:H5"	1:X:126:C:C6	2.42	0.54
1:X:1288:A:C8	12:K:16:ALA:HB2	2.43	0.54
1:X:1716:G:O6	1:X:1754:G:H1'	2.08	0.54
1:X:1967:U:H2'	1:X:1968:G:H8	1.73	0.54
1:X:1982:C:O3'	1:X:2702:G:N2	2.41	0.54
1:X:2078:G:H2'	1:X:2079:A:C8	2.43	0.54
1:X:2467:A:C2'	1:X:2468:G:H5'	2.36	0.54
7:E:83:TYR:CE2	7:E:138:LYS:HB2	2.43	0.54
21:T:21:LEU:HD11	21:T:41:ARG:NE	2.22	0.54
1:X:70:A:N3	1:X:72:A:N6	2.55	0.54



Atom-1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:347:C:H4'	19:R:15:HIS:NE2	2.23	0.54
1:X:494:A:H3'	1:X:495:C:H6	1.73	0.54
1:X:1302:C:H2'	1:X:1303:U:H6	1.72	0.54
1:X:1816:G:O2'	3:A:246:PRO:HB3	2.08	0.54
1:X:1886:G:H2'	1:X:1887:G:H8	1.72	0.54
1:X:2383:C:H2'	1:X:2384:G:O4'	2.08	0.54
1:X:2664:G:C2	1:X:2665:G:C8	2.96	0.54
1:X:2828:C:H2'	1:X:2829:A:H8	1.73	0.54
3:A:63:ARG:NH2	3:A:85:ASP:OD2	2.40	0.54
6:D:98:VAL:O	6:D:102:LYS:N	2.36	0.54
8:G:62:ILE:HD11	8:G:80:VAL:HG22	1.89	0.54
9:H:119:ARG:NH2	14:M:41:GLU:HA	2.23	0.54
10:I:83:LEU:O	10:I:87:THR:OG1	2.12	0.54
20:S:105:GLN:HG2	20:S:139:THR:O	2.07	0.54
1:X:1770:U:H5	1:X:1775:A:N7	2.06	0.54
1:X:2048:C:H1'	1:X:2428:U:N3	2.20	0.54
1:X:2568:A:H2'	1:X:2569:A:C8	2.43	0.54
1:X:2751:C:H2'	1:X:2752:C:C6	2.43	0.54
1:X:2773:G:H1	1:X:2779:A:H61	1.55	0.54
3:A:150:GLY:O	3:A:152:GLY:N	2.41	0.54
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.90	0.54
1:X:1804:U:H1'	3:A:45:ASN:HB2	1.89	0.53
1:X:1987:G:C4	1:X:1988:A:C8	2.96	0.53
1:X:2811:G:H2'	1:X:2812:A:H8	1.72	0.53
5:C:149:LEU:HD13	5:C:183:HIS:CE1	2.43	0.53
6:D:61:THR:HA	6:D:99:PHE:HZ	1.73	0.53
13:L:30:SER:O	13:L:40:ALA:CA	2.44	0.53
19:R:84:VAL:O	19:R:85:ASP:HB2	2.08	0.53
1:X:796:A:H8	1:X:797:A:H4'	1.73	0.53
1:X:1215:A:H2'	1:X:1216:G:H8	1.73	0.53
1:X:1300:A:H5"	1:X:1301:U:OP2	2.08	0.53
4:B:33:ILE:HG21	4:B:36:ARG:CZ	2.38	0.53
5:C:117:LEU:O	5:C:188:ILE:HD12	2.07	0.53
19:R:15:HIS:CE1	19:R:78:ALA:HB1	2.43	0.53
1:X:320:A:C6	1:X:341:A:C6	2.96	0.53
1:X:1033:G:H22	1:X:1153:A:H2	1.57	0.53
1:X:1047:G:C6	1:X:1131:G:C6	2.96	0.53
1:X:1428:G:N2	1:X:1601:U:H4'	2.22	0.53
1:X:1823:G:C6	1:X:1824:C:N4	2.77	0.53
1:X:1941:C:H2'	1:X:1942:G:C8	2.44	0.53
1:X:2329:C:H2'	1:X:2330:G:O4'	2.09	0.53



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:2696:A:H2'	1:X:2697:G:H5'	1.91	0.53
1:X:2705:A:C2'	1:X:2706:U:H2'	2.38	0.53
1:X:2821:G:C5	1:X:2822:U:C4	2.96	0.53
4:B:14:ILE:HG22	4:B:21:ILE:CG1	2.35	0.53
6:D:56:GLU:CD	6:D:150:ARG:HH11	2.12	0.53
1:X:767:G:H2'	1:X:768:U:H6	1.74	0.53
1:X:922:A:O2'	1:X:2243:C:O2'	2.17	0.53
1:X:1137:A:H4'	1:X:1138:A:O5'	2.07	0.53
1:X:1284:G:N2	1:X:1633:C:O4'	2.42	0.53
1:X:1381:G:H2'	1:X:1382:G:H8	1.74	0.53
8:G:116:ARG:HH21	8:G:118:ALA:HB3	1.73	0.53
14:M:55:ILE:HG22	14:M:104:LEU:HB2	1.90	0.53
19:R:64:ASN:N	19:R:64:ASN:OD1	2.38	0.53
1:X:356:A:O2'	1:X:357:A:H8	1.92	0.53
1:X:816:U:H2'	1:X:817:A:O4'	2.09	0.53
1:X:2490:U:H2'	1:X:2491:C:C6	2.43	0.53
1:X:2773:G:H1	1:X:2779:A:N6	2.06	0.53
1:X:2821:G:H2'	1:X:2822:U:C6	2.44	0.53
2:Y:14:C:H3'	21:T:72:LYS:HD2	1.91	0.53
4:B:119:ARG:CG	4:B:160:MET:HB2	2.38	0.53
5:C:72:ARG:HA	5:C:77:PHE:CD2	2.43	0.53
5:C:137:ALA:HB1	5:C:142:LEU:HD12	1.91	0.53
6:D:138:PHE:HB3	6:D:140:GLU:H	1.74	0.53
14:M:30:GLY:HA2	14:M:117:ILE:CD1	2.39	0.53
1:X:39:C:H2'	1:X:40:U:C6	2.43	0.53
1:X:568:G:H2'	1:X:569:C:O4'	2.08	0.53
1:X:595:A:N1	1:X:822:G:O2'	2.32	0.53
1:X:1267:A:H5"	1:X:1268:U:H5"	1.89	0.53
1:X:1399:C:H2'	1:X:1400:A:H8	1.72	0.53
1:X:1928:G:H2'	1:X:1929:U:H6	1.74	0.53
1:X:2322:U:O2'	1:X:2323:U:OP1	2.23	0.53
1:X:213:C:H2'	1:X:214:C:H6	1.72	0.53
1:X:694:G:C4	1:X:695:G:C8	2.97	0.53
1:X:759:C:H3'	1:X:759:C:C6	2.43	0.53
1:X:1240:G:H5"	1:X:1240:G:H8	1.74	0.53
1:X:1462:C:H2'	1:X:1463:A:H8	1.74	0.53
1:X:1656:U:C2'	1:X:1657:A:H5"	2.39	0.53
1:X:1774:A:N1	1:X:2566:A:H2'	2.23	0.53
1:X:1872:A:H2'	1:X:1873:A:C8	2.44	0.53
1:X:2039:G:N2	25:Z:5:PRO:HA	2.24	0.53
1:X:2533:U:H2'	1:X:2534:U:H6	1.74	0.53



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
3:A:231:HIS:CE1	3:A:247:VAL:HA	2.44	0.53
4:B:9:ILE:O	14:M:9:ARG:NH1	2.36	0.53
19:R:105:ARG:HD3	19:R:112:LYS:HD2	1.90	0.53
1:X:1670:G:H8	1:X:1670:G:OP2	1.91	0.53
1:X:2231:G:C4	1:X:2232:G:C8	2.97	0.53
1:X:2551:A:C5'	1:X:2553:G:H4'	2.35	0.53
24:W:4:LYS:HG2	24:W:52:GLU:HB3	1.91	0.53
1:X:1787:U:H4'	3:A:254:THR:H	1.74	0.53
1:X:1813:A:H2'	1:X:1814:G:H8	1.74	0.53
1:X:2691:C:O2'	1:X:2693:U:H5'	2.08	0.53
1:X:2807:U:H1'	1:X:2808:U:OP2	2.09	0.53
6:D:2:GLN:HA	6:D:5:LYS:HD3	1.91	0.53
10:I:71:THR:HB	10:I:105:PRO:HB2	1.91	0.53
12:K:10:LEU:O	12:K:12:ARG:HD2	2.08	0.53
17:P:32:ARG:NH1	17:P:119:LYS:HD2	2.23	0.53
22:U:19:ILE:HG22	22:U:42:GLN:HG3	1.90	0.53
1:X:68:C:O2'	1:X:72:A:O2'	2.22	0.53
1:X:216:U:H2'	1:X:217:U:C6	2.43	0.53
1:X:358:C:H2'	1:X:359:G:H5'	1.91	0.53
1:X:747:A:OP2	1:X:774[A]:A:N6	2.39	0.53
1:X:915:C:H2'	1:X:916:U:C6	2.44	0.53
1:X:1655:C:O2	1:X:2677:U:O2'	2.27	0.53
1:X:2272:A:H2'	1:X:2273:C:C6	2.44	0.53
3:A:108:PRO:HB2	3:A:127:LEU:HD11	1.90	0.53
18:Q:19:ALA:HB1	18:Q:24:VAL:HG13	1.90	0.53
19:R:56:LYS:H	19:R:56:LYS:HD2	1.73	0.53
1:X:618:A:H2'	1:X:619:A:C8	2.45	0.52
1:X:1179:A:H2'	1:X:1180:A:H8	1.74	0.52
1:X:1291:G:OP1	12:K:36:THR:OG1	2.17	0.52
1:X:1770:U:C2	1:X:1774:A:N7	2.77	0.52
1:X:1787:U:H2'	1:X:1788:C:C6	2.44	0.52
1:X:2358:C:H4'	13:L:21:THR:HG21	1.92	0.52
6:D:56:GLU:OE1	6:D:150:ARG:NH1	2.33	0.52
9:H:119:ARG:HH21	14:M:41:GLU:HA	1.74	0.52
22:U:7:LEU:HD11	22:U:46:LEU:HD13	1.90	0.52
27:2:34:ARG:CZ	27:2:39:ARG:HD2	2.40	0.52
1:X:224:G:OP2	1:X:226:C:N4	2.42	0.52
1:X:1050:G:O2'	1:X:1128:G:N2	2.42	0.52
1:X:1980:A:H5"	4:B:117:MET:CE	2.40	0.52
1:X:2282:G:H2'	1:X:2283:G:O4'	2.09	0.52
1:X:2793:G:O2'	1:X:2794:G:H5'	2.09	0.52



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:D:22:TYR:HB3	6:D:27:ALA:HB3	1.91	0.52
8:G:70:PHE:HD1	15:N:64:ARG:HH21	1.58	0.52
9:H:19:ILE:O	9:H:19:ILE:HG13	2.08	0.52
16:O:35:LEU:HD21	16:O:52:GLY:HA2	1.91	0.52
20:S:2:GLU:HG3	20:S:55:THR:HG22	1.91	0.52
21:T:19:LYS:O	21:T:21:LEU:N	2.42	0.52
25:Z:58:LEU:HD22	25:Z:59:ALA:H	1.74	0.52
1:X:591:G:H2'	1:X:592:G:C8	2.44	0.52
1:X:2002:A:N6	1:X:2018:G:H1	2.07	0.52
9:H:21:CYS:SG	9:H:51:ILE:HG13	2.49	0.52
1:X:820:U:H2'	1:X:821:A:C8	2.45	0.52
1:X:1082:G:H5'	1:X:1083:C:H5	1.74	0.52
1:X:1745:C:P	14:M:101:ARG:HH22	2.32	0.52
1:X:1982:C:H4'	1:X:2703:C:O2	2.09	0.52
2:Y:7:C:H2'	2:Y:8:C:C6	2.45	0.52
2:Y:14:C:H5	21:T:72:LYS:HB2	1.73	0.52
18:Q:14:GLU:CD	18:Q:14:GLU:H	2.12	0.52
1:X:39:C:H2'	1:X:40:U:H6	1.75	0.52
1:X:133:C:C5	1:X:134:G:H1'	2.44	0.52
1:X:528:G:H2'	1:X:529:U:C6	2.45	0.52
1:X:960:U:H2'	1:X:961:G:C8	2.45	0.52
1:X:1326:U:H2'	1:X:1626:A:C2	2.45	0.52
1:X:1816:G:O2'	3:A:252:LYS:HG2	2.08	0.52
1:X:1918:G:C6	1:X:1945:C:C5	2.98	0.52
1:X:1991:C:H2'	1:X:1992:G:C8	2.44	0.52
1:X:2272:A:H2'	1:X:2273:C:H6	1.74	0.52
5:C:2:ALA:O	5:C:112:GLN:NE2	2.41	0.52
9:H:83:ARG:HH22	9:H:134:LEU:HD11	1.74	0.52
15:N:94:VAL:HA	15:N:97:ASP:OD2	2.09	0.52
18:Q:29:VAL:HG11	18:Q:38:ILE:HD12	1.92	0.52
22:U:43:ARG:HG2	22:U:44:ALA:H	1.74	0.52
22:U:53:GLU:HA	22:U:57:VAL:HA	1.90	0.52
25:Z:45:ILE:HD12	25:Z:50:GLY:HA2	1.90	0.52
1:X:219:G:O2'	1:X:231:G:N1	2.32	0.52
1:X:463:C:OP2	5:C:46:ARG:HG2	2.10	0.52
1:X:2069:U:H2'	1:X:2070:G:H8	1.72	0.52
1:X:2085:G:N2	1:X:2171:U:O2'	2.43	0.52
1:X:2738:A:C5	7:E:67:LEU:HD11	2.45	0.52
18:Q:5:ASP:N	18:Q:5:ASP:OD1	2.42	0.52
1:X:231:G:H4'	1:X:397:U:H5"	1.92	0.52
1:X:684:C:OP1	10:I:40:ARG:HA	2.09	0.52



Atom 1	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
1:X:840:U:H4'	1:X:841:G:C2	2.45	0.52
1:X:930:A:C2	2:Y:82:U:H4'	2.43	0.52
1:X:940:G:H5'	24:W:37:THR:HG21	1.92	0.52
1:X:2175:A:H2'	1:X:2176:U:C6	2.45	0.52
1:X:2290:A:H8	1:X:2291:U:C5	2.28	0.52
1:X:2557:G:O2'	1:X:2558:C:H5'	2.09	0.52
1:X:2683:C:H2'	1:X:2684:A:H8	1.75	0.52
2:Y:39:C:H5"	2:Y:40:C:C5	2.45	0.52
1:X:219:G:H3'	28:3:5:LYS:HD3	1.90	0.52
1:X:464:G:OP2	5:C:46:ARG:NH1	2.42	0.52
1:X:576:A:H4'	1:X:821:A:OP1	2.10	0.52
1:X:829:C:H2'	1:X:830:C:C6	2.44	0.52
1:X:1429:A:C2	1:X:1603:A:H1'	2.45	0.52
1:X:2335:U:H2'	1:X:2336:G:C8	2.45	0.52
1:X:2440:C:H2'	1:X:2441:U:H6	1.74	0.52
2:Y:26:G:N2	2:Y:30:C:C2	2.77	0.52
4:B:9:ILE:O	14:M:9:ARG:HD2	2.09	0.52
6:D:149:THR:HA	6:D:150:ARG:NH2	2.25	0.52
8:G:85:ALA:HB1	8:G:127:ILE:HD12	1.92	0.52
8:G:140:GLN:O	8:G:144:MET:HG3	2.10	0.52
23:V:25:LEU:HD21	23:V:47:ARG:HG2	1.92	0.52
1:X:1050:G:N2	1:X:1127:C:H42	2.08	0.52
1:X:1122:A:O2'	1:X:1123:G:H4'	2.09	0.52
1:X:1164:C:C4	1:X:1165:G:C5	2.98	0.52
1:X:1873:A:H3'	1:X:1874:G:H8	1.75	0.52
1:X:2812:A:H2'	1:X:2813:G:H8	1.75	0.52
2:Y:59:A:H5'	2:Y:60:A:OP2	2.10	0.52
14:M:27:PHE:CD2	14:M:93:ILE:HD13	2.45	0.52
17:P:21:ARG:N	17:P:21:ARG:HD2	2.23	0.52
25:Z:42:SER:O	25:Z:44:HIS:ND1	2.43	0.52
27:2:30:ILE:O	27:2:34:ARG:HG3	2.10	0.52
1:X:38:G:H1	1:X:453:U:H3	1.57	0.52
1:X:196:A:H2'	1:X:197:G:C8	2.45	0.52
1:X:719:A:H3'	1:X:720:A:C8	2.43	0.52
1:X:1783:G:H5"	3:A:205:VAL:HG13	1.91	0.52
1:X:1833:U:C2	1:X:1834:G:C8	2.98	0.52
3:A:246:PRO:HD3	3:A:252:LYS:HE3	1.92	0.52
4:B:110:GLY:HA2	4:B:161:GLY:HA3	1.91	0.52
6:D:79:LEU:HD23	6:D:80:ARG:H	1.75	0.52
8:G:67:ARG:HH21	8:G:76:GLN:HB3	1.75	0.52
9:H:21:CYS:HB2	9:H:51:ILE:HD11	1.92	0.52



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:I:16:ARG:HG2	10:I:17:LYS:N	2.25	0.52
12:K:114:GLU:C	12:K:115:LEU:HD23	2.31	0.52
13:L:41:GLN:OE1	13:L:50:THR:HG21	2.10	0.52
14:M:33:VAL:HA	14:M:50:PHE:O	2.10	0.52
17:P:20:LEU:C	17:P:21:ARG:HD2	2.30	0.52
20:S:71:MET:HA	20:S:78:PRO:HA	1.92	0.52
1:X:2:G:H2'	1:X:3:U:C6	2.45	0.51
1:X:845:U:OP1	10:I:38:LYS:HE3	2.11	0.51
1:X:954:U:OP2	10:I:38:LYS:NZ	2.43	0.51
1:X:1996:A:H2	17:P:109:ARG:NH2	2.06	0.51
1:X:1999:U:H1'	25:Z:6:VAL:CG1	2.40	0.51
1:X:2214:G:H2'	1:X:2215:C:C6	2.44	0.51
1:X:2279:G:H2'	1:X:2280:A:C8	2.45	0.51
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.92	0.51
9:H:10:VAL:HG23	9:H:17:ARG:O	2.10	0.51
12:K:72:ASP:O	12:K:75:VAL:HG23	2.10	0.51
15:N:8:ILE:O	15:N:12:ARG:HG2	2.10	0.51
18:Q:34:THR:O	18:Q:38:ILE:HG22	2.10	0.51
25:Z:16:ARG:HD3	25:Z:20:ARG:CZ	2.40	0.51
1:X:754:G:H2'	1:X:755:C:H6	1.74	0.51
1:X:768:U:H2'	1:X:769:C:O4'	2.10	0.51
1:X:791:G:H5'	3:A:48:ARG:CZ	2.40	0.51
1:X:1006:C:OP2	15:N:54:LYS:HE3	2.11	0.51
1:X:1292:A:H4'	12:K:31:GLU:OE1	2.09	0.51
1:X:1635:G:H2'	1:X:1635:G:N3	2.24	0.51
1:X:2790:C:H2'	1:X:2791:C:C6	2.45	0.51
1:X:2795:A:O2'	12:K:3:HIS:CD2	2.62	0.51
3:A:246:PRO:HD2	3:A:250:TRP:N	2.25	0.51
6:D:101:GLU:HA	6:D:104:ILE:HG22	1.91	0.51
10:I:79:GLN:HB3	10:I:111:SER:HB2	1.91	0.51
23:V:14:PHE:O	23:V:18:ILE:HG13	2.11	0.51
1:X:263:G:N2	1:X:264:U:O4	2.39	0.51
1:X:674:U:H2'	1:X:675:C:O4'	2.11	0.51
1:X:1238:A:H4'	16:O:83:ARG:HG2	1.91	0.51
1:X:1269:G:C6	1:X:1270:C:C4	2.98	0.51
4:B:63:MET:O	4:B:67:PHE:HD1	1.94	0.51
14:M:41:GLU:CG	14:M:44:ARG:HH22	2.23	0.51
1:X:338:G:H1'	19:R:10:HIS:NE2	2.26	0.51
1:X:552:C:C2'	1:X:553:C:H5'	2.41	0.51
1:X:748:A:H5'	1:X:749:C:OP2	2.11	0.51
1:X:1354:A:H8	1:X:1354:A:O5'	1.93	0.51



A 4 1	A.L. D	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:2043:A:O2'	1:X:2481:G:O4'	2.29	0.51
1:X:2334:C:H1'	21:T:39:ARG:HH21	1.76	0.51
1:X:2386:G:H2'	1:X:2387:U:C6	2.45	0.51
1:X:2604:G:H2'	1:X:2605:C:C6	2.45	0.51
1:X:2800:C:O2	1:X:2800:C:H2'	2.11	0.51
3:A:79:VAL:HG21	3:A:111:LEU:HD21	1.92	0.51
13:L:77:ALA:O	13:L:81:GLU:HG2	2.10	0.51
14:M:38:LYS:HZ1	14:M:46:ARG:HD2	1.75	0.51
15:N:66:ASN:HB3	15:N:76:TYR:CB	2.28	0.51
20:S:28:ASN:OD1	20:S:28:ASN:N	2.41	0.51
24:W:3:ILE:O	24:W:31:SER:HA	2.10	0.51
1:X:492:G:H2'	1:X:517:A:N6	2.26	0.51
1:X:748:A:H3'	1:X:749:C:H6	1.75	0.51
1:X:847:C:C2	1:X:848:A:C8	2.98	0.51
1:X:1193:G:H2'	1:X:1194:U:C6	2.45	0.51
1:X:1307:U:H2'	1:X:1308:C:H5'	1.93	0.51
1:X:1469:U:H5'	1:X:1470:G:OP2	2.11	0.51
2:Y:78:A:H4'	20:S:20:ALA:CB	2.40	0.51
5:C:111:ARG:HB3	5:C:116:LYS:CB	2.39	0.51
17:P:54:GLU:HB3	17:P:58:ARG:HH22	1.75	0.51
17:P:59:PHE:CD2	25:Z:41:LEU:HD22	2.42	0.51
1:X:64:C:H1'	18:Q:68:PHE:CD2	2.45	0.51
1:X:222:G:H2'	1:X:223:C:C6	2.45	0.51
1:X:402:A:N3	1:X:2391:A:H2	2.09	0.51
1:X:717:G:O2'	1:X:739:G:N2	2.32	0.51
1:X:836:G:H2'	1:X:837:U:C6	2.46	0.51
1:X:1325:U:OP2	18:Q:62:ARG:NH2	2.44	0.51
1:X:1360:G:C6	1:X:1361:G:N7	2.79	0.51
1:X:1717:A:H3'	1:X:1718:A:H8	1.75	0.51
1:X:2081:U:H3	1:X:2174:G:H1	1.57	0.51
1:X:2736:U:H4'	1:X:2737:A:OP1	2.10	0.51
15:N:10:ARG:HG2	15:N:14:HIS:NE2	2.24	0.51
15:N:58:ARG:HA	15:N:61:TRP:HD1	1.73	0.51
1:X:28:A:C2	1:X:523:A:C8	2.99	0.51
1:X:494:A:H3'	1:X:495:C:C6	2.46	0.51
1:X:746:G:N7	1:X:774[B]:A:C6	2.79	0.51
1:X:2312:A:H4'	1:X:2313:G:O5'	2.11	0.51
1:X:239:A:N3	1:X:443:A:O2'	2.35	0.51
1:X:560:G:H5'	16:O:67:LYS:HE3	1.92	0.51
1:X:1063:C:H2'	1:X:1064:C:C6	2.46	0.51
1:X:1992:G:C2'	1:X:1993:G:H5'	2.41	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:B:33:ILE:HG12	4:B:89:ASP:HA	1.93	0.51
22:U:53:GLU:O	22:U:78:ILE:HG23	2.11	0.51
1:X:1377:G:C5	22:U:6:TYR:N	2.79	0.51
1:X:1573:G:H3'	1:X:1574:A:C5'	2.40	0.51
1:X:2394:G:H2'	1:X:2395:C:H6	1.75	0.51
1:X:2522:G:H2'	1:X:2523:G:C8	2.46	0.51
6:D:141:ILE:HB	6:D:146:VAL:HG21	1.92	0.51
7:E:55:PRO:HG2	7:E:61:HIS:NE2	2.26	0.51
9:H:56:LYS:O	9:H:56:LYS:NZ	2.35	0.51
1:X:503:G:H2'	1:X:504:G:O4'	2.11	0.51
1:X:831:G:C2	1:X:1204:G:C6	2.98	0.51
1:X:1448:A:H61	1:X:1574:A:N6	2.07	0.51
1:X:1802:A:H2'	1:X:1803:G:O4'	2.10	0.51
1:X:2800:C:H5'	1:X:2801:A:OP2	2.10	0.51
22:U:21:ARG:HA	22:U:39:LYS:O	2.10	0.51
1:X:393:U:H4'	22:U:19:ILE:O	2.11	0.50
1:X:393:U:H2'	1:X:394:U:C6	2.45	0.50
1:X:820:U:H2'	1:X:821:A:H8	1.75	0.50
1:X:857:U:H2'	1:X:858:G:O4'	2.11	0.50
1:X:1770:U:O2	1:X:1774:A:N6	2.45	0.50
1:X:2309:G:H2'	1:X:2310:G:O4'	2.11	0.50
6:D:149:THR:HA	6:D:150:ARG:HH21	1.76	0.50
9:H:120:ASP:OD1	9:H:120:ASP:N	2.44	0.50
12:K:96:ARG:O	12:K:113:ILE:HD12	2.11	0.50
19:R:25:LEU:O	19:R:30:LYS:HB2	2.11	0.50
1:X:198:A:O2'	1:X:243:G:N7	2.34	0.50
1:X:219:G:H8	28:3:3:LYS:O	1.95	0.50
1:X:640:C:P	28:3:17:THR:HB	2.51	0.50
1:X:1628:C:N4	1:X:1629:G:N7	2.59	0.50
1:X:1810:U:H3'	3:A:157:ARG:CG	2.41	0.50
1:X:1816:G:OP1	3:A:52:ARG:HG3	2.11	0.50
1:X:1818:G:H2'	1:X:1819:U:H6	1.76	0.50
1:X:2029:G:H2'	1:X:2030:U:C6	2.46	0.50
1:X:2049:C:O2'	1:X:2050:G:H5'	2.12	0.50
1:X:2236:U:O2'	1:X:2237:C:H5'	2.10	0.50
1:X:2369:U:O5'	1:X:2369:U:H6	1.94	0.50
1:X:2490:U:H2'	1:X:2491:C:H6	1.75	0.50
1:X:2820:C:C2	1:X:2821:G:C8	2.99	0.50
3:A:72:LYS:NZ	3:A:99:ASP:OD2	2.44	0.50
6:D:48:LYS:H	6:D:48:LYS:HD2	1.75	0.50
9:H:116:ARG:HE	9:H:134:LEU:HD11	1.76	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
11:J:36:ILE:HG22	11:J:131:LYS:O	2.11	0.50
20:S:101:THR:HG22	20:S:136:VAL:O	2.11	0.50
1:X:427:C:H2'	1:X:428:A:C8	2.46	0.50
1:X:839:U:H5"	1:X:2408:G:OP2	2.12	0.50
1:X:1364:C:H2'	1:X:1365:U:C6	2.47	0.50
1:X:1917:C:C2	1:X:1918:G:C8	3.00	0.50
1:X:1998:A:N3	25:Z:6:VAL:HG22	2.26	0.50
1:X:2509:A:H2'	1:X:2510:A:H5"	1.94	0.50
3:A:252:LYS:HZ2	3:A:253:PRO:HD2	1.75	0.50
6:D:109:PRO:HG3	6:D:137:ILE:HB	1.92	0.50
14:M:6:LYS:O	14:M:7:ILE:HD12	2.11	0.50
1:X:69:G:O2'	1:X:72:A:H1'	2.12	0.50
1:X:135:U:H2'	1:X:136:A:C8	2.47	0.50
1:X:222:G:H2'	1:X:223:C:H6	1.76	0.50
1:X:469:G:OP1	27:2:40:HIS:NE2	2.44	0.50
1:X:547:U:H2'	1:X:548:G:H8	1.75	0.50
1:X:577:U:H2'	1:X:579:G:OP2	2.11	0.50
1:X:630:G:O5'	1:X:631:G:N2	2.44	0.50
1:X:868:U:H2'	1:X:869:C:H6	1.75	0.50
1:X:1257:U:O2'	1:X:1258:G:H5'	2.12	0.50
1:X:1664:G:P	1:X:1664:G:H3'	2.52	0.50
1:X:2583:U:O2'	1:X:2584:U:H5'	2.11	0.50
7:E:98:LEU:HD12	7:E:102:ALA:O	2.12	0.50
9:H:19:ILE:HG22	9:H:55:VAL:HA	1.93	0.50
12:K:51:LEU:HD21	12:K:66:VAL:HG13	1.93	0.50
21:T:38:VAL:HG12	21:T:59:LEU:HG	1.94	0.50
1:X:166:G:H21	1:X:184:A:H62	1.60	0.50
1:X:326:A:C6	1:X:327:C:C4	3.00	0.50
1:X:1231:A:C4	1:X:1245:G:N2	2.79	0.50
1:X:1773:C:O2'	1:X:2588:U:H5"	2.12	0.50
1:X:2258:G:O6	21:T:14:ARG:HD3	2.11	0.50
1:X:2571:G:H22	1:X:2580:C:H5	1.60	0.50
1:X:2849:C:H2'	1:X:2850:U:H6	1.76	0.50
31:X:3168:SPD:H41	31:X:3168:SPD:H81	1.93	0.50
14:M:77:VAL:O	14:M:78:GLU:HG2	2.12	0.50
17:P:29:LYS:HB3	17:P:30:TYR:CD2	2.46	0.50
26:1:37:LEU:HD23	26:1:51:ARG:HA	1.94	0.50
28:3:14:ILE:HD13	28:3:22:VAL:HG13	1.94	0.50
28:3:52:LYS:NZ	28:3:56:ALA:HB2	2.26	0.50
1:X:314:G:H2'	1:X:315:G:H8	1.75	0.50
1:X:1910:A:H2'	1:X:1911:A:O4'	2.11	0.50



Atom 1	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
1:X:2274:C:C2'	1:X:2275:U:H5'	2.41	0.50
1:X:2522:G:H2'	1:X:2523:G:O4'	2.12	0.50
1:X:2696:A:C6	1:X:2697:G:N7	2.80	0.50
1:X:2786:G:C2	1:X:2787:A:C5	2.99	0.50
2:Y:45:C:H5'	6:D:95:ARG:HH12	1.75	0.50
8:G:78:ASP:OD1	8:G:78:ASP:N	2.44	0.50
12:K:10:LEU:HD13	12:K:40:LYS:HG3	1.94	0.50
14:M:68:VAL:HG21	14:M:81:PHE:HE1	1.77	0.50
1:X:455:A:C8	5:C:39:ARG:HD3	2.47	0.50
1:X:623:G:H3'	1:X:624:A:H5"	1.92	0.50
1:X:1219:C:H2'	1:X:1220:G:O4'	2.11	0.50
1:X:1281:A:C2	1:X:1282:A:H1'	2.47	0.50
1:X:1423:A:H2'	1:X:1424:U:C6	2.47	0.50
1:X:1429:A:N3	1:X:1603:A:H1'	2.27	0.50
1:X:1563:U:H2'	1:X:1564:U:C6	2.47	0.50
1:X:1628:C:O2'	27:2:5:TYR:O	2.25	0.50
1:X:1744:G:H2'	1:X:1746:A:OP2	2.12	0.50
1:X:2343:C:H2'	1:X:2344:G:O4'	2.11	0.50
1:X:2659:C:C2	1:X:2660:C:C5	3.00	0.50
1:X:2769:C:O2	1:X:2866:A:H2	1.95	0.50
3:A:24:LEU:HD21	3:A:91:ARG:HD2	1.94	0.50
4:B:188:ILE:CG2	4:B:189:PRO:HD2	2.40	0.50
1:X:547:U:H2'	1:X:548:G:C8	2.47	0.50
1:X:1037:U:O2	1:X:1037:U:H2'	2.11	0.50
1:X:1428:G:H22	1:X:1602:G:H5'	1.75	0.50
1:X:1787:U:H2'	1:X:1788:C:H6	1.76	0.50
1:X:1973:C:H6	1:X:1973:C:H3'	1.76	0.50
1:X:2277:A:H2	1:X:2300:G:H2'	1.77	0.50
1:X:2278:A:H2'	1:X:2279:G:C8	2.47	0.50
1:X:2328:G:C6	1:X:2348:A:C6	3.00	0.50
1:X:2424:G:O2'	1:X:2425:G:H5'	2.11	0.50
1:X:2594:U:H2'	1:X:2595:C:H6	1.76	0.50
1:X:2683:C:H2'	1:X:2684:A:C8	2.46	0.50
10:I:83:LEU:HD22	10:I:115:SER:HA	1.93	0.50
15:N:95:LEU:HD21	16:O:5:ILE:HG12	1.93	0.50
23:V:46:LEU:O	23:V:50:VAL:HG23	2.12	0.50
1:X:751:G:O2'	1:X:752:G:OP1	2.29	0.50
1:X:824:U:H2'	10:I:21:ARG:HA	1.94	0.50
1:X:1072:U:H4'	1:X:1081:A:O2'	2.11	0.50
1:X:1321:A:H5'	1:X:1322:G:OP2	2.12	0.50
1:X:2218:G:H5'	3:A:249:PRO:HD3	1.93	0.50



A + amo 1	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
1:X:2653:A:H4'	9:H:42:LYS:HB2	1.93	0.50
3:A:69:ARG:NH1	3:A:128:GLY:O	2.31	0.50
5:C:7:ILE:HB	5:C:122:GLY:HA2	1.92	0.50
7:E:6:LYS:HG3	7:E:69:ARG:HD3	1.94	0.50
7:E:22:GLY:O	7:E:37:TYR:HB2	2.11	0.50
1:X:58:C:OP2	18:Q:73:ASN:ND2	2.45	0.49
1:X:101:A:OP2	1:X:101:A:H8	1.95	0.49
1:X:1012:A:H62	1:X:1165:G:N2	2.09	0.49
1:X:1697:U:O2	1:X:1754:G:C8	2.65	0.49
1:X:2663:U:N3	1:X:2664:G:N7	2.60	0.49
2:Y:74:A:H1'	2:Y:108:G:N2	2.26	0.49
5:C:28:HIS:CE1	10:I:8:PRO:HB3	2.47	0.49
8:G:75:ILE:HG21	8:G:144:MET:HG2	1.94	0.49
10:I:122:VAL:O	10:I:126:SER:HB2	2.11	0.49
24:W:5:LEU:HA	24:W:51:LEU:HD23	1.93	0.49
1:X:57:G:N3	1:X:72:A:H2	2.10	0.49
1:X:1428:G:H2'	1:X:1428:G:N3	2.27	0.49
1:X:1622:G:H4'	1:X:1624:A:C2	2.47	0.49
1:X:2285:U:C4	6:D:42:SER:HB2	2.48	0.49
1:X:2724:G:C6	1:X:2741:G:C6	2.99	0.49
1:X:2859:U:P	25:Z:43:HIS:HE2	2.34	0.49
2:Y:62:C:H2'	2:Y:63:A:C8	2.46	0.49
7:E:12:PRO:HG3	7:E:80:SER:OG	2.12	0.49
7:E:105:MET:HB2	7:E:113:VAL:HG23	1.94	0.49
10:I:54:SER:HB3	10:I:55:ARG:HH22	1.77	0.49
12:K:28:LEU:HD21	12:K:115:LEU:HD21	1.94	0.49
17:P:56:LEU:O	17:P:58:ARG:N	2.45	0.49
22:U:47:HIS:CE1	22:U:64:ALA:H	2.30	0.49
28:3:13:ARG:CB	28:3:25:PHE:H	2.24	0.49
1:X:82:G:N2	1:X:100:G:H1'	2.25	0.49
1:X:405:C:H2'	1:X:406:G:H8	1.77	0.49
1:X:970:A:N6	11:J:84:MET:HE1	2.27	0.49
1:X:995:A:H5"	1:X:996:C:C5	2.47	0.49
1:X:1377:G:H5"	1:X:1800:A:O4'	2.12	0.49
1:X:2064:U:H5"	22:U:20:ARG:HH21	1.76	0.49
1:X:2407:G:H5"	1:X:2408:G:OP1	2.12	0.49
1:X:2602:G:H2'	1:X:2603:G:H8	1.77	0.49
3:A:16:MET:HG3	3:A:207:GLY:HA3	1.93	0.49
4:B:149:ARG:CB	4:B:149:ARG:HH11	2.25	0.49
6:D:65:PRO:HB2	6:D:87:ILE:CG2	2.43	0.49
12:K:52:ILE:HD11	12:K:94:TYR:CD1	2.46	0.49



