



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:31 PM GMT

PDB ID : 4WFN  
Title : Crystal structure of the large ribosomal subunit (50S) of *Deinococcus radiodurans* containing a three residue insertion in L22 in complex with erythromycin  
Authors : Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.  
Deposited on : 2014-09-16  
Resolution : 3.54 Å(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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

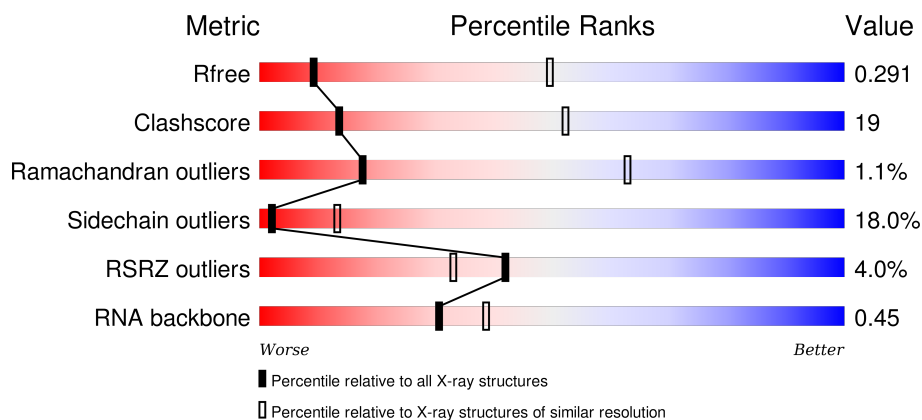
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.54 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1136 (3.68-3.40)
Clashscore	102246	1248 (3.68-3.40)
Ramachandran outliers	100387	1208 (3.68-3.40)
Sidechain outliers	100360	1208 (3.68-3.40)
RSRZ outliers	91569	1143 (3.68-3.40)
RNA backbone	2183	1052 (4.26-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>3%</div> <div>40%</div> <div>45%</div> <div>10%</div> <div>5%</div> </div>
2	B	211	<div> <div>2%</div> <div>45%</div> <div>43%</div> <div>10%</div> <div>•</div> </div>
3	C	205	<div> <div>7%</div> <div>42%</div> <div>44%</div> <div>8%</div> <div>5%</div> </div>
4	D	180	<div> <div>8%</div> <div>48%</div> <div>46%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	185	
6	G	174	
7	H	134	
8	I	156	
9	J	141	
10	K	116	
11	L	114	
12	M	165	
13	N	118	
14	O	100	
15	P	137	
16	Q	95	
17	R	115	
18	S	237	
19	T	91	
20	U	81	
21	V	67	
22	W	55	
23	Z	60	
24	1	55	
25	2	47	
26	3	65	
27	X	2880	
28	Y	124	

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
29	MG	K	201	-	-	-	X
29	MG	K	202	-	-	-	X
29	MG	X	2903	-	-	-	X
29	MG	X	2909	-	-	-	X
29	MG	X	2910	-	-	-	X
29	MG	X	2913	-	-	-	X
29	MG	X	2914	-	-	-	X
29	MG	X	2916	-	-	-	X
29	MG	X	2922	-	-	-	X
29	MG	X	2923	-	-	-	X
29	MG	X	2926	-	-	-	X
29	MG	X	2939	-	-	-	X
29	MG	X	2942	-	-	-	X
29	MG	X	2944	-	-	-	X
29	MG	X	2947	-	-	-	X
29	MG	X	2948	-	-	-	X
29	MG	X	2954	-	-	-	X
29	MG	X	2957	-	-	-	X
29	MG	X	2959	-	-	-	X
29	MG	X	2961	-	-	-	X
29	MG	X	2965	-	-	-	X

## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 84118 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1987	1235	399	350	3			

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	134	Total	C	N	O		0	0	0
			1011	619	206	186				

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 11 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	104	Total	C	N	O		0	0	0
			779	476	161	142				

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	108	Total	C	N	O		0	0	0
			871	543	172	156				

- Molecule 13 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 14 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	O	94	Total	C	N	O			
			741	465	139	137	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L22,50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	130	Total	C	N	O	S			
			1038	655	205	176	2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	110	VAL	-	linker	UNP Q9RXJ7
P	111	PRO	-	linker	UNP Q9RXJ7
P	112	ARG	-	linker	UNP Q9RXJ7

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	93	Total	C	N	O	S			
			726	458	136	130	2	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	R	110	Total	C	N	O	S			
			825	513	160	151	1	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	175	Total	C	N	O	S			
			1345	849	236	254	6	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	74	Total	C	N	O	S			
			556	351	107	97	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	U	72	Total	C	N	O			
			552	341	116	95	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	65	Total	C	N	O	S			
			525	322	106	95	2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	55	Total	C	N	O	S			
			424	264	82	76	2	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	56	Total	C	N	O	S			
			443	272	91	75	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	53	Total	C	N	O	S			
			431	274	80	76	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	46	Total	C	N	O	S			
			383	230	91	60	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	S			
			462	290	95	73	4	0	0	0

- Molecule 27 is a RNA chain called 23S ribosomal RNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	2680	Total	C	N	O	P	0	0	0
			57533	25663	10626	18564	2680			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

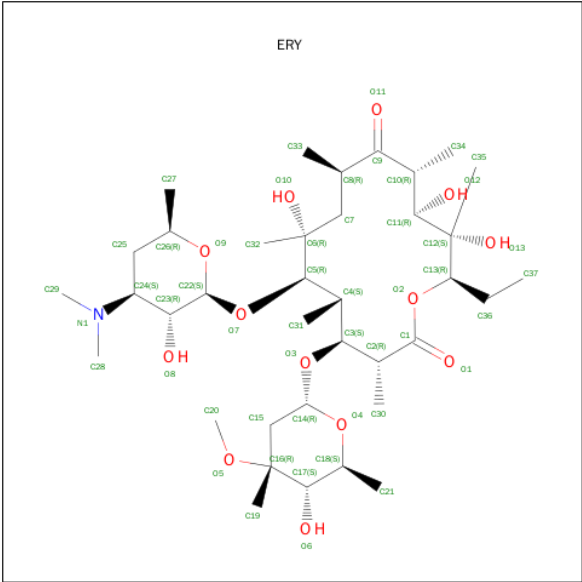
- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	122	Total	C	N	O	P	0	0	0
			2602	1161	476	843	122			

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	X	64	Total	Mg	0	0
			64	64		
29	B	1	Total	Mg	0	0
			1	1		
29	A	1	Total	Mg	0	0
			1	1		
29	K	2	Total	Mg	0	0
			2	2		
29	M	2	Total	Mg	0	0
			2	2		

- Molecule 30 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>).

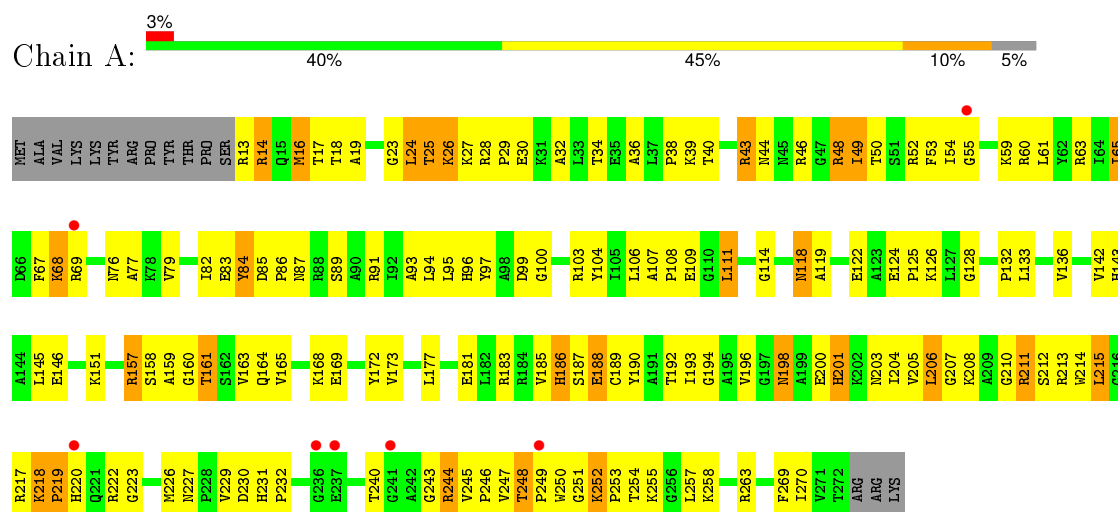


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	X	1	Total	C	N	O	0	0
			51	37	1	13		

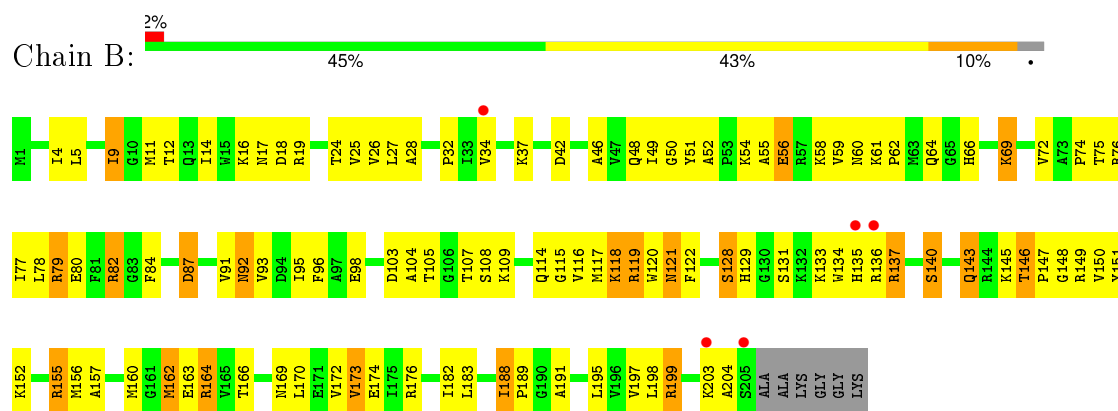
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

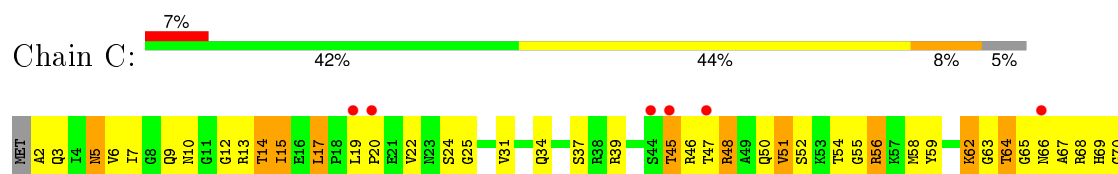
#### • Molecule 1: 50S ribosomal protein L2

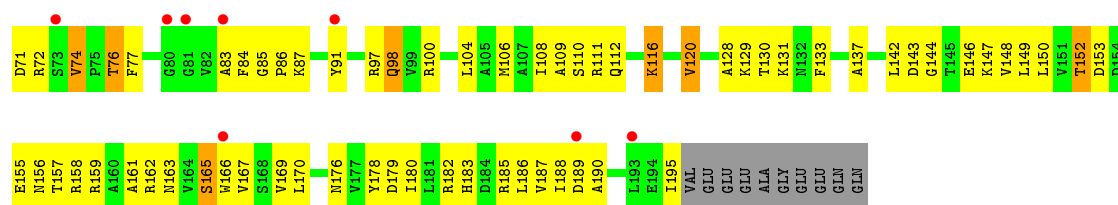


#### • Molecule 2: 50S ribosomal protein L3

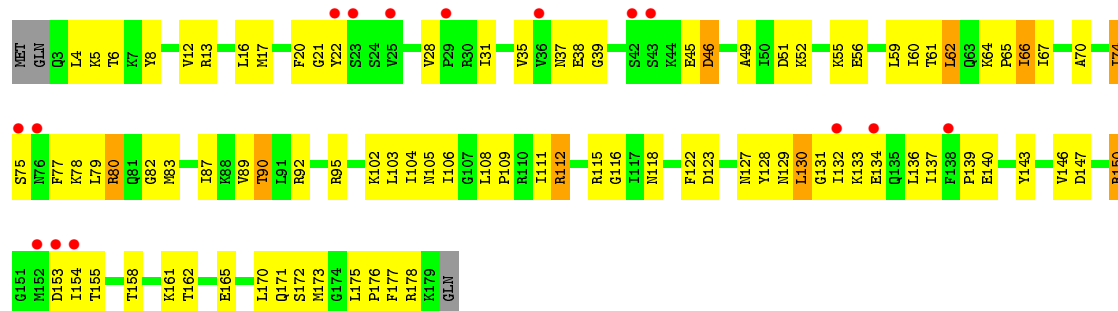


#### • Molecule 3: 50S ribosomal protein L4

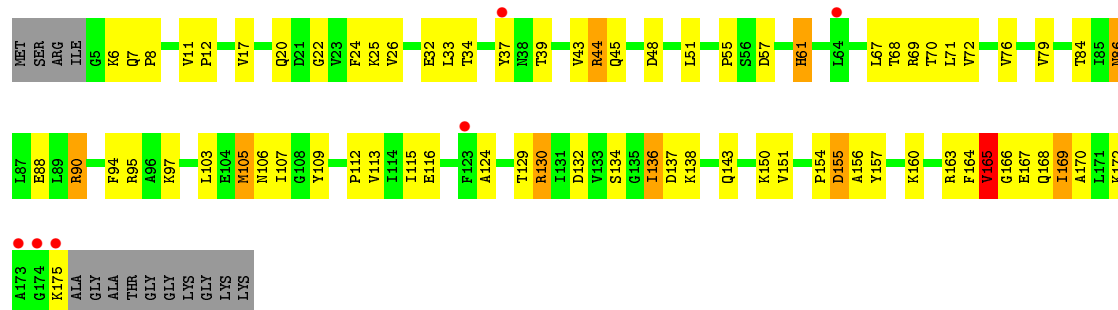




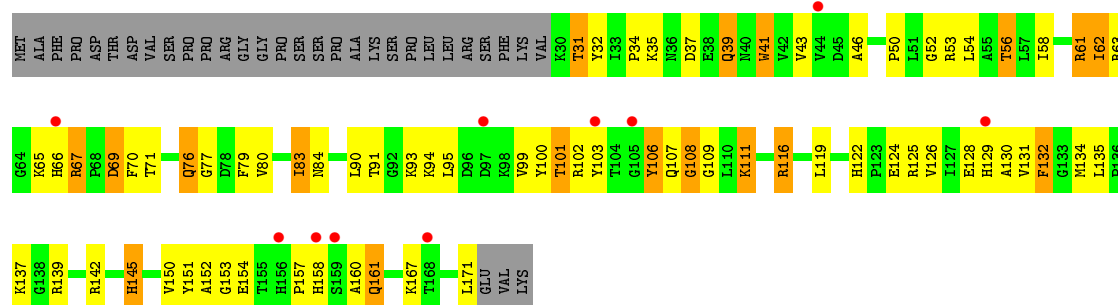
• Molecule 4: 50S ribosomal protein L5



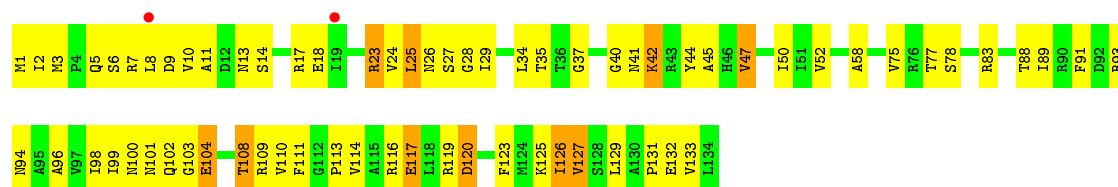
• Molecule 5: 50S ribosomal protein L6



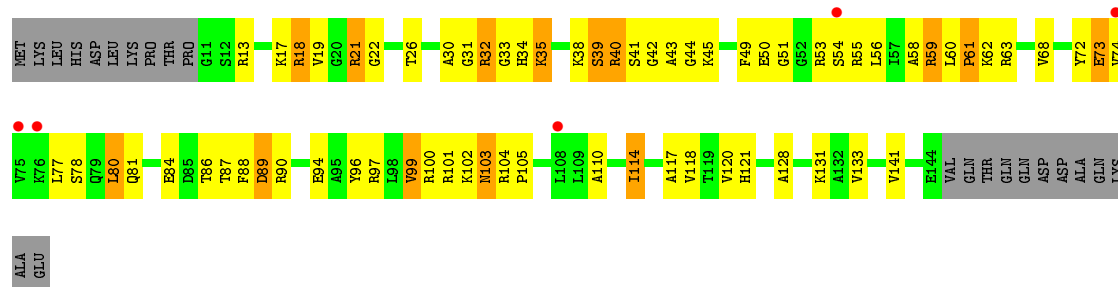
• Molecule 6: 50S ribosomal protein L13



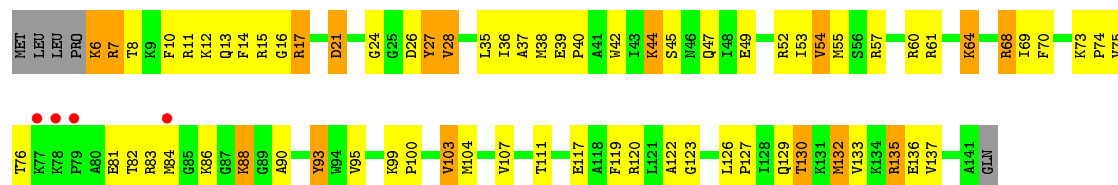
• Molecule 7: 50S ribosomal protein L14



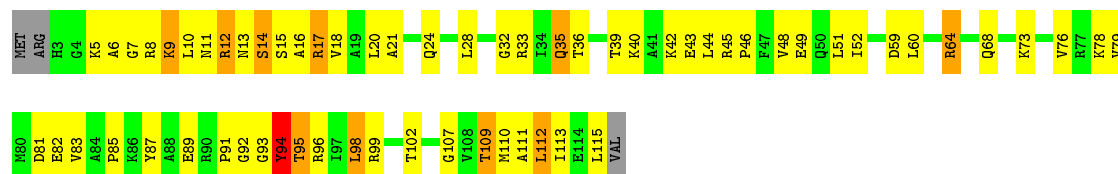
• Molecule 8: 50S ribosomal protein L15



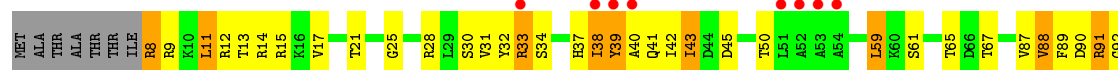
• Molecule 9: 50S ribosomal protein L16

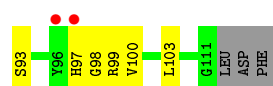


• Molecule 10: 50S ribosomal protein L17



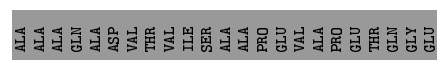
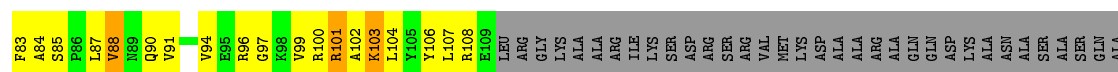
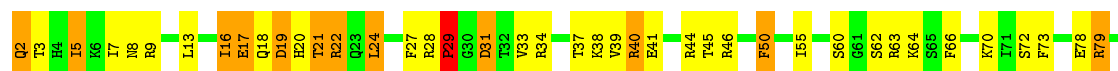
• Molecule 11: 50S ribosomal protein L18





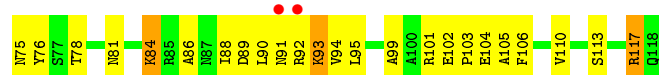
- Molecule 12: 50S ribosomal protein L19

Chain M: 29% 27% 9% 35%



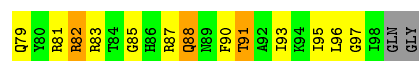
- Molecule 13: 50S ribosomal protein L20

Chain N: 2% 47% 44% 7%



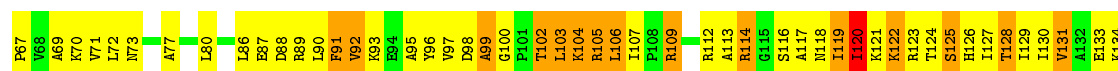
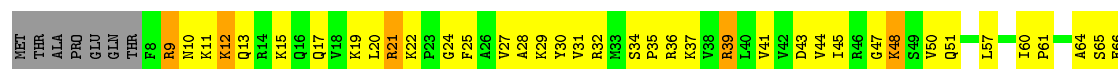
- Molecule 14: 50S ribosomal protein L21

Chain O: 4% 42% 45% 7% 6%

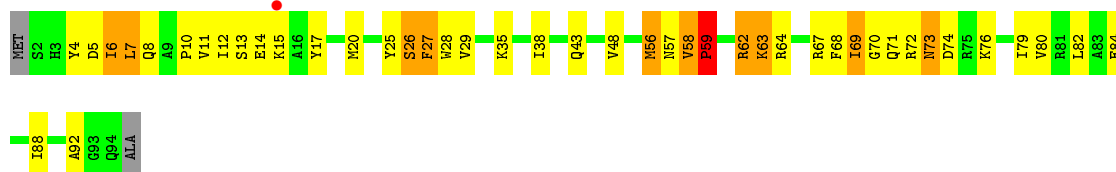


- Molecule 15: 50S ribosomal protein L22, 50S ribosomal protein L22

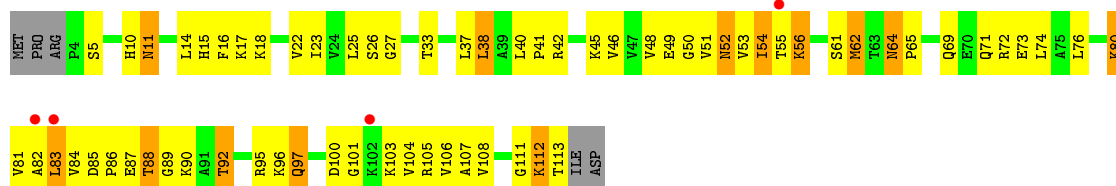
Chain P: 30% 50% 15% 5%



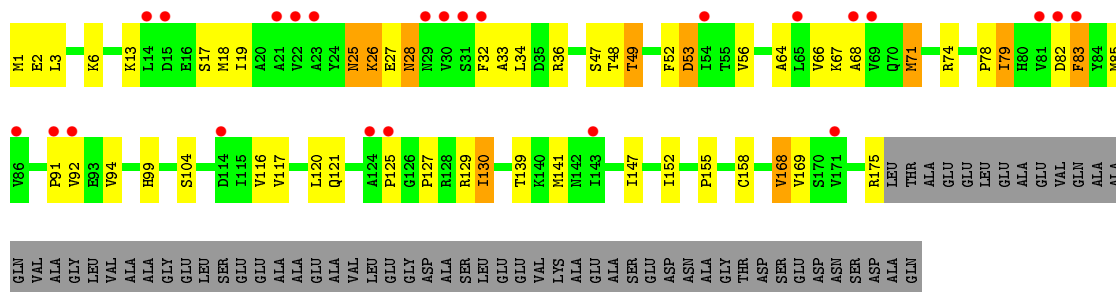
- Molecule 16: 50S ribosomal protein L23



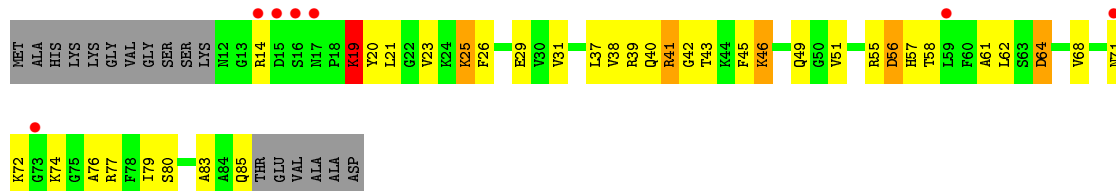
• Molecule 17: 50S ribosomal protein L24



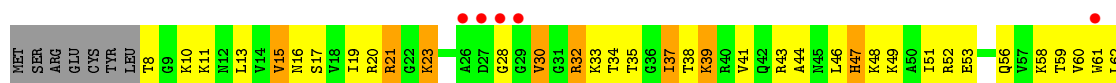
• Molecule 18: 50S ribosomal protein L25



• Molecule 19: 50S ribosomal protein L27

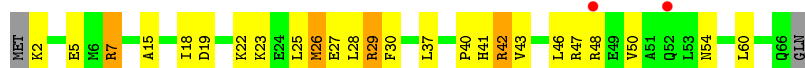


• Molecule 20: 50S ribosomal protein L28

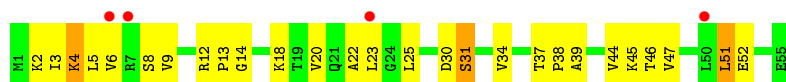




- Molecule 21: 50S ribosomal protein L29



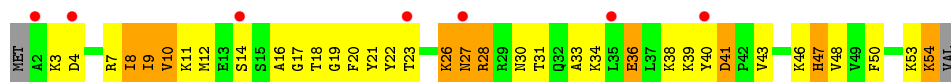
- Molecule 22: 50S ribosomal protein L30