Atom-1	Atom-2	Interatomic	Clash
		distance $(\text{\AA})$	overlap (Å)
20:S:70:GLN:N	20:S:80:HIS:O	2.41	0.49
1:X:90:G:H5'	1:X:91:A:OP2	2.12	0.49
1:X:338:G:H2'	1:X:339:U:O4'	2.12	0.49
1:X:513:A:C6	1:X:516:G:C6	3.00	0.49
1:X:530:G:H2'	1:X:531:G:C8	2.45	0.49
1:X:1194:U:H2'	1:X:1195:U:C6	2.47	0.49
1:X:1264:C:OP1	15:N:10:ARG:HG3	2.11	0.49
1:X:1779:C:H2'	1:X:1780:A:H8	1.76	0.49
1:X:2272:A:OP2	13:L:18:ARG:NH1	2.45	0.49
2:Y:31:A:H2'	2:Y:32:C:C6	2.47	0.49
2:Y:95:U:O2'	2:Y:96:C:H5'	2.12	0.49
3:A:63:ARG:HH21	3:A:65:ILE:HD11	1.77	0.49
3:A:183:ARG:NH1	3:A:184:ARG:O	2.45	0.49
4:B:134:TRP:H	4:B:134:TRP:HD1	1.60	0.49
8:G:104:THR:O	8:G:106:TYR:N	2.38	0.49
11:J:53:ILE:HG23	11:J:57:ARG:NH1	2.28	0.49
13:L:43:ILE:HG23	13:L:50:THR:HG23	1.92	0.49
19:R:38:LEU:HD22	19:R:39:ALA:H	1.76	0.49
1:X:494:A:N7	1:X:507:A:H2	2.10	0.49
1:X:1674:C:OP2	4:B:136:ARG:HG3	2.12	0.49
1:X:1681:A:C6	1:X:2706:U:C5	3.01	0.49
1:X:1817:U:O3'	3:A:233:HIS:HE1	1.95	0.49
1:X:2283:G:N2	1:X:2291:U:H3	2.08	0.49
5:C:155:GLU:O	5:C:159:ARG:HB2	2.12	0.49
12:K:102:THR:HA	12:K:109:THR:HA	1.94	0.49
17:P:41:VAL:HA	17:P:44:VAL:HG23	1.94	0.49
21:T:45:PHE:HZ	21:T:77:ARG:HH21	1.61	0.49
1:X:119:G:H5'	1:X:143:A:OP2	2.13	0.49
1:X:412:U:H2'	1:X:413:G:O4'	2.12	0.49
1:X:759:C:HO2'	1:X:760:U:P	2.36	0.49
1:X:1069:G:H2'	1:X:1070:G:C8	2.47	0.49
1:X:1468:A:C8	1:X:1468:A:OP2	2.66	0.49
1:X:1692:C:N4	1:X:1976:U:O4'	2.46	0.49
1:X:1810:U:OP2	3:A:157:ARG:NH1	2.45	0.49
1:X:1939:U:H1'	1:X:2531:U:OP1	2.11	0.49
1:X:2310:G:N2	1:X:2364:C:C4	2.81	0.49
1:X:2555:G:H8	1:X:2560:G:O6	1.95	0.49
1:X:2557:G:H2'	1:X:2558:C:H6	1.77	0.49
8:G:52:GLY:O	8:G:56:THR:HG23	2.13	0.49
15:N:24:PHE:HB3	15:N:28:ARG:HB2	1.94	0.49
16:O:26:GLN:HA	16:O:63:HIS:NE2	2.26	0.49



A 4 1	A.L. D.	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
18:Q:6:ILE:HG22	18:Q:7:LEU:HD12	1.94	0.49
25:Z:51:TYR:HE1	25:Z:55:ARG:CZ	2.26	0.49
27:2:1:MET:HG2	27:2:3:ARG:NH1	2.27	0.49
1:X:98:U:H4'	1:X:99:U:H5'	1.94	0.49
1:X:348:U:H2'	1:X:349:G:O4'	2.12	0.49
1:X:840:U:C5	1:X:2409:A:C5	3.01	0.49
1:X:852:U:H2'	1:X:853:C:C6	2.48	0.49
1:X:989:G:C2	1:X:997:C:C2	3.00	0.49
1:X:1082:G:H3'	1:X:1083:C:C6	2.46	0.49
1:X:1936:A:N6	31:X:3167:SPD:HN11	2.02	0.49
1:X:1947:G:H4'	1:X:1948:C:OP2	2.13	0.49
1:X:1956:G:H2'	1:X:1957:C:C6	2.47	0.49
1:X:2048:C:H2'	1:X:2049:C:H6	1.75	0.49
1:X:2726:U:H2'	1:X:2727:G:H5'	1.93	0.49
1:X:2781:G:O2'	1:X:2782:G:H5'	2.11	0.49
19:R:24:VAL:HA	19:R:80:LYS:HA	1.95	0.49
24:W:5:LEU:HB3	24:W:28:ILE:HA	1.94	0.49
28:3:62:LEU:HD12	28:3:63:PRO:HD2	1.95	0.49
1:X:163:A:H2'	1:X:164:G:C8	2.48	0.49
1:X:249:A:C8	1:X:381:C:H1'	2.48	0.49
1:X:563:U:H2'	1:X:564:U:O4'	2.13	0.49
1:X:627:A:H2'	1:X:628:A:H8	1.78	0.49
1:X:742:G:C5	3:A:208:LYS:HB2	2.48	0.49
1:X:790:A:H2'	1:X:791:G:H8	1.78	0.49
1:X:1016:C:H1'	1:X:1023:U:H3	1.77	0.49
1:X:1431:U:H3'	1:X:1432:G:O4'	2.13	0.49
1:X:1478:U:C2	1:X:1479:G:C8	3.01	0.49
1:X:1727:C:H4'	1:X:2833:C:O2	2.13	0.49
3:A:27:LYS:NZ	3:A:83:GLU:OE1	2.46	0.49
11:J:110:VAL:HG12	11:J:114:GLN:HB2	1.95	0.49
25:Z:45:ILE:HD13	25:Z:57:VAL:HB	1.94	0.49
26:1:9:ILE:HA	26:1:28:ARG:HA	1.94	0.49
1:X:23:G:C2	1:X:24:G:C8	3.01	0.49
1:X:33:C:O2	1:X:459:A:N6	2.46	0.49
1:X:174:A:N6	1:X:2409:A:H2'	2.28	0.49
1:X:495:C:C5'	19:R:58:VAL:HG22	2.43	0.49
1:X:930:A:N3	2:Y:82:U:O2'	2.37	0.49
1:X:1469:U:H3'	1:X:1470:G:C8	2.48	0.49
1:X:1793:A:H2'	1:X:1794:A:H8	1.70	0.49
1:X:1977:C:O2'	1:X:1978:U:H5'	2.12	0.49
4:B:120:TRP:CD1	4:B:155:ARG:HB3	2.48	0.49



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:I:16:ARG:HG2	10:I:17:LYS:H	1.78	0.49
15:N:101:ARG:O	15:N:101:ARG:HG2	2.13	0.49
1:X:334:G:C2	1:X:344:G:H1'	2.47	0.49
1:X:921:A:H4'	11:J:15:ARG:NH2	2.27	0.49
1:X:1006:C:O2	15:N:61:TRP:HH2	1.95	0.49
1:X:1268:U:C6	5:C:67:ALA:HA	2.48	0.49
1:X:1473:U:O2	1:X:1474:A:C6	2.66	0.49
1:X:1539:U:H2'	1:X:1540:C:C6	2.48	0.49
1:X:1595:A:H2'	1:X:1596:A:C8	2.48	0.49
1:X:1623:C:N4	1:X:1637:U:H2'	2.27	0.49
1:X:2280:A:H2'	1:X:2281:C:C6	2.48	0.49
1:X:2422:C:O2'	1:X:2423:G:H5'	2.13	0.49
1:X:2542:U:C5'	9:H:37:GLY:HA2	2.34	0.49
1:X:2791:C:O2	1:X:2858:A:O2'	2.25	0.49
3:A:72:LYS:HE2	3:A:97:TYR:CG	2.48	0.49
4:B:18:ASP:N	4:B:18:ASP:OD1	2.46	0.49
5:C:72:ARG:HA	5:C:77:PHE:CE2	2.47	0.49
11:J:28:VAL:N	11:J:138:TYR:HE2	2.10	0.49
16:O:4:ILE:HG13	16:O:20:ILE:HG12	1.94	0.49
1:X:542:A:H4'	1:X:543:G:C8	2.48	0.48
1:X:839:U:H1'	10:I:49:PHE:HB3	1.94	0.48
1:X:1322:G:H4'	27:2:7:PRO:HB2	1.95	0.48
1:X:2044:G:C2	1:X:2046:C:C4	3.01	0.48
1:X:2064:U:H5'	22:U:41:VAL:HG11	1.95	0.48
1:X:2398:U:OP2	28:3:41:ILE:HD11	2.12	0.48
9:H:116:ARG:HB2	9:H:134:LEU:HD21	1.95	0.48
14:M:38:LYS:HE2	14:M:46:ARG:HB3	1.94	0.48
14:M:68:VAL:CG2	14:M:81:PHE:HE1	2.26	0.48
17:P:54:GLU:HB3	17:P:58:ARG:NH2	2.28	0.48
1:X:339:U:N3	1:X:343:A:H2	2.08	0.48
1:X:590:C:OP1	15:N:31:GLN:HB3	2.13	0.48
1:X:859:U:O2	1:X:860:U:N3	2.45	0.48
1:X:2511:G:C6	1:X:2512:A:C5	3.01	0.48
1:X:2597:G:H2'	1:X:2598:C:H6	1.77	0.48
1:X:2597:G:H2'	1:X:2598:C:C6	2.47	0.48
1:X:2788:C:H2'	1:X:2789:U:H6	1.78	0.48
4:B:98:GLU:CD	4:B:174:GLU:HA	2.34	0.48
12:K:9:LYS:O	12:K:10:LEU:HD23	2.13	0.48
20:S:53:ASP:N	20:S:53:ASP:OD1	2.46	0.48
21:T:29:GLU:H	21:T:67:VAL:HG12	1.78	0.48
1:X:173:A:H2'	1:X:173:A:N3	2.28	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:215:G:H2'	1:X:216:U:O4'	2.13	0.48
1:X:596:C:P	10:I:21:ARG:NH1	2.86	0.48
1:X:753:U:O4'	1:X:1964:A:C4	2.66	0.48
1:X:1024:G:H2'	1:X:1025:A:C8	2.48	0.48
1:X:1175:A:H2'	1:X:1176:U:H6	1.78	0.48
1:X:1310:C:H2'	1:X:1311:C:H6	1.79	0.48
1:X:1620:C:O2'	1:X:1626:A:N1	2.39	0.48
1:X:2271:C:P	13:L:18:ARG:HH22	2.36	0.48
1:X:2663:U:C2	1:X:2664:G:C8	3.01	0.48
1:X:2753:C:H5"	4:B:164:ARG:HG2	1.94	0.48
1:X:2810:A:H3'	14:M:6:LYS:NZ	2.28	0.48
5:C:173:ALA:O	5:C:175:VAL:N	2.37	0.48
15:N:8:ILE:HD11	15:N:12:ARG:HH21	1.78	0.48
15:N:40:LEU:HD13	16:O:74:TYR:CE1	2.48	0.48
18:Q:17:TYR:HE2	18:Q:93:GLY:HA2	1.77	0.48
19:R:46:VAL:N	19:R:76:LEU:O	2.46	0.48
1:X:339:U:O2'	19:R:79:SER:HB3	2.13	0.48
1:X:1781:C:H2'	1:X:1782:A:C5	2.47	0.48
1:X:2044:G:H2'	1:X:2480:C:O2'	2.14	0.48
1:X:2570:C:H2'	1:X:2571:G:C8	2.47	0.48
1:X:2673:G:C6	1:X:2696:A:C6	3.01	0.48
2:Y:56:G:H21	6:D:26:MET:HG3	1.77	0.48
7:E:54:ARG:NH2	7:E:54:ARG:HB3	2.28	0.48
7:E:156:ALA:O	7:E:172:LYS:N	2.45	0.48
17:P:28:ALA:HB2	17:P:71:VAL:HG22	1.94	0.48
1:X:14:A:C5	1:X:536:A:C2	3.01	0.48
1:X:860:U:H5"	1:X:861:G:OP2	2.13	0.48
1:X:1357:U:H4'	1:X:1397:A:C5	2.49	0.48
1:X:1705:U:H1'	1:X:1718:A:C5	2.48	0.48
1:X:2672:U:H2'	1:X:2673:G:C8	2.46	0.48
1:X:2870:C:H2'	1:X:2871:U:C6	2.48	0.48
8:G:59:ALA:HB2	8:G:131:VAL:HG13	1.96	0.48
11:J:126:LEU:HD23	11:J:126:LEU:HA	1.59	0.48
1:X:524:A:H1'	1:X:590:C:O2'	2.14	0.48
1:X:559:C:O2	1:X:559:C:H2'	2.14	0.48
1:X:1164:C:H2'	1:X:1165:G:O4'	2.12	0.48
1:X:1480:G:H2'	1:X:1481:U:O4'	2.12	0.48
1:X:1683:G:N2	1:X:1686:A:N7	2.61	0.48
1:X:2306:A:H2'	1:X:2307:A:H8	1.76	0.48
1:X:2446:C:H2'	1:X:2447:G:O4'	2.14	0.48
1:X:2451:G:C6	1:X:2454:C:C5	3.01	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:2507:U:O3'	1:X:2508:G:H8	1.96	0.48
1:X:2784:A:C6	1:X:2866:A:C8	3.02	0.48
2:Y:120:G:C2	2:Y:121:G:C8	3.01	0.48
5:C:18:PRO:HD2	5:C:109:ALA:HB2	1.95	0.48
7:E:35:VAL:HB	7:E:37:TYR:CZ	2.48	0.48
8:G:56:THR:O	8:G:60:SER:OG	2.27	0.48
9:H:33:GLY:HA3	9:H:102:GLN:NE2	2.23	0.48
10:I:56:LEU:HD23	28:3:12:ARG:NH1	2.27	0.48
11:J:99:LYS:HE3	11:J:100:PRO:CD	2.44	0.48
12:K:97:ILE:HG23	12:K:113:ILE:HD13	1.96	0.48
13:L:96:TYR:CZ	13:L:101:LYS:HG3	2.48	0.48
28:3:33:ASN:OD1	28:3:34:THR:N	2.47	0.48
1:X:495:C:H5'	19:R:58:VAL:HG22	1.94	0.48
1:X:589:C:H4'	15:N:31:GLN:OE1	2.13	0.48
1:X:1034:U:H5	1:X:1035:G:C4	2.32	0.48
1:X:1782:A:O3'	3:A:206:LEU:HB2	2.13	0.48
1:X:1791:C:H42	1:X:1809:G:N2	2.11	0.48
1:X:2222:U:H2'	1:X:2223:U:C6	2.48	0.48
1:X:2274:C:H2'	1:X:2275:U:H5'	1.95	0.48
1:X:2843:A:H5'	1:X:2844:G:OP2	2.14	0.48
31:X:3167:SPD:H21	9:H:5:GLN:HE22	1.78	0.48
15:N:58:ARG:NH2	15:N:62:ILE:HD11	2.28	0.48
15:N:61:TRP:CE3	15:N:97:ASP:OD2	2.67	0.48
17:P:8:PHE:CE2	17:P:14:ARG:HG3	2.48	0.48
17:P:34:SER:O	17:P:38:VAL:HG23	2.14	0.48
1:X:24:G:H2'	1:X:25:U:C6	2.47	0.48
1:X:169:C:O2	1:X:815:A:O2'	2.22	0.48
1:X:242:A:N6	1:X:441:A:C8	2.81	0.48
1:X:959:C:H1'	1:X:995:A:N3	2.29	0.48
1:X:1050:G:H1'	1:X:1128:G:H1	1.78	0.48
1:X:1671:A:C1'	1:X:2798:A:H5'	2.44	0.48
1:X:2085:G:N2	1:X:2171:U:HO2'	2.12	0.48
1:X:2220:A:H2'	1:X:2221:G:H8	1.79	0.48
1:X:2290:A:N1	6:D:42:SER:OG	2.37	0.48
1:X:2386:G:H8	1:X:2386:G:O5'	1.97	0.48
1:X:2720:A:C8	1:X:2743:G:N2	2.81	0.48
2:Y:3:A:C6	2:Y:4:C:N4	2.82	0.48
2:Y:23:G:H2'	2:Y:24:U:H6	1.78	0.48
2:Y:34:C:H2'	2:Y:35:C:C6	2.49	0.48
3:A:6:TYR:HE2	3:A:13:ARG:HH21	1.62	0.48
4:B:12:THR:HG22	4:B:23:VAL:HG23	1.95	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
7:E:99:THR:HG23	7:E:102:ALA:HB3	1.96	0.48
9:H:3:MET:HE2	9:H:3:MET:HB3	1.72	0.48
9:H:116:ARG:HE	9:H:134:LEU:CD1	2.27	0.48
10:I:53:ARG:NH2	28:3:8:LYS:HD3	2.28	0.48
14:M:29:PRO:HG2	14:M:99:VAL:HG11	1.95	0.48
24:W:27:LYS:HG3	24:W:30:ASP:OD1	2.14	0.48
1:X:83:A:C2	1:X:101:A:C5	3.02	0.48
1:X:181:A:O3'	1:X:182:G:H4'	2.13	0.48
1:X:309:G:P	19:R:94:VAL:HG22	2.54	0.48
1:X:325:U:H2'	1:X:326:A:C8	2.49	0.48
1:X:489:A:C2'	1:X:490:A:H5"	2.42	0.48
1:X:590:C:O5'	1:X:590:C:H6	1.96	0.48
1:X:1141:U:C5	4:B:147:PRO:HD3	2.48	0.48
1:X:1210:C:H2'	1:X:1211:G:H8	1.77	0.48
1:X:1225:G:H2'	1:X:1249:G:N2	2.29	0.48
1:X:1420:A:H2'	1:X:1421:U:C6	2.48	0.48
1:X:1482:U:H2'	1:X:1483:G:C8	2.48	0.48
1:X:1561:A:H3'	1:X:1562:G:H8	1.79	0.48
1:X:2086:U:H2'	1:X:2087:U:C6	2.49	0.48
9:H:88:THR:O	14:M:79:ARG:HG3	2.14	0.48
10:I:53:ARG:HH21	28:3:12:ARG:HD3	1.76	0.48
10:I:55:ARG:NH1	28:3:25:PHE:HB2	2.28	0.48
26:1:28:ARG:C	26:1:30:ASN:H	2.16	0.48
1:X:469:G:O2'	27:2:39:ARG:HG2	2.14	0.48
1:X:659:G:H2'	1:X:660:G:C8	2.49	0.48
1:X:833:A:H8	1:X:833:A:O5'	1.97	0.48
1:X:991:A:C4	1:X:1146:G:O4'	2.67	0.48
1:X:998:C:O2'	1:X:1011:A:N3	2.34	0.48
1:X:1429:A:H1'	1:X:1603:A:C5	2.48	0.48
1:X:2230:G:C6	1:X:2231:G:C6	3.02	0.48
1:X:2270:U:H2'	1:X:2271:C:H6	1.79	0.48
1:X:2282:G:H1	1:X:2292:C:H42	1.60	0.48
3:A:252:LYS:HD2	3:A:253:PRO:HD2	1.96	0.48
13:L:9:ARG:HH11	13:L:9:ARG:C	2.16	0.48
14:M:110:LEU:HB3	14:M:115:ALA:HB1	1.94	0.48
19:R:58:VAL:HG12	19:R:68:GLY:HA2	1.95	0.48
24:W:16:GLN:OE1	24:W:49:HIS:NE2	2.44	0.48
1:X:338:G:H5'	19:R:9:HIS:ND1	2.27	0.47
1:X:462:G:H5"	1:X:463:C:OP2	2.13	0.47
1:X:534:U:H2'	1:X:535:U:C6	2.49	0.47
1:X:537:C:O2'	1:X:538:A:C4	2.65	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:588:G:C2	1:X:1275:A:C4	3.02	0.47
1:X:1030:U:H2'	1:X:1032:A:H2	1.77	0.47
1:X:1340:C:H2'	1:X:1341:G:O4'	2.13	0.47
1:X:1425:G:H2'	1:X:1426:U:H6	1.79	0.47
1:X:1606:C:H2'	1:X:1607:A:H8	1.78	0.47
1:X:1810:U:HO2'	1:X:1811:A:P	2.37	0.47
1:X:1838:G:H2'	1:X:1839:A:O4'	2.14	0.47
1:X:1919:A:H62	1:X:1946:U:H3	1.60	0.47
1:X:2358:C:H2'	1:X:2359:U:H6	1.78	0.47
1:X:2606:G:C6	1:X:2607:C:N4	2.82	0.47
1:X:2791:C:C2	1:X:2806:G:C2	3.02	0.47
1:X:2855:C:H1'	12:K:92:GLY:O	2.14	0.47
4:B:132:LYS:HA	4:B:134:TRP:NE1	2.29	0.47
5:C:2:ALA:HB3	5:C:15:ILE:HD12	1.95	0.47
6:D:63:GLN:NE2	6:D:89:VAL:HG13	2.29	0.47
1:X:89:A:H4'	1:X:90:G:O5'	2.13	0.47
1:X:144:U:H2'	1:X:145:C:H6	1.79	0.47
1:X:481:A:C6	1:X:482:A:C6	3.02	0.47
1:X:603:C:H2'	1:X:604:U:C6	2.49	0.47
1:X:737:C:H2'	1:X:738:G:O4'	2.14	0.47
1:X:1710:U:O2'	3:A:14:ARG:NH2	2.47	0.47
1:X:1865:C:H3'	1:X:1866:G:H8	1.77	0.47
1:X:2067:U:H2'	1:X:2068:C:H6	1.78	0.47
1:X:2352:A:H2'	1:X:2353:G:C8	2.49	0.47
1:X:2442:C:H2'	1:X:2443:C:C6	2.49	0.47
1:X:2493:U:H2'	1:X:2494:C:H6	1.78	0.47
1:X:2659:C:C5'	4:B:189:PRO:HA	2.37	0.47
2:Y:23:G:H2'	2:Y:24:U:C6	2.49	0.47
2:Y:36:A:H4'	2:Y:37:C:OP1	2.13	0.47
2:Y:77:G:O3'	20:S:32:PHE:HZ	1.97	0.47
6:D:22:TYR:OH	6:D:165:GLU:OE1	2.30	0.47
6:D:33:LYS:HB3	6:D:92:ARG:HG2	1.96	0.47
8:G:114:THR:O	8:G:116:ARG:NH2	2.47	0.47
15:N:106:PHE:O	15:N:110:VAL:HG23	2.13	0.47
1:X:543:G:C6	1:X:544:U:C4	3.03	0.47
1:X:1028:G:C6	1:X:1157:G:C6	3.03	0.47
1:X:1389:C:H2'	1:X:1390:G:O4'	2.14	0.47
1:X:2073:A:N6	1:X:2209:G:O6	2.47	0.47
3:A:228:PRO:HD3	3:A:235:GLY:H	1.78	0.47
4:B:55:ALA:H	4:B:58:LYS:NZ	2.11	0.47
10:I:83:LEU:HD11	10:I:99:VAL:HG11	1.96	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
20:S:43:PHE:O	20:S:47:SER:N	2.46	0.47
28:3:14:ILE:CD1	28:3:22:VAL:HG13	2.45	0.47
1:X:603:C:H2'	1:X:604:U:H6	1.78	0.47
1:X:1562:G:H5'	1:X:1563:U:H5'	1.96	0.47
2:Y:27:A:H2'	2:Y:28:A:H5"	1.96	0.47
2:Y:117:G:H2'	2:Y:118:G:O4'	2.14	0.47
3:A:246:PRO:HD2	3:A:250:TRP:O	2.14	0.47
4:B:40:GLN:OE1	4:B:41:THR:HG22	2.14	0.47
4:B:146:THR:HG22	4:B:147:PRO:CD	2.45	0.47
4:B:199:ARG:NH2	4:B:199:ARG:HB2	2.28	0.47
8:G:92:GLY:H	8:G:94:LYS:HG3	1.80	0.47
15:N:43:ALA:HB2	16:O:72:ARG:NH1	2.29	0.47
1:X:1333:G:N2	1:X:1344:C:H41	2.13	0.47
1:X:1430:G:C4	1:X:1599:G:N2	2.82	0.47
1:X:1824:C:N4	1:X:1825:C:C4	2.83	0.47
1:X:2422:C:H2'	1:X:2423:G:H8	1.79	0.47
2:Y:14:C:H3'	2:Y:14:C:H6	1.79	0.47
5:C:158:ARG:HH21	5:C:171:PRO:HA	1.79	0.47
13:L:36:LYS:HA	13:L:99:ARG:HH21	1.79	0.47
19:R:94:VAL:HG23	19:R:95:ARG:N	2.30	0.47
1:X:347:C:H4'	19:R:15:HIS:CD2	2.49	0.47
1:X:540:G:O6	1:X:2006:G:OP1	2.32	0.47
1:X:626:A:O2'	5:C:176:ASN:HB2	2.12	0.47
1:X:1104:G:H2'	1:X:1105:U:C5	2.49	0.47
1:X:1284:G:N2	1:X:1631:C:C4	2.82	0.47
1:X:1462:C:H2'	1:X:1463:A:C8	2.49	0.47
1:X:1635:G:C4	1:X:1636:G:C8	3.03	0.47
1:X:1794:A:H2	1:X:1815:G:O4'	1.97	0.47
1:X:2264:C:C2	1:X:2363:G:N2	2.82	0.47
1:X:2394:G:H2'	1:X:2395:C:C6	2.49	0.47
1:X:2434:G:H2'	1:X:2435:C:H6	1.75	0.47
1:X:2555:G:N2	1:X:2555:G:OP2	2.47	0.47
1:X:2663:U:C4	1:X:2664:G:N7	2.82	0.47
10:I:51:GLY:C	10:I:53:ARG:HE	2.17	0.47
12:K:14:SER:O	12:K:18:VAL:HG23	2.14	0.47
14:M:103:LYS:HA	14:M:103:LYS:HD3	1.58	0.47
16:O:20:ILE:HD12	16:O:21:ARG:N	2.27	0.47
1:X:186:C:H2'	1:X:187:U:C6	2.50	0.47
1:X:467:U:H2'	1:X:468:A:H2'	1.97	0.47
1:X:493:A:N6	1:X:516:G:O2'	2.46	0.47
1:X:598:U:C2	1:X:599:A:C8	3.02	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:859:U:H1'	1:X:860:U:C2	2.49	0.47
1:X:1191:G:C5	1:X:1192:A:C8	3.03	0.47
1:X:1225:G:O2'	1:X:1250:A:N6	2.48	0.47
1:X:1332:G:C2	1:X:1347:C:C2	3.03	0.47
1:X:1443:G:H2'	1:X:1444:C:C6	2.50	0.47
1:X:1705:U:H1'	1:X:1718:A:C6	2.49	0.47
1:X:1932:G:H2'	1:X:1933:G:C8	2.50	0.47
1:X:2444:C:O2'	1:X:2445:C:H5'	2.15	0.47
1:X:2530:C:OP1	31:X:3167:SPD:H81	2.14	0.47
1:X:2541:U:H1'	9:H:23:ARG:NH2	2.30	0.47
1:X:2876:C:C4	1:X:2877:A:N6	2.83	0.47
6:D:142:THR:O	6:D:146:VAL:HG22	2.15	0.47
9:H:2:ILE:O	9:H:44:TYR:HA	2.14	0.47
9:H:83:ARG:HH22	9:H:134:LEU:CD1	2.28	0.47
11:J:25:GLY:O	11:J:103:VAL:HG12	2.15	0.47
11:J:27:TYR:HB2	11:J:138:TYR:CE2	2.50	0.47
12:K:79:VAL:HA	12:K:83:VAL:HG22	1.97	0.47
18:Q:49:ARG:HG3	18:Q:49:ARG:O	2.14	0.47
20:S:116:VAL:N	20:S:168:VAL:O	2.43	0.47
20:S:154:LEU:HD11	20:S:160:LEU:HB2	1.97	0.47
21:T:12:ASN:N	21:T:12:ASN:ND2	2.62	0.47
22:U:64:ALA:HA	22:U:67:LEU:HG	1.97	0.47
1:X:24:G:H2'	1:X:25:U:O4'	2.15	0.47
1:X:689:A:C8	1:X:2422:C:H1'	2.50	0.47
1:X:783:G:H2'	1:X:784:U:O4'	2.15	0.47
1:X:1629:G:C2	1:X:1633:C:C2	3.03	0.47
1:X:2043:A:H1'	1:X:2481:G:H1'	1.97	0.47
1:X:2326:C:H2'	1:X:2327:U:H6	1.78	0.47
1:X:2590:U:C5	29:X:2901:MIV:H212	2.50	0.47
3:A:228:PRO:HD3	3:A:235:GLY:N	2.30	0.47
3:A:252:LYS:HZ2	3:A:252:LYS:H	1.63	0.47
18:Q:10:PRO:HA	18:Q:27:PHE:HB3	1.97	0.47
28:3:37:SER:HB3	28:3:40:GLU:HB2	1.96	0.47
1:X:1164:C:OP1	15:N:76:TYR:OH	2.33	0.47
1:X:1210:C:C2	1:X:1211:G:C8	3.02	0.47
1:X:1782:A:H4'	3:A:206:LEU:HB2	1.97	0.47
1:X:1845:A:H2'	1:X:1846:A:H8	1.79	0.47
1:X:2229:G:C8	1:X:2475:C:H5"	2.49	0.47
1:X:2627:G:H2'	1:X:2628:C:H6	1.80	0.47
2:Y:112:A:C6	2:Y:113:G:C5	3.03	0.47
3:A:72:LYS:HG3	3:A:97:TYR:CZ	2.50	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
6:D:13:ARG:HB2	6:D:14:PRO:HD3	1.97	0.47
11:J:42:TRP:HB3	11:J:95:VAL:HB	1.96	0.47
20:S:76:ARG:HB3	20:S:76:ARG:NH1	2.30	0.47
28:3:52:LYS:CE	28:3:56:ALA:HB2	2.44	0.47
1:X:591:G:C4	1:X:592:G:C8	3.03	0.47
1:X:621:U:H2'	1:X:622:U:H6	1.78	0.47
1:X:692:C:C2	1:X:812:G:N2	2.83	0.47
1:X:812:G:H3'	1:X:813:A:H2'	1.96	0.47
1:X:1035:G:C6	1:X:1036:G:C6	3.03	0.47
1:X:1164:C:H5'	15:N:76:TYR:CE1	2.50	0.47
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.67	0.47
1:X:1813:A:H2'	1:X:1814:G:C8	2.49	0.47
1:X:1873:A:H2'	1:X:1874:G:O4'	2.14	0.47
1:X:1959:U:O3'	1:X:1960:A:H8	1.98	0.47
1:X:1998:A:O5'	1:X:1998:A:H8	1.98	0.47
1:X:2352:A:H2'	1:X:2353:G:H8	1.80	0.47
1:X:2737:A:H2'	1:X:2738:A:H5"	1.97	0.47
1:X:326:A:H2'	1:X:327:C:O4'	2.15	0.46
1:X:526:C:O2'	1:X:527:C:H5'	2.15	0.46
1:X:806:A:OP2	1:X:2055:G:H5'	2.15	0.46
1:X:1074:G:C5	1:X:1075:C:C5	3.03	0.46
1:X:1443:G:H2'	1:X:1444:C:H6	1.80	0.46
1:X:2493:U:H2'	1:X:2494:C:C6	2.49	0.46
1:X:2594:U:N3	25:Z:7:PRO:HA	2.29	0.46
1:X:2796:A:C4	1:X:2797:G:N7	2.83	0.46
5:C:164:VAL:HB	5:C:167:VAL:HG22	1.97	0.46
6:D:53:ALA:HA	6:D:56:GLU:HG2	1.97	0.46
10:I:27:ASP:OD1	10:I:27:ASP:N	2.44	0.46
11:J:13:GLN:HG2	11:J:14:PHE:CE1	2.50	0.46
26:1:14:SER:HA	26:1:52:GLU:HA	1.96	0.46
26:1:20:PHE:HE2	26:1:42:PRO:HG2	1.80	0.46
1:X:231:G:H4'	1:X:397:U:C5'	2.45	0.46
1:X:762:A:N1	1:X:766:A:O2'	2.46	0.46
1:X:1263:G:OP2	10:I:21:ARG:NH2	2.48	0.46
1:X:1277:G:H8	1:X:1277:G:O5'	1.98	0.46
1:X:1655:C:OP1	1:X:2689:C:O2'	2.20	0.46
1:X:2708:U:H2'	1:X:2709:C:C6	2.50	0.46
1:X:2800:C:H3'	1:X:2801:A:C8	2.43	0.46
9:H:124:MET:H	9:H:125:LYS:HE3	1.80	0.46
12:K:33:ARG:HD3	12:K:112:LEU:HD22	1.97	0.46
12:K:76:VAL:O	12:K:80:MET:HB2	2.16	0.46



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
22:U:49:LYS:HA	22:U:61:TRP:HD1	1.81	0.46
1:X:405:C:H2'	1:X:406:G:C8	2.50	0.46
1:X:427:C:H1'	1:X:1856:U:H1'	1.97	0.46
1:X:525:A:OP1	31:X:3170:SPD:N10	2.49	0.46
1:X:635:C:O2'	1:X:670:U:OP1	2.27	0.46
1:X:888:G:H2'	1:X:889:C:O4'	2.16	0.46
1:X:1211:G:C2	1:X:1212:U:C4	3.03	0.46
1:X:1339:U:O2'	1:X:1993:G:H1'	2.16	0.46
1:X:1695:U:H1'	1:X:1974:U:O2'	2.15	0.46
1:X:1999:U:H1'	25:Z:6:VAL:HG11	1.96	0.46
1:X:2268:G:N2	1:X:2323:U:O2	2.49	0.46
1:X:2272:A:P	13:L:15:ARG:HH22	2.37	0.46
1:X:2345:A:H2'	1:X:2346:G:O4'	2.15	0.46
1:X:2665:G:H2'	1:X:2666:U:O4'	2.15	0.46
1:X:2695:C:H2'	1:X:2696:A:O4'	2.16	0.46
7:E:153:LYS:HG2	7:E:154:PRO:HD2	1.97	0.46
8:G:110:LEU:O	8:G:111:LYS:C	2.52	0.46
9:H:108:THR:H	9:H:108:THR:HG1	1.50	0.46
21:T:63:SER:O	21:T:81:ILE:HD12	2.14	0.46
28:3:16:ILE:HG21	28:3:63:PRO:CB	2.46	0.46
1:X:105:G:N2	1:X:357:A:H61	2.13	0.46
1:X:386:U:O2	1:X:387:A:C8	2.69	0.46
1:X:1162:A:H2'	1:X:1163:C:C6	2.50	0.46
1:X:1437:A:H2'	1:X:1438:G:C8	2.50	0.46
3:A:99:ASP:OD1	3:A:99:ASP:N	2.45	0.46
6:D:9:ASN:O	6:D:13:ARG:HG3	2.15	0.46
8:G:104:THR:C	8:G:106:TYR:H	2.19	0.46
14:M:55:ILE:HG13	14:M:67:THR:O	2.15	0.46
18:Q:25:TYR:CE2	18:Q:88:ILE:HB	2.50	0.46
1:X:526:C:H41	31:X:3170:SPD:H81	1.79	0.46
1:X:677:G:O2'	1:X:951:G:H5"	2.16	0.46
1:X:736:G:H2'	1:X:737:C:O4'	2.15	0.46
1:X:753:U:C2	1:X:754:G:N7	2.84	0.46
1:X:1143:A:H1'	8:G:101:THR:HG21	1.98	0.46
1:X:1202:U:H2'	1:X:1203:A:H8	1.79	0.46
1:X:1439:G:O2'	1:X:1440:G:OP1	2.29	0.46
1:X:2187:A:H61	1:X:2197:U:H3	1.63	0.46
1:X:2372:A:H62	1:X:2401:A:N6	2.07	0.46
1:X:2696:A:C2	1:X:2697:G:C8	3.04	0.46
1:X:2792:C:C2	1:X:2805:G:N2	2.84	0.46
4:B:4:ILE:HG12	4:B:5:LEU:H	1.81	0.46



A. 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
25:Z:30:LEU:HD23	25:Z:30:LEU:HA	1.79	0.46
1:X:598:U:H2'	1:X:599:A:H8	1.81	0.46
1:X:939:C:OP2	1:X:940:G:H8	1.98	0.46
1:X:1098:G:N2	1:X:1114:A:H1'	2.30	0.46
1:X:1223:G:H4'	1:X:1224:A:C5'	2.45	0.46
1:X:1623:C:H4'	1:X:1624:A:H5'	1.97	0.46
1:X:1670:G:O5'	1:X:2797:G:N2	2.42	0.46
1:X:2073:A:C6	1:X:2209:G:C6	3.04	0.46
1:X:2078:G:H2'	1:X:2079:A:N9	2.30	0.46
1:X:2177:U:H2'	1:X:2178:U:C6	2.50	0.46
1:X:2245:A:H4'	1:X:2246:A:C2	2.51	0.46
1:X:2324:G:N3	1:X:2360:C:H2'	2.30	0.46
1:X:2569:A:H5"	3:A:239:ARG:HH11	1.81	0.46
2:Y:49:C:H5'	2:Y:50:U:OP2	2.15	0.46
14:M:82:PRO:HG2	14:M:85:SER:CB	2.45	0.46
15:N:11:ARG:HG2	15:N:15:LYS:NZ	2.31	0.46
16:O:65:ARG:HB3	16:O:87:ARG:NH1	2.31	0.46
18:Q:34:THR:HG23	18:Q:37:GLU:OE2	2.16	0.46
19:R:81:VAL:HG21	19:R:89:GLY:HA2	1.98	0.46
22:U:11:LYS:HE3	22:U:76:LYS:HD3	1.98	0.46
1:X:268:G:C4	1:X:269:G:C8	3.04	0.46
1:X:457:C:O2'	1:X:458:G:H5'	2.16	0.46
1:X:585:U:H6	1:X:585:U:O5'	1.98	0.46
1:X:1022:A:C5	1:X:1024:G:C8	3.03	0.46
1:X:1175:A:C4	1:X:1176:U:C5	3.03	0.46
1:X:1683:G:H1'	9:H:3:MET:SD	2.56	0.46
1:X:1809:G:OP1	3:A:88:ARG:NH1	2.49	0.46
1:X:2673:G:C6	1:X:2696:A:N1	2.83	0.46
7:E:18:ASN:O	7:E:24:PHE:HB2	2.15	0.46
9:H:68:ASP:OD1	9:H:68:ASP:N	2.48	0.46
9:H:121:ARG:HB2	9:H:123:PHE:HD1	1.81	0.46
22:U:27:ASP:HB2	22:U:33:LYS:O	2.16	0.46
26:1:36:GLU:CB	26:1:52:GLU:HB2	2.44	0.46
1:X:109:A:H5"	23:V:62:ARG:NH2	2.30	0.46
1:X:123:A:OP1	27:2:14:LYS:HE2	2.15	0.46
1:X:396:U:H5'	1:X:397:U:OP2	2.16	0.46
1:X:564:U:H2'	1:X:565:A:C8	2.51	0.46
1:X:858:G:H8	1:X:858:G:OP2	1.98	0.46
1:X:960:U:H2'	1:X:961:G:H8	1.80	0.46
1:X:1369:G:C6	1:X:1370:U:C4	3.03	0.46
1:X:1656:U:H4'	1:X:2678:C:O2'	2.16	0.46



Atom 1 Atom 2		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:1976:U:C2	1:X:1977:C:C6	3.03	0.46
1:X:1976:U:N3	1:X:1977:C:C6	2.84	0.46
1:X:2011:U:H2'	1:X:2012:A:H8	1.75	0.46
1:X:2541:U:C2	1:X:2542:U:C6	3.04	0.46
4:B:33:ILE:HG21	4:B:36:ARG:NH2	2.31	0.46
6:D:30:ARG:O	6:D:158:THR:HB	2.16	0.46
6:D:115:ARG:HG3	6:D:116:GLY:O	2.15	0.46
6:D:138:PHE:HB2	6:D:141:ILE:HD12	1.98	0.46
11:J:20:GLY:O	11:J:99:LYS:HG3	2.15	0.46
11:J:28:VAL:HG12	11:J:138:TYR:CZ	2.50	0.46
17:P:41:VAL:O	17:P:44:VAL:N	2.49	0.46
19:R:64:ASN:HD21	19:R:67:GLY:HA2	1.81	0.46
28:3:52:LYS:HE3	28:3:56:ALA:HB2	1.98	0.46
1:X:21:A:C6	1:X:530:G:C6	3.03	0.46
1:X:228:A:H2'	1:X:229:G:O4'	2.16	0.46
1:X:228:A:H2'	1:X:229:G:C4'	2.46	0.46
1:X:312:G:C6	1:X:328:A:C5	3.03	0.46
1:X:441:A:H2'	1:X:442:A:C8	2.51	0.46
1:X:602:C:O2'	28:3:3:LYS:HB2	2.16	0.46
1:X:826:U:H2'	1:X:827:C:H6	1.78	0.46
1:X:857:U:H3'	1:X:858:G:C8	2.51	0.46
1:X:1332:G:C5	1:X:1333:G:C6	3.03	0.46
1:X:1496:G:O2'	1:X:1497:C:OP1	2.30	0.46
1:X:2078:G:H22	1:X:2178:U:H3	1.61	0.46
1:X:2486:C:H5"	1:X:2552:C:N4	2.30	0.46
1:X:2526:U:C5	1:X:2545:A:C8	3.04	0.46
1:X:2652:G:H2'	1:X:2653:A:H8	1.80	0.46
2:Y:9:G:H2'	2:Y:10:U:C6	2.51	0.46
9:H:114:VAL:HG23	9:H:115:ALA:O	2.14	0.46
17:P:117:ILE:HD13	17:P:118:LYS:N	2.31	0.46
20:S:72:ASP:OD2	20:S:75:LYS:N	2.33	0.46
1:X:138:G:H2'	1:X:139:A:C8	2.50	0.46
1:X:165:G:H2'	1:X:166:G:O4'	2.17	0.46
1:X:1112:U:H2'	1:X:1113:C:O4'	2.16	0.46
1:X:1229:C:O5'	1:X:1229:C:H6	1.99	0.46
1:X:1446:U:H2'	1:X:1447:U:O4'	2.16	0.46
1:X:1672:A:C6	1:X:1673:C:C2	3.04	0.46
1:X:2486:C:H5"	1:X:2552:C:H41	1.81	0.46
1:X:2690:A:OP1	1:X:2692:A:P	2.73	0.46
1:X:2708:U:C2	1:X:2709:C:C5	3.04	0.46
1:X:2728:A:H2'	1:X:2729:A:C8	2.51	0.46



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:Y:28:A:O2'	2:Y:29:C:OP1	2.29	0.46
5:C:108:ILE:O	5:C:111:ARG:HB2	2.16	0.46
5:C:130:THR:O	5:C:134:ILE:HG13	2.16	0.46
6:D:38:GLU:HB3	6:D:87:ILE:HG13	1.98	0.46
6:D:68:THR:OG1	6:D:86:GLY:O	2.19	0.46
14:M:29:PRO:HB2	14:M:99:VAL:HG11	1.98	0.46
19:R:57:ASN:HB2	19:R:60:PRO:CD	2.46	0.46
1:X:383:G:H4'	1:X:384:A:OP2	2.16	0.45
1:X:572:G:H2'	15:N:37:GLN:HE21	1.81	0.45
1:X:669:G:H2'	1:X:670:U:H6	1.81	0.45
1:X:929:A:H5"	1:X:2247:A:N6	2.31	0.45
1:X:994:A:C6	1:X:995:A:N1	2.84	0.45
1:X:1393:G:O2'	1:X:1585:A:N6	2.49	0.45
1:X:2037:A:C2	1:X:2595:C:N3	2.84	0.45
1:X:2758:A:O2'	1:X:2760:G:O2'	2.29	0.45
1:X:2813:G:O2'	12:K:46:PRO:HG3	2.15	0.45
2:Y:17:A:H1'	2:Y:112:A:C8	2.51	0.45
4:B:111:LYS:O	4:B:114:GLN:NE2	2.49	0.45
14:M:82:PRO:HG2	14:M:85:SER:HB2	1.98	0.45
22:U:16:ASN:OD1	22:U:17:SER:N	2.47	0.45
1:X:393:U:OP1	22:U:20:ARG:HB2	2.17	0.45
1:X:677:G:C6	1:X:678:G:N7	2.84	0.45
1:X:688:A:O2'	5:C:61:GLN:HG2	2.16	0.45
1:X:764:A:C4	1:X:802:A:C2	3.05	0.45
1:X:792:U:H5"	3:A:49:ILE:HD11	1.98	0.45
1:X:831:G:C2	1:X:1204:G:O6	2.70	0.45
1:X:1264:C:H5"	15:N:13:ARG:NH2	2.31	0.45
1:X:1466:C:H2'	1:X:1467:U:C1'	2.43	0.45
6:D:121:ALA:O	6:D:123:ASP:N	2.48	0.45
10:I:55:ARG:H	10:I:55:ARG:NH1	2.13	0.45
15:N:83:LEU:O	15:N:89:ASP:HB2	2.16	0.45
22:U:27:ASP:HB3	22:U:30:VAL:HB	1.97	0.45
1:X:30:G:O2'	1:X:31:C:H5'	2.17	0.45
1:X:394:U:O2'	1:X:395:G:H5'	2.16	0.45
1:X:1428:G:C2	1:X:1601:U:H4'	2.51	0.45
1:X:1439:G:H2'	1:X:1440:G:C8	2.51	0.45
1:X:2006:G:H2'	1:X:2007:G:H8	1.81	0.45
1:X:2290:A:C8	1:X:2291:U:C6	3.05	0.45
1:X:2472:U:C4	1:X:2473:G:C8	3.04	0.45
1:X:2511:G:C5	1:X:2512:A:N7	2.84	0.45
1:X:2707:G:H2'	1:X:2708:U:H6	1.81	0.45



Atom_1	Atom 2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:X:2711:G:P	4:B:169:ASN:HD22	2.38	0.45
4:B:32:PRO:O	4:B:49:ILE:HB	2.16	0.45
4:B:184:VAL:HG11	4:B:188:ILE:HD11	1.97	0.45
8:G:38:GLU:HG3	8:G:67:ARG:NH1	2.31	0.45
15:N:72:HIS:HD2	15:N:110:VAL:HG21	1.82	0.45
20:S:5:ALA:HA	20:S:31:SER:HB3	1.98	0.45
1:X:115:G:C6	1:X:117:A:N6	2.84	0.45
1:X:209:G:O2'	1:X:210:A:O5'	2.30	0.45
1:X:474:G:C2	1:X:478:G:C6	3.05	0.45
1:X:609:U:H2'	1:X:610:G:H8	1.82	0.45
1:X:777:A:H5'	3:A:210:GLY:HA3	1.97	0.45
1:X:1039:A:C2	1:X:2466:G:H1'	2.50	0.45
1:X:1084:A:H3'	1:X:1085:G:H8	1.81	0.45
1:X:1712:G:N2	1:X:1713:G:C8	2.85	0.45
1:X:1744:G:O6	1:X:1747:G:C6	2.70	0.45
1:X:2054:A:H2'	1:X:2055:G:C8	2.51	0.45
1:X:2871:U:H2'	1:X:2872:U:H6	1.81	0.45
6:D:34:ILE:HD13	6:D:34:ILE:HA	1.87	0.45
9:H:29:ILE:HD13	9:H:34:LEU:HD23	1.98	0.45
11:J:120:ARG:HE	11:J:120:ARG:HB3	1.44	0.45
17:P:89:ARG:HA	17:P:131:LYS:HG2	1.99	0.45
1:X:116:A:OP2	1:X:117:A:H5"	2.16	0.45
1:X:318:G:H21	1:X:341:A:H62	1.64	0.45
1:X:386:U:C2	1:X:387:A:C8	3.04	0.45
1:X:1805:G:H4'	3:A:44:ASN:HA	1.99	0.45
1:X:2438:A:C4	1:X:2439:U:C6	3.04	0.45
1:X:2661:G:O2'	14:M:63:ARG:HG2	2.17	0.45
1:X:2799:C:H2'	1:X:2800:C:C6	2.52	0.45
6:D:2:GLN:HG3	6:D:5:LYS:NZ	2.32	0.45
12:K:48:VAL:O	12:K:52:ILE:HG23	2.16	0.45
12:K:95:THR:HG23	12:K:113:ILE:HD11	1.98	0.45
18:Q:11:VAL:HG22	18:Q:28:TRP:NE1	2.31	0.45
1:X:60:A:C6	1:X:61:U:C4	3.05	0.45
1:X:68:C:H4'	1:X:74:G:N7	2.31	0.45
1:X:198:A:H61	1:X:441:A:N6	2.15	0.45
1:X:334:G:C6	1:X:344:G:C4	3.04	0.45
1:X:353:G:H2'	1:X:354:C:H6	1.82	0.45
1:X:769:C:C4	1:X:770:U:C5	3.05	0.45
1:X:1135:C:H2'	1:X:1136:G:O4'	2.16	0.45
1:X:1269:G:N3	1:X:1269:G:H2'	2.31	0.45
1:X:1272:G:C6	1:X:1273:G:C6	3.04	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:1327:C:P	1:X:1345:G:H5"	2.57	0.45
1:X:1467:U:O4	1:X:1473:U:C2	2.70	0.45
1:X:2061:C:H2'	1:X:2062:U:C6	2.51	0.45
1:X:2460:G:O2'	1:X:2461:G:P	2.74	0.45
1:X:2513:A:H8	1:X:2513:A:O5'	2.00	0.45
1:X:2709:C:H2'	1:X:2710:C:C6	2.52	0.45
1:X:2866:A:H3'	1:X:2867:G:C8	2.51	0.45
2:Y:27:A:H2'	2:Y:27:A:N3	2.31	0.45
2:Y:28:A:HO2'	2:Y:29:C:P	2.40	0.45
4:B:79:ARG:HD3	4:B:79:ARG:HA	1.69	0.45
4:B:159:HIS:CE1	4:B:162:MET:HB2	2.51	0.45
9:H:1:MET:HG3	9:H:46:HIS:NE2	2.32	0.45
20:S:23:ALA:HA	20:S:83:PHE:HB2	1.99	0.45
24:W:3:ILE:HD12	24:W:51:LEU:HD13	1.98	0.45
24:W:34:VAL:HG22	24:W:40:VAL:HG11	1.97	0.45
28:3:21:LYS:HA	28:3:21:LYS:HD2	1.67	0.45
1:X:48:A:H4'	1:X:49:U:O5'	2.16	0.45
1:X:173:A:O2'	1:X:818:G:O6	2.22	0.45
1:X:469:G:H3'	27:2:39:ARG:HA	1.99	0.45
1:X:805:G:N7	1:X:2419:C:H1'	2.32	0.45
1:X:1034:U:H2'	1:X:1035:G:H5'	1.98	0.45
1:X:1302:C:H2'	1:X:1303:U:C6	2.51	0.45
1:X:1403:U:HO2'	1:X:1404:C:C5'	2.30	0.45
1:X:1645:U:O2	1:X:2677:U:H5"	2.16	0.45
1:X:1993:G:P	17:P:62:ARG:HH11	2.40	0.45
1:X:2338:C:H3'	1:X:2339:A:H8	1.81	0.45
1:X:2630:C:H2'	1:X:2631:C:C6	2.51	0.45
1:X:2657:G:H2'	1:X:2658:A:O4'	2.16	0.45
1:X:2796:A:N3	1:X:2797:G:C8	2.84	0.45
2:Y:12:C:H2'	2:Y:13:C:O4'	2.17	0.45
3:A:124:GLU:O	3:A:129:ASN:ND2	2.49	0.45
4:B:55:ALA:HB3	4:B:58:LYS:CD	2.42	0.45
4:B:159:HIS:HE1	4:B:162:MET:HB2	1.82	0.45
11:J:69:ILE:HG13	11:J:70:PHE:N	2.32	0.45
18:Q:17:TYR:HE2	18:Q:93:GLY:CA	2.30	0.45
24:W:47:VAL:HB	24:W:50:LEU:HD13	1.98	0.45
1:X:148:C:HO2'	1:X:149:A:P	2.39	0.45
1:X:194:G:H2'	1:X:195:A:O4'	2.17	0.45
1:X:417:C:H4'	1:X:418:C:O5'	2.17	0.45
1:X:539:A:OP2	8:G:142:ARG:NH2	2.46	0.45
1:X:592:G:C6	1:X:593:C:N4	2.85	0.45



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:652:C:N4	1:X:657:A:H61	2.13	0.45
1:X:1164:C:N4	1:X:1165:G:C6	2.85	0.45
1:X:1321:A:H3'	1:X:1322:G:H8	1.81	0.45
1:X:1347:C:H5"	18:Q:64:ARG:HH22	1.81	0.45
1:X:1403:U:H4'	1:X:1404:C:OP1	2.15	0.45
1:X:1650:A:C6	1:X:1652:G:C5	3.04	0.45
1:X:1824:C:H2'	1:X:1825:C:O4'	2.17	0.45
1:X:2679:G:H2'	1:X:2680:U:C6	2.52	0.45
1:X:2689:C:H2'	1:X:2690:A:O4'	2.16	0.45
2:Y:93:G:O5'	11:J:19:THR:OG1	2.29	0.45
4:B:141:ILE:HD11	4:B:156:MET:CE	2.47	0.45
5:C:190:ALA:HA	5:C:194:GLU:CG	2.44	0.45
8:G:70:PHE:HA	15:N:64:ARG:NH2	2.32	0.45
16:O:14:VAL:HG12	16:O:15:SER:H	1.82	0.45
17:P:103:LEU:HB3	17:P:105:ARG:NH1	2.32	0.45
1:X:353:G:H2'	1:X:354:C:C6	2.52	0.45
1:X:540:G:HO2'	1:X:542:A:H2	1.59	0.45
1:X:572:G:C2'	15:N:37:GLN:HE21	2.30	0.45
1:X:994:A:N7	1:X:995:A:C5	2.85	0.45
1:X:1175:A:N3	1:X:1176:U:C6	2.84	0.45
1:X:1735:G:H2'	1:X:1736:C:C6	2.51	0.45
6:D:132:ILE:HG21	6:D:137:ILE:HD13	1.98	0.45
7:E:127:GLU:HB3	7:E:130:ARG:HB2	1.99	0.45
9:H:80:ALA:HA	9:H:90:ARG:HG2	1.98	0.45
14:M:97:GLY:HA3	14:M:117:ILE:CD1	2.46	0.45
15:N:92:ARG:H	16:O:5:ILE:HD13	1.82	0.45
23:V:18:ILE:HG12	23:V:53:LEU:HD13	1.99	0.45
1:X:48:A:H2'	1:X:48:A:N3	2.32	0.45
1:X:337:G:H21	19:R:10:HIS:CD2	2.34	0.45
1:X:489:A:N6	1:X:491:A:C6	2.85	0.45
1:X:783:G:C2	1:X:784:U:H1'	2.52	0.45
1:X:839:U:H5"	1:X:2408:G:P	2.57	0.45
1:X:1086:C:O2'	1:X:1087:C:OP1	2.32	0.45
1:X:1139:A:C6	1:X:2497:A:C6	3.05	0.45
1:X:1671:A:O4'	1:X:2798:A:H5'	2.16	0.45
1:X:1834:G:H2'	1:X:1835:C:H6	1.82	0.45
1:X:1836:C:C2	1:X:1837:G:C8	3.05	0.45
1:X:2035:G:P	4:B:141:ILE:HG22	2.57	0.45
1:X:2417:U:O2'	1:X:2418:A:H5"	2.17	0.45
1:X:2553:G:C6	1:X:2554:C:N3	2.84	0.45
1:X:2680:U:O2'	12:K:73:LYS:HD3	2.16	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:2833:C:H6	1:X:2833:C:O5'	2.00	0.45
2:Y:95:U:H2'	2:Y:96:C:H6	1.82	0.45
4:B:161:GLY:O	4:B:163:GLU:N	2.49	0.45
17:P:61:PRO:HD2	17:P:62:ARG:HD3	1.98	0.45
1:X:408:U:H2'	1:X:409:G:C8	2.53	0.44
1:X:694:G:C2	1:X:695:G:C4	3.04	0.44
1:X:795:A:P	1:X:795:A:H8	2.40	0.44
1:X:1045:G:H2'	1:X:1046:U:H6	1.82	0.44
1:X:1078:A:H2'	1:X:1079:G:H8	1.82	0.44
1:X:1152:C:H4'	1:X:1153:A:OP2	2.18	0.44
1:X:2057:U:H2'	1:X:2058:U:C6	2.52	0.44
1:X:2448:A:N6	1:X:2460:G:H1'	2.32	0.44
1:X:2559:U:H5"	1:X:2560:G:N2	2.32	0.44
2:Y:15:A:C6	2:Y:72:C:H5'	2.52	0.44
2:Y:64:C:H2'	2:Y:65:A:H8	1.82	0.44
2:Y:75:A:H3'	2:Y:76:U:C6	2.52	0.44
4:B:195:LEU:HB2	14:M:3:THR:HG23	1.98	0.44
9:H:88:THR:HB	14:M:80:VAL:HB	1.99	0.44
11:J:53:ILE:O	11:J:57:ARG:HG2	2.18	0.44
18:Q:77:LYS:HG3	18:Q:78:ALA:N	2.31	0.44
1:X:88:G:C8	1:X:89:A:H2'	2.52	0.44
1:X:385:G:H2'	22:U:69:THR:OG1	2.17	0.44
1:X:538:A:H2	8:G:142:ARG:HH11	1.65	0.44
1:X:934:G:H2'	1:X:935:C:O4'	2.18	0.44
1:X:1310:C:H2'	1:X:1311:C:C6	2.53	0.44
1:X:1404:C:H5'	1:X:1405:A:OP2	2.16	0.44
1:X:2007:G:N2	1:X:2023:C:C2	2.85	0.44
1:X:2286:G:N1	1:X:2287:G:C5	2.85	0.44
1:X:2395:C:C2	1:X:2396:C:C5	3.06	0.44
1:X:2495:G:C5	1:X:2496:C:C4	3.04	0.44
1:X:2539:C:C2	1:X:2540:A:C8	3.05	0.44
1:X:2805:G:C2'	1:X:2806:G:H5'	2.47	0.44
1:X:2807:U:H4'	1:X:2808:U:C5'	2.47	0.44
2:Y:116:C:H2'	2:Y:117:G:C8	2.53	0.44
5:C:13:ARG:HD3	5:C:13:ARG:HA	1.68	0.44
7:E:22:GLY:HA2	7:E:43:VAL:HB	1.98	0.44
7:E:94:PHE:HA	7:E:107:ILE:HG22	2.00	0.44
7:E:97:LYS:HD2	7:E:97:LYS:HA	1.75	0.44
9:H:83:ARG:HD2	9:H:83:ARG:N	2.32	0.44
17:P:39:ARG:HA	17:P:42:VAL:HB	1.99	0.44
1:X:32:C:O2'	1:X:33:C:H5'	2.17	0.44



Atom-1	A.L. D.	Interatomic	Clash
	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:240:U:H2'	1:X:241:C:O4'	2.18	0.44
1:X:439:C:H2'	1:X:440:U:O4'	2.17	0.44
1:X:572:G:C6	1:X:573:C:C4	3.05	0.44
1:X:673:G:H5"	5:C:93:TYR:CE2	2.52	0.44
1:X:1281:A:H2'	1:X:1282:A:O4'	2.18	0.44
1:X:1459:U:N3	1:X:1475:U:O2	2.50	0.44
1:X:1645:U:H2'	1:X:1646:G:O4'	2.17	0.44
1:X:2034:A:H4'	4:B:141:ILE:HB	1.99	0.44
1:X:2324:G:H1'	1:X:2360:C:H2'	1.99	0.44
1:X:2367:A:C8	1:X:2368:G:C5	3.06	0.44
1:X:2522:G:H2'	1:X:2523:G:H8	1.82	0.44
4:B:47:VAL:O	4:B:80:GLU:HA	2.17	0.44
4:B:84:PHE:CD1	4:B:86:PRO:HD3	2.52	0.44
11:J:6:LYS:HG3	11:J:7:ARG:H	1.82	0.44
11:J:17:ARG:CB	11:J:42:TRP:HZ2	2.30	0.44
11:J:99:LYS:HE3	11:J:100:PRO:HD2	1.99	0.44
12:K:10:LEU:HD23	12:K:10:LEU:HA	1.63	0.44
16:O:42:GLY:C	16:O:44:GLN:H	2.21	0.44
16:O:50:ASP:O	16:O:53:LYS:HB2	2.17	0.44
26:1:21:TYR:CG	26:1:42:PRO:HB3	2.52	0.44
1:X:105:G:C6	1:X:106:G:N7	2.86	0.44
1:X:923:A:C6	11:J:12:LYS:HD2	2.53	0.44
1:X:971:A:H2'	1:X:973:U:H5'	2.00	0.44
1:X:1774:A:C2	1:X:2566:A:C4	3.05	0.44
1:X:1776:A:N7	1:X:1778:U:C4	2.85	0.44
1:X:2044:G:O4'	1:X:2482:A:C6	2.70	0.44
1:X:2302:G:H2'	1:X:2303:C:O4'	2.18	0.44
1:X:2395:C:OP1	10:I:57:ILE:HA	2.17	0.44
1:X:2434:G:C4	1:X:2435:C:C5	3.06	0.44
1:X:2474:G:H2'	1:X:2475:C:O4'	2.17	0.44
1:X:2563:U:H6	1:X:2563:U:O5'	2.00	0.44
3:A:160:GLY:H	3:A:196:VAL:HB	1.82	0.44
5:C:72:ARG:HD2	5:C:77:PHE:HE2	1.82	0.44
7:E:9:ILE:HD13	7:E:9:ILE:N	2.32	0.44
14:M:29:PRO:CG	14:M:99:VAL:HG11	2.48	0.44
22:U:63:SER:HB2	22:U:66:ALA:H	1.81	0.44
1:X:249:A:H8	1:X:278:G:H21	1.65	0.44
1:X:595:A:H4'	5:C:84:PHE:HE2	1.83	0.44
1:X:853:C:C2	1:X:950:G:N1	2.86	0.44
1:X:1050:G:H2'	1:X:1051:U:C6	2.52	0.44
1:X:1271:C:H2'	1:X:1272:G:O4'	2.17	0.44



A + 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:1411:C:H2'	1:X:1412:C:C6	2.52	0.44
1:X:1650:A:C6	1:X:1652:G:C4	3.06	0.44
1:X:1846:A:H62	1:X:1871:G:H8	1.65	0.44
1:X:1880:G:H2'	1:X:1881:U:C6	2.52	0.44
1:X:1947:G:HO2'	1:X:1950:C:P	2.40	0.44
1:X:2269:G:H2'	1:X:2270:U:C6	2.52	0.44
1:X:2447:G:H22	1:X:2460:G:H2'	1.82	0.44
1:X:2447:G:N2	1:X:2460:G:H2'	2.32	0.44
1:X:2514:G:H2'	1:X:2515:G:H8	1.83	0.44
1:X:2794:G:H2'	1:X:2796:A:N7	2.32	0.44
2:Y:25:G:C2	2:Y:26:G:O6	2.70	0.44
4:B:103:ASP:OD1	4:B:168:GLN:HA	2.17	0.44
6:D:40:LEU:HD11	6:D:53:ALA:CB	2.46	0.44
6:D:148:LYS:HD2	6:D:148:LYS:O	2.18	0.44
11:J:35:LEU:O	11:J:103:VAL:HG23	2.17	0.44
12:K:9:LYS:H	12:K:9:LYS:HG2	1.40	0.44
13:L:21:THR:O	13:L:24:SER:HB3	2.16	0.44
14:M:29:PRO:HA	14:M:54:VAL:O	2.17	0.44
15:N:61:TRP:O	15:N:65:ILE:HG13	2.17	0.44
19:R:25:LEU:HG	19:R:81:VAL:CG2	2.47	0.44
19:R:25:LEU:HB2	19:R:79:SER:O	2.18	0.44
19:R:98:ILE:HG23	19:R:100:ASP:H	1.81	0.44
20:S:37:LYS:HD3	20:S:38:ALA:H	1.82	0.44
21:T:73:GLY:O	21:T:76:ALA:HB3	2.18	0.44
27:2:1:MET:HE2	27:2:3:ARG:HH12	1.81	0.44
1:X:193:A:C8	1:X:445:A:C6	3.05	0.44
1:X:480:G:OP1	5:C:54:THR:HA	2.18	0.44
1:X:571:U:O2'	1:X:581:A:H8	2.01	0.44
1:X:640:C:H4'	1:X:660:G:N2	2.26	0.44
1:X:832:A:OP2	1:X:1201:G:N2	2.50	0.44
1:X:1376:C:C2'	1:X:1377:G:H5'	2.48	0.44
1:X:1476:G:H2'	1:X:1477:C:H6	1.82	0.44
1:X:1515:U:C2	1:X:1516:A:C8	3.05	0.44
1:X:1709:U:H2'	1:X:1711:C:C4	2.53	0.44
1:X:2364:C:OP2	1:X:2364:C:H4'	2.18	0.44
1:X:2385:U:H5"	1:X:2387:U:OP2	2.18	0.44
1:X:2563:U:O2'	1:X:2564:U:O2	2.26	0.44
1:X:2845:C:O2'	1:X:2846:G:H5'	2.17	0.44
1:X:2864:C:C2	1:X:2865:G:C8	3.06	0.44
29:X:2901:MIV:H22	29:X:2901:MIV:H9	1.66	0.44
4:B:15:TRP:CE2	4:B:20:ALA:HB2	2.52	0.44


A 4 amo 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
5:C:164:VAL:HG12	5:C:166:TRP:H	1.83	0.44
9:H:1:MET:HG2	9:H:44:TYR:CG	2.53	0.44
11:J:42:TRP:HZ3	11:J:75:VAL:HG21	1.83	0.44
13:L:32:TYR:O	13:L:34:SER:OG	2.28	0.44
14:M:13:LEU:HD13	14:M:13:LEU:HA	1.83	0.44
1:X:95:G:H2'	1:X:96:C:H6	1.83	0.44
1:X:693:A:C6	1:X:811:G:N1	2.86	0.44
1:X:848:A:C4	1:X:849:G:C8	3.06	0.44
1:X:891:A:H2'	1:X:911:A:C2	2.52	0.44
1:X:931:G:C6	1:X:932:G:C5	3.05	0.44
1:X:1033:G:H4'	1:X:1034:U:H5'	2.00	0.44
1:X:1344:C:H2'	1:X:1346:C:C5	2.52	0.44
1:X:1586:A:C6	1:X:1587:A:C6	3.06	0.44
1:X:1739:G:C6	1:X:1740:G:C5	3.06	0.44
1:X:1890:G:N2	1:X:1891:C:O3'	2.42	0.44
1:X:2595:C:H2'	1:X:2596:C:C6	2.51	0.44
1:X:2661:G:N3	4:B:22:PRO:HB3	2.32	0.44
1:X:2727:G:O6	1:X:2735:C:H5"	2.16	0.44
8:G:67:ARG:NH2	8:G:76:GLN:HB3	2.32	0.44
11:J:54:VAL:HG21	11:J:121:LEU:HB3	2.00	0.44
16:O:87:ARG:HH11	16:O:87:ARG:HB3	1.82	0.44
19:R:24:VAL:HB	19:R:29:HIS:O	2.18	0.44
1:X:494:A:H4'	19:R:58:VAL:N	2.33	0.44
1:X:1192:A:H2'	1:X:1193:G:C8	2.53	0.44
1:X:1437:A:H2'	1:X:1438:G:H8	1.82	0.44
1:X:1468:A:H5'	1:X:1472:C:N4	2.32	0.44
1:X:1573:G:O5'	1:X:1574:A:H5"	2.18	0.44
1:X:1975:G:O2'	1:X:1980:A:N6	2.51	0.44
1:X:2000:U:O2	25:Z:10:LYS:HB2	2.17	0.44
1:X:2010:G:C2	1:X:2020:G:C5	3.06	0.44
1:X:2262:C:C5	1:X:2368:G:C4	3.05	0.44
1:X:2407:G:H4'	1:X:2408:G:C4	2.53	0.44
1:X:2526:U:H2'	1:X:2527:G:H8	1.83	0.44
1:X:2641:A:H2'	1:X:2642:G:O4'	2.17	0.44
2:Y:19:C:H2'	2:Y:20:A:O4'	2.18	0.44
3:A:28:ARG:NE	3:A:29:PRO:HD3	2.32	0.44
5:C:39:ARG:HG3	5:C:40:ARG:N	2.33	0.44
5:C:116:LYS:HB2	5:C:116:LYS:HE2	1.86	0.44
9:H:24:VAL:HG11	9:H:42:LYS:HG2	2.00	0.44
14:M:97:GLY:HA3	14:M:117:ILE:HD11	1.99	0.44
15:N:95:LEU:HD22	15:N:95:LEU:N	2.32	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
19:R:22:VAL:HG22	19:R:82:ALA:O	2.17	0.44
1:X:319:G:N7	17:P:12:LYS:NZ	2.66	0.44
1:X:582:G:H5'	1:X:584:A:N7	2.33	0.44
1:X:761:G:O5'	17:P:110:ALA:HB2	2.18	0.44
1:X:836:G:C4	1:X:837:U:C5	3.05	0.44
1:X:1806:G:H5"	1:X:1807:A:H2'	1.99	0.44
1:X:2066:G:H2'	1:X:2067:U:O4'	2.18	0.44
1:X:2252:A:O2'	1:X:2253:A:H5'	2.18	0.44
1:X:2300:G:H3'	1:X:2300:G:N3	2.32	0.44
2:Y:77:G:O3'	20:S:32:PHE:CZ	2.71	0.44
6:D:26:MET:CE	6:D:30:ARG:HH22	2.31	0.44
9:H:26:ASN:HB3	9:H:38:GLY:HA3	2.00	0.44
11:J:135:ARG:HA	11:J:138:TYR:CE1	2.53	0.44
13:L:95:LYS:HG2	13:L:96:TYR:N	2.33	0.44
14:M:57:ILE:H	14:M:57:ILE:HG13	1.72	0.44
16:O:19:VAL:HG13	16:O:90:PHE:CD1	2.52	0.44
18:Q:15:LYS:HA	18:Q:15:LYS:HD2	1.82	0.44
1:X:321:A:C6	1:X:341:A:C6	3.05	0.43
1:X:498:C:O2'	17:P:73:ASN:HB3	2.17	0.43
1:X:654:A:H2'	1:X:654:A:N3	2.32	0.43
1:X:659:G:H1'	28:3:46:LYS:NZ	2.33	0.43
1:X:759:C:C6	1:X:759:C:C3'	3.01	0.43
1:X:1448:A:C6	1:X:1576:G:C2	3.06	0.43
1:X:1607:A:H2'	1:X:1608:U:H6	1.83	0.43
1:X:1695:U:H3'	1:X:1696:C:H6	1.83	0.43
1:X:1772:C:H3'	1:X:1772:C:OP2	2.18	0.43
1:X:2367:A:N7	1:X:2368:G:C6	2.86	0.43
1:X:2408:G:H5'	1:X:2409:A:OP1	2.18	0.43
1:X:2659:C:N3	1:X:2660:C:C5	2.86	0.43
3:A:222:ARG:NH2	3:A:224:SER:HB2	2.33	0.43
5:C:56:ARG:HD3	5:C:57:LYS:O	2.18	0.43
5:C:155:GLU:HA	5:C:158:ARG:HG2	2.00	0.43
7:E:30:LYS:HD2	7:E:30:LYS:HA	1.91	0.43
11:J:29:ALA:O	11:J:31:GLY:N	2.45	0.43
17:P:30:TYR:CD1	17:P:123:HIS:HE1	2.36	0.43
17:P:59:PHE:CD1	25:Z:30:LEU:HD21	2.52	0.43
19:R:10:HIS:HB2	19:R:44:GLN:NE2	2.33	0.43
26:1:54:LYS:HE2	26:1:54:LYS:HB2	1.50	0.43
1:X:571:U:HO2'	1:X:581:A:H8	1.64	0.43
1:X:700:C:H2'	1:X:701:U:O4'	2.18	0.43
1:X:717:G:N3	1:X:739:G:C2	2.87	0.43