- Molecule 23: 50S ribosomal protein L32



- Molecule 24: 50S ribosomal protein L33



- Molecule 25: 50S ribosomal protein L34



- Molecule 26: 50S ribosomal protein L35



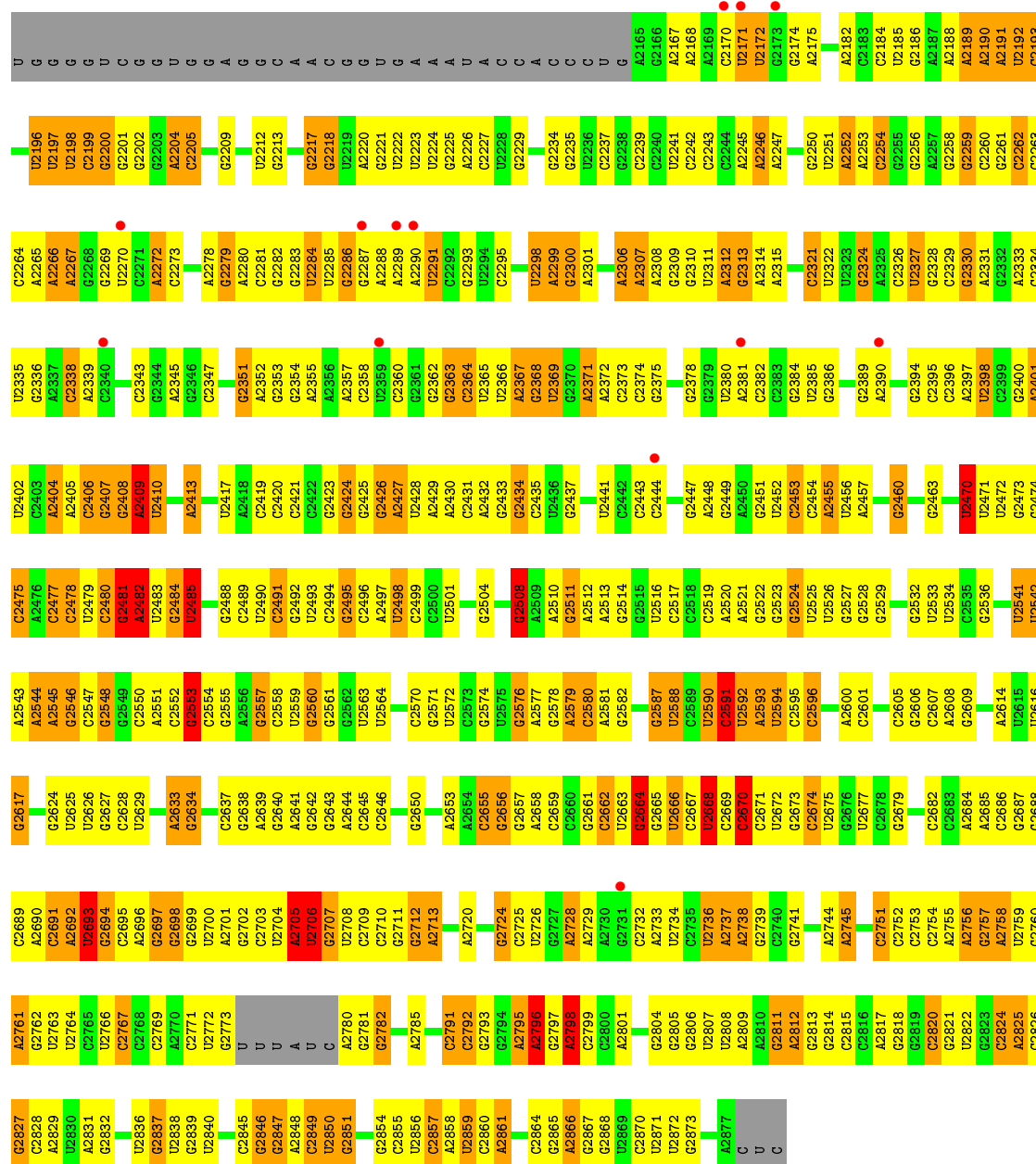
- Molecule 27: 23S ribosomal RNA



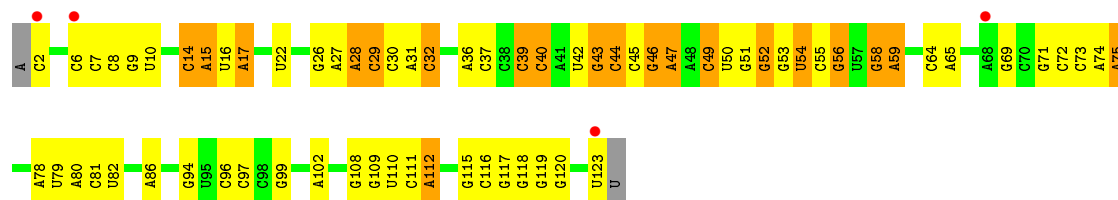
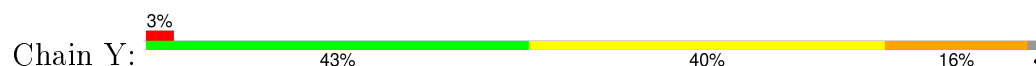


G1058	G1059	G1060	G1061	G1062	A1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	A1080	A1081	G1082	G1083	G1084	G1085	G1086	C1087	A1088	C1089	C1090	C1091	A1096	A1097	A1098	G1100	U1101	G1102	C1103	G1104	U1105	A1106	A1107	U1108	A1109	G1110	C1113	G1121	A1122	G1123	U1124	C1127	G1128	A1057																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
C	A911	C914	C914	G920	A921	A922	C923	A924	C924	G928	A929	A930	G931	G934	G935	A936	C937	G938	C939	G940	U941	U942	U943	A944	G945	U946	A1021	A1022	A1023	A1024	U1025	U1026	U1027	U1030	C1031	A1032	G1033	C959	U960	G961	C962	G963	A964	G965	A966	C967	C968	U969	A970	A971	C972	U973	C976	G977	U978	A979																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	G1263	G1264	G1265	G1266	G1267	G1268	G1269	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	G1501	G1502	G1503	G1504	G1505	G1506	G1507	G1508	G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575	G1576	G1577	G1578	G1579	G1580	G1581	G1582	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590	G1591	G1592	G1593	G1594	G1595	G1596	G1597	G1598	G1599	G1600	G1601	G1602	G1603	G1604	G1605	G1606	G1607	G1608	G1609	G1610	G1611	G1612	G1613	G1614	G1615	G1616	G1617	G1618	G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	G1635	G1636	G1637	G1638	G1639	G1640	G1641	G1642	G1643	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	G1652	G1653	G1654	G1655	G1656	G1657	G1658	G1659	G1660	G1661	G1662	G1663	G1664	G1665	G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1679	G1680	G1681	G1682	G1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733	G1734	G1735	G1736	G1737	G1738	G1739	G1740	G1741	G1742	G1743	G1744	G1745	G1746	G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1754	G1755	G1756	G1757	G1758	G1759	G1760	G1761	G1762	G1763	G1764	G1765	G1766	G1767	G1768	G1769	G1770	G1771	G1772	G1773	G1774	G1775	G1776	G1777	G1778	G1779	G1780	G1781	G1782	G1783	G1784	G1785	G1786	G1787	G1788	G1789	G1790	G1791	G1792	G1793	G1794	G1795	G1796	G1797	G1798	G1799	G1800	G1801	G1802	G1803	G1804	G1805	G1806	G1807	G1808	G1809	G1810	G1811	G1812	G1813	G1814	G1815	G1816	G1817	G1818	G1819	G1820	G1821	G1822	G1823	G1824	G1825	G1826	G1827	G1828	G1829	G1830	G1831	G1832	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1840	G1841	G1842	G1843	G1844	G1845	G1846	G1847	G1848	G1849	G1850	G1851	G1852	G1853	G1854	G1855	G1856	G1857	G1858	G1859	G1860	G1861	G1862	G1863	G1864	G1865	G1866	G1867	G1868	G1869	G1870	G1871	G1872	G1873	G1874	G1875	G1876	G1877	G1878	G1879	G1880	G1881	G1882	G1883	G1884	G1885	G1886	G1887	G1888	G1889	G1890	G1891	G1892	G1893	G1894	G1895	G1896	G1897	G1898	G1899	G1900	G1901	G1902	G1903	G1904	G1905	G1906	G1907	G1908	G1909	G1910	G1911	G1912	G1913	G1914	G1915	G1916	G1917	G1918	G1919	G1920	G1921	G1922	G1923	G1924	G1925	G1926	G1927	G1928	G1929	G1930	G1931	G1932	G1933	G1934	G1935	G1936	G1937	G1938	G1939	G1940	G1941	G1942	G1943	G1944	G1945	G1946	G1947	G1948	G1949	G1950	G1951	G1952	G1953	G1954	G1955	G1956	G1957	G1958	G1959	G1960	G1961	G1962	G1963	G1964	G1965	G1966	G1967	G1968	G1969	G1970	G1971	G1972	G1973	G1974	G1975	G1976	G1977	G1978	G1979	G1980	G1981	G1982	G1983	G1984	G1985	G1986	G1987	G1988	G1989	G1990	G1991	G1992	G1993	G1994	G1995	G1996	G1997	G1998	G1999	G2000	G2001	G2002	G2003	G2004	G2005	G2006	G2007	G2008	G2009	G2010	G2011	G2012	G2013	G2014	G2015	G2016	G2017	G2018	G2019	G2020	G2021	G2022	G2023	G2024	G2025	G2026	G2027	G2028	G2029	G2030	G2031	G2032	G2033	G2034	G2035	G2036	G2037	G2038	G2039	G2040	G2041	G2042	G2043	G2044	G2045	G2046	G2047	G2048	G2049	G2050	G2051	G2052	G2053	G2054	G2055	G2056	G2057	G2058	G2059	G2060	G2061	G2062	G2063	G2064	G2065	G2066	G2067	G2068	G2069	G2070	G2071	G2072	G2073	G2074	G2075	G2076	G2077	G2078</





• Molecule 28: 5S ribosomal RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.09Å 411.59Å 695.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.54 49.53 – 3.52	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.99-3.54) 89.6 (49.53-3.52)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.234 , 0.282 0.243 , 0.291	Depositor DCC
$R_{free}$ test set	13480 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	100.0	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 13.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 268448 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	84118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.43	0/2025	0.70	0/2726
2	B	0.55	0/1567	0.76	0/2105
3	C	0.47	0/1504	0.72	1/2036 (0.0%)
4	D	0.29	0/1419	0.52	0/1903
5	E	0.29	0/1308	0.51	0/1771
6	G	0.47	0/1138	0.78	1/1539 (0.1%)
7	H	0.61	0/1007	0.80	0/1352
8	I	0.46	0/1022	0.76	0/1366
9	J	0.52	0/1113	0.75	0/1486
10	K	0.67	0/886	0.90	1/1188 (0.1%)
11	L	0.32	0/785	0.60	0/1048
12	M	0.61	0/884	0.87	1/1186 (0.1%)
13	N	0.45	0/994	0.68	0/1323
14	O	0.44	0/750	0.74	1/1000 (0.1%)
15	P	0.58	0/1052	0.79	1/1409 (0.1%)
16	Q	0.42	0/737	0.67	1/988 (0.1%)
17	R	0.45	0/835	0.72	0/1121
18	S	0.30	0/1370	0.53	0/1862
19	T	0.44	0/563	0.70	0/747
20	U	0.41	0/556	0.69	0/741
21	V	0.31	0/529	0.51	0/704
22	W	0.36	0/426	0.61	0/568
23	Z	0.52	0/455	0.87	0/611
24	1	0.47	0/438	0.74	0/583
25	2	0.46	0/387	0.79	1/509 (0.2%)
26	3	0.53	0/468	0.85	0/614
27	X	0.63	3/64429 (0.0%)	1.22	424/100499 (0.4%)
28	Y	0.44	1/2908 (0.0%)	0.96	1/4529 (0.0%)
All	All	0.58	4/91555 (0.0%)	1.11	433/137514 (0.3%)

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
2	B	0	1
6	G	0	1
7	H	0	1
8	I	0	3
10	K	0	2
16	Q	0	1
17	R	0	1
19	T	0	1
20	U	0	1
23	Z	0	1
25	2	0	1
26	3	0	1
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	2	C	OP3-P	-10.49	1.48	1.61
27	X	1	G	OP3-P	-10.37	1.48	1.61
27	X	1981	A	N3-C4	-5.23	1.31	1.34
27	X	774	A	N3-C4	5.08	1.37	1.34

All (433) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1468	A	C8-N9-C4	-12.74	100.70	105.80
27	X	1746	A	O5'-P-OP1	-12.19	94.73	105.70
27	X	1670	G	C8-N9-C4	11.14	110.86	106.40
27	X	537	C	C6-N1-C2	-10.97	115.91	120.30
27	X	774	A	N7-C8-N9	10.55	119.08	113.80
27	X	2018	G	O5'-P-OP2	-9.92	96.77	105.70
27	X	774	A	C8-N9-C4	-9.89	101.84	105.80
27	X	2544	A	O5'-P-OP1	-9.88	96.80	105.70
27	X	1468	A	N7-C8-N9	9.40	118.50	113.80
27	X	522	G	N1-C6-O6	9.20	125.42	119.90
27	X	2705	A	C5-N7-C8	-9.11	99.35	103.90
27	X	2489	C	C6-N1-C2	-8.98	116.71	120.30
27	X	2478	C	C5-C6-N1	8.96	125.48	121.00
27	X	2705	A	N7-C8-N9	8.93	118.26	113.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2815	C	C6-N1-C2	8.84	123.83	120.30
27	X	1333	G	N3-C4-N9	-8.82	120.71	126.00
27	X	2478	C	C6-N1-C2	-8.79	116.78	120.30
27	X	2488	G	N1-C6-O6	-8.78	114.63	119.90
27	X	2018	G	O4'-C1'-N9	8.78	115.22	108.20
27	X	1668	G	N1-C6-O6	8.74	125.14	119.90
27	X	2018	G	C4-C5-N7	8.71	114.28	110.80
27	X	2705	A	N1-C6-N6	8.61	123.76	118.60
27	X	1670	G	N9-C4-C5	-8.59	101.97	105.40
27	X	538	A	C2-N3-C4	8.56	114.88	110.60
27	X	2542	U	C5-C4-O4	8.55	131.03	125.90
27	X	661	C	C6-N1-C2	-8.55	116.88	120.30
27	X	1812	U	C2-N1-C1'	8.54	127.95	117.70
27	X	2470	U	N1-C2-O2	8.33	128.63	122.80
27	X	2542	U	N1-C2-N3	8.32	119.89	114.90
27	X	2470	U	C2-N1-C1'	8.28	127.64	117.70
27	X	1992	G	C8-N9-C4	8.26	109.70	106.40
27	X	2693	U	C2-N1-C1'	-8.25	107.80	117.70
27	X	542	A	C2-N3-C4	-8.21	106.50	110.60
27	X	2495	G	N3-C4-C5	-7.82	124.69	128.60
27	X	2025	A	C8-N9-C4	-7.74	102.70	105.80
27	X	957	G	N1-C6-O6	-7.72	115.27	119.90
27	X	1467	U	C4-C5-C6	-7.72	115.07	119.70
6	G	106	TYR	N-CA-C	-7.69	90.24	111.00
27	X	774	A	C5-N7-C8	-7.69	100.06	103.90
27	X	2018	G	C5-N7-C8	-7.66	100.47	104.30
27	X	2553	G	N3-C4-C5	7.65	132.43	128.60
27	X	2548	G	C5-C6-N1	-7.56	107.72	111.50
27	X	2687	G	C8-N9-C4	7.53	109.41	106.40
27	X	2705	A	C4-C5-N7	7.49	114.44	110.70
27	X	1664	G	C4-N9-C1'	-7.43	116.83	126.50
27	X	928	G	C5-C6-O6	-7.43	124.14	128.60
27	X	343	A	C8-N9-C4	-7.42	102.83	105.80
27	X	2799	C	C6-N1-C2	-7.41	117.34	120.30
27	X	522	G	C6-C5-N7	-7.41	125.96	130.40
27	X	2690	A	C2-N3-C4	-7.41	106.90	110.60
27	X	1333	G	N3-C4-C5	7.38	132.29	128.60
27	X	860	U	C2-N1-C1'	7.33	126.50	117.70
27	X	2329	C	C5-C6-N1	7.32	124.66	121.00
27	X	774	A	C6-C5-N7	-7.27	127.21	132.30
27	X	2488	G	C5-C6-N1	7.26	115.13	111.50
27	X	1208	A	C8-N9-C4	-7.23	102.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	540	G	O4'-C1'-N9	7.23	113.98	108.20
27	X	2857	C	C6-N1-C2	-7.21	117.42	120.30
27	X	527	C	C6-N1-C2	-7.20	117.42	120.30
27	X	2591	C	C6-N1-C2	-7.19	117.42	120.30
27	X	1989	C	C5-C6-N1	7.18	124.59	121.00
27	X	2470	U	C6-N1-C1'	-7.13	111.22	121.20
27	X	2845	C	N3-C4-C5	-7.12	119.05	121.90
27	X	1283	C	N1-C2-O2	-7.11	114.63	118.90
27	X	2705	A	C2-N3-C4	-7.11	107.05	110.60
27	X	343	A	N7-C8-N9	7.09	117.35	113.80
27	X	1682	A	N1-C6-N6	7.08	122.85	118.60
27	X	462	G	C5-C6-N1	-6.96	108.02	111.50
27	X	1468	A	C2-N3-C4	6.95	114.08	110.60
10	K	92	GLY	N-CA-C	-6.94	95.74	113.10
27	X	2485	U	C2-N1-C1'	6.94	126.03	117.70
27	X	983	G	C8-N9-C4	-6.93	103.63	106.40
27	X	1270	C	C6-N1-C2	-6.92	117.53	120.30
27	X	841	G	C8-N9-C4	-6.91	103.64	106.40
27	X	774	A	N1-C6-N6	6.91	122.74	118.60
27	X	796	A	C2-N3-C4	-6.90	107.15	110.60
27	X	1724	C	C6-N1-C2	6.88	123.05	120.30
27	X	579	G	C4-C5-N7	-6.88	108.05	110.80
27	X	1468	A	C5-C6-N1	6.83	121.11	117.70
27	X	1993	G	N1-C6-O6	6.83	124.00	119.90
27	X	1235	C	C6-N1-C2	6.82	123.03	120.30
14	O	38	LEU	CA-CB-CG	6.81	130.97	115.30
27	X	1253	C	C6-N1-C2	-6.79	117.58	120.30
27	X	661	C	C5-C6-N1	6.77	124.39	121.00
27	X	1979	C	N3-C2-O2	-6.77	117.16	121.90
27	X	2815	C	C5-C6-N1	-6.76	117.62	121.00
27	X	2592	U	N3-C4-O4	6.75	124.12	119.40
27	X	2371	A	N7-C8-N9	6.72	117.16	113.80
27	X	2706	U	O5'-P-OP2	-6.72	99.65	105.70
27	X	796	A	C5-C6-N1	-6.70	114.35	117.70
27	X	1982	C	C2-N3-C4	-6.69	116.55	119.90
27	X	2553	G	N3-C4-N9	-6.69	121.98	126.00
27	X	2668	U	N1-C2-N3	6.69	118.92	114.90
27	X	1208	A	N7-C8-N9	6.69	117.15	113.80
27	X	759	C	C6-N1-C2	6.68	122.97	120.30
27	X	816	U	N3-C2-O2	-6.68	117.53	122.20
25	2	38	GLY	N-CA-C	-6.67	96.42	113.10
27	X	2845	C	C6-N1-C2	-6.65	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2478	C	C2-N1-C1'	6.63	126.09	118.80
27	X	1682	A	C4-C5-C6	6.63	120.31	117.00
27	X	2607	C	N1-C2-O2	6.62	122.87	118.90
27	X	2434	G	C4-N9-C1'	6.62	135.11	126.50
27	X	1332	G	N1-C6-O6	6.57	123.84	119.90
27	X	2488	G	N3-C4-C5	-6.52	125.34	128.60
27	X	2508	G	N1-C6-O6	6.52	123.81	119.90
27	X	1288	A	O4'-C1'-N9	6.51	113.41	108.20
27	X	957	G	N3-C4-C5	-6.50	125.35	128.60
27	X	1481	U	C2-N1-C1'	-6.49	109.91	117.70
27	X	2542	U	C6-N1-C2	-6.49	117.10	121.00
27	X	1716	G	N1-C6-O6	-6.48	116.01	119.90
27	X	538	A	N1-C2-N3	-6.48	126.06	129.30
27	X	522	G	C5-C6-O6	-6.47	124.72	128.60
27	X	2404	A	P-O3'-C3'	6.46	127.46	119.70
27	X	537	C	N3-C2-O2	-6.41	117.41	121.90
27	X	774	A	C4-C5-N7	6.41	113.91	110.70
27	X	1664	G	C8-N9-C1'	6.41	135.33	127.00
27	X	1812	U	C5-C6-N1	6.40	125.90	122.70
27	X	2705	A	C6-C5-N7	-6.38	127.84	132.30
27	X	699	G	C4-C5-N7	6.38	113.35	110.80
27	X	2670	C	C6-N1-C2	-6.38	117.75	120.30
27	X	522	G	N9-C4-C5	-6.37	102.85	105.40
27	X	2705	A	C8-N9-C4	-6.35	103.26	105.80
27	X	1467	U	C5-C6-N1	6.33	125.86	122.70
27	X	1682	A	C6-C5-N7	-6.32	127.88	132.30
27	X	1481	U	N1-C2-O2	-6.31	118.38	122.80
27	X	2541	U	N3-C2-O2	-6.29	117.80	122.20
27	X	2542	U	N3-C2-O2	-6.26	117.82	122.20
27	X	1975	G	P-O3'-C3'	6.25	127.20	119.70
27	X	1812	U	C6-N1-C1'	-6.23	112.48	121.20
27	X	522	G	C4-C5-N7	6.20	113.28	110.80
27	X	2697	G	C2-N3-C4	6.20	115.00	111.90
27	X	2421	C	C6-N1-C2	-6.19	117.82	120.30
27	X	29	U	N3-C4-O4	6.17	123.72	119.40
27	X	556	A	N1-C6-N6	6.16	122.30	118.60
27	X	928	G	C4-C5-N7	6.16	113.26	110.80
27	X	2587	G	C5-C6-O6	-6.16	124.91	128.60
27	X	346	C	C6-N1-C2	-6.15	117.84	120.30
27	X	1466	C	C6-N1-C2	-6.14	117.84	120.30
27	X	24	G	O4'-C1'-N9	6.14	113.11	108.20
27	X	1250	A	P-O3'-C3'	6.12	127.04	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	923	A	C2-N3-C4	6.11	113.66	110.60
27	X	2508	G	C4-C5-N7	6.11	113.24	110.80
27	X	968	C	C2-N1-C1'	6.10	125.51	118.80
27	X	1674	C	N1-C2-O2	6.10	122.56	118.90
27	X	2795	A	N1-C6-N6	-6.10	114.94	118.60
27	X	841	G	N7-C8-N9	6.10	116.15	113.10
27	X	843	G	C5-C6-O6	-6.10	124.94	128.60
27	X	2767	C	C6-N1-C2	-6.08	117.87	120.30
27	X	2799	C	N1-C2-O2	-6.07	115.26	118.90
27	X	816	U	C6-N1-C2	-6.07	117.36	121.00
27	X	928	G	N9-C4-C5	-6.07	102.97	105.40
27	X	1984	A	C2-N3-C4	-6.07	107.57	110.60
27	X	1305	C	C6-N1-C2	6.05	122.72	120.30
27	X	617	U	N3-C2-O2	-6.04	117.97	122.20
27	X	538	A	C5-C6-N1	6.02	120.71	117.70
27	X	1747	G	C8-N9-C4	-6.02	103.99	106.40
27	X	2867	G	N3-C4-C5	6.01	131.61	128.60
27	X	1668	G	C6-C5-N7	-6.01	126.79	130.40
27	X	1988	A	N1-C6-N6	6.01	122.21	118.60
27	X	2034	A	N1-C6-N6	-6.01	115.00	118.60
27	X	1812	U	N1-C2-O2	6.01	127.00	122.80
27	X	2279	G	N1-C6-O6	6.01	123.50	119.90
27	X	1333	G	C2-N3-C4	-6.00	108.90	111.90
27	X	2668	U	C5-C4-O4	5.99	129.50	125.90
27	X	2638	G	N3-C4-C5	5.99	131.60	128.60
27	X	2410	U	C6-N1-C2	-5.97	117.42	121.00
27	X	2398	U	C6-N1-C2	-5.97	117.42	121.00
27	X	2854	G	C4-C5-N7	5.96	113.19	110.80
27	X	2669	C	N3-C2-O2	-5.96	117.73	121.90
27	X	2806	G	N1-C6-O6	5.96	123.48	119.90
27	X	699	G	N1-C6-O6	5.96	123.47	119.90
27	X	699	G	C5-N7-C8	-5.96	101.32	104.30
27	X	2019	C	C6-N1-C2	-5.96	117.92	120.30
27	X	540	G	N1-C6-O6	-5.95	116.33	119.90
27	X	1286	U	O5'-P-OP1	-5.94	100.36	105.70
27	X	2705	A	P-O3'-C3'	5.93	126.81	119.70
27	X	1975	G	N3-C4-C5	-5.92	125.64	128.60
27	X	2799	C	N1-C2-N3	5.91	123.34	119.20
27	X	2812	A	C8-N9-C4	-5.90	103.44	105.80
27	X	2485	U	C5-C6-N1	5.89	125.65	122.70
27	X	1141	U	P-O3'-C3'	5.88	126.75	119.70
27	X	2478	C	N3-C4-N4	5.88	122.11	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	684	C	N3-C4-C5	-5.87	119.55	121.90
27	X	1674	C	N3-C4-C5	5.87	124.25	121.90
27	X	2495	G	C2-N3-C4	5.87	114.84	111.90
27	X	985	G	C8-N9-C4	-5.86	104.06	106.40
27	X	1481	U	N3-C2-O2	5.86	126.30	122.20
27	X	2049	C	C6-N1-C2	-5.85	117.96	120.30
27	X	1324	G	O4'-C1'-N9	5.83	112.86	108.20
27	X	536	A	N1-C6-N6	5.83	122.10	118.60
27	X	2021	G	C6-C5-N7	-5.82	126.91	130.40
27	X	2409	A	P-O3'-C3'	5.82	126.68	119.70
27	X	1636	G	C8-N9-C4	5.81	108.72	106.40
27	X	1647	U	N3-C4-C5	-5.81	111.11	114.60
27	X	1770	U	C5-C6-N1	-5.81	119.79	122.70
27	X	1979	C	N1-C2-O2	5.81	122.39	118.90
27	X	2508	G	C6-C5-N7	-5.81	126.92	130.40
27	X	699	G	C6-C5-N7	-5.80	126.92	130.40
27	X	1712	G	C4-N9-C1'	5.80	134.04	126.50
27	X	538	A	P-O3'-C3'	5.79	126.65	119.70
27	X	2827	G	N3-C4-N9	5.79	129.47	126.00
27	X	2488	G	C2-N3-C4	5.78	114.79	111.90
27	X	2638	G	N3-C4-N9	-5.78	122.53	126.00
27	X	479	G	N1-C6-O6	5.78	123.37	119.90
27	X	1691	G	N9-C4-C5	-5.78	103.09	105.40
27	X	1142	G	N3-C4-C5	-5.78	125.71	128.60
27	X	1982	C	C5-C6-N1	-5.78	118.11	121.00
27	X	2846	G	C8-N9-C4	5.77	108.71	106.40
12	M	17	GLU	N-CA-C	-5.77	95.43	111.00
27	X	1992	G	N7-C8-N9	-5.77	110.22	113.10
27	X	579	G	C5-C6-O6	5.76	132.06	128.60
27	X	2034	A	C8-N9-C4	-5.76	103.50	105.80
27	X	1315	A	N1-C6-N6	-5.76	115.14	118.60
27	X	2508	G	C5-C6-O6	-5.75	125.15	128.60
27	X	661	C	C2-N1-C1'	5.74	125.11	118.80
27	X	1693	A	C8-N9-C4	-5.71	103.51	105.80
27	X	1712	G	C6-C5-N7	-5.71	126.97	130.40
27	X	2563	U	C2-N1-C1'	5.71	124.55	117.70
27	X	700	C	C6-N1-C2	-5.70	118.02	120.30
27	X	841	G	C5-N7-C8	-5.69	101.46	104.30
27	X	2576	G	N1-C6-O6	5.68	123.31	119.90
27	X	2854	G	C5-N7-C8	-5.68	101.46	104.30
27	X	1934	U	C6-N1-C2	-5.68	117.59	121.00
27	X	2859	U	O5'-P-OP1	-5.68	100.59	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1746	A	C8-N9-C4	-5.67	103.53	105.80
27	X	2434	G	N3-C4-C5	-5.67	125.76	128.60
27	X	2655	C	C6-N1-C2	5.67	122.57	120.30
27	X	2634	G	O4'-C1'-N9	5.66	112.73	108.20
27	X	29	U	C5-C4-O4	-5.66	122.51	125.90
27	X	1691	G	C5-C6-O6	-5.65	125.21	128.60
27	X	2409	A	OP1-P-O3'	5.64	117.62	105.20
27	X	2587	G	C6-C5-N7	-5.64	127.01	130.40
27	X	684	C	C6-N1-C2	-5.64	118.04	120.30
27	X	2495	G	C5-C6-N1	5.63	114.32	111.50
27	X	2491	C	C6-N1-C2	-5.62	118.05	120.30
27	X	2587	G	N1-C6-O6	5.62	123.27	119.90
27	X	2813	G	C8-N9-C4	5.61	108.65	106.40
27	X	841	G	N3-C4-N9	-5.61	122.63	126.00
27	X	533	C	C2-N1-C1'	-5.61	112.63	118.80
27	X	1712	G	N3-C4-N9	5.61	129.36	126.00
27	X	2806	G	C6-C5-N7	-5.61	127.04	130.40
27	X	2656	G	OP2-P-O3'	5.60	117.52	105.20
27	X	617	U	C4-C5-C6	5.59	123.06	119.70
27	X	822	G	N3-C4-C5	-5.59	125.80	128.60
27	X	2371	A	C8-N9-C4	-5.59	103.56	105.80
27	X	1981	A	N1-C2-N3	5.59	132.10	129.30
27	X	2426	G	OP1-P-O3'	5.59	117.50	105.20
27	X	689	A	O4'-C1'-N9	5.59	112.67	108.20
27	X	1994	U	C5-C6-N1	5.58	125.49	122.70
27	X	2580	C	N1-C2-O2	-5.58	115.55	118.90
27	X	860	U	N1-C2-O2	5.57	126.70	122.80
27	X	2796	A	O5'-P-OP2	-5.57	100.69	105.70
27	X	2806	G	C5-C6-O6	-5.57	125.26	128.60
27	X	1670	G	N7-C8-N9	-5.57	110.31	113.10
27	X	1770	U	C4-C5-C6	5.57	123.04	119.70
27	X	2693	U	C6-N1-C1'	5.53	128.95	121.20
27	X	1692	C	C4-C5-C6	5.53	120.16	117.40
27	X	1713	G	N1-C6-O6	-5.52	116.59	119.90
27	X	2437	G	C8-N9-C4	-5.52	104.19	106.40
27	X	2664	G	N3-C2-N2	-5.51	116.05	119.90
27	X	542	A	N1-C2-N3	5.50	132.05	129.30
27	X	2475	C	C6-N1-C2	-5.50	118.10	120.30
27	X	522	G	C8-N9-C1'	-5.49	119.86	127.00
27	X	2481	G	C8-N9-C4	-5.49	104.20	106.40
28	Y	32	C	C6-N1-C2	-5.49	118.10	120.30
27	X	2398	U	N3-C4-C5	-5.49	111.31	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1770	U	O4'-C1'-N1	5.49	112.59	108.20
27	X	1780	A	N1-C6-N6	5.48	121.89	118.60
27	X	1982	C	N3-C4-C5	5.48	124.09	121.90
27	X	1208	A	C5-N7-C8	-5.48	101.16	103.90
27	X	1629	G	OP1-P-O3'	5.47	117.24	105.20
27	X	2796	A	N1-C6-N6	-5.47	115.32	118.60
27	X	2812	A	N7-C8-N9	5.46	116.53	113.80
27	X	2579	A	C8-N9-C4	5.46	107.98	105.80
27	X	788	G	P-O3'-C3'	5.46	126.25	119.70
27	X	1664	G	O5'-P-OP1	-5.46	100.79	105.70
27	X	2254	C	C6-N1-C2	-5.46	118.12	120.30
27	X	2382	C	C6-N1-C2	-5.46	118.12	120.30
27	X	2025	A	N9-C4-C5	5.45	107.98	105.80
27	X	1770	U	C5-C4-O4	5.45	129.17	125.90
27	X	1661	C	N3-C2-O2	-5.45	118.08	121.90
27	X	2669	C	N3-C4-C5	-5.45	119.72	121.90
27	X	1691	G	C4-C5-N7	5.45	112.98	110.80
27	X	2607	C	N3-C2-O2	-5.44	118.09	121.90
27	X	577	U	C6-N1-C2	-5.43	117.74	121.00
27	X	928	G	N1-C6-O6	5.43	123.16	119.90
27	X	2798	A	N9-C4-C5	-5.42	103.63	105.80
27	X	1923	U	P-O3'-C3'	5.42	126.21	119.70
27	X	2548	G	C4-C5-N7	-5.42	108.63	110.80
27	X	1240	G	C8-N9-C4	5.42	108.57	106.40
27	X	755	C	O5'-P-OP1	-5.41	100.83	105.70
27	X	2756	A	P-O3'-C3'	5.41	126.20	119.70
27	X	2674	C	N3-C4-N4	5.41	121.79	118.00
27	X	2706	U	C5-C6-N1	5.41	125.40	122.70
27	X	2018	G	N3-C4-C5	5.40	131.30	128.60
27	X	1682	A	C8-N9-C4	-5.39	103.64	105.80
27	X	1664	G	N3-C4-C5	5.39	131.30	128.60
27	X	2820	C	N3-C4-C5	5.39	124.06	121.90
27	X	2246	A	N1-C6-N6	-5.39	115.37	118.60
27	X	2854	G	N7-C8-N9	5.39	115.80	113.10
27	X	2837	G	C8-N9-C4	5.39	108.55	106.40
27	X	2490	U	N3-C2-O2	-5.38	118.43	122.20
27	X	519	C	C6-N1-C2	-5.38	118.15	120.30
27	X	338	G	C8-N9-C4	-5.37	104.25	106.40
27	X	2561	G	C5-C6-N1	5.37	114.19	111.50
27	X	1696	C	N1-C2-O2	-5.36	115.68	118.90
27	X	1468	A	N3-C4-C5	-5.36	123.05	126.80
27	X	2694	G	OP2-P-O3'	5.34	116.94	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2019	C	C2-N1-C1'	5.34	124.67	118.80
27	X	2023	C	C6-N1-C2	5.34	122.43	120.30
27	X	2019	C	C5-C6-N1	5.33	123.67	121.00
27	X	1657	A	C2-N3-C4	-5.33	107.93	110.60
27	X	2032	G	N3-C4-N9	5.33	129.20	126.00
27	X	2279	G	C6-C5-N7	-5.33	127.20	130.40
27	X	2025	A	N1-C6-N6	-5.32	115.41	118.60
27	X	2434	G	C8-N9-C1'	-5.32	120.08	127.00
27	X	774	A	C2-N3-C4	-5.32	107.94	110.60
27	X	1246	G	N1-C6-O6	-5.32	116.71	119.90
27	X	2470	U	N3-C2-O2	-5.32	118.48	122.20
27	X	1164	C	C6-N1-C2	-5.30	118.18	120.30
27	X	1934	U	N3-C4-O4	5.29	123.11	119.40
27	X	540	G	C8-N9-C4	-5.29	104.28	106.40
27	X	596	C	N3-C4-C5	-5.28	119.79	121.90
27	X	1742	G	N3-C4-N9	5.28	129.17	126.00
27	X	1746	A	N1-C6-N6	-5.28	115.43	118.60
27	X	1313	U	P-O3'-C3'	5.28	126.03	119.70
27	X	1679	U	N3-C2-O2	-5.28	118.50	122.20
27	X	2021	G	N1-C6-O6	5.28	123.07	119.90
27	X	2751	C	N3-C4-C5	5.28	124.01	121.90
27	X	699	G	N7-C8-N9	5.27	115.73	113.10
27	X	2693	U	N3-C4-O4	-5.26	115.72	119.40
27	X	1976	U	N3-C4-O4	-5.25	115.72	119.40
27	X	1747	G	N3-C4-C5	-5.25	125.98	128.60
27	X	833	A	C5-C6-N6	-5.24	119.50	123.70
27	X	1934	U	N3-C4-C5	-5.24	111.45	114.60
27	X	2831	A	C4-C5-C6	-5.24	114.38	117.00
27	X	1310	C	N3-C4-C5	5.24	124.00	121.90
27	X	2321	C	C6-N1-C2	-5.23	118.21	120.30
27	X	923	A	C8-N9-C4	-5.23	103.71	105.80
27	X	2239	C	C6-N1-C2	-5.22	118.21	120.30
27	X	2524	G	C4-C5-N7	5.22	112.89	110.80
27	X	1713	G	C4-C5-N7	-5.21	108.71	110.80
27	X	1993	G	C4-C5-N7	5.21	112.89	110.80
27	X	1278	A	O5'-P-OP2	-5.21	101.01	105.70
27	X	844	G	OP2-P-O3'	5.20	116.65	105.20
27	X	2662	C	C6-N1-C2	-5.20	118.22	120.30
27	X	2791	C	C6-N1-C2	5.20	122.38	120.30
27	X	2712	G	N1-C2-N2	-5.20	111.52	116.20
27	X	742	G	C4-N9-C1'	5.20	133.26	126.50
3	C	56	ARG	N-CA-C	5.20	125.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2560	G	O4'-C1'-N9	5.20	112.36	108.20
27	X	1288	A	N7-C8-N9	5.19	116.40	113.80
27	X	1391	A	P-O3'-C3'	5.19	125.93	119.70
27	X	2524	G	C5-C6-O6	-5.19	125.49	128.60
27	X	1647	U	C6-N1-C2	-5.19	117.89	121.00
27	X	1342	U	O5'-P-OP2	-5.18	101.03	105.70
27	X	2541	U	N1-C2-O2	5.18	126.43	122.80
27	X	874	A	C8-N9-C4	-5.18	103.73	105.80
27	X	2638	G	N3-C2-N2	-5.18	116.27	119.90
27	X	2827	G	N3-C4-C5	-5.18	126.01	128.60
27	X	2338	C	C6-N1-C2	-5.18	118.23	120.30
27	X	2485	U	N1-C2-O2	5.18	126.42	122.80
27	X	24	G	C4-N9-C1'	-5.17	119.78	126.50
27	X	833	A	C4-C5-N7	5.17	113.28	110.70
27	X	1223	G	C6-C5-N7	-5.17	127.30	130.40
27	X	2590	U	C2-N1-C1'	5.17	123.90	117.70
27	X	1885	C	N1-C2-O2	5.16	122.00	118.90
27	X	1712	G	C8-N9-C1'	-5.16	120.29	127.00
27	X	2815	C	N3-C4-C5	5.16	123.96	121.90
27	X	522	G	N3-C4-N9	5.16	129.09	126.00
27	X	2057	U	C6-N1-C2	-5.15	117.91	121.00
27	X	1141	U	N3-C2-O2	-5.15	118.59	122.20
27	X	1694	A	C5-N7-C8	-5.15	101.33	103.90
27	X	1623	C	N1-C2-O2	5.14	121.99	118.90
27	X	2050	G	N9-C4-C5	-5.14	103.34	105.40
27	X	1934	U	C5-C6-N1	5.14	125.27	122.70
27	X	2592	U	N3-C4-C5	-5.14	111.52	114.60
27	X	1326	U	C2-N1-C1'	5.13	123.86	117.70
27	X	593	C	C6-N1-C2	-5.13	118.25	120.30
27	X	2857	C	N3-C4-C5	-5.13	119.85	121.90
27	X	461	A	O5'-P-OP1	-5.13	101.08	105.70
27	X	1625	A	P-O3'-C3'	5.13	125.86	119.70
27	X	1232	U	N1-C2-O2	-5.13	119.21	122.80
27	X	1035	G	N3-C4-C5	-5.12	126.04	128.60
27	X	2410	U	C5-C6-N1	5.12	125.26	122.70
27	X	1992	G	N9-C4-C5	-5.12	103.35	105.40
27	X	2000	U	N3-C2-O2	5.12	125.79	122.20
27	X	2495	G	C6-N1-C2	-5.12	122.03	125.10
27	X	1211	G	N3-C4-N9	5.12	129.07	126.00
27	X	1142	G	C2-N3-C4	5.12	114.46	111.90
27	X	2668	U	N1-C2-O2	-5.12	119.22	122.80
27	X	13	A	OP2-P-O3'	5.12	116.45	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	985	G	N7-C8-N9	5.11	115.66	113.10
27	X	1223	G	C4-N9-C1'	5.11	133.14	126.50
27	X	1975	G	C4-N9-C1'	5.11	133.14	126.50
27	X	2690	A	N1-C6-N6	5.11	121.67	118.60
27	X	968	C	N1-C2-O2	5.10	121.96	118.90
27	X	1222	G	N3-C4-N9	5.10	129.06	126.00
27	X	2576	G	C6-C5-N7	-5.10	127.34	130.40
27	X	2039	G	C8-N9-C4	-5.09	104.36	106.40
27	X	2850	U	O5'-P-OP1	-5.08	101.13	105.70
27	X	537	C	P-O3'-C3'	5.08	125.80	119.70
27	X	518	A	C8-N9-C4	-5.08	103.77	105.80
27	X	1315	A	N1-C2-N3	5.08	131.84	129.30
27	X	2050	G	N1-C6-O6	5.08	122.95	119.90
27	X	2482	A	OP1-P-OP2	-5.07	112.00	119.60
27	X	2837	G	C6-C5-N7	5.07	133.44	130.40
27	X	236	C	C6-N1-C2	-5.07	118.27	120.30
27	X	479	G	C5-C6-O6	-5.06	125.56	128.60
27	X	1662	G	N3-C4-N9	5.06	129.04	126.00
27	X	1141	U	C2-N1-C1'	5.06	123.77	117.70
27	X	558	G	C4-N9-C1'	5.05	133.06	126.50
15	P	120	ILE	N-CA-C	5.04	124.62	111.00
27	X	2795	A	P-O3'-C3'	5.04	125.75	119.70
16	Q	7	LEU	CA-CB-CG	5.04	126.89	115.30
27	X	2026	C	N1-C2-O2	5.03	121.92	118.90
27	X	536	A	C5-C6-N6	-5.03	119.68	123.70
27	X	1467	U	N1-C2-N3	-5.03	111.89	114.90
27	X	1683	G	N3-C4-N9	-5.03	122.98	126.00
27	X	2371	A	C5-N7-C8	-5.03	101.39	103.90
27	X	2596	C	C6-N1-C2	5.03	122.31	120.30
27	X	69	G	C4-N9-C1'	5.02	133.03	126.50
27	X	854	G	N1-C6-O6	5.02	122.91	119.90
27	X	1240	G	N9-C4-C5	-5.02	103.39	105.40
27	X	2792	C	C6-N1-C2	5.02	122.31	120.30
27	X	2682	C	C2-N1-C1'	5.02	124.32	118.80
27	X	2693	U	C5-C6-N1	-5.02	120.19	122.70
27	X	1315	A	C5-C6-N6	5.01	127.71	123.70
27	X	2472	U	O5'-P-OP1	-5.01	101.19	105.70
27	X	770	U	C6-N1-C2	-5.01	118.00	121.00
27	X	1682	A	N7-C8-N9	5.01	116.30	113.80
27	X	1618	U	N3-C4-C5	-5.00	111.60	114.60
27	X	2687	G	N7-C8-N9	-5.00	110.60	113.10

There are no chirality outliers.



All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	2	42	LEU	Peptide
26	3	45	GLY	Peptide
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide
8	I	40	ARG	Peptide
8	I	99	VAL	Peptide
10	K	93	GLY	Peptide
10	K	94	TYR	Peptide
16	Q	59	PRO	Peptide
17	R	64	ASN	Peptide
19	T	19	LYS	Peptide
20	U	30	VAL	Peptide
23	Z	4	HIS	Peptide

## 5.2 Too-close contacts

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	A	1987	0	2056	145	0
2	B	1539	0	1600	109	0
3	C	1481	0	1504	99	0
4	D	1400	0	1481	55	0
5	E	1286	0	1336	54	0
6	G	1114	0	1144	73	0
7	H	997	0	1046	56	0
8	I	1011	0	1047	72	0
9	J	1090	0	1125	64	0
10	K	878	0	930	45	0
11	L	779	0	820	36	0
12	M	871	0	894	61	0
13	N	978	0	1020	52	0
14	O	741	0	756	51	0
15	P	1038	0	1125	85	0
16	Q	726	0	753	32	0
17	R	825	0	881	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	S	1345	0	1372	37	0
19	T	556	0	579	30	0
20	U	552	0	604	35	0
21	V	525	0	546	19	0
22	W	424	0	470	16	0
23	Z	443	0	444	26	0
24	1	431	0	456	29	0
25	2	383	0	414	26	0
26	3	462	0	506	53	0
27	X	57533	0	28987	1351	0
28	Y	2602	0	1327	61	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	K	2	0	0	0	0
29	M	2	0	0	0	0
29	X	64	0	0	0	0
30	X	51	0	67	9	0
All	All	84118	0	55290	2473	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 19.