Atom 1	Atom-2	Interatomic	Clash
Atom-1		distance $(\text{\AA})$	overlap (Å)
1:X:764:A:O2'	29:X:2901:MIV:H341	2.18	0.43
1:X:1046:U:H2'	1:X:1047:G:C8	2.54	0.43
1:X:1055:A:HO2'	1:X:1122:A:H61	1.66	0.43
1:X:1154:A:OP2	1:X:1154:A:H8	2.01	0.43
1:X:1264:C:H5"	15:N:13:ARG:CZ	2.48	0.43
1:X:1584:G:N7	3:A:28:ARG:NH2	2.52	0.43
1:X:2291:U:H2'	1:X:2292:C:H6	1.82	0.43
1:X:2495:G:C6	1:X:2548:G:C2	3.06	0.43
1:X:2843:A:H3'	1:X:2844:G:H8	1.81	0.43
2:Y:117:G:O2'	13:L:53:ALA:HB2	2.18	0.43
5:C:61:GLN:NE2	5:C:61:GLN:O	2.50	0.43
5:C:149:LEU:HB2	5:C:183:HIS:ND1	2.32	0.43
14:M:44:ARG:CZ	14:M:44:ARG:HB2	2.38	0.43
17:P:53:ALA:O	17:P:57:LEU:HB2	2.18	0.43
20:S:154:LEU:HB3	20:S:158:CYS:HB2	2.00	0.43
1:X:64:C:H1'	18:Q:68:PHE:HD2	1.82	0.43
1:X:748:A:H3'	1:X:749:C:C6	2.53	0.43
1:X:794:A:H2	1:X:1767:G:N3	2.17	0.43
1:X:1193:G:C4	1:X:1194:U:C5	3.07	0.43
1:X:2022:C:P	8:G:137:LYS:HD3	2.58	0.43
1:X:2040:A:C6	1:X:2041:A:C6	3.07	0.43
1:X:2060:A:C5	1:X:2414:A:C5	3.06	0.43
1:X:2235:G:N2	1:X:2254:C:C4	2.87	0.43
1:X:2526:U:C6	1:X:2545:A:C5	3.06	0.43
1:X:2716:G:C6	1:X:2749:A:C2	3.07	0.43
5:C:3:GLN:HG3	5:C:12:GLY:HA2	1.99	0.43
6:D:10:ASP:HA	6:D:13:ARG:CZ	2.48	0.43
8:G:136:PRO:O	8:G:141:GLY:HA3	2.18	0.43
22:U:68:ARG:O	22:U:72:LYS:HG2	2.18	0.43
23:V:14:PHE:H	23:V:14:PHE:HD1	1.65	0.43
1:X:82:G:C2	1:X:100:G:N3	2.87	0.43
1:X:669:G:H2'	1:X:670:U:C6	2.54	0.43
1:X:746:G:O6	1:X:774[B]:A:H2'	2.18	0.43
1:X:913:A:C5	1:X:914:C:C5	3.06	0.43
1:X:957:G:H2'	1:X:958:G:C8	2.49	0.43
1:X:1172:U:O5'	1:X:1172:U:H6	2.02	0.43
1:X:1197:U:H2'	1:X:1198:C:C6	2.54	0.43
1:X:1405:A:H2'	1:X:1406:A:C8	2.53	0.43
1:X:1790:G:H4'	1:X:1791:C:O5'	2.17	0.43
1:X:1935:A:H1'	1:X:2539:C:O2'	2.17	0.43
1:X:2050:G:O2'	1:X:2052:G:H5"	2.18	0.43



A . 1	A.L. D.	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:2245:A:H1'	1:X:2251:U:O4	2.19	0.43
4:B:11:MET:HG3	4:B:24:THR:OG1	2.18	0.43
5:C:59:TYR:HD1	5:C:60:GLY:N	2.16	0.43
8:G:34:PRO:CD	8:G:70:PHE:HB3	2.48	0.43
13:L:105:ASP:O	13:L:109:GLU:HB2	2.19	0.43
15:N:6:THR:O	15:N:9:VAL:HG23	2.19	0.43
17:P:45:ILE:HD11	17:P:57:LEU:CG	2.45	0.43
18:Q:20:MET:HG3	18:Q:25:TYR:CD1	2.53	0.43
28:3:5:LYS:HB3	28:3:59:LYS:O	2.18	0.43
1:X:501:G:H2'	1:X:502:A:O4'	2.19	0.43
1:X:1333:G:N2	1:X:1344:C:N4	2.67	0.43
1:X:1474:A:H2'	1:X:1474:A:N3	2.34	0.43
1:X:1672:A:C2	1:X:1673:C:H1'	2.53	0.43
1:X:1696:C:C4	1:X:1697:U:C5	3.06	0.43
1:X:1788:C:H2'	1:X:1789:U:C6	2.54	0.43
1:X:1838:G:C2'	1:X:1839:A:H5'	2.48	0.43
1:X:1919:A:C8	1:X:1928:G:O6	2.71	0.43
1:X:2225:G:C6	1:X:2405:A:C8	3.06	0.43
1:X:2323:U:O5'	1:X:2323:U:H6	2.02	0.43
1:X:2768:C:H2'	1:X:2769:C:O4'	2.18	0.43
3:A:156:ALA:HB2	3:A:163:VAL:HG23	2.00	0.43
6:D:109:PRO:HB3	6:D:137:ILE:O	2.18	0.43
9:H:2:ILE:HA	9:H:2:ILE:HD13	1.66	0.43
15:N:79:PHE:CE2	15:N:110:VAL:HG22	2.53	0.43
17:P:67:PRO:O	17:P:71:VAL:HG23	2.18	0.43
18:Q:50:VAL:HG13	18:Q:80:VAL:HG23	2.00	0.43
22:U:20:ARG:HG2	22:U:43:ARG:NH2	2.33	0.43
25:Z:57:VAL:HG22	25:Z:58:LEU:HD13	2.00	0.43
1:X:102:C:H2'	1:X:103:U:O4'	2.18	0.43
1:X:312:G:C6	1:X:328:A:C6	3.06	0.43
1:X:588:G:N2	1:X:1275:A:C4	2.86	0.43
1:X:592:G:N1	1:X:593:C:C4	2.86	0.43
1:X:874:A:H3'	1:X:875:G:H8	1.83	0.43
1:X:1599:G:H2'	1:X:1600:U:O4'	2.18	0.43
1:X:1672:A:O4'	4:B:113:THR:HG22	2.17	0.43
1:X:1823:G:C6	1:X:1958:G:C6	3.07	0.43
1:X:1832:G:C6	1:X:1833:U:C4	3.06	0.43
1:X:1835:C:H2'	1:X:1836:C:H6	1.82	0.43
1:X:2528:G:C2	1:X:2529:G:C5	3.07	0.43
2:Y:3:A:C4	2:Y:4:C:C5	3.07	0.43
7:E:17:VAL:HG13	7:E:24:PHE:HD2	1.84	0.43



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
9:H:13:ASN:HD21	9:H:109:ARG:N	2.16	0.43
9:H:55:VAL:HG12	9:H:66:ALA:HA	1.99	0.43
12:K:28:LEU:CD1	12:K:115:LEU:HD21	2.46	0.43
16:O:35:LEU:CD2	16:O:52:GLY:HA2	2.48	0.43
17:P:29:LYS:HG2	17:P:123:HIS:CD2	2.54	0.43
17:P:59:PHE:CG	25:Z:30:LEU:HD21	2.54	0.43
1:X:330:C:H2'	1:X:331:U:C6	2.54	0.43
1:X:590:C:H2'	1:X:591:G:H8	1.83	0.43
1:X:650:U:H2'	1:X:651:C:C5	2.54	0.43
1:X:922:A:H2'	1:X:923:A:C8	2.54	0.43
1:X:994:A:HO2'	1:X:995:A:P	2.41	0.43
1:X:1357:U:H4'	1:X:1397:A:C6	2.54	0.43
1:X:1464:A:H61	1:X:1477:C:H42	1.66	0.43
1:X:1833:U:H2'	1:X:1834:G:H8	1.84	0.43
1:X:1839:A:H5"	1:X:1840:A:OP1	2.19	0.43
1:X:2284:U:H1'	6:D:151:GLY:CA	2.46	0.43
1:X:2315:A:H2	1:X:2364:C:O2	2.02	0.43
1:X:2690:A:OP1	1:X:2692:A:OP1	2.36	0.43
2:Y:11:G:OP1	13:L:16:LYS:HD3	2.18	0.43
7:E:84:THR:HA	7:E:133:VAL:O	2.18	0.43
9:H:7:ARG:HA	9:H:20:MET:HA	1.99	0.43
9:H:21:CYS:SG	9:H:22:ILE:N	2.91	0.43
11:J:123:GLY:O	11:J:126:LEU:HB2	2.19	0.43
15:N:95:LEU:CD2	16:O:5:ILE:HG12	2.48	0.43
19:R:85:ASP:OD1	19:R:86:PRO:HD2	2.19	0.43
1:X:242:A:H61	1:X:440:U:HO2'	1.54	0.43
1:X:393:U:O2'	22:U:18:VAL:HB	2.19	0.43
1:X:465:C:O2'	1:X:467:U:O2'	2.24	0.43
1:X:486:U:H2'	1:X:487:G:O4'	2.18	0.43
1:X:1012:A:C8	1:X:1013:G:C8	3.07	0.43
1:X:1473:U:H6	1:X:1473:U:H2'	1.68	0.43
1:X:2550:C:N4	1:X:2553:G:C8	2.87	0.43
2:Y:80:A:H2'	2:Y:81:C:O4'	2.18	0.43
14:M:110:LEU:HA	14:M:110:LEU:HD23	1.68	0.43
1:X:3:U:H2'	1:X:4:C:H6	1.83	0.43
1:X:148:C:O2'	1:X:149:A:OP1	2.31	0.43
1:X:441:A:H3'	1:X:442:A:H8	1.84	0.43
1:X:541:C:N3	1:X:572:G:C8	2.87	0.43
1:X:592:G:OP2	15:N:10:ARG:HD2	2.18	0.43
1:X:869:C:H2'	1:X:870:C:C6	2.54	0.43
1:X:1149:G:H5"	8:G:51:LEU:HD23	2.01	0.43



A + 1	At and 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:1501:C:H2'	1:X:1502:G:O4'	2.18	0.43
1:X:1742:G:O2'	1:X:1743:C:H5'	2.18	0.43
1:X:1831:G:C6	1:X:1910:A:C2	3.07	0.43
1:X:1981:A:H4'	1:X:2704:U:O2'	2.19	0.43
1:X:2057:U:C2	1:X:2415:G:C2	3.06	0.43
1:X:2068:C:O3'	3:A:260:ARG:NH2	2.52	0.43
1:X:2222:U:H2'	1:X:2223:U:H6	1.82	0.43
1:X:2728:A:C6	1:X:2729:A:C6	3.06	0.43
1:X:2795:A:H2'	4:B:191:ALA:HB2	2.01	0.43
31:X:3168:SPD:H52	31:X:3168:SPD:H21	1.57	0.43
2:Y:3:A:C6	2:Y:4:C:C4	3.07	0.43
7:E:25:LYS:HA	7:E:34:THR:HG22	2.01	0.43
8:G:30:LYS:HA	8:G:30:LYS:HD2	1.79	0.43
8:G:75:ILE:HG13	8:G:147:ARG:NH2	2.34	0.43
9:H:104:GLU:OE1	9:H:125:LYS:HG3	2.19	0.43
17:P:38:VAL:HG12	17:P:97:VAL:HG21	2.00	0.43
28:3:48:PHE:N	28:3:48:PHE:CD1	2.87	0.43
1:X:57:G:C2	1:X:69:G:C2	3.07	0.43
1:X:165:G:H1'	1:X:1378:A:C6	2.54	0.43
1:X:524:A:H2'	1:X:525:A:O4'	2.19	0.43
1:X:529:U:H2'	1:X:530:G:C8	2.52	0.43
1:X:717:G:N2	1:X:739:G:C4	2.87	0.43
1:X:719:A:C3'	1:X:720:A:H8	2.31	0.43
1:X:1057:A:H5'	1:X:1058:G:OP2	2.19	0.43
1:X:1673:C:H2'	1:X:1674:C:H6	1.83	0.43
1:X:1685:A:N6	1:X:1976:U:C5	2.87	0.43
1:X:1811:A:H2'	3:A:178:PRO:HB2	2.01	0.43
1:X:2311:U:H4'	1:X:2315:A:H62	1.82	0.43
1:X:2394:G:H4'	10:I:58:ALA:O	2.18	0.43
1:X:2426:G:O2'	1:X:2479:U:OP2	2.23	0.43
1:X:2791:C:C2	1:X:2806:G:N2	2.87	0.43
2:Y:96:C:H2'	2:Y:97:C:H6	1.84	0.43
3:A:29:PRO:O	3:A:30:GLU:HB2	2.18	0.43
3:A:221:GLN:HE21	3:A:221:GLN:HB3	1.48	0.43
6:D:67:ILE:H	6:D:67:ILE:HG13	1.57	0.43
9:H:2:ILE:HG13	9:H:8:LEU:HD21	2.00	0.43
18:Q:53:ILE:HD12	18:Q:79:ILE:O	2.18	0.43
27:2:34:ARG:HH11	27:2:42:LEU:HA	1.82	0.43
1:X:332:C:OP1	5:C:129:LYS:NZ	2.41	0.42
1:X:543:G:C4	1:X:544:U:C5	3.07	0.42
1:X:753:U:N3	1:X:754:G:N7	2.67	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:781:G:N2	1:X:1392:U:H1'	2.34	0.42
1:X:799:C:O2'	1:X:800:U:H5'	2.18	0.42
1:X:867:G:H2'	1:X:868:U:C6	2.53	0.42
1:X:875:G:O6	1:X:928:G:N2	2.52	0.42
1:X:884:C:H2'	1:X:885:A:H8	1.84	0.42
1:X:967:G:N2	1:X:970:A:H3'	2.33	0.42
1:X:1806:G:OP2	1:X:1807:A:O2'	2.16	0.42
1:X:1810:U:H3'	3:A:157:ARG:HG3	2.01	0.42
1:X:1832:G:C5	1:X:1833:U:C5	3.06	0.42
1:X:1980:A:H5"	4:B:117:MET:HE1	2.01	0.42
1:X:1991:C:C2	1:X:1992:G:C8	3.07	0.42
1:X:2047:C:H1'	1:X:2429:A:C2	2.54	0.42
1:X:2337:A:C6	1:X:2338:C:C2	3.07	0.42
1:X:2348:A:H2'	1:X:2349:G:C8	2.54	0.42
1:X:2629:U:C2	1:X:2630:C:C6	3.07	0.42
1:X:2661:G:C6	1:X:2662:C:C4	3.07	0.42
1:X:2799:C:H2'	1:X:2800:C:H6	1.84	0.42
31:X:3171:SPD:H41	31:X:3171:SPD:H72	1.66	0.42
4:B:19:ARG:HG2	9:H:84:ALA:HB1	2.01	0.42
5:C:6:VAL:HB	5:C:7:ILE:H	1.54	0.42
20:S:72:ASP:HB3	20:S:75:LYS:O	2.18	0.42
22:U:46:LEU:HB2	22:U:47:HIS:H	1.63	0.42
27:2:41:GLN:O	27:2:42:LEU:HB3	2.19	0.42
1:X:30:G:C2	1:X:521:U:O2	2.72	0.42
1:X:79:G:H2'	1:X:80:A:H8	1.84	0.42
1:X:575:U:H4'	1:X:822:G:OP2	2.19	0.42
1:X:711:C:O2'	1:X:747:A:N6	2.52	0.42
1:X:1082:G:H3'	1:X:1083:C:H6	1.83	0.42
1:X:1378:A:P	22:U:7:LEU:HD23	2.59	0.42
1:X:1489:C:H5"	1:X:1490:U:OP2	2.19	0.42
1:X:1596:A:H2'	1:X:1597:A:O4'	2.20	0.42
1:X:2053:G:C2	1:X:2421:C:C2	3.07	0.42
1:X:2238:G:C8	1:X:2406:C:C5	3.08	0.42
1:X:2634:G:HO2'	1:X:2643:G:H1	1.67	0.42
3:A:148:VAL:HG22	3:A:149:PRO:HD2	2.02	0.42
5:C:24:SER:HB3	10:I:7:LYS:H	1.84	0.42
7:E:95:ARG:HB2	7:E:106:ASN:HB3	2.01	0.42
11:J:50:ALA:O	11:J:54:VAL:HG12	2.19	0.42
13:L:98:GLY:HA2	13:L:101:LYS:HB3	2.01	0.42
17:P:17:GLN:HG2	17:P:17:GLN:H	1.60	0.42
1:X:16:G:N1	1:X:535:U:C2	2.88	0.42



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:X:40:U:C2	1:X:41:G:C8	3.06	0.42
1:X:338:G:C2	1:X:347:C:C2	3.08	0.42
1:X:518:A:N6	17:P:30:TYR:CG	2.87	0.42
1:X:540:G:N1	1:X:2005:U:OP1	2.52	0.42
1:X:545:C:C2	1:X:546:A:C8	3.07	0.42
1:X:648:A:OP1	10:I:103:ASN:HB2	2.19	0.42
1:X:654:A:H2'	1:X:655:A:C5'	2.50	0.42
1:X:792:U:OP1	3:A:49:ILE:HG13	2.19	0.42
1:X:1071:U:H4'	1:X:1072:U:H3'	2.02	0.42
1:X:1134:C:H2'	1:X:1135:C:H6	1.85	0.42
1:X:1321:A:H3'	1:X:1322:G:C8	2.55	0.42
1:X:1377:G:C8	22:U:6:TYR:N	2.87	0.42
1:X:1745:C:H2'	1:X:1746:A:O4'	2.19	0.42
1:X:1752:U:H2'	1:X:1753:A:H5'	2.01	0.42
1:X:1886:G:H2'	1:X:1887:G:C8	2.54	0.42
1:X:2035:G:OP1	4:B:141:ILE:N	2.51	0.42
1:X:2306:A:O2'	1:X:2307:A:O5'	2.34	0.42
1:X:2644:A:C2	1:X:2645:C:C6	3.08	0.42
1:X:2837:G:C5	1:X:2838:U:C5	3.07	0.42
1:X:2855:C:O2'	12:K:90:ARG:NH1	2.52	0.42
3:A:43:ARG:CZ	3:A:49:ILE:HG12	2.49	0.42
3:A:108:PRO:CB	3:A:127:LEU:HD11	2.48	0.42
5:C:18:PRO:HB2	5:C:19:LEU:H	1.64	0.42
8:G:124:GLU:H	8:G:124:GLU:HG3	1.46	0.42
9:H:132:GLU:HB2	14:M:73:PHE:CE2	2.55	0.42
18:Q:6:ILE:HD13	18:Q:6:ILE:HA	1.93	0.42
1:X:494:A:H8	19:R:56:LYS:HG3	1.84	0.42
1:X:774[B]:A:H8	1:X:774[B]:A:O5'	2.02	0.42
1:X:817:A:H5"	1:X:818:G:OP1	2.20	0.42
1:X:846:A:H2'	1:X:847:C:C6	2.54	0.42
1:X:986:A:H1'	1:X:1001:A:C2	2.53	0.42
1:X:1195:U:H2'	1:X:1196:G:H8	1.84	0.42
1:X:1628:C:C4	1:X:1629:G:C8	3.07	0.42
3:A:63:ARG:NH2	3:A:65:ILE:HD11	2.34	0.42
4:B:141:ILE:HG21	4:B:141:ILE:HD13	1.75	0.42
7:E:169:ILE:HD13	7:E:170:ALA:H	1.85	0.42
13:L:36:LYS:O	13:L:38:ILE:HG22	2.19	0.42
14:M:55:ILE:O	14:M:103:LYS:O	2.37	0.42
17:P:33:MET:HE1	17:P:64:ALA:HA	2.01	0.42
18:Q:32:LYS:H	18:Q:32:LYS:HG2	1.56	0.42
19:R:9:HIS:CD2	19:R:9:HIS:N	2.87	0.42



A 4 amo 1	At any 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
20:S:76:ARG:HB3	20:S:76:ARG:HH11	1.83	0.42
23:V:40:PRO:O	23:V:43:VAL:HB	2.20	0.42
28:3:38:GLY:HA2	28:3:41:ILE:HG22	2.00	0.42
1:X:28:A:C4	1:X:523:A:C5	3.07	0.42
1:X:314:G:H2'	1:X:315:G:C8	2.53	0.42
1:X:533:C:H2'	1:X:534:U:O4'	2.19	0.42
1:X:567:G:H5"	8:G:140:GLN:NE2	2.35	0.42
1:X:617:U:H3'	1:X:617:U:O2	2.20	0.42
1:X:834:A:H8	1:X:834:A:O5'	2.03	0.42
1:X:888:G:H4'	20:S:167:THR:HG21	2.02	0.42
1:X:1158:A:H2'	1:X:1159:U:C6	2.54	0.42
1:X:1610:A:H2'	1:X:1611:U:C6	2.55	0.42
1:X:1623:C:H4'	1:X:1624:A:C5'	2.49	0.42
1:X:1655:C:H4'	1:X:2689:C:O2	2.18	0.42
1:X:1980:A:H5"	4:B:117:MET:HE3	2.01	0.42
1:X:2030:U:O2'	1:X:2031:A:H5'	2.19	0.42
1:X:2707:G:C4	1:X:2708:U:C5	3.07	0.42
1:X:2837:G:C6	1:X:2838:U:C4	3.07	0.42
5:C:193:LEU:O	5:C:193:LEU:HD23	2.19	0.42
9:H:5:GLN:HA	9:H:20:MET:HE2	2.01	0.42
9:H:121:ARG:HB2	9:H:123:PHE:CD1	2.54	0.42
11:J:6:LYS:HA	11:J:71:PRO:HG2	2.02	0.42
17:P:79:ALA:O	17:P:85:MET:HB2	2.20	0.42
18:Q:64:ARG:HB2	18:Q:69:ILE:HA	2.01	0.42
19:R:64:ASN:CG	19:R:67:GLY:HA2	2.39	0.42
21:T:37:LEU:HD11	21:T:61:ALA:H	1.84	0.42
1:X:706:A:H2'	1:X:707:U:O4'	2.19	0.42
1:X:1032:A:C5	1:X:1034:U:C2	3.07	0.42
1:X:1163:C:O2'	15:N:76:TYR:HE1	2.01	0.42
1:X:1211:G:N3	1:X:1212:U:C5	2.88	0.42
1:X:1264:C:H5"	15:N:13:ARG:HH22	1.84	0.42
1:X:1439:G:HO2'	1:X:1440:G:P	2.43	0.42
1:X:1774:A:H5'	1:X:2587:G:H4'	2.02	0.42
1:X:2048:C:H2'	1:X:2049:C:C6	2.53	0.42
1:X:2055:G:H2'	1:X:2056:C:H6	1.85	0.42
1:X:2355:A:H2'	1:X:2356:A:O4'	2.19	0.42
1:X:2378:G:C6	1:X:2397:A:C6	3.08	0.42
1:X:2820:C:N3	1:X:2821:G:N7	2.67	0.42
2:Y:94:G:N2	2:Y:95:U:C2	2.88	0.42
6:D:63:GLN:OE1	6:D:95:ARG:NH2	2.53	0.42
6:D:158:THR:HG21	6:D:169:LEU:HD22	2.02	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
7:E:107:ILE:HG13	7:E:107:ILE:O	2.20	0.42
7:E:157:TYR:O	7:E:171:LEU:HD12	2.20	0.42
8:G:81:VAL:HG11	8:G:156:HIS:HD2	1.84	0.42
8:G:90:LEU:HB3	8:G:94:LYS:HB2	2.01	0.42
12:K:44:LEU:HA	12:K:44:LEU:HD12	1.69	0.42
12:K:99:ARG:HA	12:K:111:ALA:CB	2.49	0.42
13:L:8:ARG:HA	13:L:8:ARG:HD2	1.69	0.42
1:X:499:G:C2	1:X:503:G:O6	2.73	0.42
1:X:555:U:O2'	1:X:556:A:OP2	2.36	0.42
1:X:790:A:O2'	3:A:48:ARG:NH2	2.52	0.42
1:X:796:A:O3'	1:X:2567:G:H5"	2.19	0.42
1:X:1326:U:H5"	1:X:1327:C:OP2	2.19	0.42
1:X:1446:U:C4	1:X:1447:U:C4	3.08	0.42
1:X:1755:G:C6	1:X:1972:G:C2	3.08	0.42
1:X:1790:G:N2	1:X:1810:U:O2'	2.52	0.42
1:X:1996:A:C2	17:P:109:ARG:NH2	2.80	0.42
1:X:2035:G:OP1	4:B:141:ILE:HG22	2.20	0.42
1:X:2627:G:C5	1:X:2628:C:C5	3.08	0.42
29:X:2901:MIV:H72C	29:X:2901:MIV:H4	1.83	0.42
2:Y:70:C:C2	2:Y:71:G:C8	3.08	0.42
2:Y:85:G:C6	2:Y:86:A:C5	3.08	0.42
3:A:182:LEU:HD12	3:A:270:ILE:HG13	2.01	0.42
4:B:176:ARG:NE	14:M:16:ILE:HG22	2.31	0.42
7:E:12:PRO:HB2	7:E:13:SER:H	1.66	0.42
8:G:81:VAL:HG11	8:G:156:HIS:CD2	2.55	0.42
13:L:95:LYS:O	13:L:100:VAL:HG11	2.20	0.42
20:S:9:THR:N	20:S:10:PRO:HD3	2.35	0.42
1:X:161:U:H2'	1:X:162:C:C6	2.54	0.42
1:X:257:G:N2	1:X:263:G:O4'	2.53	0.42
1:X:507:A:C4	1:X:508:G:C8	3.08	0.42
1:X:598:U:H2'	1:X:599:A:C8	2.54	0.42
1:X:797:A:C6	3:A:229:VAL:HG21	2.55	0.42
1:X:969:U:H5	11:J:17:ARG:CB	2.33	0.42
1:X:1084:A:H3'	1:X:1085:G:C8	2.54	0.42
1:X:1134:C:H2'	1:X:1135:C:C6	2.55	0.42
1:X:1354:A:H1'	18:Q:54:SER:HB2	2.00	0.42
1:X:1573:G:C3'	1:X:1574:A:H5"	2.46	0.42
1:X:1659:G:C2'	1:X:1660:G:H5'	2.50	0.42
1:X:2043:A:C5	1:X:2481:G:C2	3.07	0.42
1:X:2293:G:H2'	1:X:2294:U:H6	1.81	0.42
1:X:2568:A:H2'	1:X:2569:A:H8	1.83	0.42



A., 1	A.L. D	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
6:D:100:LEU:HD12	6:D:100:LEU:HA	1.82	0.42
9:H:20:MET:O	9:H:20:MET:HG2	2.19	0.42
12:K:38:LEU:HD12	12:K:38:LEU:O	2.19	0.42
17:P:35:PRO:HB2	17:P:39:ARG:HH22	1.84	0.42
19:R:58:VAL:O	19:R:58:VAL:HG23	2.19	0.42
1:X:507:A:H2'	1:X:508:G:O4'	2.20	0.42
1:X:527:C:P	25:Z:13:LYS:HE2	2.60	0.42
1:X:773:G:H2'	1:X:774[B]:A:O4'	2.19	0.42
1:X:834:A:H1'	1:X:955:G:H5'	2.02	0.42
1:X:1030:U:C2	1:X:1155:G:N2	2.88	0.42
1:X:1039:A:H62	1:X:1136:G:H2'	1.85	0.42
1:X:1282:A:H2'	1:X:1283:C:C6	2.54	0.42
1:X:1506:C:C6	3:A:99:ASP:HB3	2.54	0.42
1:X:1673:C:O5'	1:X:1673:C:H6	2.03	0.42
1:X:1745:C:O2'	1:X:1746:A:H5'	2.19	0.42
1:X:1766:U:OP1	1:X:1962:C:O2'	2.38	0.42
1:X:1821:A:N6	1:X:1960:A:N6	2.68	0.42
1:X:2043:A:H3'	5:C:62:LYS:HZ1	1.85	0.42
1:X:2043:A:H3'	5:C:62:LYS:NZ	2.35	0.42
1:X:2086:U:H2'	1:X:2087:U:C5	2.55	0.42
1:X:2238:G:C8	1:X:2406:C:C4	3.08	0.42
1:X:2283:G:H1	1:X:2291:U:H3	1.66	0.42
1:X:2598:C:H2'	1:X:2599:U:H6	1.84	0.42
5:C:6:VAL:HG23	5:C:8:GLY:H	1.85	0.42
6:D:47:SER:HA	6:D:50:ILE:HD11	2.01	0.42
6:D:96:MET:HE2	6:D:97:TYR:HA	2.02	0.42
11:J:22:ALA:HB2	11:J:99:LYS:HB2	2.02	0.42
11:J:78:LYS:HB2	11:J:78:LYS:HE3	1.64	0.42
12:K:78:LYS:O	12:K:83:VAL:HG13	2.19	0.42
13:L:67:THR:O	13:L:71:VAL:HG23	2.20	0.42
14:M:31:ASP:OD1	14:M:117:ILE:HG21	2.19	0.42
20:S:112:LEU:H	20:S:112:LEU:HD12	1.84	0.42
25:Z:45:ILE:O	25:Z:45:ILE:HG13	2.19	0.42
1:X:389:G:H2'	1:X:390:U:C6	2.55	0.42
1:X:540:G:C6	1:X:2005:U:H5"	2.54	0.42
1:X:597:U:H2'	1:X:598:U:C6	2.55	0.42
1:X:890:U:O2'	1:X:891:A:OP1	2.31	0.42
1:X:1386:A:H5"	1:X:2191:A:H62	1.84	0.42
1:X:1807:A:O4'	1:X:1809:G:C8	2.73	0.42
1:X:2271:C:OP2	13:L:18:ARG:NH2	2.53	0.42
1:X:2323:U:O2'	1:X:2324:G:H3'	2.20	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:X:2323:U:HO2'	1:X:2324:G:H3'	1.84	0.42
1:X:2675:U:H2'	1:X:2676:G:C8	2.55	0.42
1:X:2746:G:H2'	1:X:2746:G:N3	2.35	0.42
9:H:105:PRO:HD3	9:H:125:LYS:HG2	2.02	0.42
10:I:118:VAL:HG13	10:I:122:VAL:HB	2.02	0.42
12:K:68:GLN:O	12:K:71:HIS:NE2	2.52	0.42
12:K:69:ASP:C	12:K:70:ILE:HG12	2.40	0.42
14:M:41:GLU:HG2	14:M:46:ARG:NH2	2.34	0.42
14:M:108:ARG:HH11	14:M:108:ARG:HD3	1.71	0.42
24:W:3:ILE:HG23	24:W:51:LEU:HD13	2.01	0.42
25:Z:58:LEU:H	25:Z:58:LEU:CD1	2.29	0.42
28:3:29:LYS:HG2	28:3:34:THR:HG23	2.01	0.42
28:3:58:MET:H	28:3:58:MET:HG2	1.46	0.42
1:X:15:G:C6	1:X:16:G:N7	2.88	0.41
1:X:83:A:C8	1:X:98:U:C4	3.08	0.41
1:X:425:A:N7	1:X:2391:A:H1'	2.35	0.41
1:X:478:G:OP1	27:2:33:ARG:NE	2.52	0.41
1:X:1069:G:C2	1:X:1092:U:C4	3.08	0.41
1:X:1385:C:C2	1:X:1386:A:C8	3.08	0.41
1:X:1399:C:H2'	1:X:1400:A:C8	2.53	0.41
1:X:2056:C:O2'	1:X:2057:U:H5'	2.20	0.41
1:X:2228:U:H4'	1:X:2254:C:H5	1.85	0.41
1:X:2338:C:H2'	1:X:2339:A:O4'	2.20	0.41
1:X:2596:C:C2	1:X:2597:G:C8	3.08	0.41
1:X:2724:G:C2	1:X:2725:C:C5	3.08	0.41
1:X:2805:G:O2'	1:X:2806:G:H5'	2.20	0.41
2:Y:47:A:C5	2:Y:48:A:N7	2.88	0.41
5:C:111:ARG:HD3	5:C:111:ARG:HA	1.83	0.41
7:E:147:ASN:HA	7:E:150:LYS:HE2	2.01	0.41
17:P:49:SER:HB3	17:P:52:ASP:OD2	2.20	0.41
20:S:95:SER:HA	20:S:121:GLN:HA	2.02	0.41
20:S:117:VAL:HG12	20:S:119:ASN:O	2.20	0.41
21:T:57:HIS:N	21:T:57:HIS:CD2	2.87	0.41
1:X:138:G:H2'	1:X:139:A:H8	1.85	0.41
1:X:763:A:C2	1:X:766:A:H1'	2.54	0.41
1:X:797:A:N7	1:X:805:G:C4	2.89	0.41
1:X:1076:U:C2	1:X:1085:G:N2	2.88	0.41
1:X:1284:G:C2	1:X:1633:C:H4'	2.55	0.41
1:X:1563:U:H2'	1:X:1564:U:H6	1.85	0.41
1:X:1684:G:C2	1:X:1974:U:C5	3.09	0.41
1:X:1701:C:H2'	1:X:1702:C:H6	1.81	0.41



Atom 1	Atom 2	Interatomic	Clash		
Atom-1	Atom-2 distance (Å)		overlap (Å)		
1:X:1817:U:O3'	3:A:233:HIS:CE1	2.71	0.41		
1:X:2290:A:H8	1:X:2291:U:C6	2.36	0.41		
1:X:2292:C:C2	1:X:2293:G:C8	3.08	0.41		
1:X:2356:A:H8	1:X:2356:A:OP2	2.03	0.41		
1:X:2544:A:N7	1:X:2545:A:C2	2.87	0.41		
1:X:2597:G:O3'	4:B:149:ARG:NH2	2.41	0.41		
1:X:2796:A:C2	1:X:2797:G:C5	3.07	0.41		
5:C:131:LYS:HA	5:C:134:ILE:HD12	2.00	0.41		
11:J:23:LYS:HA	20:S:73:LYS:NZ	2.34	0.41		
12:K:2:ARG:C	12:K:4:GLY:H	2.23	0.41		
18:Q:10:PRO:HD3	23:V:30:PHE:CD2	2.55	0.41		
18:Q:22:ARG:NH1	18:Q:24:VAL:HG11	2.35	0.41		
26:1:14:SER:O	26:1:22:TYR:HA	2.20	0.41		
1:X:15:G:H4'	25:Z:21:SER:HB2	2.03	0.41		
1:X:306:G:H2'	1:X:307:C:C6	2.55	0.41		
1:X:334:G:OP1	1:X:349:G:N2	2.53	0.41		
1:X:467:U:O2'	1:X:483:A:N6	2.53	0.41		
1:X:515:A:H2'	1:X:516:G:H5'	2.02	0.41		
1:X:575:U:OP1	10:I:28:LYS:NZ	2.49	0.41		
1:X:738:G:C6	1:X:739:G:N1 2.88		0.41		
1:X:1034:U:OP2	1:X:1036:G:O2'	2.32	0.41		
1:X:1993:G:P	17:P:62:ARG:NH1	2.93	0.41		
1:X:2000:U:H4'	25:Z:8:LYS:O	2.20	0.41		
1:X:2371:A:H2'	1:X:2372:A:O4'	2.20	0.41		
1:X:2395:C:C5'	10:I:57:ILE:HB	2.51	0.41		
1:X:2423:G:P	5:C:62:LYS:HD2	2.60	0.41		
1:X:2595:C:C2	1:X:2596:C:C5	3.08	0.41		
1:X:2737:A:H61	7:E:67:LEU:HG	1.85	0.41		
1:X:2792:C:C2	1:X:2805:G:C2	3.08	0.41		
5:C:137:ALA:HB1	5:C:142:LEU:HB2	2.02	0.41		
6:D:117:ILE:HD11	6:D:120:ASN:HD22	1.86	0.41		
7:E:83:TYR:CD2	7:E:138:LYS:HB2	2.56	0.41		
7:E:136:ILE:HG13	7:E:137:ASP:N	2.33	0.41		
18:Q:8:GLN:O	23:V:29:ARG:HD2	2.20	0.41		
18:Q:9:ALA:HB1	8:Q:9:ALA:HB1 23:V:33:ALA:HB2		0.41		
18:Q:11:VAL:HG22	18:Q:28:TRP:CE2	2.55	0.41		
1:X:83:A:C2	1:X:101:A:C4	3.08	0.41		
1:X:89:A:H4'	1:X:90:G:C5'	2.50	0.41		
1:X:181:A:OP1	1:X:183:U:H1'	2.21	0.41		
1:X:502:A:H2'	1:X:503:G:O4'	2.20	0.41		
1:X:773:G:HO2'	1:X:774[B]:A:P	2.43	0.41		



A 4 a ma 1	Atom 2 Interatomic		Clash	
Atom-1	Atom-2 distance (Å)		overlap (Å)	
1:X:888:G:H5"	20:S:146:HIS:CE1	2.55	0.41	
1:X:1056:U:OP1	1:X:1057:A:H5"	2.20	0.41	
1:X:1163:C:H2'	1:X:1164:C:H6	1.85	0.41	
1:X:1278:A:H61	1:X:1996:A:H5"	1.85	0.41	
1:X:1496:G:HO2'	1:X:1497:C:P	2.42	0.41	
1:X:1761:G:C6	1:X:1762:C:C4	3.08	0.41	
1:X:1933:G:H2'	1:X:1934:U:C6	2.55	0.41	
1:X:2043:A:N6	5:C:68:ARG:NH2	2.68	0.41	
1:X:2210:C:C4	1:X:2211:U:C4	3.08	0.41	
1:X:2794:G:C2	1:X:2803:C:C2	3.08	0.41	
1:X:2844:G:C6	1:X:2845:C:C4	3.08	0.41	
1:X:2851:G:O5'	14:M:8:ASN:HA	2.21	0.41	
2:Y:3:A:OP1	2:Y:3:A:H3'	2.21	0.41	
2:Y:70:C:H2'	2:Y:71:G:O4'	2.20	0.41	
3:A:85:ASP:CB	3:A:92:ILE:HD12	2.51	0.41	
3:A:176:ARG:HH21	3:A:182:LEU:HD21	1.86	0.41	
3:A:258:LYS:HZ3	3:A:264:LYS:HG2	1.85	0.41	
4:B:5:LEU:HD21	4:B:79:ARG:CG	2.48	0.41	
4:B:15:TRP:NE1	14:M:86:PRO:HD2	2.36	0.41	
4:B:101:LYS:HD2	4:B:169:ASN:O	2.21	0.41	
6:D:112:ARG:HA	6:D:112:ARG:NH2	2.35	0.41	
7:E:107:ILE:HD11	7:E:151:VAL:HG12	2.02	0.41	
11:J:85:GLY:O	11:J:86:LYS:HB2	2.20	0.41	
13:L:9:ARG:NH1	13:L:9:ARG:O	2.54	0.41	
16:O:6:GLN:O	16:O:8:GLY:N	2.53	0.41	
17:P:64:ALA:O	17:P:67:PRO:HD2	2.20	0.41	
18:Q:7:LEU:HB3	23:V:30:PHE:HZ	1.85	0.41	
19:R:64:ASN:OD1	19:R:67:GLY:HA2	2.21	0.41	
20:S:49:THR:OG1	20:S:132:GLN:HA	2.21	0.41	
22:U:62:LEU:HD12	22:U:62:LEU:HA	1.87	0.41	
23:V:26:MET:O	23:V:30:PHE:HD1	2.04	0.41	
1:X:23:G:H21	17:P:98:ASP:CG	2.24	0.41	
1:X:249:A:N7	1:X:279:A:H1'	2.35	0.41	
1:X:544:U:H3	1:X:568:G:H1	1.68	0.41	
1:X:552:C:O2'	1:X:553:C:H5'	2.20	0.41	
1:X:1245:G:C5	1:X:1246:G:N7	2.88	0.41	
1:X:1446:U:H2'	1446:U:H2' 1:X:1447:U:C6		0.41	
1:X:1482:U:H2'	1:X:1483:G:H8	1.85	0.41	
1:X:1574:A:H2'	1:X:1575:C:H5"	2.01	0.41	
1:X:1940:C:H2'	1:X:1941:C:C6	2.55	0.41	
1:X:1987:G:C6	1:X:1988:A:C4	3.09	0.41	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:X:2036:G:O3'	4:B:145:LYS:HD3	0.41		
1:X:2331:A:H2'	1:X:2332:G:O4'	2.20	0.41	
1:X:2528:G:H2'	1:X:2529:G:H8 1.85		0.41	
1:X:2553:G:H8	1:X:2553:G:O5' 2.04		0.41	
1:X:2639:A:N7	7:E:175:LYS:NZ	2.63	0.41	
1:X:2770:A:H4'	1:X:2771:C:H5'	2.02	0.41	
12:K:13:ASN:ND2	12:K:13:ASN:H	2.19	0.41	
14:M:96:ARG:HH11	14:M:96:ARG:HD3	1.74	0.41	
19:R:22:VAL:HG13	19:R:81:VAL:O	2.20	0.41	
21:T:53:MET:HA	21:T:59:LEU:HA	2.02	0.41	
24:W:1:MET:N	24:W:34:VAL:O	2.53	0.41	
25:Z:41:LEU:HD12	25:Z:41:LEU:HA	1.92	0.41	
1:X:95:G:H2'	1:X:96:C:C6	2.56	0.41	
1:X:194:G:C4	1:X:195:A:C8	3.08	0.41	
1:X:213:C:H2'	1:X:214:C:C6	2.52	0.41	
1:X:386:U:HO2'	1:X:387:A:H8	1.61	0.41	
1:X:438:G:H2'	1:X:439:C:C6	2.56	0.41	
1:X:663:G:H2'	1:X:664:C:O4'	2.21	0.41	
1:X:753:U:H5'	1:X:1964:A:C6	2.55	0.41	
1:X:861:G:C6	1:X:943:U:C2	3.08	0.41	
1:X:886:A:H2'	1:X:887:G:O4'	2.21	0.41	
1:X:981:C:C4	1:X:982:C:C5	3.08	0.41	
1:X:987:G:H5'	1:X:1167:A:C6	2.56	0.41	
1:X:1174:G:C2	1:X:1175:A:N7	2.89	0.41	
1:X:1260:A:C5	1:X:1262:U:C4	3.09	0.41	
1:X:1681:A:C2	1:X:2706:U:C6	3.09	0.41	
1:X:1790:G:C6	1:X:1811:A:C8	3.08	0.41	
1:X:1998:A:C2	25:Z:6:VAL:HG13	2.55	0.41	
1:X:2029:G:C2	1:X:2030:U:C2	3.09	0.41	
1:X:2034:A:P	4:B:137:ARG:NH2	2.94	0.41	
1:X:2043:A:H1'	1:X:2481:G:O4'	2.21	0.41	
1:X:2198:U:OP2	1:X:2199:C:H5"	2.20	0.41	
1:X:2277:A:C2	1:X:2300:G:H2'	2.55	0.41	
1:X:2467:A:H2'	1:X:2468:G:H5'	1.99	0.41	
1:X:2528:G:C2	1:X:2529:G:N7	2.88	0.41	
1:X:2629:U:N3	1:X:2630:C:C5	2.88	0.41	
1:X:2754:C:H2'	1:X:2755:A:C8	2.56	0.41	
1:X:2807:U:H4'	1:X:2808:U:H5'	2.03	0.41	
2:Y:25:G:H5"	2:Y:26:G:OP1	2.20	0.41	
2:Y:52:G:C2	2:Y:53:G:H8	2.38	0.41	
2:Y:78:A:H2' 2:Y:79:U:O4'		2.21	0.41	



Atom 1 Atom 2		Interatomic	Clash		
Atom-1	Atom-2 distance (Å)		overlap (Å)		
3:A:84:TYR:CG	3:A:85:ASP:N	2.89	0.41		
4:B:61:LYS:N	4:B:62:PRO:HD2	2.34	0.41		
5:C:155:GLU:HB3	5:C:159:ARG:NH1	2.35	0.41		
6:D:103:LEU:HD23	6:D:103:LEU:HA	1.70	0.41		
8:G:68:PRO:HB3	15:N:64:ARG:HG3	2.03	0.41		
9:H:78:SER:HA	9:H:91:PHE:O	2.21	0.41		
12:K:10:LEU:HB2	12:K:12:ARG:HD3	2.02	0.41		
12:K:82:GLU:O	12:K:86:LYS:HG3	2.21	0.41		
16:O:89:ASN:OD1	16:O:89:ASN:N	2.52	0.41		
17:P:60:ILE:HG22	17:P:62:ARG:HG2	2.01	0.41		
18:Q:11:VAL:HG12	18:Q:12:ILE:O	2.20	0.41		
25:Z:33:CYS:SG	25:Z:36:CYS:N	2.93	0.41		
1:X:5:A:C6	1:X:2873:G:C6	3.09	0.41		
1:X:538:A:H3'	1:X:538:A:N3	2.36	0.41		
1:X:542:A:N6	1:X:2018:G:N2	2.68	0.41		
1:X:580:A:C5	1:X:2013:A:C6	3.09	0.41		
1:X:587:A:C2	1:X:2001:G:H1'	2.55	0.41		
1:X:748:A:H5"	1:X:749:C:H5	1.86	0.41		
1:X:810:U:C4	1:X:811:G:N7	2.88	0.41		
1:X:839:U:H5"	1:X:2407:G:O3'	2.20	0.41		
1:X:1022:A:C6	1:X:1024:G:N7	2.88	0.41		
1:X:1121:G:O2'	1:X:1122:A:O4'	2.29	0.41		
1:X:1332:G:C6	1:X:1333:G:N1	2.89	0.41		
1:X:1418:C:H2'	1:X:1419:G:H8	1.80	0.41		
1:X:1562:G:OP2	1:X:1562:G:C8	2.69	0.41		
1:X:1769:U:H2'	1:X:1775:A:C6	2.56	0.41		
1:X:2434:G:C2	1:X:2435:C:C4	3.08	0.41		
1:X:2821:G:H2'	1:X:2822:U:H6	1.85	0.41		
7:E:11:VAL:HB	7:E:50:LEU:HD11	2.01	0.41		
9:H:124:MET:O	9:H:127:VAL:HG12	2.20	0.41		
13:L:11:LEU:HD12	13:L:93:SER:HB2	2.03	0.41		
19:R:105:ARG:CZ	19:R:105:ARG:HA	2.51	0.41		
20:S:125:PRO:HD3	20:S:158:CYS:HA	2.03	0.41		
20:S:143:ILE:HA	20:S:171:VAL:HG11	2.02	0.41		
21:T:19:LYS:HA 21:T:19:LYS:HD		1.80	0.41		
21:T:37:LEU:HD11	21:T:61:ALA:N	2.35	0.41		
26:1:15:SER:HA	26:1:21:TYR:O	2.21	0.41		
1:X:69:G:H3'	1:X:111:G:O2'	2.20	0.41		
1:X:154:U:H3'	1:X:155:G:H8	1.84	0.41		
1:X:194:G:H2'	1:X:195:A:H8	1.86	0.41		
1:X:456:C:H2'	1:X:457:C:H6	1.86	0.41		



Atom 1	Atom 2	Interatomic	Clash		
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)		
1:X:555:U:H5	1:X:1232:U:H2'	1.86	0.41		
1:X:797:A:O2'	1:X:798:G:H8	2.04	0.41		
1:X:810:U:H2'	1:X:811:G:O4'	2.21	0.41		
1:X:935:C:H4'	21:T:29:GLU:HG2	2.02	0.41		
1:X:1332:G:C2	1:X:1333:G:N2	2.89	0.41		
1:X:1359:G:C6	1:X:1617:G:C6	3.09	0.41		
1:X:1421:U:H2'	1:X:1422:C:C6	2.55	0.41		
1:X:1454:U:H2'	1:X:1455:C:H6	1.82	0.41		
1:X:1631:C:H5	1:X:1633:C:C2	2.36	0.41		
1:X:1716:G:N1	1:X:1754:G:C4	2.89	0.41		
1:X:2210:C:H2'	1:X:2211:U:C6	2.55	0.41		
1:X:2290:A:C8	1:X:2291:U:C5	3.08	0.41		
1:X:2375:G:C2	1:X:2376:G:C8	3.09	0.41		
1:X:2729:A:OP1	7:E:6:LYS:NZ	2.50	0.41		
31:X:3169:SPD:HN6	31:X:3169:SPD:H32	1.38	0.41		
3:A:60:ARG:HD3	3:A:86:PRO:HB2	2.02	0.41		
3:A:132:PRO:HG2	3:A:135:PHE:HD1	1.85	0.41		
5:C:146:GLU:OE1	5:C:185:ARG:HD2	2.21	0.41		
6:D:57:LEU:HD22	6:D:89:VAL:HG21	2.02	0.41		
1:X:14:A:HO2'	25:Z:21:SER:HG	1.67	0.41		
1:X:27:G:N2	1:X:522:G:H1'	2.35	0.41		
1:X:203:G:H21	1:X:205:A:H62	1.69	0.41		
1:X:356:A:O2'	1:X:357:A:C8	2.71	0.41		
1:X:474:G:C2	1:X:478:G:C5	3.09	0.41		
1:X:487:G:H22	1:X:490:A:C5'	2.34	0.41		
1:X:705:C:C2	1:X:706:A:N7	2.89	0.41		
1:X:716:U:C4	1:X:717:G:C6	3.09	0.41		
1:X:825:C:H1'	1:X:1263:G:C2	2.56	0.41		
1:X:862:A:H2'	1:X:863:C:H6	1.82	0.41		
1:X:915:C:H2'	1:X:916:U:H6	1.86	0.41		
1:X:929:A:H2	2:Y:81:C:O2	2.04	0.41		
1:X:992:A:N1	1:X:2011:U:H5'	2.36	0.41		
1:X:1131:G:C6	1:X:1132:C:C4	3.09	0.41		
1:X:1171:A:H1'	16:O:7:THR:CG2	2.51	0.41		
1:X:1271:C:OP1	5:C:72:ARG:NH1	2.41	0.41		
1:X:1409:U:H5'	1:X:1409:U:H6	1.86	0.41		
1:X:1673:C:C2	1:X:1674:C:C5	3.09	0.41		
1:X:1726:C:H1'	1:X:2835:A:H1'	2.03	0.41		
1:X:1800:A:C6	1:X:1802:A:C6	3.09	0.41		
1:X:1986:G:C6	1:X:1987:G:C8	3.08	0.41		
1:X:2248:A:N3	1:X:2248:A:H2'	2.36	0.41		



A 4 and 1	Atom_1 Atom_2		Clash		
Atom-1	Atom-2 distance (Å)		overlap (Å)		
1:X:2401:A:C5	1:X:2403:C:C4	3.08	0.41		
1:X:2525:U:H4'	1:X:2545:A:H2	1.86	0.41		
1:X:2543:A:C5	1:X:2544:A:N1	2.88	0.41		
1:X:2717:G:H2'	1:X:2718:A:C8	2.55	0.41		
1:X:2784:A:N6	1:X:2866:A:C8	2.89	0.41		
2:Y:47:A:C4	2:Y:48:A:C8	3.09	0.41		
3:A:52:ARG:H	3:A:52:ARG:HG2	1.45	0.41		
3:A:133:LEU:HD21	3:A:145:LEU:HD11	2.03	0.41		
4:B:3:GLY:O	4:B:84:PHE:HE2	2.03	0.41		
4:B:6:GLY:HA3	4:B:27:LEU:O	2.21	0.41		
5:C:56:ARG:HB2	5:C:57:LYS:H	1.54	0.41		
6:D:34:ILE:HD11	6:D:156:ILE:HG23	2.03	0.41		
6:D:61:THR:HA	6:D:99:PHE:CE1	2.56	0.41		
7:E:102:ALA:HB2	7:E:116:GLU:OE2	2.21	0.41		
9:H:104:GLU:HA	9:H:125:LYS:HG3	2.03	0.41		
10:I:63:ARG:HE	10:I:63:ARG:HB2	1.60	0.41		
11:J:6:LYS:HD3	11:J:49:GLU:HG2	2.02	0.41		
11:J:40:PRO:HA	11:J:98:VAL:O	2.21	0.41		
13:L:37:HIS:ND1	13:L:37:HIS:O	2.53	0.41		
14:M:81:PHE:HB3	14:M:88:VAL:HG21	2.02	0.41		
18:Q:86:GLN:HB2	18:Q:87:SER:H	1.56	0.41		
20:S:142:ASN:HB3	20:S:145:ASP:OD2	2.21	0.41		
20:S:172:LEU:HD12	20:S:173:PRO:HD2	2.03	0.41		
28:3:21:LYS:NZ	28:3:53:ALA:HB2	2.35	0.41		
28:3:32:GLN:HA	28:3:32:GLN:HE21	1.86	0.41		
1:X:94:C:O2'	23:V:40:PRO:HD2	2.21	0.41		
1:X:144:U:O2'	1:X:145:C:H5'	2.21	0.41		
1:X:219:G:O2'	1:X:220:U:P	2.78	0.41		
1:X:754:G:C2	1:X:755:C:C4	3.09	0.41		
1:X:795:A:O2'	3:A:225:ALA:HB1	2.20	0.41		
1:X:2042:A:O3'	5:C:63:GLY:HA2	2.20	0.41		
1:X:2232:G:C2	1:X:2233:C:C2	3.08	0.41		
1:X:2268:G:N3	1:X:2268:G:H2'	2.36	0.41		
1:X:2408:G:H3'	1:X:2408:G:H8	1.86	0.41		
1:X:2869:U:H2'	1:X:2870:C:O4'	2.21	0.41		
31:X:3170:SPD:H42	31:X:3170:SPD:H71	1.90	0.41		
3:A:63:ARG:HH12	3:A:88:ARG:NH1	2.19	0.41		
3:A:108:PRO:HD2	3:A:111:LEU:HD12	2.03	0.41		
4:B:116:VAL:HB	4:B:122:PHE:CG	2.56	0.41		
9:H:10:VAL:HG23	9:H:17:ARG:C	2.42	0.41		
10:I:58:ALA:O	10:I:59:ARG:HG2	2.20	0.41		



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-1 Atom-2		overlap (Å)	
12:K:27:ALA:O	12:K:31:GLU:HG3	2.21	0.41	
14:M:41:GLU:HB3	14:M:44:ARG:NH2	2.37	0.41	
16:O:54:TYR:N	16:O:54:TYR:CD1	2.89	0.41	
1:X:438:G:H2'	1:X:439:C:H6	1.86	0.40	
1:X:573:C:O4'	15:N:37:GLN:NE2	2.54	0.40	
1:X:630:G:H3'	1:X:631:G:H21	1.85	0.40	
1:X:630:G:H3'	1:X:631:G:N2	2.36	0.40	
1:X:694:G:H2'	1:X:695:G:O4'	2.22	0.40	
1:X:759:C:O2'	29:X:2901:MIV:H271	2.21	0.40	
1:X:849:G:C5	1:X:850:C:C4	3.09	0.40	
1:X:921:A:H4'	11:J:15:ARG:HH22	1.86	0.40	
1:X:1160:C:H2'	1:X:1161:U:O4'	2.21	0.40	
1:X:1255:A:C6	1:X:1256:C:N4	2.89	0.40	
1:X:1302:C:O2'	1:X:1303:U:H5'	2.21	0.40	
1:X:1366:A:C5	1:X:1391:A:N6	2.90	0.40	
1:X:1643:A:H1'	1:X:1657:A:C2	2.55	0.40	
1:X:1659:G:H2'	1:X:1660:G:O4'	2.21	0.40	
1:X:1665:C:C4	1:X:1666:G:N7	2.89	0.40	
1:X:1685:A:O2'	1:X:1691:G:N7	2.45	0.40	
1:X:1888:C:H4'	1:X:1912:G:C8	2.56	0.40	
1:X:2457:A:N7	1:X:2508:G:N1	2.69	0.40	
1:X:2710:C:H4'	4:B:168:GLN:O	2.20	0.40	
4:B:135:HIS:CB	4:B:136:ARG:HG2	2.44	0.40	
4:B:181:LEU:HD13	4:B:181:LEU:HA	1.81	0.40	
5:C:116:LYS:NZ	5:C:188:ILE:HD13	2.36	0.40	
6:D:17:MET:HE3	6:D:17:MET:HB3	1.82	0.40	
8:G:113:GLU:HG3	8:G:113:GLU:H	1.70	0.40	
9:H:114:VAL:HG22	9:H:133:VAL:HG12	2.03	0.40	
9:H:125:LYS:CD	9:H:125:LYS:N	2.84	0.40	
9:H:132:GLU:HB2	14:M:73:PHE:HE2	1.86	0.40	
11:J:6:LYS:HB2	11:J:45:SER:CB	2.50	0.40	
11:J:62:GLY:O	20:S:112:LEU:HD11	2.21	0.40	
20:S:115:ILE:HG12	20:S:169:VAL:HG12	2.02	0.40	
24:W:25:LEU:HB3	24:W:30:ASP:CB	2.52	0.40	
28:3:48:PHE:N	28:3:48:PHE:HD1	2.18	0.40	
1:X:69:G:H5"	1:X:111:G:H1'	2.02	0.40	
1:X:177:U:O4	1:X:225:G:C2	2.74	0.40	
1:X:193:A:C8	1:X:445:A:N6	2.89	0.40	
1:X:405:C:C2	1:X:406:G:C8	3.09	0.40	
1:X:461:A:C4	1:X:462:G:C8	3.09	0.40	
1:X:485:G:C6 1:X:520:C:N		2.89	0.40	



Atom 1	1 Atom-2 Interatomi		Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:X:614:G:C6	1:X:636:G:C6	3.09	0.40	
1:X:940:G:HO2'	1:X:941:U:P	2.41	0.40	
1:X:1162:A:H2'	1:X:1163:C:H6	1.86	0.40	
1:X:2021:G:H2'	1:X:2022:C:C6	2.55	0.40	
3:A:89:SER:O	3:A:159:ALA:HB2	2.21	0.40	
5:C:15:ILE:O	5:C:17:LEU:HD22	2.21	0.40	
5:C:28:HIS:ND1	10:I:8:PRO:HB3	2.36	0.40	
5:C:148:VAL:HB	5:C:167:VAL:HG12	2.02	0.40	
7:E:53:GLU:HG2	7:E:54:ARG:N	2.36	0.40	
7:E:67:LEU:O	7:E:71:LEU:HG	2.21	0.40	
8:G:99:VAL:HA	8:G:115:ALA:CA	2.50	0.40	
11:J:66:TYR:HB2	11:J:106:GLU:OE1	2.22	0.40	
14:M:99:VAL:CG2	14:M:104:LEU:HD21	2.51	0.40	
17:P:79:ALA:HB1	17:P:90:LEU:HD21	2.02	0.40	
17:P:103:LEU:HB3	17:P:105:ARG:HH12	1.86	0.40	
18:Q:10:PRO:HD3	23:V:30:PHE:HA	2.03	0.40	
19:R:57:ASN:HB2	19:R:60:PRO:CG	2.52	0.40	
1:X:2:G:H2'	1:X:3:U:H6	1.85	0.40	
1:X:12:U:H6	1:X:12:U:H2'	1.64	0.40	
1:X:324:C:H2'	1:X:325:U:O4'	2.20	0.40	
1:X:1058:G:OP2	1:X:1058:G:H8 2.03		0.40	
1:X:1213:U:H2'	1:X:1214:C:C6	2.57	0.40	
1:X:1273:G:C6	1:X:1274:C:C4	3.10	0.40	
1:X:1661:C:O2	1:X:1661:C:H2'	2.22	0.40	
1:X:2034:A:OP2	4:B:137:ARG:NH2	2.43	0.40	
1:X:2250:G:H5'	21:T:20:TYR:CD2	2.56	0.40	
1:X:2340:C:P	28:3:27:SER:HG	2.44	0.40	
1:X:2357:A:H4'	13:L:26:ARG:NH2	2.36	0.40	
3:A:252:LYS:NZ	3:A:252:LYS:H	2.20	0.40	
7:E:121:VAL:HG11	7:E:144:VAL:HG11	2.03	0.40	
9:H:3:MET:HG3	9:H:4:PRO:O	2.22	0.40	
14:M:98:LYS:HD3	14:M:99:VAL:H	1.86	0.40	
19:R:49:GLU:H	19:R:49:GLU:HG3	1.63	0.40	
19:R:105:ARG:HA	19:R:105:ARG:NE	2.36	0.40	
1:X:26:G:H1'	1:X:524:A:N6	2.36	0.40	
1:X:328:A:C6	1:X:329:C:C4	3.10	0.40	
1:X:459:A:N3	1:X:484:G:C8	2.90	0.40	
1:X:575:U:H2'	1:X:576:A:O4'	2.22	0.40	
1:X:583:C:N4	1:X:2017:U:OP1	2.45	0.40	
1:X:773:G:O2'	1:X:774[B]:A:OP1	2.37	0.40	
1:X:836:G:C6	1:X:837:U:C4	3.10	0.40	



Atom 1 Atom 2		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:X:1047:G:C6	1:X:1131:G:C5	3.09	0.40	
1:X:1167:A:N7	15:N:51:ARG:HD3	2.37	0.40	
1:X:1695:U:C5	1:X:1696:C:C5	3.09	0.40	
1:X:2045:A:H61	29:X:2901:MIV:H102	1.86	0.40	
1:X:2350:G:H2'	1:X:2351:G:O4'	2.21	0.40	
1:X:2793:G:N1	1:X:2804:G:C6	2.89	0.40	
2:Y:39:C:H5"	2:Y:40:C:C6	2.57	0.40	
4:B:17:ASN:HB3	4:B:18:ASP:H	1.67	0.40	
5:C:118:VAL:HG23	5:C:190:ALA:HB2	2.04	0.40	
6:D:87:ILE:HG13	6:D:87:ILE:H	1.59	0.40	
7:E:44:ARG:NH2	7:E:44:ARG:HB2	2.36	0.40	
7:E:55:PRO:HG2	7:E:61:HIS:CE1	2.57	0.40	
26:1:20:PHE:CE2	26:1:42:PRO:HG2	2.56	0.40	
28:3:38:GLY:O	28:3:41:ILE:HG22	2.21	0.40	
1:X:400:U:H6	1:X:400:U:H5"	1.86	0.40	
1:X:759:C:OP1	1:X:2591:C:C5	2.75	0.40	
1:X:820:U:H2'	1:X:821:A:O4'	2.22	0.40	
1:X:851:C:C2	1:X:952:A:C6	3.10	0.40	
1:X:1009:C:H2'	1:X:1010:U:O4'	2.21	0.40	
1:X:1300:A:N7	12:K:106:ASP:HB3	2.37	0.40	
1:X:1704:G:C2	1:X:1719:G:O6	2.74	0.40	
1:X:1716:G:C2	1:X:1754:G:C2	3.10	0.40	
1:X:2061:C:H2'	1:X:2062:U:H6	1.86	0.40	
1:X:2407:G:H8	1:X:2407:G:O5'	2.04	0.40	
1:X:2443:C:H2'	1:X:2444:C:H6	1.87	0.40	
1:X:2597:G:C6	1:X:2598:C:C4	3.09	0.40	
1:X:2662:C:O2'	1:X:2663:U:H5'	2.22	0.40	
1:X:2824:C:N3	1:X:2842:C:H5'	2.36	0.40	
3:A:257:LEU:HD23	3:A:257:LEU:HA	1.82	0.40	
4:B:133:LYS:HB2	4:B:137:ARG:HB2	2.03	0.40	
19:R:38:LEU:HD23	19:R:38:LEU:HA	1.86	0.40	
20:S:96:VAL:HG22	20:S:97:PRO:O	2.21	0.40	
22:U:22:GLY:H	22:U:39:LYS:CB	2.35	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 X-ray entries followed by that with respect to entries of similar resolution.

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	Perce	entiles
3	А	269/271~(99%)	234 (87%)	26 (10%)	9(3%)	4	22
4	В	204/206~(99%)	176~(86%)	22~(11%)	6 (3%)	4	24
5	С	193/195~(99%)	168 (87%)	14 (7%)	11 (6%)	1	12
6	D	174/176~(99%)	147 (84%)	21 (12%)	6 (3%)	3	21
7	Е	169/171~(99%)	156 (92%)	11 (6%)	2 (1%)	13	41
8	G	140/142~(99%)	121 (86%)	14 (10%)	5 (4%)	3	21
9	Н	132/134~(98%)	122 (92%)	8 (6%)	2 (2%)	10	36
10	Ι	135/137~(98%)	103 (76%)	22~(16%)	10 (7%)	1	7
11	J	132/134~(98%)	105 (80%)	22 (17%)	5 (4%)	3	19
12	K	113/115~(98%)	103 (91%)	7~(6%)	3 (3%)	5	26
13	L	102/104~(98%)	83 (81%)	17 (17%)	2(2%)	7	30
14	М	116/118 (98%)	102 (88%)	10 (9%)	4 (3%)	3	21
15	Ν	115/117~(98%)	110 (96%)	5~(4%)	0	100	100
16	Ο	96/98~(98%)	79~(82%)	13~(14%)	4 (4%)	3	18
17	Р	127/129~(98%)	118 (93%)	7~(6%)	2(2%)	9	34
18	Q	91/93~(98%)	79 (87%)	9~(10%)	3(3%)	4	22
19	R	108/110~(98%)	92 (85%)	11 (10%)	5 (5%)	2	15
20	S	172/175~(98%)	147 (86%)	19~(11%)	6 (4%)	3	21
21	Т	70/72~(97%)	64 (91%)	5~(7%)	1 (1%)	11	37
22	U	72/74~(97%)	55 (76%)	13~(18%)	4 (6%)	2	12
23	V	52/54~(96%)	49 (94%)	2~(4%)	1 (2%)	8	31
24	W	$5\overline{3}/55~(96\%)$	51 (96%)	2 (4%)	0	100	100
25	Z	$5\overline{5}/57~(96\%)$	50 (91%)	4 (7%)	1 (2%)	8	32
26	1	47/49 (96%)	35 (74%)	7 (15%)	5 (11%)	0	3
27	2	44/46 (96%)	41 (93%)	3(7%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	erce	entile	s
28	3	61/63~(97%)	46 (75%)	13 (21%)	2(3%)		4	22	
All	All	3042/3095~(98%)	2636 (87%)	307 (10%)	99~(3%)		4	22	

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	А	30	GLU
3	А	247	VAL
3	А	254	THR
4	В	131	SER
4	В	147	PRO
4	В	149	ARG
5	С	18	PRO
5	С	120	VAL
6	D	126	GLY
8	G	69	ASP
8	G	110	LEU
8	G	111	LYS
10	Ι	30	ALA
10	Ι	43	ALA
10	Ι	105	PRO
10	Ι	130	ILE
11	J	80	ALA
11	J	86	LYS
12	K	3	HIS
13	L	33	ARG
14	М	25	PRO
14	М	28	ARG
14	М	41	GLU
19	R	78	ALA
19	R	85	ASP
20	S	18	MET
20	S	76	ARG
26	1	30	ASN
26	1	42	PRO
28	3	13	ARG
3	А	56	GLY
3	А	151	LYS
5	С	13	ARG
5	С	126	ALA
5	С	172	VAL
6	D	127	ASN



Mol	Chain	Res	Type
7	Е	7	GLN
10	Ι	83	LEU
11	J	89	GLY
12	K	88	ALA
13	L	38	ILE
14	М	42	GLY
16	0	8	GLY
18	Q	88	ILE
20	S	19	ILE
22	U	35	THR
26	1	24	THR
26	1	34	LYS
3	А	156	ALA
4	В	143	GLN
5	С	6	VAL
5	С	23	ASN
6	D	40	LEU
6	D	122	PHE
7	Е	12	PRO
8	G	34	PRO
9	Н	61	ARG
9	Н	123	PHE
16	0	36	LYS
16	0	80	TYR
19	R	84	VAL
20	S	91	PRO
28	3	29	LYS
4	В	128	SER
5	С	8	GLY
6	D	73	SER
8	G	68	PRO
10	Ι	28	LYS
10	Ι	91	ASP
10	Ι	92	THR
11	J	136	GLU
16	0	10	LYS
17	Р	20	LEU
21	Т	47	ALA
22	U	37	ILE
25	Z	53	ASP
6	D	20	PHE
12	Κ	4	GLY



Mol	Chain	Res	Type
18	Q	3	HIS
18	Q	12	ILE
20	S	66	VAL
22	U	24	ALA
22	U	46	LEU
26	1	45	LYS
3	А	235	GLY
19	R	108	VAL
4	В	52	ALA
5	С	70	GLY
10	Ι	61	PRO
11	J	71	PRO
10	Ι	60	LEU
19	R	41	PRO
23	V	43	VAL
3	А	38	PRO
3	A	121	PRO
5	C	114	GLY
5	С	174	GLY
20	S	127	PRO
17	Р	61	PRO

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	А	196/212~(92%)	168 (86%)	28 (14%)	3 13
4	В	155/155~(100%)	120 (77%)	35~(23%)	1 2
5	С	150/155~(97%)	127~(85%)	23~(15%)	2 11
6	D	147/152~(97%)	111 (76%)	36~(24%)	0 2
7	Ε	136/136~(100%)	109 (80%)	27~(20%)	1 4
8	G	116/118~(98%)	89 (77%)	27~(23%)	1 2
9	Н	102/103~(99%)	79 (78%)	23 (22%)	1 2
10	Ι	93/105~(89%)	72 (77%)	21 (23%)	1 2



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
11	J	103/109~(94%)	76 (74%)	27~(26%)	0	1
12	Κ	92/92~(100%)	63~(68%)	29~(32%)	0	1
13	L	68/74~(92%)	55 (81%)	13~(19%)	1	4
14	М	97/101~(96%)	72~(74%)	25~(26%)	0	2
15	Ν	93/96~(97%)	75 (81%)	18 (19%)	1	4
16	Ο	71/77~(92%)	51 (72%)	20 (28%)	0	1
17	Р	109/111~(98%)	82~(75%)	27~(25%)	0	2
18	Q	73/75~(97%)	49~(67%)	24 (33%)	0	1
19	R	84/91~(92%)	57~(68%)	27 (32%)	0	1
20	S	137/149~(92%)	111 (81%)	26 (19%)	1	4
21	Т	54/54~(100%)	41 (76%)	13~(24%)	0	2
22	U	52/59~(88%)	35~(67%)	17 (33%)	0	1
23	V	43/43~(100%)	36~(84%)	7~(16%)	2	9
24	W	48/48~(100%)	30~(62%)	18 (38%)	0	0
25	Ζ	50/51~(98%)	33~(66%)	17 (34%)	0	1
26	1	23/44~(52%)	15~(65%)	8~(35%)	0	1
27	2	39/39~(100%)	33~(85%)	6 (15%)	2	11
28	3	45/50~(90%)	24~(53%)	$2\overline{1}$ (47%)	0	0
All	All	2376/2499 (95%)	1813~(76%)	563~(24%)	1	2