All (2473) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.32	1.11
23:Z:19:ARG:NH2	27:X:1277:G:OP1	1.90	1.04
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.46	0.97
27:X:854:G:H1	27:X:948:C:H42	1.04	0.96
7:H:40:GLY:HA3	27:X:2545:A:H61	1.29	0.95
8:I:21:ARG:HE	8:I:22:GLY:H	1.08	0.95
6:G:109:GLY:HA2	6:G:111:LYS:HE3	1.46	0.95
27:X:517:A:H5''	27:X:518:A:H5'	1.50	0.94
1:A:250:TRP:O	1:A:255:LYS:NZ	2.01	0.93
27:X:2447:G:HO2'	27:X:2448:A:H8	1.07	0.92
9:J:82:THR:HA	27:X:2474:G:H5''	1.53	0.90
27:X:4:C:H42	27:X:2873:G:H1	1.17	0.89
1:A:55:GLY:H	1:A:217:ARG:HB2	1.38	0.88
27:X:571:U:HO2'	27:X:581:A:H8	1.21	0.87
10:K:60:LEU:HG	10:K:64:ARG:HD2	1.55	0.86
27:X:2281:C:H42	27:X:2293:G:H1	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:38:THR:HB	27:X:2063:A:H5'	1.58	0.85
15:P:80:LEU:HD11	15:P:87:GLU:HB3	1.58	0.85
8:I:21:ARG:HE	8:I:22:GLY:N	1.75	0.85
24:1:41:ASP:HB2	24:1:46:LYS:HE3	1.56	0.85
27:X:538:A:H62	27:X:2026:C:H5'	1.40	0.84
27:X:832:A:OP2	27:X:1201:G:N2	2.10	0.84
1:A:218:LYS:NZ	1:A:219:PRO:O	2.10	0.84
27:X:2016:A:O2'	27:X:2018:G:OP2	1.95	0.84
27:X:2225:G:H2'	27:X:2226:A:H8	1.41	0.83
27:X:833:A:N3	27:X:954:U:O2'	2.10	0.83
27:X:2757:G:H5''	27:X:2758:A:H5'	1.60	0.83
9:J:83:ARG:HH22	27:X:971:A:H61	1.22	0.83
26:3:13:ARG:HE	26:3:25:PHE:H	1.27	0.83
15:P:100:GLY:HA3	15:P:124:THR:HA	1.58	0.83
2:B:14:ILE:HG12	12:M:20:HIS:HD2	1.43	0.82
27:X:2811:G:H2'	27:X:2812:A:C8	2.13	0.82
2:B:146:THR:HG1	27:X:2550:C:HO2'	1.19	0.82
14:O:12:TYR:HB3	14:O:40:VAL:H	1.45	0.81
1:A:252:LYS:HZ2	1:A:252:LYS:H	1.28	0.81
27:X:649:G:H22	27:X:661:C:H1'	1.45	0.81
22:W:8:SER:HB2	27:X:999:A:H5''	1.62	0.81
27:X:1173:G:H2'	27:X:1174:G:H8	1.46	0.80
6:G:37:ASP:O	6:G:39:GLN:NE2	2.15	0.79
27:X:841:G:H2'	27:X:842:A:C8	2.16	0.79
27:X:2259:G:H4'	27:X:2306:A:H5'	1.65	0.79
27:X:415:A:H61	27:X:436:A:H61	1.30	0.79
15:P:99:ALA:HB2	27:X:24:G:O2'	1.83	0.78
26:3:26:LYS:HD3	26:3:28:GLY:H	1.45	0.78
2:B:82:ARG:NH2	27:X:2617:G:OP2	2.16	0.78
9:J:17:ARG:NH1	27:X:966:A:OP2	2.17	0.78
15:P:30:TYR:H	15:P:126:HIS:HD2	1.32	0.78
14:O:57:GLN:H	14:O:97:GLY:HA3	1.47	0.78
27:X:538:A:O2'	27:X:539:A:O5'	2.00	0.78
2:B:51:TYR:HE2	12:M:3:THR:HG21	1.49	0.77
18:S:125:PRO:O	18:S:129:ARG:NH1	2.18	0.77
1:A:157:ARG:NH1	27:X:1810:U:OP2	2.17	0.77
9:J:100:PRO:HB2	18:S:74:ARG:HG2	1.67	0.77
7:H:23:ARG:NH1	27:X:2526:U:O2	2.17	0.77
27:X:2796:A:H2'	27:X:2797:G:C8	2.19	0.77
27:X:89:A:H4'	27:X:90:G:H5'	1.68	0.76
27:X:1856:U:OP1	27:X:2389:G:O2'	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1882:G:N2	27:X:1885:C:H41	1.83	0.76
27:X:215:G:H21	27:X:632:A:H8	1.30	0.76
3:C:163:ASN:HD21	3:C:167:VAL:H	1.31	0.76
20:U:21:ARG:HD3	20:U:23:LYS:HG2	1.66	0.76
27:X:2002:A:N6	27:X:2018:G:O6	2.19	0.76
27:X:1329:U:H2'	27:X:1330:G:H8	1.49	0.76
3:C:162:ARG:O	3:C:162:ARG:NH1	2.19	0.76
8:I:40:ARG:NH2	27:X:820:U:OP1	2.18	0.76
1:A:14:ARG:HG3	1:A:24:LEU:HG	1.68	0.76
27:X:2761:A:H5'	27:X:2762:G:H5'	1.67	0.75
3:C:161:ALA:HB1	3:C:167:VAL:HG21	1.69	0.75
27:X:2543:A:H5'	27:X:2627:G:H4'	1.66	0.75
2:B:176:ARG:HH21	12:M:16:ILE:HG23	1.51	0.75
1:A:243:GLY:C	1:A:244:ARG:HE	1.89	0.75
1:A:24:LEU:HB2	1:A:205:VAL:HG22	1.68	0.75
15:P:45:ILE:HD11	15:P:57:LEU:HD11	1.68	0.75
27:X:965:G:O2'	27:X:2253:A:N1	2.20	0.75
3:C:137:ALA:HB1	3:C:142:LEU:HB2	1.68	0.75
27:X:1327:C:H42	27:X:1351:G:H1	1.32	0.75
1:A:210:GLY:HA2	1:A:213:ARG:HG2	1.69	0.75
16:Q:14:GLU:OE2	27:X:1405:A:N6	2.18	0.75
17:R:56:LYS:HB3	17:R:69:GLN:HG2	1.69	0.75
24:1:27:ASN:ND2	24:1:36:GLU:OE1	2.20	0.75
27:X:2225:G:H2'	27:X:2226:A:C8	2.20	0.75
27:X:27:G:N2	27:X:522:G:H1'	2.02	0.75
26:3:32:GLN:HB3	27:X:2400:G:N7	2.02	0.75
27:X:2796:A:H2'	27:X:2797:G:H8	1.50	0.74
11:L:90:ASP:OD2	11:L:91:ARG:N	2.20	0.74
15:P:30:TYR:H	15:P:126:HIS:CD2	2.05	0.74
1:A:91:ARG:HB2	1:A:107:ALA:HB3	1.69	0.74
27:X:1673:C:H2'	27:X:1674:C:H6	1.52	0.74
27:X:1278:A:H2	27:X:1997:A:H62	1.35	0.74
2:B:91:VAL:HB	2:B:93:VAL:HG12	1.70	0.74
27:X:1922:U:H3'	27:X:1923:U:H5'	1.70	0.74
27:X:591:G:H3'	27:X:592:G:H8	1.51	0.74
27:X:2757:G:OP2	27:X:2761:A:O2'	2.06	0.74
9:J:117:GLU:OE1	9:J:120:ARG:NH1	2.21	0.74
12:M:60:SER:HA	12:M:64:LYS:HB2	1.69	0.74
6:G:34:PRO:HB3	6:G:71:THR:HG21	1.69	0.74
22:W:5:LEU:HB2	22:W:25:LEU:HD13	1.68	0.74
27:X:465:C:O2'	27:X:483:A:N6	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:19:ARG:HG2	27:X:123:A:H5'	1.68	0.74
27:X:2820:C:H2'	27:X:2821:G:H8	1.52	0.73
27:X:1337:G:N2	27:X:1343:C:O2	2.20	0.73
11:L:65:THR:OG1	28:Y:52:G:OP1	2.06	0.73
2:B:137:ARG:NH2	27:X:2034:A:OP1	2.19	0.73
27:X:854:G:N2	27:X:948:C:N3	2.32	0.73
2:B:9:ILE:HD11	2:B:27:LEU:HB2	1.70	0.73
27:X:872:G:O2'	27:X:928:G:O6	2.07	0.73
27:X:613:A:N6	27:X:668:A:O2'	2.22	0.73
12:M:100:ARG:HD2	27:X:1744:G:OP1	1.89	0.73
27:X:115:G:OP2	27:X:117:A:O2'	2.07	0.73
2:B:128:SER:HB3	27:X:1976:U:H4'	1.71	0.73
4:D:116:GLY:HA2	4:D:176:PRO:HB2	1.71	0.73
15:P:35:PRO:HD3	15:P:124:THR:OG1	1.89	0.73
27:X:1963:G:O2'	27:X:1965:U:OP2	2.07	0.73
27:X:2708:U:H2'	27:X:2709:C:C6	2.23	0.73
27:X:2484:G:H22	30:X:2902:ERY:H191	1.54	0.72
17:R:17:LYS:NZ	27:X:83:A:OP2	2.16	0.72
17:R:105:ARG:HH22	17:R:113:THR:H	1.37	0.72
27:X:313:U:H2'	27:X:314:G:H8	1.54	0.72
2:B:152:LYS:HB3	6:G:106:TYR:HB2	1.71	0.72
1:A:63:ARG:HH21	1:A:86:PRO:HD2	1.55	0.72
16:Q:35:LYS:NZ	27:X:1615:C:OP2	2.23	0.72
27:X:1399:C:OP2	27:X:1409:U:N3	2.21	0.72
27:X:2324:G:HO2'	27:X:2360:C:HO2'	1.35	0.72
27:X:1744:G:N2	27:X:1747:G:OP2	2.18	0.72
14:O:68:LYS:NZ	27:X:1238:A:OP1	2.18	0.72
23:Z:16:ARG:NH1	23:Z:17:ASP:OD2	2.22	0.72
24:1:28:ARG:NH1	27:X:2264:C:OP2	2.22	0.72
27:X:1643:A:H61	27:X:1656:U:H3	1.38	0.72
1:A:54:ILE:HA	1:A:217:ARG:H	1.55	0.71
27:X:168:A:H2'	27:X:169:C:C6	2.24	0.71
27:X:209:G:N2	27:X:433:G:OP1	2.22	0.71
14:O:66:GLY:O	14:O:87:ARG:NH2	2.23	0.71
3:C:6:VAL:HG13	3:C:7:ILE:HG12	1.72	0.71
27:X:1030:U:H3	27:X:1153:A:H62	1.38	0.71
26:3:30:ARG:HE	26:3:31:HIS:CE1	2.09	0.71
16:Q:64:ARG:NH2	27:X:1348:C:O2'	2.22	0.71
27:X:2048:C:O2	27:X:2428:U:N3	2.20	0.71
9:J:16:GLY:HA2	9:J:17:ARG:HH11	1.55	0.71
27:X:2020:G:H2'	27:X:2021:G:C8	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:O	1:A:252:LYS:NZ	2.20	0.71
27:X:1551:U:OP2	27:X:1553:G:N2	2.24	0.71
8:I:38:LYS:NZ	27:X:954:U:OP2	2.20	0.71
27:X:2354:G:N2	27:X:2357:A:OP2	2.22	0.71
22:W:25:LEU:HD22	22:W:30:ASP:HB3	1.73	0.71
3:C:149:LEU:HD11	3:C:170:LEU:HB2	1.73	0.71
27:X:1466:C:H2'	27:X:1467:U:O4'	1.91	0.71
8:I:31:GLY:O	8:I:32:ARG:NH2	2.23	0.71
6:G:116:ARG:HA	6:G:119:LEU:HD23	1.73	0.70
28:Y:51:G:H2'	28:Y:52:G:H8	1.56	0.70
8:I:18:ARG:NH2	8:I:18:ARG:O	2.23	0.70
27:X:1845:A:N3	27:X:2212:U:O2'	2.24	0.70
27:X:1361:G:H1	27:X:1614:C:H42	1.39	0.70
6:G:100:TYR:HB2	6:G:116:ARG:NH1	2.06	0.70
7:H:28:GLY:HA3	7:H:35:THR:OG1	1.91	0.70
24:1:41:ASP:N	24:1:41:ASP:OD1	2.24	0.70
8:I:17:LYS:HG3	8:I:19:VAL:H	1.57	0.70
26:3:13:ARG:NE	26:3:25:PHE:H	1.89	0.70
5:E:33:LEU:HD21	5:E:136:ILE:HB	1.73	0.70
27:X:538:A:HO2'	27:X:539:A:P	2.15	0.69
27:X:661:C:H2'	27:X:662:G:C8	2.27	0.69
27:X:113:C:HO2'	27:X:125:A:HO2'	1.40	0.69
1:A:96:HIS:NE2	27:X:1517:C:O2'	2.21	0.69
5:E:124:ALA:HB3	5:E:132:ASP:HB3	1.73	0.69
27:X:27:G:H22	27:X:522:G:H1'	1.58	0.69
10:K:24:GLN:HB3	10:K:44:LEU:HD22	1.74	0.69
27:X:2241:U:H2'	27:X:2242:C:H6	1.56	0.69
1:A:249:PRO:HD3	27:X:2218:G:H5'	1.73	0.69
27:X:793:G:H21	27:X:796:A:H62	1.38	0.69
1:A:231:HIS:CD2	1:A:232:PRO:HD2	2.26	0.69
27:X:2237:C:O2'	27:X:2406:C:OP2	2.11	0.69
27:X:953:G:O2'	27:X:1203:A:N3	2.24	0.69
12:M:31:ASP:HB2	12:M:94:VAL:HB	1.75	0.69
14:O:23:GLU:HB2	14:O:91:THR:HG21	1.75	0.69
27:X:2617:G:H1	27:X:2755:A:H2'	1.58	0.68
6:G:106:TYR:CD2	6:G:108:GLY:HA2	2.28	0.68
27:X:1030:U:O2	27:X:1155:G:N2	2.26	0.68
27:X:224:G:OP2	27:X:226:C:N4	2.26	0.68
27:X:105:G:H21	27:X:357:A:H61	1.42	0.68
11:L:28:ARG:NH1	11:L:90:ASP:OD1	2.27	0.68
27:X:1342:U:H5''	27:X:1343:C:H5	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:41:ARG:HH12	27:X:2366:U:H1'	1.59	0.68
4:D:66:ILE:HD11	28:Y:43:G:H3'	1.75	0.68
21:V:48:ARG:NH2	27:X:76:C:OP1	2.27	0.68
6:G:50:PRO:HG2	6:G:53:ARG:HB2	1.76	0.68
1:A:55:GLY:N	1:A:217:ARG:HB2	2.07	0.68
11:L:39:TYR:OH	28:Y:118:G:N3	2.27	0.68
9:J:61:ARG:HH11	18:S:175:ARG:HB2	1.58	0.68
25:2:33:ARG:NE	27:X:478:G:OP1	2.25	0.68
8:I:51:GLY:HA3	26:3:59:LYS:HE3	1.74	0.68
26:3:19:THR:OG1	27:X:661:C:OP1	2.12	0.67
27:X:226:C:OP2	27:X:2373:C:O2'	2.12	0.67
27:X:2200:G:H2'	27:X:2201:G:C8	2.29	0.67
9:J:81:GLU:HG2	9:J:82:THR:HG23	1.76	0.67
3:C:48:ARG:NH1	3:C:51:VAL:HG13	2.09	0.67
2:B:78:LEU:O	2:B:79:ARG:NE	2.27	0.67
27:X:1573:G:O6	27:X:1574:A:N6	2.27	0.67
3:C:111:ARG:NH1	3:C:180:ILE:O	2.27	0.67
10:K:12:ARG:HD3	10:K:16:ALA:HB1	1.77	0.67
27:X:1202:U:H2'	27:X:1203:A:H8	1.60	0.67
8:I:56:LEU:HB3	26:3:52:LYS:HZ1	1.60	0.67
15:P:28:ALA:HB2	15:P:71:VAL:HG21	1.76	0.67
2:B:26:VAL:HB	2:B:182:ILE:HG23	1.77	0.67
27:X:760:U:O2'	27:X:761:G:OP2	2.12	0.67
27:X:2672:U:H2'	27:X:2673:G:H8	1.60	0.67
4:D:115:ARG:HH22	4:D:178:ARG:HH12	1.43	0.67
7:H:40:GLY:HA3	27:X:2545:A:N6	2.08	0.67
27:X:2040:A:H2'	27:X:2041:A:C8	2.29	0.67
27:X:203:G:O2'	27:X:205:A:N1	2.23	0.67
23:Z:36:CYS:SG	23:Z:49:CYS:N	2.67	0.67
3:C:59:TYR:OH	3:C:67:ALA:HB1	1.93	0.67
15:P:99:ALA:HB1	27:X:25:U:H5'	1.76	0.67
14:O:10:LYS:HG3	14:O:13:ARG:HH22	1.60	0.66
4:D:62:LEU:O	4:D:95:ARG:NH1	2.28	0.66
10:K:28:LEU:HD21	10:K:115:LEU:HG	1.78	0.66
27:X:1287:A:N1	27:X:1661:C:O2'	2.26	0.66
18:S:47:SER:OG	18:S:48:THR:N	2.18	0.66
27:X:1278:A:N6	27:X:1996:A:H5''	2.10	0.66
9:J:38:MET:HB2	9:J:129:GLN:HB2	1.76	0.66
27:X:571:U:O2'	27:X:581:A:H8	1.77	0.66
27:X:1173:G:H2'	27:X:1174:G:C8	2.30	0.66
27:X:617:U:H5	27:X:632:A:C2	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:16:HIS:HB3	25:2:43:THR:HG21	1.77	0.66
27:X:18:U:O2'	27:X:563:U:OP1	2.14	0.66
23:Z:31:THR:OG1	27:X:2861:A:O2'	2.12	0.66
27:X:854:G:H1	27:X:948:C:N4	1.86	0.66
27:X:1850:G:O2'	27:X:1867:A:N6	2.29	0.66
3:C:46:ARG:HB3	3:C:51:VAL:HB	1.77	0.66
27:X:2298:U:O2	27:X:2299:A:N6	2.28	0.66
17:R:61:SER:HA	17:R:65:PRO:HG3	1.77	0.66
12:M:101:ARG:NH2	27:X:1745:C:OP1	2.29	0.66
2:B:77:ILE:HD13	2:B:195:LEU:HD22	1.77	0.66
27:X:2324:G:N3	27:X:2360:C:H2'	2.10	0.66
27:X:1089:C:O2'	27:X:1099:A:OP1	2.10	0.66
6:G:122:HIS:HB3	6:G:125:ARG:HB2	1.78	0.66
27:X:2284:U:H5'	27:X:2286:G:H1	1.59	0.66
28:Y:46:G:N3	28:Y:49:C:N4	2.44	0.65
7:H:13:ASN:HD21	7:H:109:ARG:HG2	1.61	0.65
3:C:83:ALA:HB3	27:X:595:A:H5'	1.77	0.65
27:X:1283:C:H5''	27:X:1284:G:H5'	1.78	0.65
17:R:84:VAL:HG11	17:R:90:LYS:H	1.59	0.65
6:G:103:TYR:CG	6:G:111:LYS:HB2	2.31	0.65
1:A:183:ARG:NH1	27:X:1790:G:O2'	2.29	0.65
27:X:1329:U:H2'	27:X:1330:G:C8	2.30	0.65
9:J:36:ILE:HG12	9:J:103:VAL:HA	1.78	0.65
7:H:13:ASN:ND2	7:H:109:ARG:HG2	2.11	0.65
6:G:130:ALA:O	27:X:1148:G:O2'	2.14	0.65
19:T:74:LYS:HA	19:T:77:ARG:HG3	1.77	0.65
1:A:52:ARG:HD3	27:X:1816:G:OP1	1.96	0.65
27:X:1466:C:H42	27:X:1476:G:H1	1.45	0.65
27:X:1109:A:H3'	27:X:1110:G:H8	1.62	0.65
13:N:93:LYS:HE2	14:O:10:LYS:HD3	1.76	0.65
27:X:2015:G:OP2	27:X:2433:G:O2'	2.09	0.65
6:G:61:ARG:HH12	6:G:66:HIS:H	1.45	0.65
27:X:578:U:O2'	27:X:994:A:N1	2.26	0.65
27:X:1562:G:H5'	27:X:1563:U:H5'	1.78	0.65
27:X:840:U:H4'	27:X:841:G:C2	2.32	0.65
27:X:1082:G:O2'	27:X:1100:G:OP2	2.14	0.65
2:B:140:SER:HB3	27:X:2554:C:O2'	1.96	0.65
23:Z:6:VAL:HG22	23:Z:7:PRO:HD2	1.79	0.65
7:H:1:MET:HE2	27:X:1682:A:H1'	1.78	0.65
2:B:76:ARG:NH2	27:X:2804:G:O3'	2.30	0.65
17:R:56:LYS:HD2	27:X:494:A:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:219:G:HO2'	27:X:231:G:H1	1.44	0.65
27:X:87:G:H2'	27:X:88:G:H5''	1.77	0.65
3:C:163:ASN:ND2	3:C:167:VAL:H	1.95	0.65
15:P:105:ARG:O	15:P:105:ARG:NE	2.29	0.65
27:X:812:G:H3'	27:X:813:A:H2'	1.79	0.65
27:X:545:C:H2'	27:X:546:A:C8	2.32	0.65
27:X:1067:G:H5''	27:X:1068:A:H5'	1.77	0.65
27:X:308:C:O2	27:X:352:G:N2	2.23	0.65
27:X:1401:G:O6	27:X:1412:C:N4	2.30	0.65
27:X:403:A:H4'	27:X:404:A:H5'	1.79	0.65
6:G:132:PHE:CZ	6:G:145:HIS:HB2	2.32	0.64
3:C:9:GLN:HG2	3:C:120:VAL:HG21	1.79	0.64
27:X:1225:G:O2'	27:X:1250:A:N6	2.30	0.64
27:X:1742:G:HO2'	27:X:2836:U:HO2'	1.43	0.64
8:I:40:ARG:NH1	27:X:576:A:O3'	2.30	0.64
27:X:304:A:N6	27:X:356:A:N7	2.44	0.64
11:L:38:ILE:HD11	11:L:40:ALA:HB2	1.77	0.64
27:X:1373:G:H22	27:X:2192:U:H3	1.45	0.64
10:K:87:TYR:HE1	10:K:94:TYR:HD1	1.46	0.64
27:X:2432:A:H61	27:X:2479:U:H3	1.45	0.64
19:T:40:GLN:NE2	19:T:42:GLY:O	2.30	0.64
27:X:759:C:H5''	27:X:761:G:H1'	1.79	0.64
27:X:800:U:H5''	27:X:801:A:H5'	1.79	0.64
5:E:94:PHE:HB3	5:E:107:ILE:HG22	1.80	0.64
2:B:16:LYS:HD3	2:B:173:VAL:HG12	1.80	0.64
20:U:47:HIS:ND1	27:X:410:A:OP1	2.30	0.64
2:B:5:LEU:HD11	2:B:79:ARG:HB2	1.79	0.64
27:X:1225:G:H2'	27:X:1249:G:N2	2.12	0.64
27:X:542:A:OP1	27:X:570:G:N2	2.29	0.64
4:D:92:ARG:CZ	28:Y:47:A:H1'	2.27	0.64
7:H:104:GLU:OE2	7:H:125:LYS:NZ	2.31	0.64
10:K:68:GLN:NE2	27:X:2686:C:O3'	2.28	0.64
10:K:102:THR:HA	10:K:109:THR:HA	1.80	0.64
27:X:1017:C:H2'	27:X:1018:C:H6	1.60	0.64
27:X:1504:G:N2	27:X:1517:C:O2	2.31	0.64
17:R:90:LYS:HG3	17:R:108:VAL:HG21	1.79	0.64
9:J:84:MET:HG2	27:X:2229:G:H5'	1.80	0.64
9:J:15:ARG:HD3	9:J:74:PRO:HD2	1.79	0.64
12:M:103:LYS:HG2	27:X:2698:G:H4'	1.79	0.64
27:X:1882:G:H21	27:X:1885:C:H41	1.45	0.64
27:X:2811:G:H2'	27:X:2812:A:H8	1.58	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:5:A:H2'	27:X:6:A:C8	2.33	0.64
3:C:2:ALA:HA	3:C:13:ARG:HA	1.80	0.64
2:B:14:ILE:HG12	12:M:20:HIS:CD2	2.29	0.63
6:G:70:PHE:HB3	13:N:64:ARG:HG2	1.78	0.63
5:E:8:PRO:HD2	5:E:69:ARG:HH11	1.62	0.63
27:X:619:A:N6	27:X:630:G:O2'	2.31	0.63
16:Q:48:VAL:HG21	16:Q:82:LEU:HD13	1.79	0.63
2:B:92:ASN:HA	2:B:95:ILE:HB	1.78	0.63
27:X:874:A:H2'	27:X:875:G:O4'	1.99	0.63
5:E:90:ARG:HH21	5:E:163:ARG:HD2	1.64	0.63
14:O:5:ILE:HG23	14:O:13:ARG:NH1	2.13	0.63
16:Q:88:ILE:HG13	16:Q:92:ALA:HB2	1.80	0.63
3:C:58:MET:HG2	3:C:59:TYR:CD1	2.33	0.63
1:A:159:ALA:HB3	27:X:1812:U:H3'	1.80	0.63
27:X:1827:G:H1	27:X:1888:C:H42	1.45	0.63
1:A:254:THR:OG1	27:X:1835:C:O2'	2.15	0.63
26:3:17:THR:HG22	26:3:21:LYS:H	1.62	0.63
7:H:123:PHE:HB3	7:H:126:ILE:HG13	1.80	0.63
27:X:826:U:H2'	27:X:827:C:C6	2.33	0.63
27:X:1422:C:H2'	27:X:1423:A:H8	1.63	0.63
27:X:584:A:OP2	27:X:2038:C:N4	2.31	0.63
27:X:1030:U:H2'	27:X:1032:A:H2	1.63	0.63
27:X:2039:G:C2	27:X:2040:A:C8	2.87	0.63
27:X:646:C:O2'	27:X:650:U:OP1	2.17	0.63
27:X:748:A:H5'	27:X:749:C:OP2	1.99	0.63
27:X:160:C:O2'	27:X:445:A:N3	2.28	0.62
27:X:1554:G:H2'	27:X:1555:A:H8	1.64	0.62
28:Y:27:A:O2'	28:Y:28:A:O5'	2.17	0.62
27:X:1502:G:H22	27:X:1518:C:H42	1.46	0.62
14:O:21:ARG:HH22	27:X:1005:U:H1'	1.64	0.62
19:T:51:VAL:HG21	19:T:79:ILE:HG22	1.80	0.62