All (563) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	А	10	THR
3	А	18	THR
3	А	24	LEU
3	А	52	ARG
3	А	54	ILE
3	А	63	ARG
3	А	69	ARG
3	А	71	ASP
3	А	92	ILE
3	А	111	LEU
3	А	147	LEU
3	А	148	VAL
3	А	157	ARG



3       A       169       GLU $3$ A       171       ASP $3$ A       203       ASN $3$ A       203       ASN $3$ A       206       LEU $3$ A       211       ARG $3$ A       221       GLN $3$ A       220       ASP $3$ A       240       THR $3$ A       245       VAL $3$ A       252       LYS $3$ A       265       THR $3$ A       266       SER $3$ A       265       THR $4$ B       14       ILE $4$ B       14       ILE $4$ B       23       VAL	Mol	Chain	Res	Type
3       A       171       ASP         3       A       185       VAL         3       A       203       ASN         3       A       206       LEU         3       A       211       ARG         3       A       221       GLN         3       A       221       GLN         3       A       240       THR         3       A       245       VAL         3       A       245       VAL         3       A       252       LYS         3       A       265       THR         3       A       266       SER         4       B       14       ILE         4       B       14       ILE         4       B       19       ARG         4       B       23       VAL         4 <td< th=""><th>3</th><th>А</th><th>169</th><th>GLU</th></td<>	3	А	169	GLU
3       A       185       VAL         3       A       203       ASN         3       A       206       LEU         3       A       211       ARG         3       A       221       GLN         3       A       230       ASP         3       A       240       THR         3       A       245       VAL         3       A       252       LYS         3       A       254       THR         3       A       265       THR         3       A       266       SER         3       A       266       SER         3       A       266       SER         3       A       266       SER         3       A       269       PHE         4       B       14       ILE         4       B       14       ILE         4       B       19       ARG         4       B       23       VAL         4       B       24       THR         4       B       25       VAL         4       B<	3	А	171	ASP
3       A       203       ASN         3       A       206       LEU         3       A       211       ARG         3       A       221       GLN         3       A       230       ASP         3       A       240       THR         3       A       245       VAL         3       A       252       LYS         3       A       265       THR         3       A       266       SER         4       B       14       ILE         4       B       14       ILE         4       B       14       ILE         4       B       19       ARG         4       B       23       VAL         4       B       25       VAL         4       B	3	А	185	VAL
3       A       206       LEU         3       A       211       ARG         3       A       221       GLN         3       A       230       ASP         3       A       240       THR         3       A       245       VAL         3       A       252       LYS         3       A       254       THR         3       A       265       THR         3       A       266       SER         3       A       269       PHE         4       B       14       ILE         4       B       14       ILE         4       B       14       ILE         4       B       11       MET         4       B       23       VAL         4       B       25       VAL         4       B       42       ASP         4       B<	3	А	203	ASN
3       A       211       ARG         3       A       221       GLN         3       A       230       ASP         3       A       240       THR         3       A       245       VAL         3       A       252       LYS         3       A       254       THR         3       A       265       THR         3       A       266       SER         4       B       14       ILE         4       B       14       ILE         4       B       14       ILE         4       B       23       VAL         4       B       24       THR         4       B       25       VAL         4       B<	3	А	206	LEU
3 $A$ $221$ $GLN$ $3$ $A$ $230$ $ASP$ $3$ $A$ $240$ $THR$ $3$ $A$ $245$ $VAL$ $3$ $A$ $252$ $LYS$ $3$ $A$ $254$ $THR$ $3$ $A$ $265$ $THR$ $3$ $A$ $266$ $SER$ $3$ $A$ $269$ $PHE$ $4$ $B$ $11$ $MET$ $4$ $B$ $114$ $ILE$ $4$ $B$ $114$ $ILE$ $4$ $B$ $23$ $VAL$ $4$ $B$ $24$ $THR$ $4$ $B$ $25$ $VAL$ $4$ $B$	3	А	211	ARG
3       A       230       ASP         3       A       240       THR         3       A       245       VAL         3       A       252       LYS         3       A       254       THR         3       A       265       THR         3       A       266       SER         3       A       269       PHE         4       B       2       LYS         4       B       1       MET         4       B       14       ILE         4       B       14       ILE         4       B       14       ILE         4       B       23       VAL         4       B       23       VAL         4       B       23       VAL         4       B       24       THR         4       B       25       VAL         4       B       25       VAL         4       B       40       GLN         4       B       42       ASP         4       B       48       GLN         4       B	3	А	221	GLN
3       A       240       THR         3       A       245       VAL         3       A       252       LYS         3       A       254       THR         3       A       265       THR         3       A       266       SER         3       A       266       SER         3       A       269       PHE         4       B       2       LYS         4       B       1       MET         4       B       14       ILE         4       B       14       ILE         4       B       13       VAL         4       B       23       VAL         4       B       23       VAL         4       B       25       VAL         4       B       38       THR         4       B       40       GLN         4       B       42       ASP         4       B       48       GLN         4       B       49       ILE         4       B       66       HIS         4       B	3	А	230	ASP
3 $A$ $245$ $VAL$ $3$ $A$ $252$ $LYS$ $3$ $A$ $265$ $THR$ $3$ $A$ $266$ $SER$ $3$ $A$ $266$ $SER$ $3$ $A$ $269$ $PHE$ $4$ $B$ $2$ $LYS$ $4$ $B$ $11$ $MET$ $4$ $B$ $14$ $ILE$ $4$ $B$ $12$ $LYS$ $4$ $B$ $12$ $LYS$ $4$ $B$ $12$ $ILE$ $4$ $B$ $23$ $VAL$ $4$ $B$ $23$ $VAL$ $4$ $B$ $25$ $VAL$ $4$ $B$ $25$ $VAL$ $4$ $B$ $40$ $GLN$ $4$ $B$ $42$ $ASP$ $4$ $B$ $48$ $GLN$ $4$ $B$ $66$ $HIS$ $4$ $B$ $66$	3	А	240	THR
3       A $252$ LYS $3$ A $254$ THR $3$ A $265$ THR $3$ A $266$ SER $3$ A $266$ SER $3$ A $266$ PHE $4$ B $2$ LYS $4$ B $11$ MET $4$ B $14$ ILE $4$ B $14$ ILE $4$ B $21$ ILE $4$ B $23$ VAL $4$ B $25$ VAL $4$ B $40$ GLN $4$ B $42$ ASP $4$ B $42$ ASP $4$ B $49$ ILE $4$ B $63$ MET $4$ B $66$ HIS $4$ B $66$ HIS $4$ B $69$ LYS $4$ B <td< th=""><th>3</th><th>А</th><th>245</th><th>VAL</th></td<>	3	А	245	VAL
3       A $254$ THR $3$ A $265$ THR $3$ A $266$ SER $3$ A $269$ PHE $4$ B $2$ LYS $4$ B $11$ MET $4$ B $14$ ILE $4$ B $14$ ILE $4$ B $12$ IXS $4$ B $12$ IXE $4$ B $23$ VAL $4$ B $23$ VAL $4$ B $24$ THR $4$ B $25$ VAL $4$ B $25$ VAL $4$ B $40$ GLN $4$ B $40$ GLN $4$ B $42$ ASP $4$ B $49$ ILE $4$ B $63$ MET $4$ B $66$ HIS $4$ B	3	А	252	LYS
3       A       265       THR         3       A       266       SER         3       A       269       PHE         4       B       2       LYS         4       B       11       MET         4       B       14       ILE         4       B       14       ILE         4       B       18       ASP         4       B       19       ARG         4       B       23       VAL         4       B       24       THR         4       B       25       VAL         4       B       38       THR         4       B       40       GLN         4       B       42       ASP         4       B       40       GLN         4       B       42       ASP         4       B       49       ILE         4       B       49       ILE         4       B       63       MET         4       B       69       LYS         4       B       77       ILE         4       B <td< th=""><th>3</th><th>А</th><th>254</th><th>THR</th></td<>	3	А	254	THR
3       A       266       SER         3       A       269       PHE         4       B       11       MET         4       B       11       MET         4       B       14       ILE         4       B       14       ILE         4       B       19       ARG         4       B       23       VAL         4       B       24       THR         4       B       25       VAL         4       B       38       THR         4       B       40       GLN         4       B       42       ASP         4       B       42       ASP         4       B       42       ASP         4       B       49       ILE         4       B       63       MET         4       B       66       HIS         4       B       69       LYS         4       B       69       LYS         4       B       90       SER         4       B       92       ASN         4       B <td< th=""><th>3</th><th>А</th><th>265</th><th>THR</th></td<>	3	А	265	THR
3 $A$ $269$ PHE $4$ $B$ $2$ $LYS$ $4$ $B$ $11$ MET $4$ $B$ $14$ $ILE$ $4$ $B$ $14$ $ILE$ $4$ $B$ $19$ $ARG$ $4$ $B$ $21$ $ILE$ $4$ $B$ $23$ $VAL$ $4$ $B$ $23$ $VAL$ $4$ $B$ $23$ $VAL$ $4$ $B$ $23$ $VAL$ $4$ $B$ $25$ $VAL$ $4$ $B$ $25$ $VAL$ $4$ $B$ $40$ $GLN$ $4$ $B$ $40$ $GLN$ $4$ $B$ $49$ $ILE$ $4$ $B$ $63$ $MET$ $4$ $B$ $66$ $HIS$ $4$ $B$ $69$ $LYS$ $4$ $B$ $90$ $SER$ $4$ $B$ $92$	3	А	266	SER
4B $2$ LYS $4$ B11MET $4$ B14ILE $4$ B18ASP $4$ B19ARG $4$ B21ILE $4$ B23VAL $4$ B24THR $4$ B25VAL $4$ B38THR $4$ B40GLN $4$ B42ASP $4$ B48GLN $4$ B49ILE $4$ B58LYS $4$ B66HIS $4$ B66HIS $4$ B69LYS $4$ B90SER $4$ B90SER $4$ B94ASP $4$ B98GLU $4$ B116VAL $4$ B119ARG $4$ B129HIS	3	А	269	PHE
4       B       11       MET         4       B       14       ILE         4       B       18       ASP         4       B       19       ARG         4       B       21       ILE         4       B       23       VAL         4       B       23       VAL         4       B       25       VAL         4       B       38       THR         4       B       40       GLN         4       B       42       ASP         4       B       42       ASP         4       B       42       ASP         4       B       42       ASP         4       B       49       ILE         4       B       58       LYS         4       B       66       HIS         4       B       69       LYS         4       B       69       LYS         4       B       90       SER         4       B       92       ASN         4       B       94       ASP         4       B       9	4	В	2	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	11	MET
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	14	ILE
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	18	ASP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	19	ARG
4       B       23       VAL         4       B       24       THR         4       B       25       VAL         4       B       38       THR         4       B       38       THR         4       B       40       GLN         4       B       42       ASP         4       B       42       ASP         4       B       49       ILE         4       B       58       LYS         4       B       63       MET         4       B       66       HIS         4       B       69       LYS         4       B       69       LYS         4       B       69       SER         4       B       90       SER         4       B       92       ASN         4       B       94       ASP         4       B       98       GLU         4       B       116       VAL         4       B       119       ARG         4       B       129       HIS	4	В	21	ILE
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	23	VAL
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	24	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	25	VAL
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	38	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	40	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	42	ASP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	48	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	В	49	ILE
4       B       63       MET         4       B       66       HIS         4       B       69       LYS         4       B       77       ILE         4       B       84       PHE         4       B       90       SER         4       B       92       ASN         4       B       94       ASP         4       B       98       GLU         4       B       116       VAL         4       B       119       ARG         4       B       129       HIS	4	В	58	LYS
4       B       66       HIS         4       B       69       LYS         4       B       77       ILE         4       B       84       PHE         4       B       90       SER         4       B       92       ASN         4       B       94       ASP         4       B       98       GLU         4       B       116       VAL         4       B       129       HIS	4	В	63	MET
4       B       69       LYS         4       B       77       ILE         4       B       84       PHE         4       B       90       SER         4       B       92       ASN         4       B       94       ASP         4       B       98       GLU         4       B       116       VAL         4       B       119       ARG         4       B       129       HIS	4	В	66	HIS
4     B     77     ILE       4     B     84     PHE       4     B     90     SER       4     B     92     ASN       4     B     94     ASP       4     B     98     GLU       4     B     116     VAL       4     B     129     HIS	4	В	69	LYS
4         B         84         PHE           4         B         90         SER           4         B         92         ASN           4         B         94         ASP           4         B         98         GLU           4         B         116         VAL           4         B         119         ARG           4         B         129         HIS	4	В	77	ILE
4         B         90         SER           4         B         92         ASN           4         B         94         ASP           4         B         98         GLU           4         B         116         VAL           4         B         119         ARG           4         B         129         HIS	4	В	84	PHE
4         B         92         ASN           4         B         94         ASP           4         B         98         GLU           4         B         116         VAL           4         B         119         ARG           4         B         129         HIS	4	В	90	SER
4         B         94         ASP           4         B         98         GLU           4         B         116         VAL           4         B         119         ARG           4         B         129         HIS	4	В	92	ASN
4         B         98         GLU           4         B         116         VAL           4         B         119         ARG           4         B         129         HIS	4	В	94	ASP
4         B         116         VAL           4         B         119         ARG           4         B         129         HIS	4	В	98	GLU
4         B         119         ARG           4         B         129         HIS	4	В	116	VAL
4 B 129 HIS	4	В	119	ARG
	4	В	129	HIS

Continued from previous page...



Mol	Chain	Res	Type
4	В	135	HIS
4	В	137	ARG
4	В	143	GLN
4	В	149	ARG
4	В	156	MET
4	В	163	GLU
4	В	184	VAL
4	В	199	ARG
5	С	4	ILE
5	С	16	GLU
5	С	17	LEU
5	С	44	SER
5	С	45	THR
5	С	46	ARG
5	С	52	SER
5	C	53	LYS
5	С	56	ARG
5	С	62	LYS
5	С	74	VAL
5	С	76	THR
5	С	90	SER
5	С	92	ASP
5	С	95	LEU
5	С	104	LEU
5	С	116	LYS
5	С	118	VAL
5	С	129	LYS
5	С	136	TRP
5	C	153	ASP
5	С	163	ASN
5	C	181	LEU
6	D	10	ASP
6	D	18	GLN
6	D	20	PHE
6	D	30	ARG
6	D	31	ILE
6	D	38	GLU
6	D	42	SER
6	D	44	LYS
6	D	51	ASP
6	D	57	LEU
6	D	62	LEU



Mol	Chain	Res	Type
6	D	64	LYS
6	D	67	ILE
6	D	72	LYS
6	D	79	LEU
6	D	81	GLN
6	D	87	ILE
6	D	96	MET
6	D	102	LYS
6	D	103	LEU
6	D	104	ILE
6	D	108	LEU
6	D	111	ILE
6	D	114	PHE
6	D	117	ILE
6	D	123	ASP
6	D	125	ARG
6	D	128	TYR
6	D	130	LEU
6	D	141	ILE
6	D	148	LYS
6	D	149	THR
6	D	150	ARG
6	D	158	THR
6	D	159	THR
6	D	163	ASP
7	Е	6	LYS
7	Е	9	ILE
7	Е	11	VAL
7	Е	24	PHE
7	Е	33	LEU
7	Е	40	GLU
7	Е	44	ARG
7	Ε	45	GLN
7	Е	46	ASP
7	Е	49	GLN
7	E	50	LEU
7	Е	51	LEU
7	Е	62	ARG
7	E	67	LEU
7	Е	69	ARG
7	Е	84	THR
7	Е	85	ILE

Continued from previous page...



Mol	Chain	Res	Type
7	Е	86	ASN
7	Е	87	LEU
7	Е	89	LEU
7	Е	113	VAL
7	Е	127	GLU
7	Е	129	THR
7	Е	132	ASP
7	Е	140	LEU
7	Е	153	LYS
7	Е	169	ILE
8	G	33	ILE
8	G	35	LYS
8	G	43	VAL
8	G	44	VAL
8	G	51	LEU
8	G	60	SER
8	G	63	ARG
8	G	67	ARG
8	G	71	THR
8	G	78	ASP
8	G	91	THR
8	G	94	LYS
8	G	95	LEU
8	G	100	TYR
8	G	102	ARG
8	G	116	ARG
8	G	119	LEU
8	G	121	LYS
8	G	124	GLU
8	G	132	PHE
8	G	137	LYS
8	G	140	GLN
8	G	142	ARG
8	G	154	GLU
8	G	159	SER
8	G	165	VAL
8	G	166	LEU
9	Н	7	ARG
9	Н	10	VAL
9	Н	23	ARG
9	Н	35	THR
9	Н	47	VAL



Mol	Chain	Res	Type
9	Н	51	ILE
9	Н	56	LYS
9	Н	70	VAL
9	Н	76	ARG
9	Н	78	SER
9	Н	81	ILE
9	Н	83	ARG
9	Н	87	SER
9	Н	97	VAL
9	Н	104	GLU
9	Н	108	THR
9	Н	114	VAL
9	Н	120	ASP
9	Н	121	ARG
9	Н	125	LYS
9	Н	126	ILE
9	Н	127	VAL
9	Н	133	VAL
10	Ι	4	HIS
10	Ι	5	ASP
10	Ι	19	VAL
10	Ι	21	ARG
10	Ι	38	LYS
10	Ι	45	LYS
10	Ι	54	SER
10	Ι	55	ARG
10	Ι	56	LEU
10	Ι	57	ILE
10	Ι	63	ARG
10	Ι	71	THR
10	Ι	77	LEU
10	Ι	80	LEU
10	Ι	81	GLN
10	Ι	87	THR
10	Ι	89	ASP
10	Ι	90	ARG
10	Ι	93	LEU
10	Ι	103	ASN
10	Ι	109	LEU
11	J	6	LYS
11	J	9	LYS
11	J	18	MET

Continued from previous page...



Mol	Chain	Res	Type
11	J	19	THR
11	J	23	LYS
11	J	38	MET
11	J	44	LYS
11	J	46	ASN
11	J	48	ILE
11	J	52	ARG
11	J	64	LYS
11	J	69	ILE
11	J	77	LYS
11	J	84	MET
11	J	86	LYS
11	J	88	LYS
11	J	91	VAL
11	J	95	VAL
11	J	96	SER
11	J	106	GLU
11	J	112	GLU
11	J	116	LYS
11	J	121	LEU
11	J	130	THR
11	J	134	LYS
11	J	135	ARG
11	J	136	GLU
12	K	1	MET
12	K	2	ARG
12	K	5	LYS
12	K	8	ARG
12	K	9	LYS
12	K	12	ARG
12	K	28	LEU
12	K	36	THR
12	K	37	THR
12	K	39	THR
12	K	45	ARG
12	K	52	ILE
12	K	59	ASP
12	K	63	ARG
12	K	64	ARG
12	K	70	ILE
12	K	71	HIS
12	K	75	VAL



Mol	Chain	Res	Type
12	K	76	VAL
12	K	83	VAL
12	K	89	GLU
12	K	95	THR
12	K	97	ILE
12	K	98	LEU
12	K	99	ARG
12	K	102	THR
12	K	104	ARG
12	K	109	THR
12	K	110	MET
13	L	8	ARG
13	L	9	ARG
13	L	14	ARG
13	L	17	VAL
13	L	19	THR
13	L	20	THR
13	L	31	VAL
13	L	34	SER
13	L	43	ILE
13	L	46	SER
13	L	47	ARG
13	L	85	LYS
13	L	94	TYR
14	М	5	ILE
14	М	7	ILE
14	М	11	GLU
14	М	14	ARG
14	М	18	GLN
14	М	24	LEU
14	М	26	ASP
14	М	27	PHE
14	М	31	ASP
14	М	38	LYS
14	М	41	GLU
14	М	44	ARG
14	М	46	ARG
14	М	50	PHE
14	М	55	ILE
14	М	57	ILE
14	М	85	SER
14	М	87	LEU



Mol	Chain	Res	Type
14	М	93	ILE
14	М	95	GLU
14	М	98	LYS
14	М	109	GLU
14	М	113	LYS
14	М	116	ARG
14	М	119	SER
15	Ν	8	ILE
15	N	15	LYS
15	N	18	LEU
15	N	22	LYS
15	N	28	ARG
15	Ν	34	ASN
15	N	51	ARG
15	Ν	53	LYS
15	N	58	ARG
15	N	60	LEU
15	N	64	ARG
15	N	80	ILE
15	N	84	LYS
15	N	85	ARG
15	N	88	ILE
15	N	94	VAL
15	Ν	101	ARG
15	Ν	113	SER
16	0	4	ILE
16	0	11	GLN
16	0	16	GLU
16	0	20	ILE
16	0	22	VAL
16	0	24	SER
16	0	25	LEU
16	0	26	GLN
16	0	31	ASP
16	0	33	VAL
16	0	35	LEU
16	0	54	TYR
16	0	65	ARG
16	0	72	ARG
16	0	81	ARG
16	0	83	ARG
16	0	84	THR



Mol	Chain	Res	Type
16	0	87	ARG
16	0	89	ASN
16	0	96	LEU
17	Р	12	LYS
17	Р	17	GLN
17	Р	20	LEU
17	Р	21	ARG
17	Р	22	LYS
17	Р	32	ARG
17	Р	34	SER
17	Р	36	ARG
17	Р	41	VAL
17	Р	43	ASP
17	Р	46	ARG
17	Р	49	SER
17	Р	51	GLN
17	Р	55	ASP
17	Р	57	LEU
17	Р	61	PRO
17	Р	62	ARG
17	Р	63	SER
17	Р	65	SER
17	Р	86	LEU
17	Р	104	LYS
17	Р	106	LEU
17	Р	107	ILE
17	Р	113	SER
17	Р	117	ILE
17	Р	118	LYS
17	Р	125	THR
18	Q	3	HIS
18	Q	5	ASP
18	Q	8	GLN
18	Q	13	SER
18	Q	14	GLU
18	Q	18	SER
18	Q	27	PHE
18	Q	29	VAL
18	Q	32	LYS
18	Q	34	THR
18	Q	36	THR
10	0	20	ILE

Continued from previous page..



Mol	Chain	Res	Type
18	Q	40	ASP
18	Q	49	ARG
18	$\frac{\tilde{Q}}{Q}$	51	ILE
18	0	56	MET
18	$\frac{\tilde{Q}}{Q}$	64	ARG
18	Q	65	VAL
18	Q	72	ARG
18	Q	80	VAL
18	Q	86	GLN
18	Q	88	ILE
18	Q	89	GLU
18	Q	91	LEU
19	R	5	SER
19	R	14	LEU
19	R	15	HIS
19	R	16	PHE
19	R	21	THR
19	R	25	LEU
19	R	26	SER
19	R	30	LYS
19	R	38	LEU
19	R	44	GLN
19	R	49	GLU
19	R	52	ASN
19	R	56	LYS
19	R	57	ASN
19	R	58	VAL
19	R	64	ASN
19	R	70	GLU
19	R	74	LEU
19	R	80	LYS
19	R	84	VAL
19	R	85	ASP
19	R	87	GLU
19	R	88	THR
19	R	92	THR
19	R	102	LYS
19	R	104	VAL
19	R	113	THR
20	S	13	LYS
20	S	31	SER
20	S	37	LYS


Mol	Chain	Res	Type
20	S	48	THR
20	S	49	THR
20	S	51	LEU
20	S	53	ASP
20	S	56	VAL
20	S	57	GLU
20	S	60	GLU
20	S	61	THR
20	S	65	LEU
20	S	74	ARG
20	S	90	GLU
20	S	93	GLU
20	S	99	HIS
20	S	104	SER
20	S	117	VAL
20	S	120	LEU
20	S	121	GLN
20	S	128	ARG
20	S	130	ILE
20	S	132	GLN
20	S	146	HIS
20	S	159	THR
20	S	169	VAL
21	Т	12	ASN
21	Т	19	LYS
21	Т	20	TYR
21	Т	37	LEU
21	Т	38	VAL
21	Т	46	LYS
21	Т	57	HIS
21	Т	59	LEU
21	Т	62	LEU
21	Т	64	ASP
21	Т	68	VAL
21	Т	72	LYS
21	Т	77	ARG
22	U	6	TYR
22	U	11	LYS
22	U	17	SER
22	U	19	ILE
22	U	20	ARG
22	U	34	THR



Mol	Chain	Res	Type
22	U	40	ARG
22	U	43	ARG
22	U	46	LEU
22	U	54	ASN
22	U	57	VAL
22	U	58	LYS
22	U	60	VAL
22	U	62	LEU
22	U	63	SER
22	U	65	ASN
22	U	78	ILE
23	V	19	ASP
23	V	25	LEU
23	V	26	MET
23	V	28	LEU
23	V	37	LEU
23	V	53	LEU
23	V	57	LYS
24	W	2	LYS
24	W	4	LYS
24	W	5	LEU
24	W	10	ILE
24	W	12	ARG
24	W	17	VAL
24	W	20	VAL
24	W	23	LEU
24	W	25	LEU
24	W	26	ARG
24	W	27	LYS
24	W	28	ILE
24	W	30	ASP
24	W	31	SER
24	W	34	VAL
24	W	35	SER
24	W	41	ARG
24	W	45	LYS
25	Z	4	HIS
25	Z	15	LYS
25	Z	16	ARG
25	Z	18	MET
25	Z	19	ARG
25	Z	31	THR

Continued from previous page..



Mol	Chain	Res	Type
25	Ζ	32	GLU
25	Ζ	33	CYS
25	Ζ	36	CYS
25	Ζ	41	LEU
25	Ζ	42	SER
25	Ζ	45	ILE
25	Ζ	46	CYS
25	Ζ	53	ASP
25	Ζ	56	GLN
25	Ζ	57	VAL
25	Ζ	58	LEU
26	1	7	ARG
26	1	8	ILE
26	1	9	ILE
26	1	20	PHE
26	1	30	ASN
26	1	36	GLU
26	1	41	ASP
26	1	54	LYS
27	2	12	ARG
27	2	14	LYS
27	2	19	ARG
27	2	21	ARG
27	2	24	THR
27	2	42	LEU
28	3	5	LYS
28	3	8	LYS
28	3	11	LYS
28	3	14	ILE
28	3	31	HIS
28	3	32	GLN
28	3	34	THR
28	3	36	LYS
28	3	39	ASP
28	3	40	GLU
28	3	44	LYS
28	3	46	LYS
28	3	48	PHE
28	3	49	VAL
28	3	50	LEU
28	3	52	LYS
28	3	58	MET



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Mol	Chain	Res	Type
28	3	59	LYS
28	3	60	LEU
28	3	61	MET
28	3	64	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	А	231	HIS
4	В	66	HIS
5	С	3	GLN
6	D	76	ASN
7	Е	45	GLN
8	G	140	GLN
9	Н	5	GLN
9	Н	102	GLN
14	М	2	GLN
15	Ν	31	GLN
15	Ν	72	HIS
21	Т	71	ASN
22	U	47	HIS
28	3	32	GLN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Х	2685/2699~(99%)	770 (28%)	65~(2%)
2	Y	121/122~(99%)	28~(23%)	4(3%)
All	All	2806/2821~(99%)	798~(28%)	69~(2%)

All (798) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Х	2	G
1	Х	13	А
1	Х	19	С
1	Х	23	G
1	Х	25	U
1	Х	28	А
1	Х	34	U



Continued from previous page				
Mol	Chain	$\mathbf{Res}$	Type	
1	Х	39	С	
1	Х	45	С	
1	Х	49	U	
1	Х	50	G	
1	Х	51	А	
1	Х	54	G	
1	Х	56	С	
1	Х	59	G	
1	Х	60	А	
1	Х	63	А	
1	Х	69	G	
1	Х	70	А	
1	Х	71	А	
1	X	72	A	
1	Х	73	A	
1	Х	74	G	
1	Х	83	А	
1	Х	87	G	
1	Х	89	А	
1	Х	98	U	
1	Х	99	U	
1	Х	100	G	
1	Х	101	А	
1	Х	102	С	
1	Х	106	G	
1	Х	107	G	
1	Х	108	G	
1	Х	109	А	
1	Х	111	G	
1	Х	116	А	
1	Х	118	U	
1	X	119	G	
1	X	126	С	
1	Х	127	С	
1	Х	132	U	
1	X	133	С	
1	X	134	G	
1	Х	138	G	
1	X	146	C	
1	X	147	G	
1	Х	148	С	
1	Х	149	А	



Mol	Chain	Res	Type
1	Х	150	A
1	Х	158	А
1	Х	170	U
1	Х	173	А
1	Х	176	А
1	Х	181	А
1	Х	192	G
1	Х	193	А
1	Х	198	А
1	Х	199	А
1	Х	200	А
1	Х	201	G
1	Х	202	А
1	Х	205	А
1	Х	206	U
1	Х	207	U
1	Х	210	А
1	Х	219	G
1	Х	220	U
1	Х	222	G
1	Х	225	G
1	Х	229	G
1	Х	241	С
1	Х	242	А
1	Х	243	G
1	Х	245	С
1	Х	249	А
1	Х	253	А
1	Х	255	А
1	Х	256	С
1	Х	257	G
1	Х	259	U
1	Х	260	U
1	Х	261	G
1	Х	262	С
1	Х	263	G
1	Х	264	U
1	Х	265	U
1	Х	266	U
1	Х	268	G
1	Х	272	U
1	Х	273	U
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Mol	Chain	Res	Type
1	Х	274	G
1	Х	275	U
1	Х	276	А
1	Х	277	G
1	Х	279	А
1	Х	280	С
1	Х	303	С
1	Х	304	А
1	Х	305	А
1	Х	306	G
1	Х	310	А
1	Х	319	G
1	Х	321	А
1	Х	322	A
1	X	327	C
1	Х	340	G
1	Х	341	A
1	Х	342	G
1	X	344	G
1	Х	349	G
1	Х	358	C
1	Х	360	А
1	Х	362	С
1	Х	384	А
1	Х	385	G
1	Х	386	U
1	Х	387	А
1	Х	399	G
1	Х	400	U
1	Х	401	G
1	Х	403	A
1	Х	405	С
1	Х	408	U
1	Х	409	G
1	Х	413	G
1	Х	416	U
1	Х	418	С
1	Х	419	G
1	Х	424	G
1	Х	425	A
1	Х	441	A
1	X	456	C



Mol	Chain	Res	Type
1	Х	461	A
1	Х	463	С
1	Х	467	U
1	Х	469	G
1	Х	478	G
1	Х	482	А
1	Х	483	А
1	Х	484	G
1	Х	486	U
1	Х	492	G
1	Х	508	G
1	Х	514	G
1	Х	515	A
1	Х	516	G
1	Х	518	A
1	Х	519	С
1	Х	520	С
1	Х	521	U
1	Х	526	С
1	Х	534	U
1	Х	537	С
1	Х	540	G
1	Х	541	С
1	Х	542	А
1	Х	543	G
1	Х	544	U
1	Х	551	А
1	Х	553	С
1	Х	554	U
1	X	555	U
1	X	556	A
1	X	559	С
1	Х	560	G
1	Х	571	U
1	X	572	G
1	X	577	U
1	Х	578	U
1	Х	580	А
1	Х	582	G
1	Х	584	А
1	X	587	A
1	Х	589	С



$\mathbf{Mol}$	Chain	Res	Type
1	Х	595	А
1	Х	596	С
1	Х	600	G
1	Х	601	А
1	Х	613	А
1	Х	614	G
1	Х	615	С
1	Х	624	А
1	Х	625	А
1	Х	626	А
1	Х	627	А
1	Х	628	А
1	Х	631	G
1	Х	632	А
1	Х	642	А
1	Х	645	G
1	Х	646	С
1	Х	648	А
1	Х	649	G
1	Х	653	G
1	Х	654	А
1	Х	655	А
1	Х	657	А
1	Х	665	А
1	Х	666	U
1	Х	667	U
1	Х	668	А
1	Х	682	G
1	Х	699	G
1	X	733	G
1	X	743	A
1	Х	747	А
1	Х	752	G
1	Х	753	U
1	Х	754	G
1	Х	759	С
1	Х	760	U
1	X	761	G
1	Х	766	А
1	Х	767	G
1	Х	775	U
1	Х	778	G



Mol	Chain	Res	Type
1	Х	788	G
1	Х	789	G
1	Х	795	A
1	Х	797	A
1	Х	798	G
1	Х	802	A
1	Х	803	С
1	Х	804	С
1	Х	805	G
1	Х	806	A
1	Х	818	G
1	Х	825	С
1	Х	832	A
1	Х	840	U
1	Х	841	G
1	Х	843	G
1	Х	844	G
1	Х	859	U
1	Х	860	U
1	Х	872	G
1	Х	877	G
1	Х	878	С
1	Х	879	А
1	Х	887	G
1	Х	890	U
1	Х	891	А
1	Х	921	А
1	Х	922	А
1	Х	924	С
1	Х	926	С
1	X	927	C
1	Х	929	А
1	X	939	С
1	Х	941	U
1	Х	945	G
1	Х	949	G
1	Х	952	A
1	X	955	G
1	Х	957	G
1	X	961	G
1	Х	964	A
1	Х	969	U



Mol	Chain	Res	Type
1	Х	970	A
1	X	972	C
1	X	973	U
1	X	983	G
1	X	984	A
1	X	985	G
1	Х	994	A
1	Х	995	А
1	Х	1000	G
1	Х	1004	А
1	Х	1006	С
1	Х	1007	A
1	Х	1010	U
1	Х	1014	G
1	Х	1016	С
1	Х	1017	С
1	Х	1021	А
1	Х	1022	А
1	Х	1023	U
1	Х	1024	G
1	Х	1027	С
1	Х	1033	G
1	Х	1034	U
1	Х	1036	G
1	Х	1042	G
1	Х	1043	А
1	Х	1044	U
1	Х	1047	G
1	Х	1049	С
1	Х	1054	С
1	X	1055	A
1	Х	1056	U
1	Х	1057	А
1	X	1058	G
1	X	1060	C
1	X	1061	A
1	Х	1064	С
1	X	1068	А
1	X	1069	G
1	X	1070	G
1	X	1071	U
1	X	1073	G



Mol	Chain	Res	Type
1	Х	1075	С
1	Х	1076	U
1	Х	1081	А
1	Х	1082	G
1	Х	1083	С
1	Х	1084	А
1	Х	1085	G
1	Х	1087	С
1	Х	1090	С
1	Х	1094	С
1	Х	1097	А
1	Х	1098	G
1	Х	1099	А
1	Х	1100	G
1	Х	1101	U
1	X	1102	G
1	Х	1103	С
1	Х	1105	U
1	Х	1106	А
1	Х	1114	А
1	Х	1115	С
1	Х	1122	А
1	Х	1123	G
1	Х	1124	U
1	Х	1127	С
1	Х	1128	G
1	Х	1129	A
1	Х	1130	U
1	Х	1142	G
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	Х	1154	A
1	X	1155	G
1	X	1156	U
1	X	1161	U
1	Х	1180	A
1	Х	1182	U
1	X	1183	C
1	Х	1192	A
1	Х	1193	G
1	X	1223	G



Mol	Chain	Res	Type
1	Х	1224	A
1	Х	1225	G
1	Х	1227	А
1	Х	1231	A
1	Х	1232	U
1	Х	1234	С
1	Х	1240	G
1	Х	1247	U
1	Х	1249	G
1	Х	1251	G
1	Х	1253	С
1	Х	1260	А
1	Х	1261	G
1	Х	1263	G
1	Х	1266	G
1	Х	1267	A
1	Х	1268	U
1	Х	1269	G
1	Х	1284	G
1	Х	1285	А
1	Х	1288	А
1	Х	1300	А
1	Х	1301	U
1	Х	1302	С
1	Х	1311	С
1	Х	1313	U
1	Х	1314	А
1	Х	1315	А
1	Х	1319	С
1	Х	1326	U
1	Х	1332	G
1	Х	1334	A
1	Х	1337	G
1	Х	1342	U
1	X	1345	G
1	Х	1351	G
1	Х	1354	А
1	X	1365	U
1	Х	1372	A
1	Х	1377	G
1	Х	1378	А
1	Х	1379	А