8:I:61:PRO:HB2	26:3:30:ARG:HD3	1.80	0.62
27:X:661:C:H2'	27:X:662:G:H8	1.62	0.62
6:G:119:LEU:HD12	6:G:122:HIS:HB2	1.80	0.62
28:Y:42:U:O2'	28:Y:47:A:N6	2.32	0.62
18:S:91:PRO:HD3	18:S:127:PRO:HD3	1.80	0.62
4:D:16:LEU:O	4:D:20:PHE:N	2.27	0.62
15:P:70:LYS:NZ	27:X:500:G:O6	2.31	0.62
8:I:59:ARG:HB2	27:X:2371:A:H8	1.63	0.62
2:B:51:TYR:CE2	12:M:3:THR:HG21	2.33	0.62
27:X:2200:G:H2'	27:X:2201:G:H8	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:725:C:O2	27:X:732:G:N2	2.26	0.62
1:A:46:ARG:NE	27:X:1383:C:OP1	2.32	0.62
8:I:59:ARG:HB2	27:X:2371:A:C8	2.34	0.62
15:P:57:LEU:HD13	15:P:69:ALA:HA	1.82	0.62
27:X:2679:G:H1	27:X:2686:C:H42	1.48	0.62
27:X:772:G:H2'	27:X:773:G:H8	1.65	0.62
27:X:313:U:H2'	27:X:314:G:C8	2.35	0.62
4:D:39:GLY:O	4:D:150:ARG:NH2	2.33	0.62
6:G:157:PRO:O	6:G:161:GLN:NE2	2.32	0.62
27:X:1919:A:N6	27:X:1946:U:H3	1.97	0.62
7:H:25:LEU:HD21	7:H:52:VAL:HG23	1.81	0.62
27:X:588:G:O2'	27:X:2002:A:OP1	2.14	0.62
5:E:45:GLN:NE2	5:E:48:ASP:O	2.32	0.62
2:B:115:GLY:HA2	2:B:136:ARG:HD2	1.81	0.62
27:X:1361:G:H1	27:X:1614:C:N4	1.97	0.62
17:R:22:VAL:HG22	17:R:82:ALA:HA	1.81	0.62
8:I:102:LYS:O	8:I:104:ARG:N	2.32	0.62
23:Z:51:TYR:CE1	23:Z:55:ARG:HB2	2.35	0.62
20:U:53:GLU:HB3	20:U:58:LYS:H	1.65	0.62
19:T:41:ARG:NH2	27:X:2366:U:O2'	2.25	0.61
27:X:2617:G:N1	27:X:2755:A:H2'	2.15	0.61
13:N:66:ASN:ND2	27:X:1021:A:OP1	2.33	0.61
27:X:2417:U:O2'	27:X:2419:C:OP1	2.16	0.61
10:K:6:ALA:HB1	27:X:2848:A:H2	1.63	0.61
4:D:4:LEU:HG	4:D:5:LYS:H	1.66	0.61
1:A:252:LYS:NZ	1:A:252:LYS:H	1.97	0.61
27:X:1140:A:O2'	27:X:2494:C:O2'	2.15	0.61
27:X:605:G:H2'	27:X:606:A:H8	1.66	0.61
15:P:25:PHE:HD1	15:P:130:ILE:HD11	1.66	0.61
4:D:106:ILE:HG21	4:D:139:PRO:HB3	1.81	0.61
28:Y:78:A:H2'	28:Y:79:U:O4'	2.01	0.61
5:E:86:ASN:HB2	5:E:165:VAL:HG13	1.82	0.61
7:H:13:ASN:OD1	7:H:108:THR:N	2.32	0.61
27:X:2191:A:OP1	27:X:2193:C:N4	2.32	0.61
27:X:1440:G:H5''	27:X:1441:A:H2'	1.83	0.61
12:M:18:GLN:HA	12:M:21:THR:HB	1.82	0.61
13:N:50:ARG:HA	13:N:53:LYS:HE2	1.83	0.61
27:X:165:G:H1	27:X:185:C:H42	1.47	0.61
12:M:17:GLU:HG3	12:M:62:SER:H	1.65	0.61
2:B:189:PRO:HA	27:X:2659:C:H5'	1.82	0.61
14:O:36:LYS:HB2	14:O:51:ALA:HB1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:ARG:HB3	27:X:1673:C:H5''	1.81	0.61
27:X:1070:G:H5''	27:X:1071:U:H2'	1.82	0.61
22:W:4:LYS:HG3	22:W:52:GLU:HB3	1.83	0.61
12:M:66:PHE:HB3	12:M:83:PHE:HE1	1.66	0.61
25:2:7:PRO:HB2	27:X:1322:G:H4'	1.81	0.61
27:X:540:G:HO2'	27:X:542:A:H2	1.48	0.61
1:A:246:PRO:HD3	1:A:252:LYS:HE3	1.82	0.61
6:G:35:LYS:N	6:G:69:ASP:OD2	2.34	0.61
27:X:1514:C:H4'	27:X:1592:U:O2'	2.01	0.61
21:V:15:ALA:HA	21:V:18:ILE:HD12	1.83	0.61
20:U:51:ILE:HG23	20:U:59:THR:HA	1.82	0.61
13:N:5:LYS:HG2	13:N:7:GLY:H	1.64	0.61
27:X:635:C:O2'	27:X:670:U:OP1	2.17	0.61
27:X:810:U:H2'	27:X:811:G:O4'	2.01	0.61
17:R:42:ARG:NH2	27:X:86:U:OP2	2.33	0.61
2:B:174:GLU:HB3	2:B:183:LEU:HD12	1.82	0.61
11:L:28:ARG:NH2	28:Y:10:U:O3'	2.34	0.60
27:X:2820:C:H2'	27:X:2821:G:C8	2.36	0.60
20:U:49:LYS:HD3	20:U:61:TRP:CE2	2.36	0.60
7:H:99:ILE:HD12	7:H:103:GLY:HA2	1.83	0.60
27:X:2591:C:H2'	27:X:2592:U:H5	1.65	0.60
3:C:15:ILE:HD11	3:C:195:ILE:H	1.66	0.60
27:X:2191:A:H5''	27:X:2192:U:H5	1.66	0.60
20:U:52:ARG:HD2	20:U:79:GLU:HA	1.82	0.60
7:H:47:VAL:HG23	7:H:77:THR:HG23	1.83	0.60
8:I:81:GLN:HB3	8:I:114:ILE:HG23	1.84	0.60
27:X:1073:G:H22	27:X:1087:C:H42	1.48	0.60
27:X:1301:U:O2'	27:X:1664:G:N2	2.34	0.60
11:L:50:THR:N	28:Y:116:C:O2'	2.33	0.60
8:I:62:LYS:HB3	26:3:12:ARG:HA	1.83	0.60
27:X:2591:C:H2'	27:X:2592:U:C5	2.35	0.60
18:S:117:VAL:HB	18:S:168:VAL:HG22	1.82	0.60
1:A:252:LYS:N	1:A:252:LYS:HZ2	1.99	0.60
27:X:482:A:H2'	27:X:483:A:O4'	2.02	0.60
4:D:45:GLU:OE1	4:D:78:LYS:NZ	2.30	0.60
27:X:623:G:C2	27:X:624:A:H1'	2.37	0.60
5:E:103:LEU:HD23	5:E:115:ILE:HD12	1.83	0.60
13:N:13:ARG:NH1	27:X:1264:C:H5''	2.17	0.60
15:P:118:ASN:HA	27:X:1996:A:O2'	2.01	0.60
16:Q:13:SER:OG	16:Q:14:GLU:N	2.32	0.60
2:B:169:ASN:HD21	2:B:204:ALA:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1430:G:H1	27:X:1598:C:H42	1.50	0.60
18:S:28:ASN:OD1	18:S:28:ASN:N	2.34	0.60
2:B:52:ALA:O	2:B:76:ARG:N	2.25	0.60
3:C:71:ASP:OD1	3:C:72:ARG:N	2.34	0.60
9:J:6:LYS:HB3	9:J:45:SER:HB2	1.84	0.60
7:H:11:ALA:O	7:H:111:PHE:N	2.30	0.60
18:S:26:LYS:HG3	18:S:27:GLU:HG3	1.83	0.60
27:X:663:G:H3'	27:X:664:C:H5''	1.84	0.60
1:A:68:LYS:H	1:A:68:LYS:HD3	1.67	0.60
3:C:48:ARG:HB2	3:C:50:GLN:HB3	1.82	0.60
27:X:615:C:O2	27:X:670:U:O2'	2.17	0.60
7:H:9:ASP:O	7:H:96:ALA:N	2.34	0.60
27:X:1451:C:H2'	27:X:1452:U:H6	1.67	0.60
26:3:17:THR:HG23	26:3:19:THR:H	1.67	0.60
27:X:2707:G:H2'	27:X:2708:U:C6	2.36	0.60
4:D:133:LYS:HE2	27:X:2284:U:H4'	1.83	0.60
2:B:105:THR:HB	2:B:166:THR:HG23	1.84	0.60
3:C:158:ARG:HB3	3:C:169:VAL:HG11	1.83	0.60
6:G:62:ILE:O	6:G:77:GLY:HA3	2.02	0.60
12:M:3:THR:HG22	12:M:5:ILE:HG13	1.84	0.60
27:X:1350:G:H2'	27:X:1351:G:H8	1.66	0.60
1:A:63:ARG:HE	1:A:85:ASP:HB3	1.67	0.60
27:X:2767:C:HO2'	27:X:2785:A:HO2'	1.49	0.60
12:M:27:PHE:HA	12:M:96:ARG:NH2	2.16	0.60
27:X:13:A:O2'	27:X:15:G:N7	2.35	0.60
27:X:2330:G:H21	27:X:2345:A:H62	1.50	0.59
27:X:1777:A:H1'	27:X:1921:A:N6	2.17	0.59
10:K:10:LEU:HD11	10:K:17:ARG:HE	1.66	0.59
18:S:71:MET:HA	18:S:78:PRO:HA	1.84	0.59
27:X:1997:A:H2'	27:X:1998:A:C8	2.37	0.59
4:D:171:GLN:HE21	4:D:177:PHE:HE1	1.49	0.59
27:X:242:A:N6	27:X:441:A:N7	2.50	0.59
27:X:2279:G:N2	27:X:2295:C:O2	2.33	0.59
14:O:85:GLY:O	27:X:1237:G:H4'	2.02	0.59
13:N:93:LYS:HE3	14:O:6:GLN:HG3	1.84	0.59
4:D:112:ARG:NH2	4:D:134:GLU:OE2	2.35	0.59
4:D:70:ALA:HB3	4:D:82:GLY:HA2	1.83	0.59
28:Y:7:C:O2'	28:Y:29:C:O2	2.14	0.59
2:B:136:ARG:HD3	27:X:1673:C:H5'	1.84	0.59
13:N:20:ARG:HD2	13:N:39:LEU:HD13	1.84	0.59
1:A:163:VAL:HG22	1:A:177:LEU:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:26:THR:OG1	27:X:676:G:OP1	2.15	0.59
27:X:2174:G:H2'	27:X:2175:A:H8	1.68	0.59
8:I:30:ALA:CA	27:X:824:U:H2'	2.33	0.59
27:X:721:C:H42	27:X:736:G:H1	1.51	0.59
25:2:3:ARG:O	25:2:6:GLN:NE2	2.30	0.59
27:X:243:G:O6	27:X:439:C:N4	2.29	0.59
2:B:56:GLU:HG2	2:B:74:PRO:HG3	1.83	0.59
7:H:2:ILE:HD12	7:H:8:LEU:HD21	1.85	0.59
27:X:1563:U:H2'	27:X:1564:U:C6	2.38	0.59
2:B:60:ASN:HB3	2:B:62:PRO:HD2	1.85	0.59
5:E:22:GLY:HA3	5:E:39:THR:HG22	1.85	0.59
27:X:2837:G:H2'	27:X:2838:U:H6	1.67	0.59
1:A:168:LYS:HD3	1:A:173:VAL:HG22	1.83	0.59
14:O:70:TYR:OH	27:X:1236:G:O6	2.21	0.59
17:R:107:ALA:HB2	17:R:111:GLY:HA2	1.83	0.59
5:E:107:ILE:HD11	5:E:151:VAL:HG12	1.85	0.59
27:X:711:C:O2'	27:X:747:A:N6	2.36	0.59
27:X:2283:G:H1	27:X:2291:U:H3	1.51	0.59
27:X:1141:U:O5'	27:X:1141:U:H6	1.86	0.59
27:X:2571:G:O6	27:X:2580:C:N4	2.32	0.59
27:X:1479:G:H2'	27:X:1480:G:C8	2.38	0.59
2:B:128:SER:OG	27:X:1976:U:O3'	2.21	0.59
27:X:2849:C:H2'	27:X:2850:U:H6	1.68	0.59
27:X:1937:G:O2'	27:X:1939:U:O4	2.14	0.59
16:Q:26:SER:HB3	16:Q:79:ILE:HG12	1.85	0.59
24:1:14:SER:HB2	24:1:23:THR:H	1.68	0.59
2:B:121:ASN:O	2:B:122:PHE:HB2	2.03	0.59
1:A:172:TYR:HA	1:A:186:HIS:HA	1.84	0.59
13:N:49:ASP:HA	13:N:52:ASN:HB2	1.85	0.59
15:P:30:TYR:O	15:P:123:ARG:NE	2.27	0.58
27:X:2201:G:H2'	27:X:2202:G:H8	1.68	0.58
3:C:48:ARG:NE	3:C:51:VAL:HG22	2.18	0.58
10:K:79:VAL:HA	10:K:83:VAL:HB	1.85	0.58
3:C:68:ARG:NH1	27:X:687:G:H1'	2.18	0.58
2:B:5:LEU:HD22	2:B:195:LEU:HD11	1.85	0.58
27:X:1854:G:H2'	27:X:1855:G:H8	1.69	0.58
27:X:2522:G:H2'	27:X:2523:G:C8	2.38	0.58
27:X:139:A:H2'	27:X:140:G:H8	1.68	0.58
2:B:133:LYS:HG3	2:B:137:ARG:HB3	1.85	0.58
13:N:24:PHE:CE1	27:X:543:G:H5'	2.38	0.58
2:B:76:ARG:HH22	27:X:2805:G:P	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:SER:CB	27:X:1976:U:H4'	2.34	0.58
10:K:10:LEU:HD23	10:K:13:ASN:O	2.03	0.58
17:R:26:SER:OG	17:R:27:GLY:N	2.34	0.58
1:A:245:VAL:HB	1:A:249:PRO:HA	1.85	0.58
27:X:154:U:H3'	27:X:155:G:H8	1.68	0.58
20:U:51:ILE:HG12	20:U:59:THR:HB	1.84	0.58
4:D:122:PHE:HA	27:X:2282:G:H4'	1.85	0.58
27:X:1785:A:H2'	27:X:1786:C:H6	1.66	0.58
1:A:16:MET:SD	1:A:17:THR:N	2.74	0.58
27:X:1468:A:H8	27:X:1468:A:O5'	1.87	0.58
17:R:84:VAL:HG21	17:R:89:GLY:HA2	1.85	0.58
27:X:500:G:C2	27:X:501:G:H1'	2.39	0.58
27:X:1210:C:H2'	27:X:1211:G:H8	1.68	0.58
27:X:312:G:HO2'	27:X:313:U:H6	1.52	0.58
9:J:61:ARG:HB3	18:S:175:ARG:H	1.69	0.58
6:G:61:ARG:NH1	6:G:65:LYS:HB3	2.19	0.58
10:K:68:GLN:HG2	27:X:2686:C:O2'	2.04	0.58
27:X:1554:G:H2'	27:X:1555:A:C8	2.38	0.58
7:H:75:VAL:HG22	7:H:96:ALA:HA	1.84	0.58
27:X:2245:A:H4'	27:X:2246:A:N3	2.18	0.58
1:A:76:ASN:ND2	1:A:118:ASN:OD1	2.37	0.58
1:A:252:LYS:HZ2	1:A:253:PRO:HD2	1.67	0.58
27:X:1019:U:O2'	27:X:1020:A:O5'	2.19	0.58
27:X:1501:C:H42	27:X:1519:G:H1	1.50	0.58
27:X:1140:A:HO2'	27:X:2494:C:HO2'	1.42	0.58
4:D:64:LYS:O	28:Y:44:C:O2'	2.20	0.58
27:X:1919:A:H2	27:X:1926:U:H3	1.52	0.58
6:G:103:TYR:CD2	6:G:111:LYS:HB2	2.39	0.58
2:B:176:ARG:HH21	12:M:16:ILE:CG2	2.17	0.58
27:X:712:A:H2'	27:X:713:G:O4'	2.04	0.58
6:G:84:ASN:O	6:G:152:ALA:HA	2.03	0.58
13:N:37:GLN:HB3	27:X:1265:G:H1	1.69	0.58
27:X:670:U:H2'	27:X:671:A:C8	2.38	0.58
27:X:163:A:H2'	27:X:164:G:C8	2.39	0.58
27:X:2006:G:H5'	27:X:2596:C:H4'	1.85	0.58
27:X:70:A:H4'	27:X:71:A:H5''	1.85	0.58
12:M:7:ILE:HD12	12:M:8:ASN:H	1.68	0.58
27:X:222:G:O2'	27:X:397:U:O2	2.18	0.57
27:X:2492:G:C2	27:X:2493:U:C2	2.92	0.57
19:T:68:VAL:HB	19:T:80:SER:HB2	1.86	0.57
19:T:72:LYS:HD3	28:Y:14:C:H5''	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1699:A:H61	27:X:1723:U:H3	1.52	0.57
26:3:15:LYS:O	26:3:23:MET:N	2.35	0.57
3:C:176:ASN:HB3	3:C:179:ASP:H	1.68	0.57
8:I:73:GLU:HG3	8:I:101:ARG:HG3	1.84	0.57
27:X:1443:G:H2'	27:X:1444:C:C6	2.39	0.57
27:X:1454:U:H2'	27:X:1455:C:C6	2.40	0.57
15:P:95:ALA:HB2	15:P:129:ILE:HG23	1.86	0.57
2:B:143:GLN:O	27:X:2035:G:H4'	2.03	0.57
6:G:69:ASP:H	6:G:76:GLN:HE22	1.51	0.57
27:X:2594:U:H2'	27:X:2595:C:H6	1.69	0.57
9:J:15:ARG:HH21	9:J:73:LYS:HZ2	1.51	0.57
11:L:32:TYR:CZ	11:L:34:SER:HB3	2.39	0.57
5:E:6:LYS:HB2	5:E:69:ARG:HG3	1.85	0.57
27:X:346:C:H2'	27:X:347:C:C6	2.40	0.57
3:C:69:HIS:HE2	27:X:1270:C:P	2.27	0.57
4:D:60:ILE:HG13	4:D:61:THR:HG23	1.86	0.57
18:S:3:LEU:HD23	18:S:56:VAL:HG13	1.86	0.57
28:Y:17:A:H1'	28:Y:112:A:C8	2.39	0.57
27:X:1342:U:H5''	27:X:1343:C:C5	2.37	0.57
19:T:74:LYS:C	19:T:76:ALA:H	2.07	0.57
27:X:303:C:H3'	27:X:304:A:H5''	1.86	0.57
1:A:158:SER:OG	1:A:159:ALA:N	2.35	0.57
27:X:1310:C:H2'	27:X:1311:C:C6	2.39	0.57
27:X:1422:C:H2'	27:X:1423:A:C8	2.38	0.57
13:N:78:THR:HG23	13:N:117:ARG:CZ	2.34	0.57
13:N:105:ALA:HB2	14:O:45:THR:HG21	1.86	0.57
27:X:2570:C:H2'	27:X:2571:G:C8	2.40	0.57
27:X:2528:G:H2'	27:X:2529:G:H8	1.69	0.57
27:X:1373:G:N2	27:X:2192:U:H3	2.03	0.57
27:X:2493:U:H2'	27:X:2494:C:C6	2.40	0.57
27:X:1185:C:H2'	27:X:1186:G:H2'	1.85	0.57
27:X:554:U:H5''	27:X:556:A:C2	2.39	0.57
27:X:751:G:H2'	27:X:752:G:C8	2.40	0.57
17:R:92:THR:O	17:R:92:THR:OG1	2.21	0.57
9:J:81:GLU:HB2	27:X:2473:G:O2'	2.05	0.57
27:X:2590:U:H1'	30:X:2902:ERY:H361	1.85	0.57
10:K:32:GLY:HA2	10:K:115:LEU:HD12	1.86	0.57
6:G:132:PHE:HZ	6:G:142:ARG:HA	1.70	0.57
27:X:772:G:H2'	27:X:773:G:C8	2.40	0.57
27:X:992:A:N1	27:X:2010:G:O2'	2.32	0.57
24:1:16:ALA:HB2	24:1:50:PHE:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:3:ILE:HD11	22:W:44:VAL:HG11	1.86	0.57
27:X:1645:U:H2'	27:X:1646:G:C8	2.40	0.57
27:X:859:U:H3	27:X:944:A:N6	2.03	0.57
2:B:136:ARG:HB3	27:X:1673:C:C5'	2.34	0.57
1:A:252:LYS:O	27:X:1787:U:O2'	2.22	0.57
27:X:436:A:H5''	27:X:437:G:H5''	1.85	0.57
27:X:82:G:H1	27:X:100:G:HO2'	1.52	0.57
10:K:87:TYR:CE1	10:K:94:TYR:HD1	2.23	0.57
10:K:76:VAL:HA	10:K:79:VAL:HG12	1.87	0.57
1:A:223:GLY:HA2	1:A:226:MET:HG3	1.87	0.57
27:X:638:A:H4'	27:X:639:G:H5'	1.86	0.57
18:S:64:ALA:HB2	18:S:85:MET:HG2	1.86	0.57
27:X:1333:G:N7	27:X:1342:U:H5'	2.20	0.56
27:X:1982:C:H5''	27:X:2703:C:O2'	2.05	0.56
1:A:89:SER:C	1:A:198:ASN:HD21	2.08	0.56
8:I:30:ALA:HA	27:X:824:U:H2'	1.87	0.56
27:X:1455:C:H2'	27:X:1456:C:H6	1.70	0.56
27:X:1774:A:H5'	27:X:2587:G:H4'	1.87	0.56
27:X:2025:A:H5''	27:X:2026:C:OP2	2.05	0.56
27:X:1033:G:H22	27:X:1153:A:H2	1.53	0.56
27:X:2336:G:N2	27:X:2339:A:OP2	2.38	0.56
9:J:26:ASP:OD1	9:J:27:TYR:N	2.38	0.56
12:M:17:GLU:OE2	12:M:63:ARG:NH2	2.31	0.56
13:N:13:ARG:HH12	27:X:1264:C:H5''	1.70	0.56
27:X:2222:U:H2'	27:X:2223:U:C6	2.39	0.56
27:X:2085:G:H22	27:X:2171:U:H1'	1.69	0.56
27:X:540:G:C6	27:X:2005:U:H5''	2.40	0.56
27:X:1830:C:N4	27:X:1882:G:OP2	2.39	0.56
27:X:2708:U:H2'	27:X:2709:C:H6	1.70	0.56
27:X:1017:C:H2'	27:X:1018:C:C6	2.40	0.56
27:X:726:G:H21	27:X:731:A:H2	1.53	0.56
27:X:2736:U:H1'	27:X:2737:A:H5''	1.87	0.56
27:X:2763:U:H2'	27:X:2764:U:H6	1.70	0.56
9:J:86:LYS:O	9:J:88:LYS:HE3	2.05	0.56
27:X:1327:C:N4	27:X:1351:G:H1	2.02	0.56
19:T:21:LEU:HD11	19:T:41:ARG:HG2	1.87	0.56
9:J:26:ASP:H	9:J:103:VAL:HG12	1.70	0.56
12:M:22:ARG:HB2	12:M:84:ALA:HB2	1.87	0.56
20:U:63:SER:O	20:U:67:LEU:N	2.38	0.56
4:D:13:ARG:HG3	4:D:28:VAL:HG11	1.87	0.56
27:X:1674:C:H2'	27:X:1675:C:C6	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:NH1	27:X:704:G:O2'	2.39	0.56
27:X:2431:C:H2'	27:X:2432:A:C8	2.40	0.56
12:M:22:ARG:NH1	12:M:83:PHE:O	2.39	0.56
27:X:705:C:O2'	27:X:1367:A:O2'	2.21	0.56
27:X:2871:U:H2'	27:X:2872:U:C6	2.40	0.56
2:B:87:ASP:OD2	2:B:87:ASP:N	2.38	0.56
15:P:117:ALA:O	15:P:118:ASN:ND2	2.38	0.56
15:P:117:ALA:HB3	27:X:1997:A:H5''	1.87	0.56
27:X:2174:G:H2'	27:X:2175:A:C8	2.41	0.56
2:B:176:ARG:NH2	12:M:16:ILE:HG23	2.18	0.56
10:K:7:GLY:N	27:X:2848:A:N3	2.52	0.56
3:C:54:THR:HG21	3:C:72:ARG:HB2	1.88	0.56
13:N:104:GLU:OE2	13:N:104:GLU:N	2.37	0.56
27:X:1467:U:C6	27:X:1468:A:H5'	2.41	0.56
27:X:2492:G:H2'	27:X:2493:U:C6	2.40	0.56
17:R:54:ILE:HG12	17:R:71:GLN:HG3	1.86	0.56
27:X:597:U:H2'	27:X:598:U:C6	2.41	0.56
27:X:1174:G:H2'	27:X:1175:A:H8	1.71	0.56
27:X:75:C:H2'	27:X:76:C:C6	2.41	0.56
12:M:28:ARG:HB2	12:M:29:PRO:HD3	1.87	0.56
15:P:44:VAL:HG11	23:Z:27:ALA:HB2	1.86	0.56
24:1:12:MET:HB2	24:1:27:ASN:ND2	2.21	0.56
24:1:9:ILE:HA	24:1:28:ARG:HA	1.87	0.56
28:Y:51:G:H2'	28:Y:52:G:C8	2.38	0.56
27:X:388:G:H2'	27:X:389:G:C8	2.41	0.56
27:X:1501:C:H2'	27:X:1502:G:O4'	2.06	0.56
1:A:43:ARG:HH21	1:A:55:GLY:HA2	1.71	0.55
21:V:23:LYS:O	21:V:27:GLU:HG2	2.06	0.55
7:H:117:GLU:O	7:H:120:ASP:HB2	2.05	0.55
2:B:143:GLN:NE2	2:B:151:TYR:OH	2.39	0.55
3:C:144:GLY:HA3	3:C:166:TRP:CD1	2.42	0.55
25:2:39:ARG:O	27:X:469:G:H3'	2.07	0.55
3:C:152:THR:OG1	3:C:153:ASP:O	2.22	0.55
13:N:58:ARG:O	13:N:62:ILE:HG13	2.07	0.55
27:X:1795:C:H2'	27:X:1796:A:H8	1.71	0.55
6:G:132:PHE:CZ	6:G:142:ARG:HA	2.41	0.55
23:Z:42:SER:O	23:Z:44:HIS:HD2	1.88	0.55
27:X:533:C:O2	27:X:563:U:O2'	2.23	0.55
27:X:388:G:H2'	27:X:389:G:H8	1.72	0.55
25:2:1:MET:HB3	25:2:3:ARG:HH12	1.71	0.55
27:X:1918:G:H1'	27:X:1947:G:N2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:16:PHE:CZ	17:R:46:VAL:HG22	2.42	0.55
24:1:30:ASN:ND2	27:X:2264:C:OP2	2.40	0.55
27:X:1336:G:H2'	27:X:1337:G:H5'	1.88	0.55
17:R:83:LEU:HD13	17:R:113:THR:HB	1.87	0.55
27:X:1348:C:H2'	27:X:1349:A:C8	2.41	0.55
6:G:151:TYR:CE1	6:G:160:ALA:HB3	2.41	0.55
18:S:3:LEU:HB3	18:S:56:VAL:HA	1.88	0.55
1:A:28:ARG:HD2	27:X:1583:A:N6	2.22	0.55
27:X:542:A:O2'	27:X:543:G:OP1	2.25	0.55
15:P:90:LEU:HD22	15:P:131:VAL:HG12	1.88	0.55
27:X:1825:C:O2'	27:X:1952:A:N1	2.33	0.55
2:B:4:ILE:HD13	2:B:28:ALA:HB1	1.88	0.55
17:R:11:ASN:O	17:R:11:ASN:ND2	2.36	0.55
2:B:146:THR:OG1	27:X:2550:C:O2'	2.00	0.55
1:A:48:ARG:H	1:A:48:ARG:HD2	1.72	0.55
28:Y:39:C:N4	28:Y:51:G:O4'	2.40	0.55
27:X:2828:C:H2'	27:X:2829:A:H8	1.71	0.55
15:P:27:VAL:HG13	27:X:504:G:H4'	1.88	0.55
3:C:48:ARG:HB2	3:C:50:GLN:H	1.72	0.55
27:X:1480:G:C2	27:X:1481:U:O2	2.59	0.55
10:K:96:ARG:NE	27:X:2857:C:OP1	2.39	0.55
4:D:123:ASP:HB3	4:D:127:ASN:H	1.71	0.55
15:P:47:GLY:H	15:P:92:VAL:HG23	1.71	0.55
14:O:12:TYR:HD2	14:O:40:VAL:HB	1.72	0.55
27:X:2594:U:H2'	27:X:2595:C:C6	2.42	0.55
18:S:168:VAL:HG12	18:S:169:VAL:HG23	1.89	0.55
27:X:2856:U:H2'	27:X:2857:C:C6	2.41	0.55
13:N:54:LYS:NZ	27:X:1006:C:OP2	2.40	0.55
1:A:60:ARG:HD3	1:A:86:PRO:HB2	1.89	0.54
14:O:83:ARG:NH2	27:X:1239:A:OP1	2.40	0.54
27:X:2860:C:H2'	27:X:2861:A:O4'	2.07	0.54
19:T:40:GLN:HE22	19:T:43:THR:HA	1.71	0.54
11:L:8:ARG:HG3	11:L:9:ARG:H	1.71	0.54
27:X:2235:G:N2	27:X:2254:C:C4	2.75	0.54
27:X:228:A:C5	27:X:229:G:H1'	2.42	0.54
2:B:118:LYS:HG2	2:B:160:MET:SD	2.48	0.54
27:X:1412:C:O2'	27:X:1413:U:O5'	2.25	0.54
27:X:188:G:H2'	27:X:189:A:C8	2.43	0.54
27:X:1454:U:H3	27:X:1567:A:H61	1.53	0.54
3:C:66:ASN:HA	27:X:1268:U:H2'	1.89	0.54
4:D:74:ILE:HA	4:D:79:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:130:LEU:HD13	4:D:131:GLY:H	1.71	0.54
2:B:104:ALA:HB3	2:B:170:LEU:HD12	1.88	0.54
28:Y:58:G:H4'	28:Y:59:A:O5'	2.07	0.54
27:X:540:G:N1	27:X:2005:U:OP1	2.40	0.54
1:A:44:ASN:HB3	1:A:49:ILE:HA	1.89	0.54
13:N:93:LYS:HB3	27:X:1007:A:H4'	1.89	0.54
27:X:1919:A:H2	27:X:1926:U:N3	2.04	0.54
5:E:86:ASN:HB3	5:E:130:ARG:HH21	1.72	0.54
27:X:1279:G:O2'	27:X:1995:G:O6	2.11	0.54
27:X:946:U:H2'	27:X:947:C:H6	1.72	0.54
3:C:65:GLY:HA3	27:X:2042:A:H5''	1.90	0.54
1:A:93:ALA:HB2	1:A:107:ALA:HB2	1.88	0.54
23:Z:51:TYR:CE1	23:Z:55:ARG:HD3	2.43	0.54
27:X:2384:G:N2	27:X:2390:A:N7	2.56	0.54
3:C:129:LYS:C	3:C:131:LYS:H	2.11	0.54
1:A:146:GLU:HB2	1:A:189:CYS:HB3	1.88	0.54
27:X:1673:C:H2'	27:X:1674:C:C6	2.38	0.54
27:X:219:G:N2	27:X:231:G:H2'	2.23	0.54
12:M:29:PRO:HB3	12:M:99:VAL:HG12	1.90	0.54
28:Y:27:A:N6	28:Y:56:G:OP2	2.41	0.54
27:X:825:C:H5''	27:X:1263:G:O2'	2.07	0.54
27:X:1785:A:H2'	27:X:1786:C:C6	2.42	0.54
27:X:627:A:H2'	27:X:628:A:C8	2.43	0.54
1:A:27:LYS:HZ3	1:A:29:PRO:HB3	1.72	0.54
15:P:13:GLN:O	15:P:17:GLN:HG2	2.07	0.54
15:P:116:SER:OG	15:P:117:ALA:N	2.40	0.54
27:X:1141:U:O2	27:X:2008:C:H5''	2.08	0.54
27:X:1787:U:H2'	27:X:1788:C:C6	2.43	0.54
11:L:32:TYR:CE2	28:Y:9:G:H5'	2.43	0.54
27:X:1827:G:H1'	27:X:1914:U:C2	2.43	0.54
27:X:1991:C:H2'	27:X:1992:G:H8	1.72	0.54
27:X:317:U:O2'	27:X:1224:A:N7	2.40	0.54
27:X:963:G:H1	27:X:976:C:H42	1.56	0.54
27:X:1790:G:H5'	27:X:1811:A:N6	2.23	0.54
27:X:838:A:H4'	27:X:2407:G:C5	2.42	0.54
2:B:62:PRO:O	27:X:2766:U:O2'	2.22	0.54
4:D:17:MET:HA	4:D:21:GLY:H	1.72	0.54
25:2:12:ARG:NH2	25:2:46:ASP:O	2.36	0.54
27:X:653:G:H2'	27:X:654:A:H5''	1.89	0.54
27:X:2054:A:H2'	27:X:2055:G:H8	1.71	0.54
27:X:490:A:H1'	27:X:491:A:H5'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:19:LYS:NZ	27:X:507:A:OP2	2.23	0.54
3:C:48:ARG:HD2	3:C:50:GLN:HB3	1.90	0.54
14:O:5:ILE:HG23	14:O:13:ARG:HH12	1.73	0.54
27:X:343:A:H1'	27:X:346:C:H41	1.73	0.54
25:2:26:SER:O	25:2:30:ILE:HG13	2.08	0.54
27:X:684:C:H2'	27:X:685:U:C6	2.42	0.54
27:X:2705:A:H1'	27:X:2706:U:H2'	1.89	0.54
15:P:97:VAL:HG22	15:P:127:ILE:HA	1.90	0.54
27:X:2791:C:O2'	27:X:2792:C:H5'	2.08	0.54
5:E:44:ARG:HH22	5:E:51:LEU:HB3	1.72	0.54
27:X:1484:G:H2'	27:X:1485:U:C6	2.43	0.54
24:1:33:ALA:O	24:1:34:LYS:HD2	2.08	0.54
27:X:2707:G:H2'	27:X:2708:U:H6	1.72	0.54
1:A:61:LEU:HG	27:X:1584:G:H5''	1.90	0.54
27:X:805:G:O2'	27:X:2419:C:N3	2.35	0.54
27:X:774:A:H8	27:X:774:A:O5'	1.90	0.54
27:X:946:U:H2'	27:X:947:C:C6	2.43	0.54
3:C:74:VAL:HG23	3:C:76:THR:H	1.72	0.54
27:X:1296:G:H22	27:X:1299:A:H5'	1.73	0.54
27:X:1974:U:H2'	27:X:1975:G:H5''	1.90	0.54
3:C:67:ALA:HB2	15:P:112:ARG:HH22	1.73	0.53
8:I:62:LYS:H	26:3:12:ARG:HG3	1.72	0.53
17:R:56:LYS:HD3	17:R:69:GLN:HE21	1.73	0.53
3:C:48:ARG:O	3:C:51:VAL:HG23	2.07	0.53
13:N:93:LYS:HB3	27:X:1007:A:O3'	2.08	0.53
27:X:171:G:H2'	27:X:172:A:O4'	2.08	0.53
27:X:2378:G:H1	27:X:2396:C:H42	1.56	0.53
27:X:455:A:H2	27:X:1258:G:N3	2.06	0.53
27:X:2555:G:OP2	27:X:2555:G:N2	2.41	0.53
20:U:21:ARG:HH12	27:X:400:U:H2'	1.74	0.53
5:E:160:LYS:HZ1	27:X:2637:C:H5'	1.72	0.53
25:2:19:ARG:HG2	27:X:123:A:C5'	2.36	0.53
27:X:2241:U:H2'	27:X:2242:C:C6	2.38	0.53
2:B:118:LYS:NZ	27:X:2704:U:OP1	2.24	0.53
3:C:50:GLN:HE22	3:C:56:ARG:HH12	1.56	0.53
27:X:1374:G:N2	27:X:1384:G:H1'	2.23	0.53
27:X:2374:C:H42	27:X:2400:G:H1	1.56	0.53
27:X:2572:U:H3	27:X:2579:A:H61	1.57	0.53
27:X:75:C:H2'	27:X:76:C:H6	1.73	0.53
27:X:1854:G:H2'	27:X:1855:G:C8	2.44	0.53
4:D:75:SER:H	4:D:79:LEU:HD12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:41:GLN:NE2	27:X:470:U:OP1	2.36	0.53
10:K:40:LYS:NZ	27:X:1290:A:OP1	2.42	0.53
10:K:14:SER:HB3	27:X:2693:U:OP1	2.08	0.53
27:X:605:G:H2'	27:X:606:A:C8	2.44	0.53
27:X:1714:A:OP2	27:X:1715:A:O2'	2.26	0.53
18:S:68:ALA:HB3	18:S:82:ASP:HB2	1.91	0.53
8:I:89:ASP:HB2	8:I:120:VAL:HG13	1.90	0.53
17:R:52:ASN:HA	17:R:74:LEU:H	1.72	0.53
27:X:978:U:H2'	27:X:979:A:C8	2.43	0.53
1:A:50:THR:HG21	27:X:1805:G:N3	2.24	0.53
27:X:538:A:H62	27:X:2026:C:C5'	2.16	0.53
26:3:15:LYS:HZ3	26:3:60:LEU:HD11	1.73	0.53
3:C:148:VAL:HB	3:C:167:VAL:HG12	1.91	0.53
17:R:26:SER:HB2	27:X:321:A:H5''	1.90	0.53
3:C:106:MET:O	3:C:110:SER:OG	2.19	0.53
13:N:84:LYS:HB2	13:N:92:ARG:HH12	1.74	0.53
10:K:81:ASP:O	10:K:85:PRO:HG2	2.09	0.53
18:S:6:LYS:HD3	18:S:32:PHE:HD2	1.73	0.53
28:Y:16:U:H1'	28:Y:109:G:H21	1.74	0.53
5:E:155:ASP:N	5:E:155:ASP:OD1	2.36	0.53
27:X:542:A:H62	27:X:2002:A:H2	1.55	0.53
15:P:122:LYS:HB3	15:P:124:THR:HG23	1.90	0.53
6:G:132:PHE:CE2	6:G:145:HIS:HB2	2.44	0.53
27:X:746:G:OP2	27:X:774:A:N6	2.32	0.53
27:X:1184:G:H1	27:X:1190:C:H42	1.57	0.53
1:A:25:THR:HG22	1:A:26:LYS:H	1.74	0.53
11:L:91:ARG:HG2	11:L:92:GLY:O	2.08	0.53
27:X:746:G:N7	27:X:774:A:C5	2.76	0.53
12:M:63:ARG:HD3	27:X:2661:G:H4'	1.90	0.53
27:X:2870:C:H2'	27:X:2871:U:C6	2.44	0.53
1:A:28:ARG:HD3	1:A:84:TYR:HB3	1.90	0.53
3:C:112:GLN:HE22	3:C:116:LYS:HG3	1.73	0.53
9:J:44:LYS:HA	9:J:95:VAL:HG12	1.91	0.53
27:X:5:A:H2'	27:X:6:A:H8	1.71	0.53
28:Y:7:C:H2'	28:Y:8:C:H6	1.74	0.53
1:A:186:HIS:HB2	1:A:188:GLU:HG2	1.91	0.53
27:X:2083:G:H1	27:X:2172:U:H3	1.56	0.53
27:X:2633:A:N1	27:X:2644:A:H5''	2.23	0.53
1:A:108:PRO:HB3	1:A:143:HIS:CE1	2.45	0.52
27:X:1348:C:H2'	27:X:1349:A:H8	1.73	0.52
6:G:100:TYR:HB2	6:G:116:ARG:HH11	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:THR:HG1	27:X:1835:C:HO2'	1.56	0.52
15:P:24:GLY:O	15:P:130:ILE:HA	2.09	0.52
27:X:754:G:H2'	27:X:755:C:H6	1.74	0.52
5:E:7:GLN:N	5:E:7:GLN:OE1	2.42	0.52
27:X:88:G:H3'	27:X:89:A:H5''	1.91	0.52
13:N:39:LEU:HA	13:N:42:ALA:HB3	1.92	0.52
27:X:2245:A:H4'	27:X:2246:A:C2	2.44	0.52
24:1:7:ARG:NH2	27:X:2262:C:OP1	2.42	0.52
9:J:83:ARG:HH22	27:X:971:A:N6	1.99	0.52
27:X:90:G:H3'	27:X:91:A:C8	2.45	0.52
1:A:91:ARG:NH1	1:A:109:GLU:OE1	2.43	0.52
27:X:872:G:OP2	27:X:872:G:H8	1.91	0.52
27:X:1744:G:N2	27:X:1746:A:H3'	2.25	0.52
26:3:6:THR:OG1	26:3:7:HIS:N	2.42	0.52
27:X:1250:A:H5'	27:X:1250:A:H8	1.73	0.52
27:X:732:G:H2'	27:X:733:G:H8	1.74	0.52
27:X:2837:G:H2'	27:X:2838:U:C6	2.45	0.52
27:X:2856:U:H2'	27:X:2857:C:H6	1.74	0.52
21:V:28:LEU:HD21	21:V:42:ARG:HG2	1.91	0.52
21:V:7:ARG:HB2	21:V:60:LEU:HD11	1.91	0.52
15:P:104:LYS:HE2	15:P:119:ILE:HD12	1.90	0.52
18:S:74:ARG:HH22	28:Y:94:G:H5''	1.75	0.52
1:A:108:PRO:HB3	1:A:143:HIS:HE1	1.75	0.52
27:X:1333:G:N2	27:X:1344:C:H41	2.08	0.52
27:X:2014:A:C6	27:X:2477:C:H1'	2.44	0.52
27:X:1556:A:H2'	27:X:1557:G:H8	1.74	0.52
27:X:2062:U:H2'	27:X:2063:A:C8	2.45	0.52
1:A:212:SER:O	1:A:215:LEU:HD12	2.10	0.52
11:L:89:PHE:O	11:L:91:ARG:NH2	2.43	0.52
1:A:227:ASN:ND2	27:X:797:A:H5''	2.24	0.52
17:R:51:VAL:HG12	17:R:74:LEU:HD21	1.91	0.52
19:T:23:VAL:HB	19:T:26:PHE:HE2	1.74	0.52
28:Y:64:C:H2'	28:Y:65:A:H8	1.75	0.52
19:T:64:ASP:N	19:T:64:ASP:OD1	2.41	0.52
28:Y:36:A:H61	28:Y:46:G:H2'	1.74	0.52
2:B:120:TRP:CD2	2:B:155:ARG:HD2	2.44	0.52
10:K:45:ARG:HD3	10:K:95:THR:HG22	1.91	0.52
16:Q:71:GLN:NE2	27:X:64:C:OP1	2.42	0.52
5:E:76:VAL:HA	5:E:79:VAL:HG22	1.91	0.52
15:P:31:VAL:N	15:P:125:SER:OG	2.43	0.52
1:A:48:ARG:HB2	27:X:792:U:P	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2306:A:O2'	27:X:2307:A:O4'	2.26	0.52
12:M:5:ILE:HD12	12:M:5:ILE:H	1.75	0.52
27:X:1350:G:H2'	27:X:1351:G:C8	2.45	0.52
9:J:15:ARG:NH2	9:J:73:LYS:HZ2	2.08	0.52
27:X:447:U:O2'	27:X:449:C:N4	2.42	0.52
20:U:48:LYS:HE3	27:X:2074:U:H1'	1.92	0.52
2:B:55:ALA:HB3	2:B:58:LYS:HD2	1.92	0.52
7:H:44:TYR:OH	27:X:1978:U:O2	2.28	0.52
27:X:1762:C:H2'	27:X:1763:G:C8	2.45	0.52
27:X:2335:U:H2'	27:X:2336:G:C8	2.45	0.52
27:X:1441:A:H4'	27:X:1442:C:O5'	2.10	0.52
16:Q:29:VAL:HG21	16:Q:38:ILE:HD11	1.91	0.52
20:U:39:LYS:HA	27:X:2063:A:H4'	1.92	0.52
1:A:49:ILE:HD11	1:A:52:ARG:HA	1.92	0.52
8:I:55:ARG:HH21	27:X:846:A:H4'	1.74	0.52
9:J:15:ARG:HH21	9:J:73:LYS:NZ	2.07	0.52
12:M:29:PRO:HG2	12:M:97:GLY:H	1.75	0.52
14:O:36:LYS:HE2	14:O:56:VAL:HB	1.92	0.52
27:X:2309:G:H2'	27:X:2310:G:O4'	2.10	0.52
5:E:67:LEU:HD21	27:X:2738:A:C4	2.45	0.52
1:A:94:LEU:HD12	1:A:95:LEU:H	1.75	0.52
27:X:1655:C:H5''	27:X:2689:C:O2'	2.10	0.52
1:A:43:ARG:O	27:X:1805:G:O2'	2.28	0.52
27:X:2299:A:H4'	27:X:2300:G:O5'	2.09	0.52
27:X:188:G:H2'	27:X:189:A:H8	1.73	0.52
16:Q:17:TYR:HA	16:Q:20:MET:HB2	1.92	0.52
7:H:116:ARG:NH2	12:M:41:GLU:OE2	2.35	0.52
27:X:1316:G:H5'	27:X:1659:G:H21	1.75	0.52
3:C:187:VAL:HG12	3:C:189:ASP:HB2	1.92	0.52
2:B:52:ALA:HB3	2:B:76:ARG:HB2	1.91	0.51
27:X:1573:G:O5'	27:X:1574:A:H5''	2.10	0.51
6:G:43:VAL:HG21	6:G:158:HIS:HE1	1.75	0.51
14:O:36:LYS:NZ	14:O:54:TYR:HB3	2.25	0.51
3:C:34:GLN:O	3:C:37:SER:OG	2.19	0.51
27:X:2234:G:H2'	27:X:2235:G:O4'	2.10	0.51
25:2:34:ARG:HD3	25:2:37:LYS:HD2	1.92	0.51
27:X:1662:G:H5''	27:X:1663:C:H5'	1.92	0.51
7:H:42:LYS:HA	27:X:2653:A:O3'	2.10	0.51
8:I:35:LYS:NZ	27:X:575:U:H5''	2.25	0.51
11:L:91:ARG:NH2	27:X:2355:A:H61	2.08	0.51
12:M:55:ILE:O	12:M:103:LYS:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:185:C:H2'	27:X:186:C:H6	1.74	0.51
27:X:1296:G:N2	27:X:1299:A:H5'	2.25	0.51
28:Y:96:C:H2'	28:Y:97:C:H6	1.76	0.51
26:3:20:GLY:O	26:3:57:ARG:NH1	2.43	0.51
15:P:103:LEU:HB2	15:P:121:LYS:O	2.10	0.51
16:Q:62:ARG:O	16:Q:70:GLY:HA2	2.09	0.51
15:P:50:VAL:HG23	15:P:91:PHE:HA	1.92	0.51
7:H:129:LEU:O	7:H:131:PRO:HD3	2.11	0.51
9:J:15:ARG:HE	9:J:73:LYS:HZ2	1.58	0.51
20:U:61:TRP:O	20:U:62:LEU:HD12	2.10	0.51
27:X:2007:G:C2	27:X:2023:C:C2	2.98	0.51
27:X:2451:G:O2'	27:X:2457:A:N6	2.42	0.51
26:3:62:LEU:HD13	27:X:603:C:H5''	1.91	0.51
27:X:939:C:OP2	27:X:940:G:H8	1.94	0.51
4:D:102:LYS:NZ	4:D:140:GLU:OE2	2.33	0.51
27:X:2171:U:H2'	27:X:2172:U:C5	2.46	0.51
27:X:2826:C:H2'	27:X:2827:G:O4'	2.11	0.51
27:X:503:G:H2'	27:X:504:G:O4'	2.10	0.51
18:S:17:SER:HB2	18:S:36:ARG:HB3	1.93	0.51
27:X:2:G:O2'	27:X:3:U:H5'	2.10	0.51
27:X:746:G:C8	27:X:774:A:C6	2.98	0.51
6:G:58:ILE:HG12	6:G:80:VAL:HG11	1.93	0.51
15:P:36:ARG:HD3	27:X:1279:G:N7	2.26	0.51
27:X:2824:C:H4'	27:X:2825:A:O5'	2.10	0.51
27:X:636:G:O2'	27:X:669:G:H4'	2.10	0.51
5:E:24:PHE:HB2	5:E:37:TYR:CD1	2.45	0.51
27:X:3:U:O2'	27:X:4:C:O5'	2.26	0.51
14:O:12:TYR:CD2	14:O:40:VAL:HB	2.46	0.51
23:Z:4:HIS:HB2	23:Z:5:PRO:HD3	1.93	0.51
6:G:61:ARG:HH22	6:G:65:LYS:H	1.59	0.51
2:B:54:LYS:HD3	2:B:59:VAL:HG22	1.92	0.51
4:D:46:ASP:HB2	4:D:49:ALA:H	1.75	0.51
17:R:100:ASP:HB3	17:R:103:LYS:HB2	1.93	0.51
27:X:474:G:N2	27:X:477:A:OP2	2.38	0.51
9:J:86:LYS:NZ	27:X:2256:G:OP2	2.29	0.51
27:X:1316:G:N2	27:X:1317:G:H1'	2.26	0.51
7:H:27:SER:HB2	7:H:50:ILE:HB	1.93	0.51
27:X:1599:G:C2	27:X:1600:U:H1'	2.46	0.51
12:M:50:PHE:HE2	12:M:70:LYS:HB2	1.76	0.51
27:X:2250:G:H2'	27:X:2251:U:C6	2.45	0.51
27:X:1692:C:N4	27:X:1976:U:O4'	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:35:GLN:HG3	23:Z:51:TYR:HB3	1.91	0.51
3:C:39:ARG:HG3	27:X:455:A:C8	2.46	0.51
19:T:26:PHE:HD1	27:X:934:G:H1'	1.76	0.51
27:X:959:C:H42	27:X:980:G:H1	1.59	0.51
27:X:2167:A:H2	27:X:2168:A:H62	1.59	0.51
21:V:40:PRO:HD2	27:X:94:C:H1'	1.92	0.51
3:C:67:ALA:HB2	15:P:112:ARG:HH12	1.76	0.51
27:X:577:U:O5'	27:X:956:A:N6	2.44	0.51
27:X:796:A:C8	27:X:797:A:H4'	2.45	0.51
3:C:48:ARG:CZ	3:C:51:VAL:HG13	2.41	0.51
6:G:67:ARG:CG	6:G:70:PHE:HA	2.41	0.51
5:E:154:PRO:HA	5:E:160:LYS:O	2.10	0.51
5:E:109:TYR:HD2	27:X:2646:C:H1'	1.75	0.51
3:C:58:MET:HG2	3:C:59:TYR:HD1	1.76	0.51
3:C:25:GLY:HA3	8:I:18:ARG:NH1	2.26	0.51
27:X:1443:G:H2'	27:X:1444:C:H6	1.75	0.51
15:P:36:ARG:NH2	27:X:1279:G:O5'	2.44	0.51
20:U:20:ARG:HB2	20:U:43:ARG:HD2	1.92	0.51
15:P:119:ILE:HG13	15:P:120:ILE:H	1.76	0.50
27:X:541:C:H4'	27:X:542:A:H5''	1.92	0.50
3:C:162:ARG:HH21	27:X:333:A:H2'	1.76	0.50
18:S:25:ASN:HD22	18:S:85:MET:HB2	1.75	0.50
11:L:15:ARG:HH21	27:X:2272:A:P	2.34	0.50
6:G:101:THR:HG23	6:G:103:TYR:CE1	2.46	0.50
27:X:493:A:H5''	27:X:494:A:OP1	2.10	0.50
3:C:149:LEU:HD23	3:C:180:ILE:HG22	1.92	0.50
5:E:136:ILE:HD12	5:E:137:ASP:H	1.76	0.50
2:B:117:MET:HA	2:B:121:ASN:O	2.11	0.50
27:X:943:U:H2'	27:X:944:A:C8	2.46	0.50
27:X:1539:U:H2'	27:X:1540:C:C6	2.45	0.50
18:S:13:LYS:HA	18:S:18:MET:HB2	1.93	0.50
16:Q:56:MET:HG2	27:X:1354:A:H4'	1.93	0.50
17:R:15:HIS:CE1	17:R:80:LYS:HE2	2.45	0.50
25:2:17:GLY:O	25:2:21:ARG:HG2	2.11	0.50
15:P:35:PRO:HD3	15:P:124:THR:CB	2.41	0.50
27:X:116:A:N3	27:X:155:G:H1'	2.26	0.50
27:X:2020:G:H2'	27:X:2021:G:H8	1.76	0.50
6:G:53:ARG:NH2	27:X:1150:C:O3'	2.43	0.50
26:3:6:THR:N	26:3:9:MET:HG2	2.26	0.50
27:X:2664:G:H2'	27:X:2665:G:H8	1.74	0.50
27:X:2380:U:H3	27:X:2394:G:H1	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:90:ARG:HG2	8:I:121:HIS:CE1	2.47	0.50
11:L:30:SER:HB2	11:L:43:ILE:HD11	1.93	0.50
27:X:1843:U:H3	27:X:1874:G:H1	1.58	0.50
19:T:39:ARG:NH2	27:X:2334:C:O2	2.44	0.50
27:X:1870:U:H3'	27:X:1871:G:H21	1.77	0.50
27:X:633:G:H2'	27:X:634:G:H8	1.77	0.50
9:J:68:ARG:CZ	9:J:103:VAL:HG11	2.42	0.50