Mol	Chain	Res	Type
1	Х	1381	G
1	Х	1391	А
1	Х	1392	U
1	Х	1393	G
1	Х	1398	G
1	Х	1403	U
1	Х	1404	С
1	Х	1405	А
1	Х	1408	А
1	Х	1409	U
1	Х	1410	U
1	Х	1428	G
1	Х	1429	А
1	Х	1430	G
1	Х	1432	G
1	Х	1433	А
1	Х	1434	U
1	Х	1435	G
1	Х	1440	G
1	Х	1442	С
1	Х	1443	G
1	Х	1447	U
1	Х	1460	G
1	Х	1463	А
1	Х	1466	С
1	Х	1467	U
1	Х	1468	А
1	Х	1469	U
1	Х	1470	G
1	X	1471	G
1	X	1474	A
1	X	1476	G
1	Х	1482	U
1	Х	1490	U
1	X	1497	С
1	X	1498	G
1	Х	1500	U
1	X	1505	U
1	X	1509	A
1	X	1513	U
1	Х	1519	G
1	Х	1522	С



Mol	Chain	Res	Type
1	Х	1529	С
1	Х	1531	С
1	Х	1544	А
1	Х	1545	G
1	Х	1562	G
1	Х	1571	G
1	Х	1574	А
1	Х	1575	С
1	Х	1576	G
1	Х	1581	С
1	Х	1582	А
1	Х	1585	А
1	Х	1594	U
1	Х	1599	G
1	Х	1601	U
1	Х	1602	G
1	Х	1603	А
1	Х	1623	С
1	Х	1624	А
1	Х	1626	А
1	Х	1632	А
1	Х	1642	G
1	Х	1648	С
1	Х	1651	U
1	Х	1656	U
1	Х	1657	А
1	Х	1660	G
1	Х	1661	С
1	Х	1662	G
1	Х	1664	G
1	X	1665	C
1	X	1668	G
1	X	1669	А
1	X	1670	G
1	X	1671	A
1	X	1676	U
1	X	1688	U
1	X	1689	U
1	X	1691	G
1	X	1692	С
1	Х	1693	А
1	Х	1695	U



Mol	Chain	Res	Type
1	Х	1699	A
1	Х	1705	U
1	Х	1710	U
1	Х	1713	G
1	Х	1714	A
1	Х	1717	А
1	Х	1739	G
1	Х	1747	G
1	Х	1749	G
1	Х	1753	А
1	Х	1754	G
1	Х	1755	G
1	Х	1764	A
1	Х	1770	U
1	Х	1771	A
1	Х	1772	С
1	Х	1773	С
1	Х	1782	А
1	Х	1788	С
1	Х	1790	G
1	Х	1791	С
1	Х	1792	С
1	Х	1793	А
1	Х	1799	А
1	Х	1801	С
1	Х	1802	А
1	Х	1805	G
1	Х	1807	А
1	Х	1808	С
1	X	1811	А
1	X	1819	U
1	X	1821	A
1	X	1825	C
1	X	1826	U
1	Х	1827	G
1	X	1830	C
1	X	1831	G
1	X	1832	G
1	X	1835	C
1	X	1839	A
1	X	1840	A
1	X	1850	G



Mol	Chain	Res	Type
1	Х	1855	G
1	Х	1857	G
1	Х	1867	А
1	Х	1871	G
1	Х	1872	А
1	Х	1883	А
1	Х	1885	С
1	Х	1887	G
1	Х	1888	С
1	Х	1889	G
1	Х	1890	G
1	Х	1891	С
1	Х	1909	U
1	Х	1910	A
1	Х	1911	A
1	Х	1912	G
1	Х	1920	А
1	Х	1921	А
1	Х	1922	U
1	Х	1924	С
1	Х	1928	G
1	Х	1934	U
1	Х	1938	U
1	Х	1939	U
1	Х	1945	С
1	Х	1946	U
1	Х	1947	G
1	Х	1948	С
1	Х	1949	А
1	X	1950	С
1	X	1951	G
1	Х	1953	А
1	Х	1954	A
1	Х	1955	G
1	Х	1957	С
1	Х	1958	G
1	X	1959	U
1	Х	1960	A
1	Х	1965	U
1	X	1971	C
1	Х	1975	G
1	X	1976	U



$\mathbf{Mol}$	Chain	Res	Type
1	Х	1979	C
1	Х	1980	A
1	Х	1993	G
1	Х	2003	A
1	Х	2006	G
1	Х	2014	A
1	Х	2015	G
1	Х	2026	С
1	Х	2033	С
1	Х	2038	С
1	Х	2039	G
1	Х	2043	A
1	Х	2044	G
1	Х	2046	C
1	Х	2047	С
1	Х	2052	G
1	Х	2076	G
1	Х	2077	G
1	Х	2079	A
1	Х	2082	С
1	Х	2088	U
1	Х	2089	С
1	Х	2090	U
1	Х	2167	А
1	Х	2168	А
1	Х	2170	С
1	Х	2171	U
1	Х	2172	U
1	Х	2176	U
1	Х	2181	A
1	Х	2188	A
1	Х	2189	A
1	Х	2190	A
1	Х	2191	A
1	Х	2192	U
1	Х	2196	U
1	Х	2197	U
1	Х	2198	U
1	Х	2199	С
1	Х	2204	A
1	Х	2205	С
1	Х	2217	G



Mol	Chain	Res	Type
1	Х	2218	G
1	Х	2222	U
1	Х	2226	A
1	Х	2231	G
1	Х	2245	А
1	Х	2247	A
1	Х	2252	А
1	Х	2258	G
1	Х	2262	С
1	Х	2265	А
1	Х	2266	А
1	Х	2267	А
1	Х	2268	G
1	Х	2269	G
1	Х	2274	С
1	Х	2275	U
1	Х	2283	G
1	Х	2284	U
1	Х	2286	G
1	Х	2287	G
1	Х	2290	A
1	Х	2294	U
1	Х	2298	U
1	Х	2299	A
1	Х	2301	А
1	Х	2304	G
1	Х	2305	С
1	Х	2306	A
1	Х	2307	А
1	Х	2313	G
1	X	2314	A
1	Х	2315	A
1	X	2322	U
1	X	2323	U
1	X	2324	G
1	X	2326	C
1	X	2329	C
1	X	2331	A
1	X	2333	A
1	X	2339	A
1	X	2351	G
1	X	2358	C
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Mol	Chain	Res	Type
1	Х	2361	G
1	Х	2362	G
1	Х	2363	G
1	Х	2364	С
1	Х	2367	A
1	Х	2368	G
1	Х	2369	U
1	Х	2373	С
1	Х	2375	G
1	Х	2386	G
1	Х	2389	G
1	Х	2399	С
1	Х	2401	A
1	Х	2402	U
1	Х	2403	С
1	Х	2404	A
1	Х	2407	G
1	Х	2408	G
1	Х	2409	А
1	Х	2410	U
1	Х	2413	А
1	Х	2415	G
1	Х	2420	С
1	Х	2424	G
1	Х	2426	G
1	Х	2427	А
1	Х	2429	А
1	Х	2449	G
1	Х	2452	U
1	X	2455	A
1	X	2461	G
1	Х	2464	G
1	X	2466	G
1	X	2468	G
1	Х	2469	G
1	X	2471	U
1	X	2473	G
1	X	2477	C
1	X	2479	U
1	X	2480	C
1	Х	2481	G
1	Х	2482	A



1       X $2483$ U         1       X $2484$ G         1       X $2492$ G         1       X $2497$ A         1       X $2497$ A         1       X $2508$ G         1       X $2509$ A         1       X $2509$ A         1       X $2522$ G         1       X $2533$ U         1       X $2533$ U         1       X $2535$ C         1       X $2543$ A         1       X $2545$ A         1       X $2545$ A         1       X $2551$ A         1       X $2553$ G         1       X $2556$ A         1       X $2556$ A         1       X $2566$ A         1       X $2566$ A         1       X $2578$ G	Mol	Chain	Res	Type
1       X $2484$ G         1       X $2486$ C         1       X $2492$ G         1       X $2497$ A         1       X $2508$ G         1       X $2509$ A         1       X $2522$ G         1       X $2523$ G         1       X $2533$ U         1       X $2533$ U         1       X $2543$ A         1       X $2545$ A         1       X $2546$ G         1       X $2551$ A         1       X $2552$ C         1       X $2553$ G         1       X $2556$ A         1       X $2556$ A         1       X $2566$ A         1       X $2566$ A         1       X $2573$ C         1       X $25778$ G	1	Х	2483	U
1       X $2486$ C         1       X $2492$ G         1       X $2497$ A         1       X $2508$ G         1       X $2509$ A         1       X $2522$ G         1       X $2523$ G         1       X $2533$ U         1       X $2533$ U         1       X $2533$ U         1       X $2543$ A         1       X $2545$ A         1       X $2545$ A         1       X $2548$ G         1       X $2545$ A         1       X $2552$ C         1       X $2553$ G         1       X $2555$ A         1       X $2556$ A         1       X $2566$ A         1       X $2566$ A         1       X $2578$ G	1	Х	2484	G
1         X $2492$ G           1         X $2497$ A           1         X $2508$ G           1         X $2509$ A           1         X $2522$ G           1         X $2523$ G           1         X $2533$ U           1         X $2533$ U           1         X $2533$ U           1         X $2543$ A           1         X $2543$ A           1         X $2545$ A           1         X $2545$ A           1         X $2551$ A           1         X $2552$ C           1         X $2553$ G           1         X $2553$ G           1         X $2553$ G           1         X $2559$ U           1         X $2566$ A           1         X </td <td>1</td> <td>Х</td> <td>2486</td> <td>С</td>	1	Х	2486	С
1         X         2497         A           1         X         2508         G           1         X         2509         A           1         X         2522         G           1         X         2528         G           1         X         2531         U           1         X         2533         U           1         X         2535         C           1         X         2543         A           1         X         2543         A           1         X         2545         A           1         X         2545         A           1         X         2546         G           1         X         2551         A           1         X         2553         G           1         X         2556         A           1         X         2559         U           1         X         2566         A           1         X         2566         A           1         X         2566         A           1         X         2573         C<	1	Х	2492	G
1       X       2508       G         1       X       2509       A         1       X       2522       G         1       X       2528       G         1       X       2531       U         1       X       2533       U         1       X       2535       C         1       X       2543       A         1       X       2545       A         1       X       2545       A         1       X       2546       G         1       X       2548       G         1       X       2551       A         1       X       2553       G         1       X       2553       G         1       X       2553       G         1       X       2553       G         1       X       2559       U         1       X       2560       G         1       X       2564       U         1       X       2566       A         1       X       2578       G         1       X	1	Х	2497	А
1         X         2509         A           1         X         2522         G           1         X         2531         U           1         X         2533         U           1         X         2533         U           1         X         2535         C           1         X         2543         A           1         X         2545         A           1         X         2551         A           1         X         2552         C           1         X         2553         G           1         X         2559         U           1         X         2559         U           1         X         2564         U           1         X         2565         C           1         X         2573         C           1         X         2579         A<	1	Х	2508	G
1       X $2522$ G         1       X $2528$ G         1       X $2531$ U         1       X $2533$ U         1       X $2535$ C         1       X $2535$ C         1       X $2543$ A         1       X $2545$ A         1       X $2546$ G         1       X $2546$ G         1       X $2551$ A         1       X $2553$ G         1       X $2555$ C         1       X $2556$ A         1       X $2559$ U         1       X $2560$ G         1       X $2564$ U         1       X $2566$ A         1       X $2573$ C         1       X $2578$ G         1       X $2579$ A         1       X $2591$ C      1	1	Х	2509	А
1       X       2528       G         1       X       2531       U         1       X       2533       U         1       X       2535       C         1       X       2543       A         1       X       2545       A         1       X       2545       A         1       X       2546       G         1       X       2548       G         1       X       2551       A         1       X       2552       C         1       X       2553       G         1       X       2556       A         1       X       2556       A         1       X       2560       G         1       X       2564       U         1       X       2565       C         1       X       2573       C         1       X       2566       A         1       X       2578       G         1       X       2579       A         1       X       2580       C         1       X	1	Х	2522	G
1       X $2531$ U         1       X $2533$ U         1       X $2535$ C         1       X $2543$ A         1       X $2545$ A         1       X $2546$ G         1       X $2546$ G         1       X $2548$ G         1       X $2551$ A         1       X $2552$ C         1       X $2556$ A         1       X $2556$ A         1       X $2566$ G         1       X $2561$ G         1       X $2564$ U         1       X $2566$ A         1       X $2573$ C         1       X $2578$ G         1       X $2579$ A         1       X $2580$ C         1       X $2591$ C         1       X $2609$ G	1	Х	2528	G
1       X $2533$ U         1       X $2535$ C         1       X $2543$ A         1       X $2545$ A         1       X $2546$ G         1       X $2546$ G         1       X $2546$ G         1       X $2551$ A         1       X $2552$ C         1       X $2553$ G         1       X $2556$ A         1       X $2556$ A         1       X $2560$ G         1       X $2564$ U         1       X $2565$ C         1       X $2566$ A         1       X $2573$ C         1       X $2578$ G         1       X $2580$ C         1       X $2591$ C         1       X $2619$ G         1       X $2619$ G	1	Х	2531	U
1       X       2535       C         1       X       2543       A         1       X       2545       A         1       X       2546       G         1       X       2546       G         1       X       2548       G         1       X       2551       A         1       X       2552       C         1       X       2553       G         1       X       2556       A         1       X       2559       U         1       X       2560       G         1       X       2561       G         1       X       2565       C         1       X       2566       A         1       X       2566       A         1       X       2573       C         1       X       2578       G         1       X       2580       C         1       X       2588       U         1       X       2609       G         1       X       2611       A         1       X	1	Х	2533	U
1       X       2543       A         1       X       2545       A         1       X       2546       G         1       X       2548       G         1       X       2551       A         1       X       2552       C         1       X       2553       G         1       X       2556       A         1       X       2559       U         1       X       2560       G         1       X       2561       G         1       X       2565       C         1       X       2566       A         1       X       2566       A         1       X       2566       A         1       X       2573       C         1       X       2578       G         1       X       2580       C         1       X       2588       U         1       X       2609       G         1       X       2611       A         1       X       2619       G         1       X	1	Х	2535	С
1       X       2545       A         1       X       2546       G         1       X       2548       G         1       X       2551       A         1       X       2552       C         1       X       2553       G         1       X       2556       A         1       X       2556       A         1       X       2557       U         1       X       2556       A         1       X       2560       G         1       X       2561       G         1       X       2565       C         1       X       2566       A         1       X       2566       A         1       X       2566       A         1       X       2573       C         1       X       2579       A         1       X       2579       A         1       X       2580       C         1       X       2609       G         1       X       2611       A         1       X	1	Х	2543	A
1       X       2546       G         1       X       2548       G         1       X       2551       A         1       X       2552       C         1       X       2553       G         1       X       2553       G         1       X       2556       A         1       X       2556       A         1       X       2560       G         1       X       2561       G         1       X       2565       C         1       X       2566       A         1       X       2573       C         1       X       2579       A         1       X       2580       C         1       X       2591       C         1       X       2609       G         1       X       2611       A         1       X	1	Х	2545	A
1       X       2548       G         1       X       2551       A         1       X       2552       C         1       X       2553       G         1       X       2556       A         1       X       2559       U         1       X       2560       G         1       X       2561       G         1       X       2565       C         1       X       2566       A         1       X       2566       A         1       X       2566       A         1       X       2566       A         1       X       2573       C         1       X       2578       G         1       X       2579       A         1       X       2580       C         1       X       2588       U         1       X       2609       G         1       X       2611       A         1       X       2612       G         1       X       2633       A         1       X	1	Х	2546	G
1       X $2551$ A         1       X $2552$ C         1       X $2553$ G         1       X $2553$ G         1       X $2556$ A         1       X $2559$ U         1       X $2559$ U         1       X $2560$ G         1       X $2561$ G         1       X $2565$ C         1       X $2566$ A         1       X $2566$ A         1       X $2566$ A         1       X $2566$ A         1       X $2573$ C         1       X $2579$ A         1       X $2580$ C         1       X $2591$ C         1       X $2609$ G         1       X $2609$ G         1       X $2611$ A         1       X $2660$ C	1	Х	2548	G
1X $2552$ C1X $2553$ G1X $2556$ A1X $2556$ A1X $2550$ U1X $2560$ G1X $2561$ G1X $2564$ U1X $2565$ C1X $2566$ A1X $2573$ C1X $2578$ G1X $2579$ A1X $2580$ C1X $2580$ C1X $2591$ C1X $2609$ G1X $2611$ A1X $2611$ A1X $2611$ A1X $2660$ C1X $2660$ C1X $2660$ C1X $2677$ U1X $2678$ C1X $2678$ C1X $2692$ A	1	Х	2551	А
1X $2553$ G1X $2556$ A1X $2559$ U1X $2560$ G1X $2561$ G1X $2564$ U1X $2565$ C1X $2566$ A1X $2573$ C1X $2578$ G1X $2579$ A1X $2579$ A1X $2580$ C1X $2588$ U1X $2591$ C1X $2609$ G1X $2611$ A1X $2612$ G1X $2660$ C1X $2660$ C1X $2660$ C1X $2668$ U1X $2677$ U1X $2678$ C1X $2692$ A	1	Х	2552	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2553	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2556	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2559	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2560	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2561	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2564	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2565	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2566	A
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2573	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2578	G
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2579	A
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2580	С
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Х	2588	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2591	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2609	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2611	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2619	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2621	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2633	А
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2660	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2668	U
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Х	2677	U
1 X 2692 A	1	Х	2678	С
	1	Х	2692	A



Mol	Chain	Res	Type
1	Х	2693	U
1	Х	2694	G
1	Х	2697	G
1	Х	2698	G
1	Х	2705	A
1	Х	2706	U
1	Х	2707	G
1	Х	2711	G
1	Х	2713	А
1	Х	2714	А
1	Х	2728	А
1	Х	2731	G
1	Х	2732	С
1	Х	2736	U
1	Х	2737	A
1	Х	2738	A
1	Х	2743	G
1	Х	2744	A
1	Х	2745	А
1	Х	2746	G
1	Х	2751	С
1	Х	2757	G
1	Х	2758	А
1	Х	2759	U
1	Х	2760	G
1	Х	2769	С
1	Х	2771	C
1	Х	2772	U
1	X	2783	U
1	Х	2792	С
1	X	2795	A
1	X	2796	A
1	Х	2807	U
1	Х	2808	U
1	Х	2809	A
1	Х	2810	A
1	Х	2825	A
1	Х	2838	U
1	Х	2843	A
1	Х	2847	G
1	X	2851	G
1	Х	2855	С



Mol	Chain	Res	Type
1	Х	2858	А
1	Х	2860	С
1	Х	2861	А
1	Х	2864	С
1	Х	2866	А
1	Х	2867	G
1	Х	2868	G
2	Y	3	А
2	Y	6	С
2	Y	15	А
2	Y	16	U
2	Y	17	А
2	Y	18	G
2	Y	26	G
2	Y	27	А
2	Y	28	А
2	Y	29	С
2	Y	37	С
2	Y	39	С
2	Y	40	С
2	Y	43	G
2	Y	44	С
2	Y	45	С
2	Y	49	С
2	Y	54	U
2	Y	58	G
2	Y	68	A
2	Y	69	G
2	Y	84	G
2	Y	102	A
2	Y	108	G
2	Y	112	A
2	Y	121	G
2	Y	122	U
2	Y	123	U

Continued from previous page...

All (69) RNA pucker outliers are listed below:

Mol	Chain	Res	Type	
1	Х	38	G	
1	Х	48	А	
1	Х	50	G	



Mol	Chain	Res	Type		
1	Х	100	G		
1	Х	148	С		
1	Х	209	G		
1	Х	219	G		
1	Х	265	U		
1	Х	341	А		
1	Х	343	А		
1	Х	490	А		
1	Х	518	А		
1	Х	537	С		
1	Х	540	G		
1	Х	555	U		
1	Х	559	С		
1	Х	600	G		
1	Х	751	G		
1	Х	759	С		
1	Х	788	G		
1	Х	797	А		
1	Х	803	С		
1	Х	804	С		
1	Х	813	А		
1	Х	843	G		
1	Х	859	U		
1	Х	890	U		
1	Х	971	А		
1	Х	972	С		
1	Х	994	А		
1	Х	1053	G		
1	Х	1086	С		
1	X	1096	A		
1	Х	1122	А		
1	Х	1145	С		
1	X	1153	A		
1	Х	1299	А		
1	Х	1391	А		
1	Х	1403	U		
1	Х	1439	G		
1	X	1473	U		
1	Х	1475	U		
1	Х	1496	G		
1	Х	1691	G		
1	X	1749	G		



Mol	Chain	Res	Type
1	Х	1790	G
1	Х	1800	А
1	Х	1830	С
1	Х	1909	U
1	Х	1910	А
1	Х	2043	А
1	Х	2180	U
1	Х	2190	А
1	Х	2312	А
1	Х	2322	U
1	Х	2323	U
1	Х	2402	U
1	Х	2414	А
1	Х	2437	G
1	Х	2460	G
1	Х	2469	G
1	Х	2564	U
1	Х	2705	А
1	Х	2807	U
1	Х	2848	А
2	Y	14	С
2	Y	28	А
2	Y	36	А
2	Y	68	А

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 285 ligands modelled in this entry, 277 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



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Mal	Turne	Chain	Dec Link		Bond lengths			Bond angles		
10101	Tor Type Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
29	MIV	Х	2901	-	51,51,51	0.72	2 (3%)	62,71,71	1.42	7 (11%)
31	SPD	Х	3166	-	9,9,9	0.38	0	8,8,8	0.64	0
31	SPD	Х	3167	1	9,9,9	0.32	0	8,8,8	1.00	0
31	SPD	Х	3168	1	9,9,9	0.42	0	8,8,8	0.96	0
31	SPD	Х	3170	1	9,9,9	0.47	0	8,8,8	1.19	1 (12%)
31	SPD	Х	3171	-	9,9,9	0.28	0	8,8,8	0.66	0
31	SPD	V	101	-	9,9,9	0.29	0	8,8,8	0.85	0
31	SPD	X	3169	1	9,9,9	0.37	0	8,8,8	1.08	1 (12%)

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).

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
29	MIV	Х	2901	-	-	25/55/91/91	0/2/3/3
31	SPD	Х	3166	-	-	3/7/7/7	-
31	SPD	Х	3167	1	-	2/7/7/7	-
31	SPD	Х	3168	1	-	3/7/7/7	-
31	SPD	Х	3170	1	-	4/7/7/7	-
31	SPD	Х	3171	-	-	3/7/7/7	-
31	SPD	V	101	-	-	5/7/7/7	_
31	SPD	Х	3169	1	-	3/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
29	Х	2901	MIV	O6-C24	2.84	1.40	1.34
29	Х	2901	MIV	C31-C33	2.81	1.58	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
29	Х	2901	MIV	O6-C25-C26	-5.97	97.39	106.92
29	Х	2901	MIV	O6-C25-C28	4.22	116.68	107.42
29	Х	2901	MIV	C32-O8-C31	3.85	124.64	114.52



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
29	Х	2901	MIV	O11-C30-C31	3.55	116.55	109.51
31	Х	3170	SPD	C8-C7-N6	2.87	119.88	112.14
29	Х	2901	MIV	C30-O11-C36	2.23	117.50	113.67
31	Х	3169	SPD	C7-N6-C5	2.16	123.65	113.45
29	Х	2901	MIV	C13-C14-N	2.03	116.71	110.83
29	Х	2901	MIV	C27-C26-C25	-2.03	107.69	113.27

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
29	Х	2901	MIV	C17-C14-N-C15
29	Х	2901	MIV	C13-C14-N-C15
29	Х	2901	MIV	C5-C6-C8-C9
29	Х	2901	MIV	O1-C5-C6-C7
29	Х	2901	MIV	C4-C5-C6-C7
29	Х	2901	MIV	C2-C1-C28-C29
29	Х	2901	MIV	O6-C25-C28-C1
29	Х	2901	MIV	C26-C25-C28-C1
29	Х	2901	MIV	C26-C25-C28-C29
29	Х	2901	MIV	C1-C28-C29-O7
29	Х	2901	MIV	C25-C28-C29-O7
29	Х	2901	MIV	O11-C30-O7-C29
29	Х	2901	MIV	C30-C31-O8-C32
31	Х	3170	SPD	C4-C5-N6-C7
31	Х	3171	SPD	C4-C5-N6-C7
31	V	101	SPD	C3-C4-C5-N6
31	Х	3168	SPD	C2-C3-C4-C5
29	Х	2901	MIV	C17-C14-N-C16
29	Х	2901	MIV	C31-C30-O7-C29
31	Х	3169	SPD	C3-C4-C5-N6
29	Х	2901	MIV	C11-C20-C22-C23
31	V	101	SPD	C7-C8-C9-N10
31	Х	3169	SPD	C2-C3-C4-C5
29	Х	2901	MIV	C1-C2-C3-C4
29	Х	2901	MIV	C22-C23-C24-O6
31	Х	3166	SPD	C2-C3-C4-C5
31	Х	3170	SPD	C2-C3-C4-C5
31	Х	3166	SPD	N6-C7-C8-C9
29	Х	2901	MIV	C21-C20-C22-C23
31	Х	3169	SPD	C7-C8-C9-N10
31	Х	3166	SPD	N1-C2-C3-C4

All (48) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
29	Х	2901	MIV	C22-C23-C24-O5
29	Х	2901	MIV	C7-C6-C8-C9
29	Х	2901	MIV	C2-C1-C28-C25
29	Х	2901	MIV	O1-C5-C6-C8
31	Х	3167	SPD	C7-C8-C9-N10
31	Х	3170	SPD	C7-C8-C9-N10
31	Х	3171	SPD	C2-C3-C4-C5
31	Х	3170	SPD	C8-C7-N6-C5
31	Х	3171	SPD	C8-C7-N6-C5
29	Х	2901	MIV	C6-C8-C9-C10
31	V	101	SPD	C8-C7-N6-C5
31	Х	3168	SPD	N1-C2-C3-C4
31	Х	3167	SPD	C2-C3-C4-C5
31	Х	3168	SPD	C8-C7-N6-C5
31	V	101	SPD	C4-C5-N6-C7
31	V	101	SPD	N6-C7-C8-C9
29	Х	2901	MIV	C28-C25-C26-C27

Continued from previous page...

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Х	2901	MIV	8	0
31	Х	3167	SPD	6	0
31	Х	3168	SPD	3	0
31	Х	3170	SPD	3	0
31	Х	3171	SPD	2	0
31	Х	3169	SPD	1	0

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





# 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	Х	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Х	282:A	O3'	302:U	Р	65.10
1	Х	362:C	O3'	380:C	Р	54.16
1	Х	2090:U	O3'	2165:A	Р	19.14
1	Х	1184:G	O3'	1191:G	Р	18.52
1	Х	2773:G	O3'	2779:A	Р	17.92
1	Х	1522:C	O3'	1526:U	Р	17.66
1	Х	725:C	O3'	732:G	Р	16.37
1	Х	1546:C	O3'	1558:C	Р	15.65
1	Х	1891:C	O3'	1908:C	Р	14.39
1	Х	1732:U	O3'	1735:G	Р	9.97
1	X	891:A	O3'	911:A	P	7.98



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Х	724:C	O3'	725:C	Р	4.77



# 6 Fit of model and data (i)

# 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	Х	2699/2699~(100%)	0.43	183 (6%) 17 19	37, 96, 191, 312	0
2	Y	122/122~(100%)	0.51	10 (8%) 11 13	95, 183, 226, 251	0
3	А	271/271~(100%)	0.76	39 (14%) 2 3	79, 131, 162, 170	0
4	В	206/206~(100%)	0.16	8 (3%) 39 38	40, 64, 80, 85	0
5	С	195/195~(100%)	0.47	22 (11%) 5 6	60, 122, 150, 159	0
6	D	176/176~(100%)	0.80	33 (18%) 1 1	168, 207, 227, 235	0
7	Е	171/171~(100%)	0.76	35~(20%) 1 1	98, 144, 186, 190	0
8	G	142/142~(100%)	0.22	5 (3%) 44 43	60, 95, 107, 115	0
9	Н	134/134~(100%)	0.04	2 (1%) 73 72	46, 57, 64, 69	0
10	Ι	137/137~(100%)	0.78	21 (15%) 2 2	67, 141, 180, 192	0
11	J	134/134~(100%)	0.43	9 (6%) 17 19	71, 103, 126, 132	0
12	Κ	115/115~(100%)	-0.01	0 100 100	40, 47, 54, 58	0
13	L	104/104~(100%)	0.72	18 (17%) 1 1	159, 198, 226, 237	0
14	М	118/118~(100%)	-0.14	1 (0%) 86 85	46, 56, 69, 74	0
15	Ν	117/117~(100%)	0.42	5 (4%) 35 35	59, 94, 121, 127	0
16	Ο	98/98~(100%)	0.32	6 (6%) 21 22	66, 114, 134, 138	0
17	Р	129/129~(100%)	-0.13	0 100 100	49, 59, 82, 97	0
18	Q	93/93~(100%)	0.34	6 (6%) 18 20	85, 109, 125, 126	0
19	R	110/110~(100%)	0.35	9 (8%) 11 13	86, 103, 146, 156	0
20	S	175/175~(100%)	1.15	48 (27%) 0 0	113, 157, 176, 182	0
21	Т	72/72~(100%)	0.54	6 (8%) 11 13	87, 133, 147, 153	0
22	U	74/74~(100%)	0.88	12 (16%) 1 2	106, 144, 175, 178	0
23	V	54/54~(100%)	0.48	6 (11%) 5 6	116, 127, 154, 162	0
24	W	55/55~(100%)	0.83	7(12%) 3 4	88, 108, 128, 133	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(A^2)$	Q<0.9
25	Z	57/57~(100%)	0.02	0 100 100	47, 56, 70, 74	0
26	1	49/49~(100%)	0.69	$8\ (16\%)\ 1\ 2$	132, 148, 166, 168	0
27	2	46/46~(100%)	0.11	0 100 100	63, 86, 94, 96	0
28	3	63/63~(100%)	0.44	0 100 100	105, 115, 128, 134	0
All	All	5916/5916~(100%)	0.45	499 (8%) 11 13	37, 105, 203, 312	0

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#### All (499) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	S	82	ASP	9.5
1	Х	248	А	8.9
7	Е	123	PHE	8.6
6	D	153	ASP	8.6
1	Х	1095	А	8.1
20	S	93	GLU	7.8
1	Х	1602	G	7.7
1	Х	1072	U	7.7
1	Х	2089	С	7.5
10	Ι	67	ASN	7.4
20	S	68	ALA	7.3
3	А	101	GLU	7.1
3	А	100	GLY	7.0
1	Х	1085	G	6.9
13	L	30	SER	6.8
1	Х	1115	С	6.7
3	А	99	ASP	6.7
13	L	97	HIS	6.6
1	Х	250	С	6.6
20	S	81	VAL	6.4
6	D	94	GLU	6.4
10	Ι	72	TYR	6.3
13	L	40	ALA	6.1
1	Х	1099	А	6.1
4	В	206	ALA	6.1
20	S	67	LYS	5.9
20	S	86	VAL	5.8
1	Х	1080	А	5.6
1	Х	1073	G	5.6
20	S	83	PHE	5.6
1	Х	2088	U	5.5
1	Х	249	А	5.5



Mol	Chain	Res	Type	RSRZ
20	S	92	VAL	5.5
1	Х	1068	А	5.4
1	Х	2166	G	5.4
6	D	39	GLY	5.3
1	Х	1116	U	5.3
19	R	68	GLY	5.2
11	J	82	THR	5.2
1	Х	2169	А	5.1
1	Х	1516	А	5.1
22	U	47	HIS	5.1
3	А	98	ALA	5.1
20	S	51	LEU	5.0
1	Х	263	G	5.0
5	С	94	THR	4.9
1	Х	74	G	4.9
10	Ι	115	SER	4.9
19	R	69	GLN	4.9
6	D	23	SER	4.9
1	Х	1081	А	4.8
20	S	3	LEU	4.8
19	R	56	LYS	4.8
1	Х	192	G	4.8
7	Е	120	GLY	4.7
1	Х	75	С	4.7
1	Х	2090	U	4.7
6	D	22	TYR	4.7
1	Х	251	С	4.7
10	Ι	68	VAL	4.7
20	S	30	VAL	4.7
22	U	50	ALA	4.7
1	Х	427	С	4.7
3	А	171	ASP	4.7
20	S	69	VAL	4.7
22	U	7	LEU	4.7
1	Х	1059	A	4.7
26	1	40	TYR	4.6
1	Х	247	A	4.6
6	D	20	PHE	4.6
6	D	25	VAL	4.6
3	A	97	TYR	4.6
20	S	130	ILE	4.6
20	S	114	ASP	4.6



Mol	Chain	Res	Type	RSRZ
2	Y	2	С	4.5
19	R	54	ILE	4.5
1	Х	1060	С	4.5
1	Х	1071	U	4.4
1	Х	1057	А	4.4
1	Х	2170	С	4.4
7	Е	133	VAL	4.4
26	1	24	THR	4.4
1	Х	1098	G	4.4
1	Х	1082	G	4.3
1	Х	1507	А	4.3
20	S	171	VAL	4.3
3	А	72	LYS	4.3
1	Х	2290	A	4.3
20	S	65	LEU	4.2
1	Х	2082	С	4.2
16	0	23	GLU	4.2
20	S	14	LEU	4.2
1	Х	1603	А	4.1
20	S	21	ALA	4.1
24	W	43	MET	4.1
6	D	136	LEU	4.1
13	L	34	SER	4.1
24	W	40	VAL	4.1
6	D	144	ASP	4.1
22	U	61	TRP	4.1
11	J	122	ALA	4.1
1	Х	2171	U	4.0
7	Е	15	VAL	4.0
7	Е	68	THR	4.0
10	Ι	103	ASN	4.0
6	D	129	ASN	3.9
3	A	21	PHE	3.9
5	C	92	ASP	3.9
13	L	31	VAL	3.8
1	X	1084	A	3.8
15	N	91	ASN	3.8
23	V	36	GLN	3.8
1	Х	2270	U	3.7
24	W	7	ARG	3.7
4	В	139	GLY	3.7
1	Х	1079	G	3.7



Mol	Chain	Res	Type	RSRZ
1	Х	2280	А	3.7
10	Ι	24	GLY	3.7
7	Е	136	ILE	3.7
5	С	44	SER	3.7
22	U	35	THR	3.7
1	Х	2167	А	3.7
1	Х	1117	G	3.6
10	Ι	48	PHE	3.6
2	Y	111	С	3.6
1	Х	1094	С	3.6
1	Х	1515	U	3.6
4	В	135	HIS	3.6
3	А	19	ALA	3.6
13	L	8	ARG	3.6
3	А	132	PRO	3.5
1	Х	1888	С	3.5
26	1	27	ASN	3.5
1	Х	1114	А	3.5
1	Х	2174	G	3.5
3	А	12	SER	3.5
5	С	45	THR	3.5
5	С	193	LEU	3.5
7	Е	135	GLY	3.5
26	1	21	TYR	3.5
10	Ι	92	THR	3.5
9	Н	20	MET	3.5
1	Х	2731	G	3.4
6	D	141	ILE	3.4
19	R	55	THR	3.4
20	S	148	THR	3.4
10	Ι	49	PHE	3.4
18	Q	17	TYR	3.4
1	Х	1090	С	3.4
1	Х	431	G	3.4
1	X	260	U	3.4
1	Х	76	С	3.4
6	D	72	LYS	3.4
10	Ι	47	ALA	3.4
8	G	91	THR	3.3
20	S	63	PRO	3.3
22	U	49	LYS	3.3
23	V	48	ARG	3.3



Mol	Chain	Res	Type	RSRZ
5	С	133	PHE	3.3
1	Х	429	С	3.3
20	S	15	ASP	3.3
1	Х	2078	G	3.3
13	L	96	TYR	3.3
13	L	89	PHE	3.3
2	Y	42	U	3.3
24	W	23	LEU	3.3
15	Ν	89	ASP	3.3
3	А	90	ALA	3.3
1	Х	430	С	3.3
10	Ι	63	ARG	3.3
20	S	166	LEU	3.3
1	Х	2165	A	3.3
5	С	161	ALA	3.3
22	U	58	LYS	3.3
1	Х	2279	G	3.3
1	Х	2610	G	3.3
21	Т	37	LEU	3.3
4	В	84	PHE	3.3
5	С	81	GLY	3.3
8	G	171	LEU	3.3
6	D	71	LYS	3.3
6	D	119	PRO	3.3
7	Е	131	ILE	3.3
20	S	19	ILE	3.3
24	W	26	ARG	3.2
16	0	22	VAL	3.2
13	L	52	ALA	3.2
1	Х	1517	С	3.2
1	Х	1913	G	3.2
3	А	162	SER	3.2
5	С	123	PHE	3.2
1	Х	1877	C	3.2
1	Х	$1\overline{604}$	A	3.2
1	Х	160	С	3.2
21	Т	22	GLY	3.2
6	D	3	GLN	3.2
1	Х	1062	G	3.2
1	Х	1599	G	3.2
1	Х	$2\overline{444}$	C	3.2
1	Х	259	U	3.2