7:H:10:VAL:HA	7:H:96:ALA:O	2.11	0.50
6:G:84:ASN:HD21	6:G:154:GLU:HG2	1.74	0.50
19:T:23:VAL:HG13	19:T:38:VAL:HG22	1.92	0.50
8:I:35:LYS:HZ2	27:X:575:U:H5''	1.75	0.50
15:P:134:LYS:HG3	15:P:136:ASN:H	1.75	0.50
2:B:11:MET:HG2	2:B:24:THR:OG1	2.10	0.50
27:X:1332:G:O2'	27:X:1333:G:H5'	2.11	0.50
1:A:63:ARG:O	1:A:65:ILE:HG22	2.12	0.50
27:X:1867:A:O2'	27:X:1868:A:H8	1.95	0.50
27:X:163:A:H2'	27:X:164:G:H8	1.76	0.50
27:X:700:C:H2'	27:X:701:U:O4'	2.11	0.50
27:X:461:A:C4	27:X:462:G:C8	2.99	0.50
27:X:2674:C:H2'	27:X:2675:U:C6	2.46	0.50
10:K:35:GLN:HB3	10:K:112:LEU:HD23	1.94	0.50
27:X:2067:U:H2'	27:X:2068:C:C6	2.47	0.50
27:X:1770:U:H5	27:X:1775:A:N7	2.10	0.50
26:3:30:ARG:HE	26:3:31:HIS:HE1	1.57	0.50
15:P:28:ALA:HB2	15:P:71:VAL:CG2	2.42	0.50
6:G:106:TYR:CE2	6:G:108:GLY:HA2	2.47	0.50
9:J:44:LYS:HB2	9:J:47:GLN:NE2	2.26	0.50
21:V:42:ARG:O	21:V:46:LEU:HG	2.11	0.50
22:W:20:VAL:HG23	22:W:47:VAL:HG11	1.94	0.50
27:X:2270:U:O2'	27:X:2353:G:N3	2.43	0.50
1:A:244:ARG:HD2	27:X:1884:A:O2'	2.11	0.50
4:D:170:LEU:HB2	4:D:175:LEU:HD22	1.92	0.50
27:X:358:C:H2'	27:X:359:G:O4'	2.11	0.50
14:O:64:GLY:HA3	14:O:90:PHE:CZ	2.46	0.50
27:X:857:U:H2'	27:X:858:G:O4'	2.11	0.50
8:I:38:LYS:HE3	8:I:41:SER:OG	2.12	0.50
27:X:2482:A:H4'	27:X:2483:U:OP1	2.10	0.50
3:C:163:ASN:HD21	3:C:167:VAL:N	2.03	0.50
15:P:66:GLU:HB3	15:P:67:PRO:HD3	1.93	0.50
27:X:1399:C:H2'	27:X:1400:A:H8	1.77	0.50
6:G:125:ARG:HD2	6:G:129:HIS:CE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:32:TYR:CE1	11:L:34:SER:HB3	2.46	0.50
27:X:2828:C:H2'	27:X:2829:A:C8	2.47	0.50
21:V:5:GLU:HA	21:V:7:ARG:HH21	1.77	0.50
27:X:1001:A:H1'	27:X:1167:A:N3	2.26	0.50
12:M:85:SER:O	12:M:88:VAL:N	2.42	0.50
27:X:806:A:OP2	27:X:806:A:H8	1.94	0.50
2:B:115:GLY:CA	2:B:136:ARG:HD2	2.42	0.50
27:X:1098:G:N2	27:X:1114:A:H1'	2.27	0.50
28:Y:43:G:H5'	28:Y:44:C:H5''	1.94	0.50
27:X:1148:G:H5''	27:X:1149:G:OP2	2.11	0.50
27:X:1481:U:O2'	27:X:1562:G:O2'	2.18	0.50
20:U:51:ILE:O	20:U:52:ARG:HD3	2.11	0.50
27:X:958:G:H2'	27:X:959:C:H6	1.77	0.50
27:X:2557:G:H2'	27:X:2558:C:H6	1.77	0.50
1:A:161:THR:H	1:A:196:VAL:HG23	1.76	0.50
27:X:121:G:H2'	27:X:122:G:O4'	2.12	0.50
27:X:1059:A:O2'	27:X:1060:C:OP1	2.26	0.50
27:X:2628:C:H2'	27:X:2629:U:H6	1.77	0.50
3:C:146:GLU:OE2	3:C:185:ARG:NH2	2.45	0.50
15:P:21:ARG:HG3	15:P:22:LYS:H	1.77	0.50
26:3:11:LYS:HD2	26:3:11:LYS:H	1.77	0.50
27:X:820:U:H2'	27:X:821:A:H8	1.76	0.49
17:R:105:ARG:NH2	17:R:111:GLY:O	2.43	0.49
27:X:1383:C:H3'	27:X:1384:G:H8	1.76	0.49
1:A:169:GLU:N	1:A:172:TYR:O	2.36	0.49
27:X:2528:G:H2'	27:X:2529:G:C8	2.47	0.49
27:X:1060:C:O2	27:X:1124:U:H4'	2.12	0.49
10:K:39:THR:O	10:K:42:LYS:N	2.45	0.49
6:G:103:TYR:HD2	27:X:1142:G:O4'	1.94	0.49
15:P:102:THR:HA	15:P:123:ARG:H	1.76	0.49
1:A:244:ARG:HD3	27:X:1885:C:O4'	2.12	0.49
1:A:160:GLY:HA3	27:X:1812:U:C4	2.47	0.49
3:C:14:THR:HG22	3:C:15:ILE:H	1.77	0.49
27:X:1665:C:H42	27:X:1992:G:H1	1.59	0.49
1:A:132:PRO:HD3	1:A:190:TYR:CE2	2.47	0.49
27:X:116:A:OP2	27:X:117:A:H2'	2.12	0.49
28:Y:6:C:H2'	28:Y:7:C:C6	2.47	0.49
1:A:169:GLU:HB3	1:A:172:TYR:HB2	1.94	0.49
27:X:1310:C:H2'	27:X:1311:C:H6	1.76	0.49
27:X:705:C:HO2'	27:X:1367:A:HO2'	1.52	0.49
27:X:520:C:H2'	27:X:521:U:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:2:LYS:HZ1	22:W:31:SER:HB2	1.76	0.49
1:A:145:LEU:HD21	1:A:185:VAL:HG11	1.93	0.49
16:Q:63:LYS:HD3	16:Q:69:ILE:H	1.78	0.49
27:X:50:G:O2'	27:X:51:A:OP2	2.30	0.49
27:X:1938:U:H5	27:X:2536:G:N2	2.10	0.49
4:D:111:ILE:HG23	4:D:137:ILE:HG21	1.94	0.49
27:X:1277:G:H2'	27:X:1997:A:N6	2.28	0.49
6:G:103:TYR:O	6:G:107:GLN:NE2	2.46	0.49
9:J:21:ASP:C	9:J:99:LYS:HG2	2.33	0.49
15:P:41:VAL:HG21	15:P:64:ALA:HB3	1.94	0.49
24:1:8:ILE:HG12	24:1:9:ILE:HG23	1.93	0.49
27:X:2484:G:N2	30:X:2902:ERY:H191	2.26	0.49
27:X:2324:G:O2'	27:X:2360:C:O2'	2.13	0.49
3:C:56:ARG:NE	27:X:814:G:OP2	2.45	0.49
27:X:562:G:H2'	27:X:563:U:O4'	2.12	0.49
27:X:1482:U:HO2'	27:X:1483:G:H8	1.60	0.49
16:Q:73:ASN:OD1	16:Q:73:ASN:N	2.44	0.49
27:X:1703:C:H2'	27:X:1704:G:O4'	2.12	0.49
27:X:1035:G:C6	27:X:1036:G:C6	3.00	0.49
16:Q:15:LYS:HG2	27:X:1404:C:O2	2.13	0.49
27:X:1313:U:H4'	27:X:1314:A:H5'	1.93	0.49
27:X:1790:G:H5'	27:X:1811:A:H62	1.77	0.49
27:X:1922:U:H1'	27:X:2571:G:O4'	2.12	0.49
13:N:20:ARG:NH1	14:O:83:ARG:HH11	2.11	0.49
14:O:10:LYS:HE3	14:O:13:ARG:HH22	1.77	0.49
10:K:6:ALA:HB1	27:X:2848:A:C2	2.47	0.49
27:X:2839:G:H2'	27:X:2840:U:C6	2.48	0.49
4:D:37:ASN:ND2	27:X:2291:U:O2'	2.39	0.49
27:X:1255:A:H2'	27:X:1256:C:C6	2.48	0.49
1:A:226:MET:HB3	1:A:230:ASP:HB2	1.93	0.49
23:Z:44:HIS:CD2	23:Z:44:HIS:N	2.80	0.49
17:R:45:LYS:HA	17:R:76:LEU:O	2.12	0.49
28:Y:58:G:O2'	28:Y:59:A:H5''	2.13	0.49
27:X:2457:A:C8	27:X:2508:G:C5	3.01	0.49
27:X:2557:G:H2'	27:X:2558:C:C6	2.47	0.49
27:X:2189:A:H3'	27:X:2190:A:H5''	1.93	0.49
2:B:50:GLY:HA3	2:B:75:THR:HG21	1.93	0.49
27:X:1640:C:H2'	27:X:1641:C:H6	1.78	0.49
27:X:2520:A:H2	27:X:2745:A:H61	1.58	0.49
3:C:3:GLN:N	3:C:12:GLY:O	2.30	0.49
27:X:1787:U:H2'	27:X:1788:C:H6	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HD3	27:X:1797:C:H4'	1.94	0.49
27:X:828:C:H2'	27:X:829:C:C6	2.47	0.49
12:M:27:PHE:HA	12:M:96:ARG:HH22	1.78	0.49
27:X:32:C:O2'	27:X:33:C:H5'	2.13	0.49
27:X:2053:G:H2'	27:X:2054:A:C8	2.48	0.49
27:X:1979:C:H4'	27:X:1980:A:OP1	2.13	0.49
8:I:72:TYR:CE2	8:I:105:PRO:HG2	2.48	0.49
17:R:37:LEU:HD11	17:R:49:GLU:HG2	1.95	0.49
28:Y:73:C:H2'	28:Y:74:A:O4'	2.13	0.49
27:X:2226:A:H2'	27:X:2227:C:C6	2.47	0.49
1:A:252:LYS:H	1:A:252:LYS:CE	2.26	0.49
24:1:9:ILE:HB	24:1:27:ASN:O	2.13	0.49
1:A:38:PRO:HA	1:A:61:LEU:HD22	1.93	0.49
3:C:111:ARG:NH1	3:C:183:HIS:O	2.45	0.49
7:H:10:VAL:HG23	7:H:17:ARG:O	2.12	0.49
27:X:2605:C:H2'	27:X:2606:G:H8	1.76	0.49
2:B:37:LYS:HB2	2:B:46:ALA:HB3	1.95	0.49
24:1:38:LYS:HE2	24:1:40:TYR:HE1	1.78	0.49
27:X:538:A:N6	27:X:2025:A:H3'	2.28	0.49
18:S:155:PRO:HG2	18:S:158:CYS:SG	2.53	0.49
27:X:104:C:H2'	27:X:105:G:H8	1.78	0.49
27:X:2198:U:C2	27:X:2199:C:H1'	2.48	0.49
17:R:84:VAL:HG11	17:R:89:GLY:HA2	1.95	0.49
27:X:2553:G:N1	27:X:2554:C:O2	2.45	0.49
26:3:42:ARG:NE	27:X:2328:G:OP1	2.46	0.49
27:X:1699:A:H2'	27:X:1700:C:C6	2.48	0.49
27:X:346:C:C6	27:X:347:C:H5	2.30	0.49
27:X:1184:G:H3'	27:X:1185:C:H5''	1.95	0.49
2:B:104:ALA:HB1	2:B:188:ILE:HD11	1.93	0.49
1:A:161:THR:O	1:A:196:VAL:HG22	2.13	0.49
8:I:42:GLY:N	8:I:45:LYS:HE3	2.27	0.49
3:C:128:ALA:C	3:C:130:THR:H	2.16	0.49
27:X:960:U:H2'	27:X:961:G:C8	2.47	0.49
27:X:1672:A:C6	27:X:1673:C:C2	3.00	0.49
26:3:30:ARG:HB3	26:3:31:HIS:ND1	2.28	0.49
26:3:14:ILE:HG23	26:3:60:LEU:HD22	1.95	0.49
1:A:143:HIS:ND1	1:A:194:GLY:O	2.35	0.49
27:X:2427:A:HO2'	27:X:2428:U:H5	1.61	0.49
10:K:12:ARG:HH11	10:K:12:ARG:HG2	1.78	0.49
17:R:62:MET:O	17:R:65:PRO:HA	2.12	0.49
5:E:24:PHE:HB2	5:E:37:TYR:HD1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD23	1:A:211:ARG:HD2	1.94	0.49
4:D:56:GLU:HA	4:D:59:LEU:HD12	1.95	0.49
9:J:16:GLY:C	9:J:17:ARG:HD3	2.33	0.49
28:Y:39:C:H5'	28:Y:40:C:OP2	2.12	0.49
7:H:28:GLY:O	7:H:35:THR:HG23	2.13	0.49
28:Y:15:A:O2'	28:Y:16:U:H5''	2.12	0.49
27:X:1802:A:H2'	27:X:1803:G:O4'	2.13	0.49
27:X:830:C:O2'	27:X:852:U:H5''	2.13	0.49
4:D:38:GLU:HB3	4:D:87:ILE:HB	1.95	0.49
2:B:136:ARG:HG2	2:B:137:ARG:N	2.27	0.48
27:X:2543:A:C2	27:X:2626:U:H4'	2.47	0.48
27:X:1351:G:H2'	27:X:1352:G:C8	2.48	0.48
6:G:69:ASP:H	6:G:76:GLN:NE2	2.10	0.48
17:R:86:PRO:HG2	17:R:90:LYS:HE2	1.95	0.48
11:L:32:TYR:O	11:L:38:ILE:HA	2.13	0.48
12:M:104:LEU:HA	12:M:106:TYR:CE2	2.47	0.48
6:G:67:ARG:HG2	6:G:70:PHE:HA	1.95	0.48
28:Y:96:C:H2'	28:Y:97:C:C6	2.47	0.48
27:X:1498:G:N2	27:X:1522:C:O2	2.40	0.48
13:N:66:ASN:HB2	13:N:70:ARG:NH1	2.28	0.48
15:P:41:VAL:HG11	15:P:65:SER:HA	1.95	0.48
14:O:85:GLY:N	27:X:1238:A:H5'	2.27	0.48
27:X:836:G:H2'	27:X:837:U:H6	1.78	0.48
2:B:145:LYS:HB2	27:X:2551:A:N7	2.29	0.48
27:X:2261:G:H5''	27:X:2262:C:O4'	2.14	0.48
27:X:2204:A:H4'	27:X:2205:C:O5'	2.13	0.48
8:I:33:GLY:HA2	14:O:79:GLN:HG3	1.95	0.48
1:A:251:GLY:HA3	1:A:255:LYS:NZ	2.27	0.48
27:X:543:G:C5	27:X:544:U:C4	3.02	0.48
3:C:163:ASN:HD21	3:C:166:TRP:HB2	1.78	0.48
19:T:41:ARG:HA	19:T:41:ARG:HD2	1.52	0.48
27:X:1283:C:H5''	27:X:1284:G:C5'	2.42	0.48
12:M:102:ALA:C	12:M:103:LYS:HD2	2.33	0.48
6:G:43:VAL:HG12	6:G:167:LYS:HE3	1.96	0.48
27:X:346:C:H2'	27:X:347:C:C5	2.48	0.48
2:B:203:LYS:HG2	27:X:2713:A:H61	1.78	0.48
27:X:38:G:H1	27:X:453:U:H3	1.61	0.48
27:X:558:G:C8	27:X:560:G:C8	3.01	0.48
27:X:514:G:H4'	27:X:515:A:OP2	2.11	0.48
27:X:2532:G:C2	27:X:2533:U:H1'	2.47	0.48
18:S:104:SER:HA	18:S:139:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:26:LYS:NZ	26:3:28:GLY:HA3	2.28	0.48
24:1:30:ASN:OD1	24:1:31:THR:N	2.47	0.48
27:X:2040:A:H2'	27:X:2041:A:H8	1.73	0.48
27:X:2407:G:H5''	27:X:2408:G:O5'	2.12	0.48
27:X:165:G:H1	27:X:185:C:N4	2.11	0.48
27:X:2278:A:H2'	27:X:2279:G:C8	2.47	0.48
27:X:736:G:H2'	27:X:737:C:O4'	2.14	0.48
27:X:2655:C:O2	27:X:2712:G:N2	2.38	0.48
27:X:2498:U:C5	27:X:2520:A:C6	3.01	0.48
11:L:21:THR:O	11:L:25:GLY:N	2.33	0.48
4:D:80:ARG:NE	4:D:83:MET:SD	2.81	0.48
9:J:99:LYS:HG3	9:J:100:PRO:HD2	1.94	0.48
2:B:128:SER:HB2	2:B:129:HIS:ND1	2.29	0.48
3:C:182:ARG:NH1	3:C:183:HIS:HE1	2.10	0.48
27:X:224:G:H4'	27:X:399:G:C5	2.48	0.48
2:B:172:VAL:HG22	2:B:182:ILE:HD11	1.96	0.48
27:X:1019:U:HO2'	27:X:1020:A:P	2.35	0.48
28:Y:7:C:H2'	28:Y:8:C:C6	2.49	0.48
26:3:58:MET:HA	26:3:61:MET:HB2	1.94	0.48
16:Q:62:ARG:NH1	16:Q:73:ASN:HD21	2.11	0.48
27:X:459:A:H4'	27:X:461:A:N7	2.28	0.48
1:A:30:GLU:HB2	1:A:82:ILE:O	2.14	0.48
27:X:1437:A:H2'	27:X:1438:G:C8	2.47	0.48
27:X:1623:C:H4'	27:X:1624:A:O5'	2.13	0.48
6:G:56:THR:HA	6:G:134:MET:HE1	1.96	0.48
5:E:37:TYR:CZ	5:E:72:VAL:HG22	2.48	0.48
3:C:104:LEU:O	3:C:108:ILE:HG13	2.12	0.48
5:E:143:GLN:NE2	27:X:2724:G:H21	2.12	0.48
7:H:14:SER:OG	7:H:98:ILE:HD12	2.13	0.48
16:Q:28:TRP:HZ3	16:Q:58:VAL:HG21	1.78	0.48
27:X:936:A:H2'	27:X:937:C:O4'	2.13	0.48
9:J:57:ARG:NE	27:X:2448:A:O2'	2.38	0.48
27:X:537:C:O2'	27:X:538:A:C4	2.66	0.48
3:C:62:LYS:HD2	27:X:2044:G:OP1	2.13	0.48
15:P:39:ARG:HD2	15:P:97:VAL:HB	1.94	0.48
27:X:1815:G:H2'	27:X:1816:G:H8	1.79	0.48
27:X:2013:A:H4'	27:X:2014:A:C8	2.49	0.48
20:U:20:ARG:N	20:U:41:VAL:O	2.38	0.48
20:U:20:ARG:HH21	20:U:43:ARG:HG2	1.79	0.48
27:X:1653:C:H2'	27:X:1654:A:C8	2.49	0.48
27:X:764:A:H2	27:X:802:A:HO2'	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:492:G:H2'	27:X:517:A:N1	2.29	0.48
24:1:28:ARG:HB2	24:1:30:ASN:ND2	2.28	0.48
27:X:1333:G:N2	27:X:1344:C:N4	2.61	0.48
27:X:2590:U:C1'	30:X:2902:ERY:H361	2.44	0.48
27:X:1586:A:H2'	27:X:1587:A:C8	2.49	0.48
27:X:2199:C:H2'	27:X:2200:G:H8	1.79	0.48
17:R:61:SER:HA	17:R:65:PRO:CG	2.42	0.48
27:X:1451:C:H2'	27:X:1452:U:C6	2.47	0.48
10:K:82:GLU:O	10:K:85:PRO:HD2	2.14	0.48
27:X:603:C:H2'	27:X:604:U:H6	1.79	0.48
27:X:1404:C:C2	27:X:1406:A:N7	2.81	0.48
16:Q:58:VAL:HA	16:Q:59:PRO:HD2	1.61	0.48
27:X:2657:G:H2'	27:X:2658:A:O4'	2.14	0.48
8:I:94:GLU:HA	8:I:97:ARG:NE	2.28	0.48
27:X:568:G:H2'	27:X:569:C:O4'	2.14	0.48
15:P:70:LYS:HE2	27:X:499:G:O2'	2.14	0.48
27:X:732:G:H2'	27:X:733:G:C8	2.48	0.48
5:E:165:VAL:HB	5:E:166:GLY:H	1.46	0.48
3:C:72:ARG:CZ	3:C:77:PHE:HE2	2.27	0.48
4:D:134:GLU:HG2	4:D:136:LEU:H	1.79	0.48
27:X:2260:C:O2'	27:X:2261:G:H5'	2.14	0.48
6:G:137:LYS:HD2	27:X:2022:C:OP2	2.14	0.48
5:E:24:PHE:CD1	5:E:37:TYR:HB2	2.49	0.48
13:N:74:MET:HE1	13:N:113:SER:HB3	1.95	0.48
27:X:227:G:C6	27:X:228:A:C6	3.01	0.48
23:Z:7:PRO:HA	27:X:2594:U:C6	2.49	0.48
27:X:2190:A:H61	27:X:2196:U:H3	1.60	0.48
1:A:206:LEU:HA	1:A:211:ARG:HH11	1.79	0.48
5:E:143:GLN:HG2	27:X:2725:C:H1'	1.95	0.48
1:A:200:GLU:HB2	1:A:203:ASN:ND2	2.29	0.48
3:C:62:LYS:HE2	3:C:63:GLY:N	2.29	0.47
8:I:38:LYS:HG3	27:X:954:U:OP2	2.14	0.47
1:A:212:SER:OG	1:A:213:ARG:N	2.48	0.47
24:1:36:GLU:HG3	24:1:53:LYS:HA	1.96	0.47
8:I:31:GLY:HA3	8:I:34:HIS:ND1	2.29	0.47
27:X:114:C:O2'	27:X:124:A:N3	2.43	0.47
27:X:773:G:H2'	27:X:774:A:H5'	1.95	0.47
27:X:824:U:O2	27:X:1263:G:H3'	2.14	0.47
13:N:81:ASN:HD22	13:N:117:ARG:HH12	1.61	0.47
27:X:1107:A:H3'	27:X:1108:U:H5''	1.96	0.47
27:X:1417:C:H2'	27:X:1418:C:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:38:LYS:HG3	27:X:954:U:P	2.53	0.47
30:X:2902:ERY:H2	30:X:2902:ERY:H312	1.63	0.47
9:J:28:VAL:HG11	9:J:135:ARG:HB3	1.95	0.47
18:S:67:LYS:NZ	18:S:92:VAL:HG21	2.28	0.47
2:B:108:SER:HB3	2:B:163:GLU:H	1.79	0.47
27:X:66:U:H2'	27:X:67:G:C8	2.49	0.47
27:X:1672:A:H3'	27:X:1673:C:C6	2.49	0.47
8:I:62:LYS:HB3	26:3:13:ARG:H	1.77	0.47
27:X:1074:G:H1	27:X:1086:C:N4	2.12	0.47
7:H:11:ALA:N	7:H:96:ALA:O	2.37	0.47
21:V:46:LEU:O	21:V:50:VAL:HG23	2.14	0.47
27:X:1655:C:H4'	27:X:2689:C:O2	2.14	0.47
16:Q:59:PRO:HA	16:Q:74:ASP:OD1	2.15	0.47
19:T:83:ALA:HB1	19:T:85:GLN:HE21	1.79	0.47
27:X:1636:G:H2'	27:X:1637:U:C6	2.49	0.47
27:X:2542:U:O2	27:X:2544:A:H8	1.98	0.47
1:A:97:TYR:HE2	1:A:103:ARG:HB2	1.79	0.47
19:T:56:ASP:OD1	27:X:2343:C:H4'	2.15	0.47
2:B:136:ARG:HH21	2:B:157:ALA:H	1.62	0.47
27:X:2258:G:C2	27:X:2259:G:C8	3.02	0.47
9:J:16:GLY:HA2	9:J:17:ARG:NH1	2.25	0.47
27:X:91:A:H2'	27:X:92:U:C6	2.49	0.47
27:X:333:A:H5'	27:X:351:A:H1'	1.95	0.47
27:X:760:U:OP1	27:X:2591:C:H1'	2.15	0.47
27:X:2701:A:C2	27:X:2848:A:C4	3.03	0.47
21:V:54:ASN:HB3	27:X:71:A:C5	2.49	0.47
27:X:2691:C:O2'	27:X:2693:U:H5'	2.13	0.47
27:X:1171:A:H2'	27:X:1172:U:C6	2.49	0.47
8:I:128:ALA:HA	8:I:131:LYS:HB3	1.95	0.47
27:X:2312:A:N7	27:X:2314:A:N6	2.62	0.47
27:X:2184:C:H2'	27:X:2185:U:O4'	2.14	0.47
27:X:1052:C:N4	27:X:1053:G:N7	2.63	0.47
9:J:70:PHE:C	9:J:70:PHE:CD2	2.87	0.47
27:X:540:G:C5	27:X:2005:U:H5''	2.49	0.47
27:X:525:A:N1	27:X:1273:G:O2'	2.40	0.47
4:D:4:LEU:C	4:D:6:THR:H	2.18	0.47
27:X:2363:G:H3'	27:X:2365:U:OP1	2.14	0.47
23:Z:45:ILE:HD13	23:Z:57:VAL:HG23	1.96	0.47
8:I:56:LEU:CB	26:3:52:LYS:HZ1	2.25	0.47
15:P:122:LYS:HB3	15:P:124:THR:CG2	2.45	0.47
27:X:1468:A:H8	27:X:1468:A:P	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:153:ASP:OD1	27:X:2283:G:O2'	2.28	0.47
27:X:2363:G:HO2'	27:X:2364:C:P	2.37	0.47
27:X:2368:G:H5''	27:X:2369:U:H5'	1.97	0.47
15:P:21:ARG:HH21	27:X:506:G:H5'	1.79	0.47
27:X:552:C:H2'	27:X:553:C:H5''	1.96	0.47
27:X:2576:G:C6	27:X:2577:A:C6	3.03	0.47
27:X:1750:A:H4'	27:X:2695:C:O4'	2.14	0.47
27:X:682:G:H3'	27:X:683:A:C8	2.50	0.47
4:D:31:ILE:HA	4:D:158:THR:HA	1.97	0.47
27:X:1673:C:C2	27:X:1674:C:C5	3.02	0.47
10:K:60:LEU:HD11	10:K:64:ARG:HH11	1.80	0.47
7:H:23:ARG:HD2	7:H:24:VAL:O	2.15	0.47
17:R:62:MET:H	17:R:65:PRO:HA	1.79	0.47
7:H:110:VAL:HB	7:H:129:LEU:HB3	1.97	0.47
27:X:536:A:N6	27:X:2605:C:H4'	2.30	0.47
27:X:1164:C:H2'	27:X:1165:G:O4'	2.15	0.47