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Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	Х	1069	G	3.2
1	Х	2168	А	3.2
10	Ι	65	PHE	3.2
1	Х	1183	С	3.2
3	А	170	SER	3.2
1	Х	2087	U	3.1
1	Х	48	А	3.1
1	Х	1077	U	3.1
7	Е	43	VAL	3.1
1	Х	1083	С	3.1
1	Х	190	А	3.1
1	Х	1086	С	3.1
24	W	22	ALA	3.1
20	S	22	VAL	3.1
7	Е	134	SER	3.1
18	Q	93	GLY	3.1
7	E	34	THR	3.0
1	Х	1087	С	3.0
11	J	123	GLY	3.0
22	U	73	GLY	3.0
1	Х	362	С	3.0
7	Е	174	GLY	3.0
1	Х	271	G	3.0
11	J	84	MET	3.0
1	Х	1097	А	3.0
20	S	20	ALA	3.0
1	Х	426	С	3.0
3	А	137	PRO	3.0
1	Х	381	С	3.0
3	А	242	ALA	3.0
26	1	14	SER	3.0
1	Х	2361	G	3.0
10	Ι	69	GLY	3.0
5	С	95	LEU	3.0
1	Х	732	G	2.9
1	Х	667	U	2.9
11	J	121	LEU	2.9
24	W	39	ALA	2.9
1	Х	1526	U	2.9
7	Е	83	TYR	2.9
1	Х	2291	U	2.9
1	Х	725	С	2.9



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Mol	Chain	Res	Type	RSRZ
1	Х	2390	А	2.9
1	Х	278	G	2.9
5	С	96	PRO	2.9
16	0	78	VAL	2.9
1	Х	1514	С	2.9
10	Ι	19	VAL	2.9
1	Х	1513	U	2.9
1	Х	1845	А	2.9
7	Е	121	VAL	2.8
6	D	120	ASN	2.8
1	Х	1120	С	2.8
10	Ι	15	ASP	2.8
22	U	60	VAL	2.8
1	Х	1050	G	2.8
4	В	138	PRO	2.8
6	D	152	MET	2.8
1	Х	382	U	2.8
11	J	14	PHE	2.8
1	Х	1912	G	2.8
26	1	41	ASP	2.8
7	Е	67	LEU	2.8
4	В	205	SER	2.8
3	А	254	THR	2.8
1	Х	653	G	2.8
1	Х	1430	G	2.8
6	D	26	MET	2.8
13	L	86	GLN	2.7
2	Y	123	U	2.7
6	D	145	MET	2.7
13	L	51	LEU	2.7
20	S	31	SER	2.7
7	Е	16	THR	2.7
1	Х	1154	А	2.7
3	А	91	ARG	2.7
20	S	85	MET	2.7
7	Е	52	VAL	2.7
13	L	32	TYR	2.7
1	Х	1427	G	2.7
2	Y	43	G	2.7
3	А	136	VAL	2.7
1	Х	1844	С	2.7
13	L	39	TYR	2.7



Mol	Chain	Res	Type	RSRZ
3	А	76	ASN	2.7
3	А	77	ALA	2.7
10	Ι	73	GLU	2.7
13	L	55	SER	2.7
2	Y	29	С	2.7
19	R	53	VAL	2.7
3	А	172	TYR	2.6
3	А	186	HIS	2.7
10	Ι	18	ARG	2.6
3	А	229	VAL	2.6
7	Е	175	LYS	2.6
11	J	80	ALA	2.6
3	А	102	LYS	2.6
7	Е	27	LYS	2.6
1	Х	191	G	2.6
11	J	107	VAL	2.6
19	R	57	ASN	2.6
1	Х	2077	G	2.6
1	Х	1522	С	2.6
10	Ι	81	GLN	2.6
1	Х	1887	G	2.6
6	D	30	ARG	2.6
5	С	91	TYR	2.6
22	U	46	LEU	2.6
1	Х	2323	U	2.6
7	Е	41	LEU	2.6
7	Е	42	THR	2.6
6	D	177	PHE	2.5
5	С	43	ALA	2.5
1	Х	2084	G	2.5
13	L	99	ARG	2.5
20	S	24	TYR	2.5
6	D	84	PRO	2.5
15	N	2	PRO	2.5
10	Ι	41	SER	2.5
1	X	116	A	2.5
1	X	428	A	2.5
1	X	2199	C	2.5
1	Х	1508	G	2.5
15	Ν	88	ILE	2.5
2	Y	68	A	2.5
20	S	66	VAL	2.5



Mol	Chain	Res	Type	RSRZ
1	Х	1056	U	2.5
1	Х	2389	G	2.5
1	Х	435	А	2.5
1	Х	1063	С	2.5
1	Х	1089	С	2.5
3	А	228	PRO	2.5
20	S	144	GLY	2.5
1	Х	225	G	2.5
6	D	132	ILE	2.5
6	D	85	VAL	2.4
7	Е	140	LEU	2.4
19	R	67	GLY	2.4
20	S	80	HIS	2.4
1	Х	1390	G	2.4
26	1	52	GLU	2.4
7	Е	101	LYS	2.4
20	S	2	GLU	2.4
1	Х	1106	A	2.4
20	S	147	ILE	2.4
4	В	168	GLN	2.4
7	Е	64	LEU	2.4
20	S	87	THR	2.4
1	Х	2326	С	2.4
5	С	84	PHE	2.4
19	R	28	LYS	2.4
1	Х	665	A	2.4
1	Х	1367	А	2.4
7	Е	50	LEU	2.4
20	S	94	VAL	2.4
7	Е	124	ALA	2.4
1	Х	436	А	2.4
23	V	52	GLN	2.4
7	Е	60	LYS	2.4
6	D	92	ARG	2.4
7	Е	122	THR	2.4
1	Х	1832	G	2.4
1	Х	1023	U	2.4
8	G	90	LEU	2.4
1	Х	1100	G	2.4
23	V	17	GLU	2.4
3	А	45	ASN	2.4
1	Х	2182	А	2.3

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Mol	Chain	Res	Type	RSRZ
1	Х	2325	А	2.3
3	А	168	LYS	2.3
1	Х	1096	А	2.3
16	0	6	GLN	2.3
1	Х	275	U	2.3
3	А	133	LEU	2.3
3	А	58	HIS	2.3
6	D	122	PHE	2.3
8	G	43	VAL	2.3
3	А	82	ILE	2.3
20	S	172	LEU	2.3
6	D	62	LEU	2.3
20	S	50	GLY	2.3
1	Х	154	U	2.3
7	Е	150	LYS	2.3
11	J	126	LEU	2.3
20	S	23	ALA	2.3
26	1	35	LEU	2.3
6	D	162	THR	2.3
1	Х	878	С	2.3
1	Х	1049	С	2.3
20	S	112	LEU	2.3
13	L	33	ARG	2.3
21	Т	61	ALA	2.3
1	Х	246	С	2.3
7	Е	30	LYS	2.3
1	Х	2269	G	2.3
3	А	9	TYR	2.3
20	S	84	TYR	2.3
5	С	157	THR	2.3
9	Н	8	LEU	2.3
1	Х	1872	А	2.3
22	U	6	TYR	2.3
1	Х	1067	G	2.2
1	Х	184	A	2.2
1	Х	270	G	2.2
3	А	59	LYS	2.2
23	V	37	LEU	2.2
18	Q	50	VAL	2.2
1	Х	2198	U	2.2
1	Х	1078	A	2.2
1	Х	1406	А	2.2



Mol	Chain	Res	Type	RSRZ
13	L	104	ALA	2.2
3	А	73	SER	2.2
1	Х	2866	А	2.2
3	А	224	SER	2.2
20	S	54	ILE	2.2
20	S	108	VAL	2.2
1	Х	2085	G	2.2
1	Х	2197	U	2.2
14	М	88	VAL	2.2
21	Т	38	VAL	2.2
1	Х	151	G	2.2
1	Х	1066	G	2.2
5	С	54	THR	2.2
3	А	96	HIS	2.2
1	Х	1030	U	2.2
5	С	173	ALA	2.2
5	С	20	PRO	2.2
20	S	70	GLN	2.2
1	Х	2173	G	2.2
20	S	149	ALA	2.2
20	S	109	GLN	2.2
15	Ν	44	THR	2.2
1	Х	1118	G	2.2
5	С	169	VAL	2.2
23	V	51	ALA	2.1
1	Х	1494	G	2.1
1	Х	2328	G	2.1
7	Е	89	LEU	2.1
7	Е	69	ARG	2.1
1	Х	1585	A	2.1
2	Y	58	G	2.1
6	D	93	GLY	2.1
20	S	58	GLY	2.1
6	D	143	TYR	2.1
7	Е	143	GLN	2.1
1	X	724	C	2.1
1	Х	2359	U	2.1
7	Е	37	TYR	2.1
7	Е	26	VAL	2.1
5	С	80	GLY	2.1
20	S	6	LYS	2.1
16	0	47	PHE	2.1



Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	Х	238	G	2.1
1	Х	1058	G	2.1
1	Х	1831	G	2.1
1	Х	863	С	2.1
1	Х	1885	С	2.1
5	С	42	THR	2.1
1	Х	86	U	2.1
1	Х	2385	U	2.1
1	Х	2433	G	2.1
6	D	155	THR	2.1
18	Q	13	SER	2.1
5	С	99	VAL	2.1
13	L	48	GLY	2.1
18	Q	94	GLN	2.1
16	0	7	THR	2.1
1	Х	424	G	2.1
1	Х	1589	G	2.1
20	S	141	MET	2.1
10	Ι	118	VAL	2.1
3	А	24	LEU	2.1
3	А	145	LEU	2.1
3	А	236	GLY	2.1
6	D	128	TYR	2.1
10	Ι	70	THR	2.1
18	Q	31	PRO	2.1
1	Х	1512	A	2.1
1	Х	1920	A	2.1
4	В	144	ARG	2.0
1	Х	1121	G	2.0
1	Х	199	А	2.0
2	Y	41	A	2.0
1	Х	1104	G	2.0
1	Х	1384	G	2.0
2	Y	23	G	2.0
1	X	277	G	2.0
1	X	361	G	2.0
1	Х	2353	G	2.0
1	Х	303	C	2.0
1	Х	420	С	2.0
1	X	2329	С	2.0
6	D	40	LEU	2.0
8	G	78	ASP	2.0



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Mol	Chain	Res	Type	RSRZ
21	Т	24	LYS	2.0
21	Т	21	LEU	2.0
22	U	36	GLY	2.0
1	Х	1061	А	2.0
1	Х	1952	А	2.0

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
30	MG	Х	2976	1/1	0.39	0.78	125,125,125,125	0
30	MG	Х	3060	1/1	0.40	0.85	54,54,54,54	0
30	MG	Х	3097	1/1	0.44	0.64	102,102,102,102	0
30	MG	Х	3154	1/1	0.46	1.29	74,74,74,74	0
30	MG	Х	3050	1/1	0.54	0.63	108,108,108,108	0
31	SPD	Х	3166	10/10	0.56	0.69	92,95,99,99	0
30	MG	Х	3104	1/1	0.58	1.46	119,119,119,119	0
30	MG	Х	3002	1/1	0.59	0.48	138,138,138,138	0
30	MG	Х	3096	1/1	0.61	0.44	71,71,71,71	0
30	MG	Х	3146	1/1	0.61	0.82	178,178,178,178	0
30	MG	Y	202	1/1	0.62	0.58	98,98,98,98	0
30	MG	Х	3074	1/1	0.63	0.46	59, 59, 59, 59, 59	0
30	MG	Х	3121	1/1	0.63	0.38	79,79,79,79	0
30	MG	Х	3090	1/1	0.64	0.55	81,81,81,81	0
31	SPD	V	101	10/10	0.67	0.28	126,128,135,136	0
30	MG	Х	3109	1/1	0.68	0.54	63,63,63,63	0
30	MG	Х	3122	1/1	0.68	0.52	$65,\!65,\!65,\!65$	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(A <sup>2</sup> )	Q<0.9
30	MG	X	3141	1/1	0.68	0.44	145,145,145,145	0
30	MG	<u>X</u>	3115	1/1	0.68	0.73	54,54,54,54	0
30	MG	X	3144	1/1	0.69	1.39	105,105,105,105	0
30	MG	Х	3151	1/1	0.69	0.89	53,53,53,53	0
30	MG	Х	3163	1/1	0.70	0.52	60,60,60,60	0
30	MG	X	3113	1/1	0.70	0.39	55,55,55,55	0
30	MG	X	2969	1/1	0.73	0.81	55,55,55,55	0
30	MG	Х	3102	1/1	0.73	0.76	112,112,112,112	0
30	MG	Х	3130	1/1	0.73	0.39	60,60,60,60	0
30	MG	Х	2950	1/1	0.73	0.45	88,88,88,88	0
30	MG	Х	3052	1/1	0.74	0.74	$105,\!105,\!105,\!105$	0
30	MG	Х	3057	1/1	0.74	0.51	80,80,80,80	0
30	MG	Х	2984	1/1	0.74	0.36	62,62,62,62	0
30	MG	Х	3071	1/1	0.75	0.54	$95,\!95,\!95,\!95$	0
30	MG	Х	3131	1/1	0.76	0.59	98,98,98,98	0
30	MG	Х	3149	1/1	0.76	0.56	83,83,83,83	0
30	MG	Х	3086	1/1	0.76	0.72	78,78,78,78	0
30	MG	Х	3045	1/1	0.76	0.55	92,92,92,92	0
30	MG	Х	2979	1/1	0.77	0.71	83,83,83,83	0
30	MG	Х	3116	1/1	0.77	0.26	60,60,60,60	0
30	MG	Х	3105	1/1	0.78	0.54	69,69,69,69	0
30	MG	Х	3017	1/1	0.79	0.34	114,114,114,114	0
30	MG	Х	3159	1/1	0.79	0.49	93,93,93,93	0
30	MG	Х	3018	1/1	0.79	0.30	76,76,76,76	0
30	MG	Х	2988	1/1	0.79	0.35	87,87,87,87	0
30	MG	2	101	1/1	0.79	1.45	80,80,80,80	0
30	MG	Х	3048	1/1	0.79	0.30	124,124,124,124	0
30	MG	Х	2925	1/1	0.79	0.71	50,50,50,50	0
30	MG	Х	3046	1/1	0.80	0.47	78,78,78,78	0
30	MG	Х	3145	1/1	0.80	0.37	77,77,77,77	0
30	MG	Х	3123	1/1	0.81	0.34	85,85,85,85	0
30	MG	Х	3110	1/1	0.81	0.71	41,41,41,41	0
30	MG	Х	3032	1/1	0.81	0.74	112,112,112,112	0
30	MG	Х	3051	1/1	0.81	0.37	118,118,118,118	0
30	MG	Х	2958	1/1	0.81	0.46	77,77,77,77	0
30	MG	X	3120	1/1	0.81	0.37	78,78,78,78	0
30	MG	X	3026	1/1	0.81	0.43	81,81,81,81	0
30	MG	Х	3030	1/1	0.81	0.40	48,48,48,48	0
30	MG	X	2944	1/1	0.82	1.21	102,102,102,102	0
30	MG	X	3091	1/1	0.82	0.90	$53,\!53,\!53,\!53$	0
30	MG	X	3139	1/1	0.82	0.41	182,182,182,182	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B$ -factors $(A^2)$	$Q{<}0.9$
30	MG	X	3095	1/1	0.82	0.40	$65,\!65,\!65,\!65$	0
30	MG	Х	3164	1/1	0.82	0.42	39,39,39,39	0
30	MG	Х	3082	1/1	0.82	0.86	112,112,112,112	0
30	MG	Х	3003	1/1	0.82	0.25	77, 77, 77, 77	0
30	MG	Х	3098	1/1	0.82	0.36	120,120,120,120	0
30	MG	Х	3124	1/1	0.82	0.81	$67,\!67,\!67,\!67$	0
30	MG	Х	3021	1/1	0.83	0.63	$73,\!73,\!73,\!73$	0
30	MG	3	101	1/1	0.83	1.69	126, 126, 126, 126, 126	0
30	MG	Х	2989	1/1	0.83	0.39	$103,\!103,\!103,\!103$	0
31	SPD	Х	3170	10/10	0.83	0.29	62,63,64,64	0
30	MG	Х	3044	1/1	0.83	0.55	73,73,73,73	0
30	MG	Х	2923	1/1	0.84	0.34	75,75,75,75	0
30	MG	Y	203	1/1	0.84	0.45	132,132,132,132	0
30	MG	N	201	1/1	0.84	1.01	75,75,75,75	0
30	MG	Q	101	1/1	0.84	0.56	104,104,104,104	0
30	MG	Х	3153	1/1	0.84	0.57	47,47,47,47	0
30	MG	Х	2914	1/1	0.84	0.31	$65,\!65,\!65,\!65$	0
30	MG	Х	2920	1/1	0.84	0.55	74,74,74,74	0
30	MG	Х	3077	1/1	0.84	1.50	56,56,56,56	0
30	MG	Х	3093	1/1	0.84	0.23	117,117,117,117	0
30	MG	Х	3117	1/1	0.85	0.26	48,48,48,48	0
30	MG	Х	3152	1/1	0.85	0.65	49,49,49,49	0
30	MG	Х	2903	1/1	0.85	0.54	60,60,60,60	0
30	MG	Х	3055	1/1	0.85	0.39	66,66,66,66	0
30	MG	Х	2939	1/1	0.85	0.26	50,50,50,50	0
30	MG	Х	2990	1/1	0.85	0.15	62,62,62,62	0
30	MG	Х	3040	1/1	0.85	0.60	103,103,103,103	0
30	MG	Х	2971	1/1	0.85	0.49	59, 59, 59, 59, 59	0
30	MG	Х	3010	1/1	0.86	0.52	111,111,111,111	0
30	MG	Х	3034	1/1	0.86	0.16	66,66,66,66	0
30	MG	Х	3036	1/1	0.86	0.28	75,75,75,75	0
30	MG	Х	2924	1/1	0.86	0.26	80,80,80,80	0
30	MG	Х	2959	1/1	0.86	0.49	78,78,78,78	0
30	MG	W	101	1/1	0.86	0.32	111,111,111,111	0
30	MG	Х	2999	1/1	0.86	0.61	81,81,81,81	0
30	MG	Х	3111	1/1	0.86	0.30	53,53,53,53	0
30	MG	Х	3065	1/1	0.86	0.46	99,99,99,99	0
30	MG	Х	2986	1/1	0.86	0.47	57,57,57,57	0
30	MG	Х	2961	1/1	0.86	0.39	78,78,78,78	0
30	MG	Х	3004	1/1	0.87	0.52	61,61,61,61	0
30	MG	Х	3158	1/1	0.87	0.25	64,64,64,64	0
30	MG	Х	3009	1/1	0.87	0.31	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B$ -factors $(A^2)$	$Q{<}0.9$
30	MG	Х	2981	1/1	0.87	0.30	$79,\!79,\!79,\!79$	0
30	MG	Х	3140	1/1	0.87	0.20	$159,\!159,\!159,\!159$	0
30	MG	Y	201	1/1	0.87	0.33	114,114,114,114	0
30	MG	Х	2934	1/1	0.87	0.18	58, 58, 58, 58	0
30	MG	Х	2964	1/1	0.87	0.34	$67,\!67,\!67,\!67$	0
30	MG	Х	2982	1/1	0.88	0.15	101,101,101,101	0
30	MG	Х	3023	1/1	0.88	0.75	$70,\!70,\!70,\!70$	0
30	MG	Х	3056	1/1	0.88	0.32	$47,\!47,\!47,\!47$	0
30	MG	Х	2937	1/1	0.88	0.42	83,83,83,83	0
30	MG	Х	3035	1/1	0.88	0.39	104,104,104,104	0
30	MG	Q	102	1/1	0.88	0.44	75,75,75,75	0
30	MG	Х	2917	1/1	0.89	0.40	71,71,71,71	0
30	MG	Х	2985	1/1	0.89	0.23	63,63,63,63	0
30	MG	Х	3062	1/1	0.89	0.30	109,109,109,109	0
30	MG	Х	3022	1/1	0.89	0.12	64,64,64,64	0
30	MG	Х	3119	1/1	0.89	0.30	69,69,69,69	0
30	MG	Х	2977	1/1	0.89	0.23	66,66,66,66	0
30	MG	Х	2957	1/1	0.89	0.70	73,73,73,73	0
30	MG	Х	3008	1/1	0.89	0.32	49,49,49,49	0
29	MIV	Х	2901	49/49	0.89	0.26	52,53,57,58	0
30	MG	Х	2936	1/1	0.89	0.25	69,69,69,69	0
30	MG	Х	3127	1/1	0.89	0.16	49,49,49,49	0
30	MG	Х	3016	1/1	0.89	0.73	72,72,72,72	0
30	MG	Х	2993	1/1	0.89	0.26	128,128,128,128	0
30	MG	Х	3160	1/1	0.89	0.50	40,40,40,40	0
30	MG	Х	3069	1/1	0.90	0.27	90,90,90,90	0
30	MG	Y	204	1/1	0.90	0.28	151,151,151,151	0
30	MG	А	301	1/1	0.90	0.69	94,94,94,94	0
30	MG	Х	3112	1/1	0.90	0.60	54,54,54,54	0
30	MG	Х	2962	1/1	0.90	0.70	97,97,97,97	0
30	MG	Х	2911	1/1	0.90	0.36	39,39,39,39	0
30	MG	Х	3143	1/1	0.90	0.72	133,133,133,133	0
30	MG	Х	3007	1/1	0.90	0.19	71,71,71,71	0
30	MG	X	3125	1/1	0.90	0.62	71,71,71,71	0
30	MG	Х	3126	1/1	0.90	0.51	76,76,76,76	0
31	SPD	X	3167	10/10	0.90	0.32	56,56,57,57	0
30	MG	X	2912	1/1	0.90	0.80	64,64,64,64	0
30	MG	X	3068	1/1	0.90	0.27	97,97.97.97	0
30	MG	X	3033	1/1	0.91	0.24	45,45,45,45	0
30	MG	X	3132	1/1	0.91	0.28	88.88.88.88	0
30	MG	X	2908	1/1	0.91	0.47	39,39,39,39	0
30	MG	X	2910	1/1	0.91	0.37	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	$\mathbf{Q} < 0.9$
30	MG	Х	2978	1/1	0.91	0.85	$85,\!85,\!85,\!85$	0
30	MG	Х	3094	1/1	0.91	1.22	$69,\!69,\!69,\!69$	0
30	MG	Х	2913	1/1	0.91	0.36	$59,\!59,\!59,\!59$	0
30	MG	Х	2927	1/1	0.91	0.60	$69,\!69,\!69,\!69$	0
30	MG	Х	3067	1/1	0.91	0.21	94,94,94,94	0
30	MG	Х	3000	1/1	0.91	0.26	$67,\!67,\!67,\!67$	0
30	MG	Х	2928	1/1	0.91	0.20	$68,\!68,\!68,\!68$	0
30	MG	Х	2983	1/1	0.91	0.56	89,89,89,89	0
30	MG	2	102	1/1	0.91	0.57	62,62,62,62	0
30	MG	Х	2956	1/1	0.91	0.35	69,69,69,69	0
30	MG	Х	2970	1/1	0.91	0.34	61,61,61,61	0
30	MG	Х	2921	1/1	0.91	0.46	66,66,66,66	0
30	MG	Х	3129	1/1	0.91	0.15	86,86,86,86	0
31	SPD	Х	3171	10/10	0.91	0.26	45,47,50,50	0
30	MG	Х	3084	1/1	0.91	0.79	82,82,82,82	0
30	MG	Х	3059	1/1	0.92	0.36	55,55,55,55	0
30	MG	Х	3006	1/1	0.92	0.32	44,44,44,44	0
30	MG	Х	3061	1/1	0.92	0.18	95,95,95,95	0
30	MG	Х	2922	1/1	0.92	0.76	51,51,51,51	0
30	MG	Х	3092	1/1	0.92	0.20	77,77,77,77	0
30	MG	Х	2902	1/1	0.92	0.64	82,82,82,82	0
30	MG	Х	2951	1/1	0.92	0.39	54,54,54,54	0
30	MG	Х	2942	1/1	0.92	0.28	49,49,49,49	0
30	MG	Х	3012	1/1	0.92	0.31	47,47,47,47	0
30	MG	Х	3118	1/1	0.92	0.54	45,45,45,45	0
30	MG	Х	3053	1/1	0.92	0.22	53,53,53,53	0
30	MG	Х	3039	1/1	0.92	0.29	67,67,67,67	0
31	SPD	X	3169	10/10	0.92	0.21	77,79,80,81	0
30	MG	X	3165	1/1	0.92	0.29	39.39.39.39	0
30	MG	X	3015	1/1	0.92	0.66	105,105,105,105	0
30	MG	X	3028	1/1	0.92	0.76	69.69.69.69	0
30	MG	X	2987	1/1	0.93	0.26	54,54,54,54	0
30	MG	X	3064	1/1	0.93	0.30	113.113.113.113	0
30	MG	X	3088	1/1	0.93	0.17	78.78.78.78	0
30	MG	X	3108	1/1	0.93	0.31	61.61.61.61	0
30	MG	X	2906	1/1	0.93	0.33	75.75.75.75	0
30	MG	X	2941	1/1	0.93	0.23	73.73.73.73	0
30	MG	X	2918	1/1	0.93	0.91	71.71.71.71	0
30	MG	X	3147	1/1	0.93	1.02	95.95.95.95	0
30	MG	X	2963	1/1	0.93	0.48	96.96.96.96	0
30	MG	X	3058	1/1	0.93	0.36	63 63 63 63	0
30	MG	X	3128	1/1	0.00	0.00	95 95 95 95	0
50	MU	~ ~ ~	0120	<b>T</b>   <b>T</b>	0.00	0.10	55,55,55,55	U



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	$Q{<}0.9$
30	MG	Х	3073	1/1	0.93	0.20	118,118,118,118	0
30	MG	Х	2995	1/1	0.93	0.23	54,54,54,54	0
30	MG	Х	3156	1/1	0.93	0.44	71,71,71,71	0
30	MG	Х	2930	1/1	0.93	0.52	$50,\!50,\!50,\!50$	0
30	MG	Х	2948	1/1	0.93	0.40	83,83,83,83	0
31	SPD	Х	3168	10/10	0.93	0.43	44,45,46,46	0
30	MG	Х	3134	1/1	0.93	0.40	39,39,39,39	0
30	MG	Х	3161	1/1	0.93	0.47	38,38,38,38	0
30	MG	Х	3162	1/1	0.93	0.43	69,69,69,69	0
30	MG	Х	3136	1/1	0.93	0.27	79,79,79,79	0
30	MG	Х	3080	1/1	0.94	0.28	51,51,51,51	0
30	MG	Х	3107	1/1	0.94	0.17	83,83,83,83	0
30	MG	Х	2947	1/1	0.94	0.15	87,87,87,87	0
30	MG	Х	3150	1/1	0.94	0.18	70,70,70,70	0
30	MG	Ι	201	1/1	0.94	0.27	81,81,81,81	0
30	MG	Х	3014	1/1	0.94	0.49	75,75,75,75	0
30	MG	Х	2974	1/1	0.94	0.20	61,61,61,61	0
30	MG	Х	3031	1/1	0.94	0.55	38,38,38,38	0
30	MG	Х	3049	1/1	0.94	0.56	124,124,124,124	0
30	MG	Х	2953	1/1	0.94	0.28	57,57,57,57	0
30	MG	Х	2968	1/1	0.94	0.47	75,75,75,75	0
30	MG	X	2915	1/1	0.94	0.47	57,57,57,57	0
30	MG	Х	2996	1/1	0.94	0.27	76,76,76,76	0
30	MG	Х	2935	1/1	0.94	0.33	90,90,90,90	0
30	MG	Х	3072	1/1	0.94	0.15	115,115,115,115	0
30	MG	Х	2980	1/1	0.94	0.50	88,88,88,88	0
30	MG	X	3024	1/1	0.94	0.31	41,41,41,41	0
30	MG	X	3076	1/1	0.94	0.43	65,65,65,65	0
30	MG	Х	3042	1/1	0.94	0.20	58,58,58,58	0
30	MG	X	2972	1/1	0.95	0.40	81,81,81,81	0
30	MG	X	2946	1/1	0.95	0.21	51,51,51,51	0
30	MG	X	3078	1/1	0.95	0.22	59,59,59,59	0
30	MG	X	3037	1/1	0.95	0.36	104,104,104,104	0
30	MG	X	3038	1/1	0.95	0.30	67.67.67.67	0
30	MG	X	2975	1/1	0.95	0.32	84,84,84,84	0
30	MG	X	3029	1/1	0.95	0.39	66,66.66.66	0
30	MG	X	3001	1/1	0.95	0.08	91,91.91.91	0
30	MG	X	3089	1/1	0.95	0.29	61.61.61.61	0
30	MG	X	3019	1/1	0.95	0.45	91.91.91.91	0
30	MG	X	2992	1/1	0.95	0.55	73.73.73.73	0
30	MG	X	2904	1/1	0.95	0.32	49.49.49.49	0
30	MG	X	2931	1/1	0.95	0.42	68.68.68.68	0
$\begin{array}{r} 30\\ 30\\ 30\\ 30\\ 30\\ 30\\ 30\\ 30\\ 30\\ 30\\$	MG MG MG MG MG MG MG MG MG MG MG MG MG	X X X X X X X X X X X X X X X X X X X	2980 3024 3076 2972 2946 3078 3037 3038 2975 3029 3001 3089 3019 2992 2904 2931	$\begin{array}{c} 1/1\\ 1/1\\ 1/1\\ 1/1\\ 1/1\\ 1/1\\ 1/1\\ 1/1$	$\begin{array}{c} 0.94 \\ 0.94 \\ 0.94 \\ 0.94 \\ 0.95 \\ 0.$	$\begin{array}{c} 0.50\\ 0.31\\ 0.43\\ 0.20\\ 0.40\\ 0.21\\ 0.22\\ 0.36\\ 0.30\\ 0.32\\ 0.39\\ 0.08\\ 0.29\\ 0.45\\ 0.55\\ 0.32\\ 0.42\\ \end{array}$	$\begin{array}{r} 88,88,88,88\\ 41,41,41,41\\ 65,65,65,65\\ 58,58,58,58\\ 81,81,81,81\\ 51,51,51,51\\ 59,59,59,59\\ 104,104,104,104\\ 67,67,67,67\\ 84,84,84,84\\ 66,66,66,66\\ 91,91,91,91\\ 91,91,91,91\\ 61,61,61,61\\ 91,91,91,91\\ 73,73,73,73\\ 49,49,49,49\\ 68,68,68,68\\ \end{array}$	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 $\alpha$ 1 L.



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Conti	nued from	m previoi	is page.					
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
30	MG	Х	3135	1/1	0.96	0.18	148,148,148,148	0
30	MG	Х	2938	1/1	0.96	0.17	$52,\!52,\!52,\!52$	0
30	MG	Х	3137	1/1	0.96	0.12	83,83,83,83	0
30	MG	Х	3066	1/1	0.96	0.37	81,81,81,81	0
30	MG	Х	2998	1/1	0.96	0.47	78,78,78,78	0
30	MG	Х	2960	1/1	0.96	0.37	62,62,62,62	0
30	MG	Х	3011	1/1	0.96	0.48	53,53,53,53	0
30	MG	Х	3070	1/1	0.96	0.14	136,136,136,136	0
30	MG	Х	3025	1/1	0.96	0.64	38,38,38,38	0
30	MG	Х	3054	1/1	0.96	0.26	101,101,101,101	0
30	MG	Х	2926	1/1	0.96	0.28	$55,\!55,\!55,\!55$	0
30	MG	Х	2954	1/1	0.96	0.42	56,56,56,56	0
30	MG	Х	3101	1/1	0.96	0.26	95,95,95,95	0
30	MG	Х	3041	1/1	0.96	0.17	114,114,114,114	0
30	MG	Х	2940	1/1	0.96	0.38	60,60,60,60	0
30	MG	Х	2905	1/1	0.96	0.48	62,62,62,62	0
30	MG	Х	2966	1/1	0.96	0.49	101,101,101,101	0
30	MG	Х	2994	1/1	0.96	0.29	88,88,88,88	0
30	MG	Х	3047	1/1	0.96	0.38	92,92,92,92	0
30	MG	Х	3063	1/1	0.96	0.16	112,112,112,112	0
30	MG	Х	3087	1/1	0.96	0.68	116,116,116,116	0
30	MG	Х	3133	1/1	0.96	0.13	50,50,50,50	0
30	MG	Х	2919	1/1	0.96	0.54	44,44,44,44	0
30	MG	Х	3100	1/1	0.97	0.11	77,77,77,77	0
30	MG	Х	2929	1/1	0.97	0.20	71,71,71,71	0
30	MG	Х	2952	1/1	0.97	0.51	52,52,52,52	0
30	MG	Х	2945	1/1	0.97	1.19	104,104,104,104	0
30	MG	Х	2916	1/1	0.97	0.96	62,62,62,62	0
30	MG	Х	2965	1/1	0.97	0.51	117,117,117,117	0
30	MG	Х	2973	1/1	0.97	0.41	69,69,69,69	0
30	MG	Х	3083	1/1	0.97	0.63	79,79,79,79	0
30	MG	Х	2955	1/1	0.97	0.23	68,68,68,68	0
30	MG	Х	3085	1/1	0.97	0.53	75,75,75,75	0
30	MG	Х	3005	1/1	0.97	0.17	101,101,101,101	0
30	MG	Х	2997	1/1	0.97	0.18	99,99,99,99	0
30	MG	Х	3099	1/1	0.97	0.21	69,69,69,69	0
30	MG	Х	3027	1/1	0.98	0.10	50,50,50,50	0
30	MG	Х	3020	1/1	0.98	0.20	88,88,88,88	0
30	MG	Х	3114	1/1	0.98	0.38	48,48,48,48	0
30	MG	Х	3103	1/1	0.98	0.12	61,61,61,61	0
30	MG	Х	3138	1/1	0.98	0.10	39,39,39,39	0
30	MG	Х	2907	1/1	0.98	0.45	46,46,46,46	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
30	MG	Х	2949	1/1	0.98	0.65	56, 56, 56, 56	0
30	MG	Х	2991	1/1	0.98	0.09	80,80,80,80	0
30	MG	Х	2943	1/1	0.98	0.35	67,67,67,67	0
30	MG	Х	2967	1/1	0.98	0.24	86,86,86,86	0
30	MG	Х	2909	1/1	0.98	0.18	44,44,44,44	0
30	MG	Х	3043	1/1	0.98	0.09	$47,\!47,\!47,\!47$	0
30	MG	Х	3013	1/1	0.99	0.24	62,62,62,62	0
30	MG	Х	2933	1/1	0.99	0.25	61,61,61,61	0
30	MG	Х	3155	1/1	0.99	0.15	54,54,54,54	0
30	MG	Х	3079	1/1	0.99	0.07	$55,\!55,\!55,\!55$	0
30	MG	Х	3157	1/1	0.99	0.10	45,45,45,45	0
30	MG	Х	3075	1/1	0.99	0.21	72,72,72,72	0
30	MG	Х	3148	1/1	0.99	0.13	72,72,72,72	0
30	MG	Х	3081	1/1	0.99	0.14	76,76,76,76	0
30	MG	Х	3106	1/1	0.99	0.21	64,64,64,64	0
30	MG	Х	3142	1/1	0.99	0.10	83,83,83,83	0
30	MG	Х	2932	1/1	0.99	0.31	49,49,49,49	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers (i)

There are no such residues in this entry.