27:X:469:G:N2	27:X:480:G:H2'	2.30	0.47
15:P:47:GLY:H	15:P:92:VAL:CG2	2.27	0.47
27:X:2512:A:OP1	27:X:2644:A:O2'	2.26	0.47
27:X:1779:C:O5'	27:X:1779:C:H6	1.97	0.47
27:X:1419:G:H2'	27:X:1420:A:C8	2.50	0.47
27:X:2684:A:H2'	27:X:2685:A:O4'	2.14	0.47
27:X:2524:G:C6	27:X:2525:U:C4	3.02	0.47
27:X:136:A:H2'	27:X:137:A:O4'	2.15	0.47
27:X:1353:A:H4'	27:X:1407:G:H1'	1.95	0.47
1:A:79:VAL:HB	1:A:114:GLY:H	1.80	0.47
27:X:2670:C:H5'	27:X:2847:G:H5''	1.97	0.47
27:X:742:G:H2'	27:X:1766:U:H1'	1.96	0.47
27:X:582:G:O2'	27:X:583:C:H3'	2.14	0.47
27:X:2280:A:H2'	27:X:2281:C:C6	2.49	0.47
27:X:1332:G:C6	27:X:1333:G:N1	2.82	0.47
27:X:835:U:H2'	27:X:836:G:C8	2.50	0.47
27:X:343:A:H1'	27:X:346:C:N4	2.29	0.47
11:L:8:ARG:HE	11:L:9:ARG:HG2	1.79	0.47
28:Y:16:U:O2'	28:Y:110:U:H1'	2.15	0.47
27:X:1838:G:N2	27:X:1878:C:N3	2.63	0.47
1:A:181:GLU:HG3	1:A:270:ILE:HA	1.95	0.47
16:Q:57:ASN:HD21	16:Q:76:LYS:HE3	1.80	0.47
11:L:59:LEU:HD23	11:L:61:SER:HB3	1.97	0.47
5:E:138:LYS:HG2	27:X:2726:U:H5''	1.97	0.47
15:P:34:SER:O	15:P:37:LYS:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PRO:O	2:B:49:ILE:HA	2.15	0.47
26:3:23:MET:HB3	26:3:25:PHE:CE2	2.49	0.47
26:3:30:ARG:HB2	27:X:2372:A:OP1	2.15	0.47
27:X:1813:A:H5''	27:X:1814:G:OP2	2.15	0.47
27:X:640:C:H1'	27:X:650:U:H1'	1.97	0.47
1:A:38:PRO:HG3	27:X:1586:A:H5'	1.97	0.47
19:T:46:LYS:HE3	19:T:76:ALA:HA	1.96	0.47
17:R:22:VAL:HG13	17:R:81:VAL:O	2.15	0.47
3:C:54:THR:HG22	3:C:55:GLY:O	2.15	0.47
27:X:1727:C:H2'	27:X:1728:A:C8	2.50	0.47
11:L:33:ARG:HH21	11:L:103:LEU:HD12	1.79	0.47
27:X:393:U:H2'	27:X:394:U:C6	2.49	0.47
27:X:649:G:C5	27:X:650:U:C5	3.02	0.47
27:X:1643:A:N6	27:X:1656:U:H3	2.08	0.47
27:X:203:G:H21	27:X:205:A:H62	1.63	0.47
9:J:28:VAL:HG21	9:J:135:ARG:HB3	1.97	0.47
27:X:2781:G:H2'	27:X:2782:G:H5''	1.96	0.47
6:G:151:TYR:HE1	6:G:161:GLN:HE21	1.63	0.47
1:A:118:ASN:HD22	1:A:119:ALA:N	2.12	0.47
20:U:64:ALA:O	20:U:67:LEU:HB3	2.15	0.47
23:Z:42:SER:O	23:Z:44:HIS:CD2	2.67	0.47
3:C:129:LYS:O	3:C:131:LYS:N	2.47	0.47
15:P:9:ARG:HD2	15:P:13:GLN:HG3	1.96	0.47
27:X:2266:A:H5''	27:X:2267:A:OP1	2.15	0.47
28:Y:53:G:N3	28:Y:53:G:H2'	2.29	0.47
18:S:1:MET:N	18:S:53:ASP:O	2.42	0.47
14:O:88:GLN:HB3	14:O:88:GLN:HE21	1.48	0.47
27:X:879:A:H2'	27:X:879:A:N3	2.30	0.47
9:J:21:ASP:N	9:J:21:ASP:OD1	2.36	0.46
15:P:45:ILE:O	15:P:48:LYS:HG2	2.15	0.46
27:X:1467:U:H3'	27:X:1467:U:H6	1.80	0.46
26:3:6:THR:N	26:3:59:LYS:HB3	2.30	0.46
27:X:1448:A:H61	27:X:1574:A:H61	1.61	0.46
1:A:159:ALA:HA	1:A:198:ASN:CG	2.35	0.46
8:I:102:LYS:C	8:I:104:ARG:H	2.17	0.46
27:X:1301:U:C2	27:X:1340:C:O2	2.68	0.46
27:X:2170:C:H3'	27:X:2171:U:H5''	1.97	0.46
6:G:83:ILE:HG22	6:G:153:GLY:O	2.15	0.46
4:D:103:LEU:HG	4:D:108:LEU:HG	1.97	0.46
11:L:11:LEU:HD21	27:X:2273:C:H5''	1.97	0.46
7:H:29:ILE:HB	7:H:34:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:132:GLU:HB2	12:M:73:PHE:CE1	2.49	0.46
27:X:1141:U:O2'	27:X:1142:G:O5'	2.23	0.46
27:X:540:G:O2'	27:X:542:A:H2	1.97	0.46
27:X:522:G:OP1	27:X:1247:U:O2'	2.23	0.46
27:X:758:G:H2'	27:X:759:C:H5'	1.98	0.46
8:I:31:GLY:O	8:I:32:ARG:HD2	2.15	0.46
12:M:99:VAL:HG21	12:M:104:LEU:HD11	1.97	0.46
27:X:747:A:H2'	27:X:748:A:O4'	2.14	0.46
27:X:1919:A:C6	27:X:1928:G:C4	3.03	0.46
10:K:13:ASN:OD1	10:K:15:SER:N	2.43	0.46
1:A:133:LEU:HB3	1:A:173:VAL:HG21	1.97	0.46
10:K:78:LYS:O	10:K:83:VAL:HG23	2.15	0.46
27:X:687:G:N2	27:X:2423:G:O3'	2.48	0.46
27:X:1781:C:H2'	27:X:1782:A:C5	2.50	0.46
27:X:2312:A:H4'	27:X:2313:G:O5'	2.15	0.46
27:X:1407:G:C6	27:X:1408:A:C6	3.03	0.46
27:X:179:U:H2'	27:X:180:C:O4'	2.15	0.46
1:A:18:THR:HG22	1:A:19:ALA:H	1.79	0.46
5:E:84:THR:HG22	5:E:134:SER:OG	2.15	0.46
3:C:19:LEU:HA	3:C:20:PRO:C	2.34	0.46
27:X:218:A:H61	27:X:232:A:H5''	1.80	0.46
9:J:37:ALA:O	9:J:100:PRO:HA	2.14	0.46
2:B:162:MET:SD	27:X:2796:A:H4'	2.55	0.46
1:A:25:THR:HG22	1:A:26:LYS:N	2.30	0.46
27:X:2020:G:C6	27:X:2021:G:C6	3.03	0.46
26:3:6:THR:N	26:3:59:LYS:HD3	2.31	0.46
27:X:1388:C:H2'	27:X:1389:C:C6	2.50	0.46
12:M:22:ARG:HH22	12:M:24:LEU:HD23	1.80	0.46
5:E:68:THR:O	5:E:72:VAL:HG23	2.15	0.46
1:A:222:ARG:HD3	27:X:1820:G:O6	2.16	0.46
5:E:150:LYS:HZ1	27:X:2724:G:H1'	1.81	0.46
16:Q:8:GLN:O	21:V:29:ARG:HG2	2.15	0.46
27:X:1840:A:H2'	27:X:1841:G:O4'	2.15	0.46
7:H:5:GLN:HG2	27:X:1685:A:H5''	1.97	0.46
12:M:90:GLN:OE1	12:M:90:GLN:N	2.34	0.46
3:C:5:ASN:N	3:C:5:ASN:OD1	2.48	0.46
27:X:2026:C:H2'	27:X:2027:C:H6	1.80	0.46
27:X:2226:A:H2'	27:X:2227:C:H6	1.81	0.46
15:P:28:ALA:O	15:P:126:HIS:HA	2.16	0.46
27:X:835:U:H2'	27:X:836:G:H8	1.80	0.46
9:J:6:LYS:HE2	9:J:6:LYS:HB2	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2605:C:H2'	27:X:2606:G:C8	2.50	0.46
27:X:962:C:H2'	27:X:963:G:H8	1.81	0.46
27:X:1975:G:H22	27:X:1979:C:H6	1.63	0.46
6:G:31:THR:HG21	13:N:61:TRP:HE1	1.81	0.46
27:X:1159:U:H2'	27:X:1160:C:C6	2.51	0.46
27:X:571:U:C2	27:X:581:A:C8	3.03	0.46
27:X:2425:G:C2	27:X:2480:C:C4	3.03	0.46
7:H:2:ILE:HG22	7:H:6:SER:HB3	1.98	0.46
27:X:89:A:H4'	27:X:90:G:C5'	2.42	0.46
14:O:68:LYS:HA	14:O:87:ARG:HG2	1.97	0.46
27:X:2406:C:H5''	27:X:2407:G:OP1	2.15	0.46
27:X:104:C:H2'	27:X:105:G:C8	2.50	0.46
14:O:5:ILE:N	14:O:10:LYS:HE2	2.30	0.46
19:T:74:LYS:HG2	19:T:77:ARG:NE	2.30	0.46
14:O:20:ILE:HG22	14:O:21:ARG:H	1.80	0.46
17:R:40:LEU:HB2	17:R:45:LYS:HB2	1.98	0.46
27:X:958:G:H2'	27:X:959:C:C6	2.51	0.46
13:N:74:MET:SD	13:N:110:VAL:HG13	2.55	0.46
27:X:2030:U:H2'	27:X:2031:A:H8	1.81	0.46
27:X:769:C:C4	27:X:770:U:C4	3.03	0.46
18:S:94:VAL:O	18:S:121:GLN:HA	2.15	0.46
9:J:37:ALA:HB2	9:J:104:MET:SD	2.55	0.46
27:X:1040:A:C8	27:X:1041:G:C8	3.04	0.46
27:X:1030:U:H2'	27:X:1032:A:C2	2.48	0.46
27:X:54:G:O2'	27:X:125:A:N1	2.43	0.46
27:X:2197:U:H2'	27:X:2198:U:C5	2.51	0.46
3:C:46:ARG:HD3	27:X:463:C:OP1	2.15	0.46
27:X:1018:C:H5''	27:X:1019:U:H5''	1.98	0.46
18:S:19:ILE:HG23	18:S:79:ILE:O	2.16	0.46
27:X:1073:G:H8	27:X:1073:G:OP2	1.99	0.46
27:X:824:U:H1'	27:X:1264:C:O4'	2.15	0.46
27:X:2522:G:H2'	27:X:2523:G:H8	1.79	0.46
27:X:2692:A:H5''	27:X:2693:U:OP2	2.16	0.46
22:W:12:ARG:HG2	22:W:12:ARG:HH11	1.81	0.46
27:X:1806:G:H5''	27:X:1807:A:H2'	1.97	0.46
8:I:118:VAL:HG23	8:I:133:VAL:HG13	1.98	0.46
27:X:817:A:H2'	27:X:819:C:C4	2.50	0.46
14:O:15:SER:N	14:O:95:ILE:O	2.49	0.46
19:T:25:LYS:HD3	19:T:31:VAL:HG12	1.98	0.46
27:X:2485:U:O2	27:X:2485:U:H2'	2.15	0.46
3:C:58:MET:HB2	3:C:70:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:31:ASP:N	12:M:31:ASP:OD2	2.49	0.46
2:B:98:GLU:HA	2:B:172:VAL:HG12	1.97	0.46
10:K:28:LEU:HD12	10:K:113:ILE:HG23	1.96	0.46
15:P:105:ARG:HG3	15:P:107:ILE:HB	1.97	0.46
27:X:308:C:H2'	27:X:309:G:O4'	2.15	0.46
27:X:1412:C:H2'	27:X:1412:C:H6	1.61	0.46
5:E:90:ARG:HB3	5:E:160:LYS:HA	1.97	0.46
27:X:603:C:H2'	27:X:604:U:C6	2.51	0.46
27:X:2051:U:H3	27:X:2409:A:H62	1.63	0.46
25:2:21:ARG:O	25:2:28:ARG:HD3	2.16	0.46
5:E:169:ILE:HD13	5:E:170:ALA:H	1.81	0.46
15:P:89:ARG:HB3	15:P:133:GLU:HB3	1.97	0.46
2:B:129:HIS:CD2	27:X:1692:C:C2	3.03	0.46
27:X:82:G:N1	27:X:100:G:O2'	2.42	0.46
27:X:839:U:H5''	27:X:2408:G:P	2.56	0.46
27:X:2546:G:H2'	27:X:2547:C:C6	2.51	0.46
27:X:1681:A:C2	27:X:2706:U:C2	3.04	0.46
7:H:132:GLU:HB2	12:M:73:PHE:HE1	1.80	0.46
6:G:94:LYS:HE3	6:G:95:LEU:HG	1.98	0.46
4:D:22:TYR:OH	4:D:165:GLU:OE1	2.34	0.46
27:X:2753:C:H2'	27:X:2754:C:H6	1.81	0.46
26:3:29:LYS:HD2	26:3:33:ASN:O	2.16	0.46
27:X:2696:A:O2'	27:X:2697:G:H5'	2.15	0.46
27:X:2516:U:H2'	27:X:2517:C:C6	2.51	0.46
13:N:24:PHE:HB3	13:N:28:ARG:HB2	1.97	0.46
3:C:59:TYR:CD2	3:C:64:THR:HG21	2.51	0.46
26:3:13:ARG:O	26:3:13:ARG:HG3	2.16	0.46
15:P:97:VAL:HG13	15:P:125:SER:O	2.16	0.46
27:X:2526:U:H2'	27:X:2527:G:C8	2.50	0.46
27:X:330:C:H2'	27:X:331:U:O4'	2.16	0.46
27:X:312:G:C4	27:X:313:U:C5	3.04	0.46
27:X:1223:G:H5'	27:X:1225:G:O4'	2.16	0.46
27:X:2309:G:H1	27:X:2364:C:H42	1.63	0.46
27:X:2453:C:H5'	27:X:2454:C:OP2	2.16	0.46
27:X:1770:U:C5	27:X:1775:A:N7	2.84	0.46
27:X:1096:A:H5''	27:X:1116:U:H4'	1.98	0.46
16:Q:11:VAL:HG23	16:Q:27:PHE:HA	1.97	0.46
1:A:201:HIS:HA	1:A:204:ILE:HD12	1.97	0.46
27:X:1998:A:O5'	27:X:1998:A:H8	1.99	0.46
27:X:820:U:H2'	27:X:821:A:C8	2.51	0.46
27:X:2372:A:H62	27:X:2401:A:N6	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:NZ	1:A:253:PRO:HD2	2.31	0.46
27:X:650:U:H2'	27:X:651:C:C6	2.51	0.46
12:M:16:ILE:H	12:M:16:ILE:HD12	1.81	0.46
27:X:1981:A:O3'	27:X:2704:U:H4'	2.15	0.46
3:C:34:GLN:NE2	3:C:176:ASN:OD1	2.49	0.46
2:B:37:LYS:NZ	2:B:80:GLU:OE2	2.42	0.46
27:X:2434:G:H2'	27:X:2435:C:C6	2.51	0.46
27:X:984:A:O4'	27:X:1202:U:C6	2.69	0.45
27:X:1793:A:H2'	27:X:1794:A:C8	2.51	0.45
27:X:658:G:H2'	27:X:659:G:H8	1.81	0.45
27:X:2048:C:H1'	27:X:2428:U:H3	1.81	0.45
27:X:1478:U:H2'	27:X:1479:G:C8	2.51	0.45
27:X:787:A:H2	27:X:800:U:HO2'	1.63	0.45
12:M:104:LEU:HD23	12:M:106:TYR:CZ	2.51	0.45
27:X:746:G:N7	27:X:774:A:C6	2.85	0.45
27:X:825:C:H5''	27:X:1263:G:HO2'	1.81	0.45
28:Y:16:U:H4'	28:Y:72:C:O2	2.16	0.45
27:X:939:C:OP2	27:X:940:G:C8	2.70	0.45
27:X:1782:A:N6	27:X:1820:G:O2'	2.49	0.45
2:B:164:ARG:HD2	27:X:2753:C:H5''	1.98	0.45
27:X:666:U:H2'	27:X:667:U:H5''	1.98	0.45
10:K:89:GLU:O	10:K:91:PRO:HD3	2.15	0.45
1:A:252:LYS:HD3	27:X:1817:U:O4'	2.16	0.45
2:B:52:ALA:HB2	12:M:3:THR:HG23	1.98	0.45
27:X:2797:G:H2'	27:X:2798:A:H5''	1.99	0.45
27:X:88:G:C3'	27:X:89:A:H5''	2.47	0.45
27:X:2849:C:H2'	27:X:2850:U:C6	2.51	0.45
27:X:2736:U:H4'	27:X:2737:A:OP1	2.17	0.45
16:Q:10:PRO:HA	16:Q:27:PHE:HB3	1.98	0.45
13:N:8:ILE:HG22	13:N:11:ARG:NH2	2.31	0.45
27:X:982:C:H2'	27:X:983:G:O4'	2.16	0.45
7:H:91:PHE:N	7:H:91:PHE:CD1	2.84	0.45
15:P:104:LYS:HG3	15:P:106:LEU:H	1.82	0.45
9:J:82:THR:HA	27:X:2474:G:C5'	2.34	0.45
8:I:59:ARG:CB	27:X:2371:A:H8	2.30	0.45
15:P:99:ALA:CB	27:X:25:U:H5'	2.43	0.45
2:B:9:ILE:HD11	2:B:27:LEU:CB	2.43	0.45
27:X:115:G:P	27:X:117:A:HO2'	2.40	0.45
27:X:1763:G:H2'	27:X:1764:A:H4'	1.97	0.45
25:2:38:GLY:HA3	27:X:469:G:H8	1.82	0.45
27:X:2477:C:O2'	27:X:2478:C:H5'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:68:PHE:O	16:Q:70:GLY:N	2.42	0.45
5:E:150:LYS:NZ	27:X:2741:G:H21	2.13	0.45
8:I:94:GLU:HA	8:I:97:ARG:HG3	1.97	0.45
27:X:2640:G:H2'	27:X:2641:A:C8	2.51	0.45
24:1:39:LYS:NZ	24:1:47:HIS:HA	2.31	0.45
27:X:1230:C:H2'	27:X:1231:A:C8	2.52	0.45
27:X:324:C:H2'	27:X:325:U:O4'	2.17	0.45
13:N:45:TYR:HH	27:X:570:G:HO2'	1.64	0.45
27:X:2044:G:C8	27:X:2482:A:C8	3.04	0.45
3:C:133:PHE:CE1	3:C:161:ALA:HB2	2.51	0.45
27:X:2590:U:C5	30:X:2902:ERY:H312	2.51	0.45
27:X:577:U:H2'	27:X:579:G:OP2	2.17	0.45
28:Y:43:G:OP1	28:Y:45:C:N4	2.40	0.45
5:E:44:ARG:NH2	5:E:51:LEU:HB3	2.32	0.45
12:M:50:PHE:CE2	12:M:70:LYS:HB2	2.52	0.45
27:X:2645:C:H3'	27:X:2646:C:H6	1.82	0.45
27:X:2674:C:H2'	27:X:2675:U:H6	1.81	0.45
1:A:206:LEU:HD22	1:A:211:ARG:HB3	1.98	0.45
27:X:768:U:C4	27:X:769:C:C4	3.05	0.45
9:J:13:GLN:HG3	9:J:14:PHE:CD1	2.51	0.45
2:B:69:LYS:HB3	2:B:69:LYS:HE2	1.80	0.45
26:3:14:ILE:HD11	26:3:56:ALA:HB1	1.98	0.45
8:I:56:LEU:HD21	8:I:59:ARG:HH21	1.82	0.45
7:H:24:VAL:HG22	7:H:45:ALA:HB2	1.97	0.45
27:X:90:G:H3'	27:X:91:A:H8	1.80	0.45
27:X:1724:C:N3	27:X:1747:G:C6	2.85	0.45
17:R:105:ARG:HH22	17:R:112:LYS:HA	1.82	0.45
2:B:152:LYS:HB3	6:G:106:TYR:CB	2.44	0.45
27:X:1083:C:H42	27:X:1103:C:N4	2.15	0.45
27:X:2499:C:C4	27:X:2546:G:C8	3.04	0.45
27:X:1225:G:H2'	27:X:1249:G:H22	1.81	0.45
27:X:2519:C:O2	27:X:2720:A:H2	2.00	0.45
27:X:172:A:H5''	27:X:173:A:OP2	2.17	0.45
9:J:42:TRP:CZ2	27:X:969:U:H5	2.35	0.45
27:X:1751:A:H2'	27:X:1752:U:C6	2.51	0.45
1:A:43:ARG:H	1:A:43:ARG:NH1	2.14	0.45
26:3:52:LYS:O	26:3:56:ALA:HB2	2.17	0.45
27:X:2306:A:O2'	27:X:2307:A:O5'	2.34	0.45
27:X:2579:A:H2'	27:X:2580:C:H6	1.81	0.45
1:A:231:HIS:CG	1:A:232:PRO:HD2	2.52	0.45
27:X:16:G:H2'	27:X:17:G:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1223:G:N2	27:X:1249:G:O2'	2.49	0.45
20:U:46:LEU:O	27:X:2209:G:O2'	2.28	0.45
13:N:64:ARG:O	13:N:67:ALA:HB3	2.16	0.45
27:X:725:C:H2'	27:X:726:G:C8	2.52	0.45
27:X:1646:G:C5	27:X:1647:U:C5	3.04	0.45
9:J:76:THR:HB	9:J:88:LYS:O	2.17	0.45
28:Y:71:G:C6	28:Y:72:C:C4	3.05	0.45
1:A:208:LYS:HD3	27:X:1782:A:H1'	1.99	0.45
25:2:25:LYS:HD3	25:2:25:LYS:HA	1.74	0.45
10:K:43:GLU:O	10:K:46:PRO:HD2	2.17	0.45
27:X:1736:C:H2'	27:X:1737:G:C8	2.52	0.45
27:X:2220:A:H2'	27:X:2221:G:H8	1.81	0.45
2:B:145:LYS:HB2	27:X:2551:A:C8	2.51	0.45
4:D:129:ASN:ND2	27:X:2282:G:O2'	2.49	0.45
24:1:16:ALA:HB2	24:1:50:PHE:CE1	2.51	0.45
27:X:36:G:N3	27:X:462:G:O2'	2.50	0.45
3:C:65:GLY:O	15:P:112:ARG:NH2	2.50	0.45
7:H:23:ARG:HH11	27:X:2541:U:H1'	1.82	0.45
27:X:838:A:H2'	27:X:839:U:O4'	2.17	0.45
27:X:1098:G:C5	27:X:1100:G:H1'	2.51	0.45
27:X:1982:C:OP1	27:X:2704:U:H5'	2.16	0.45
27:X:2859:U:C5	27:X:2860:C:C2	3.05	0.45
27:X:231:G:H4'	27:X:397:U:H5''	1.99	0.45
27:X:828:C:H2'	27:X:829:C:H6	1.82	0.45
27:X:186:C:H2'	27:X:187:U:O4'	2.17	0.45
21:V:15:ALA:O	21:V:18:ILE:HB	2.17	0.45
20:U:78:ILE:HG12	20:U:79:GLU:H	1.81	0.45
27:X:809:C:H2'	27:X:810:U:C6	2.52	0.45
27:X:242:A:C8	27:X:441:A:N6	2.84	0.45
27:X:346:C:H2'	27:X:347:C:H6	1.80	0.45
27:X:587:A:OP1	27:X:1268:U:O2'	2.26	0.45
27:X:2368:G:H5''	27:X:2369:U:C5'	2.47	0.45
26:3:62:LEU:HD12	26:3:62:LEU:HA	1.86	0.45
27:X:2668:U:OP2	27:X:2847:G:N2	2.36	0.45
27:X:742:G:N2	27:X:1766:U:O4'	2.50	0.45
5:E:25:LYS:HG3	5:E:34:THR:HG22	1.98	0.45
27:X:1286:U:O2	27:X:1985:G:O2'	2.35	0.45
27:X:2513:A:C2	27:X:2514:G:H1'	2.50	0.45
22:W:14:GLY:O	22:W:18:LYS:HG2	2.17	0.45
10:K:98:LEU:O	10:K:111:ALA:HB1	2.17	0.45
27:X:1987:G:C6	27:X:1988:A:C4	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:120:ILE:HG12	27:X:1996:A:OP1	2.17	0.45
27:X:658:G:H1'	27:X:2330:G:OP1	2.17	0.45
27:X:659:G:H2'	27:X:660:G:C8	2.51	0.45
11:L:88:VAL:HG11	27:X:2357:A:H1'	1.99	0.45
1:A:107:ALA:HA	1:A:108:PRO:HD2	1.82	0.45
27:X:2579:A:H2'	27:X:2580:C:C6	2.52	0.45
17:R:105:ARG:HH22	17:R:113:THR:N	2.10	0.45
26:3:7:HIS:NE2	27:X:220:U:OP2	2.47	0.45
9:J:15:ARG:NE	9:J:73:LYS:HZ2	2.15	0.45
17:R:38:LEU:HD22	17:R:40:LEU:HG	1.99	0.45
27:X:2706:U:OP1	27:X:2706:U:C6	2.70	0.45
27:X:2738:A:H2'	27:X:2739:G:O4'	2.17	0.45
27:X:1418:C:H2'	27:X:1419:G:C8	2.52	0.45
27:X:2656:G:H1	27:X:2710:C:H42	1.63	0.45
6:G:124:GLU:O	6:G:128:GLU:HG2	2.17	0.45
27:X:2034:A:H2	27:X:2035:G:O6	1.99	0.45
27:X:2792:C:C2	27:X:2805:G:C2	3.05	0.45
27:X:2796:A:O2'	27:X:2801:A:N1	2.46	0.45
24:1:9:ILE:HG13	24:1:10:VAL:N	2.32	0.45
14:O:83:ARG:HG2	27:X:1238:A:H4'	1.99	0.45
2:B:109:LYS:NZ	27:X:2703:C:OP2	2.50	0.45
2:B:95:ILE:HA	2:B:95:ILE:HD13	1.82	0.45
5:E:109:TYR:CD2	27:X:2646:C:H1'	2.51	0.45
27:X:513:A:H5''	27:X:514:G:H5'	1.99	0.45
19:T:29:GLU:HG2	27:X:935:C:H1'	1.98	0.45
3:C:17:LEU:HG	3:C:109:ALA:HB2	1.99	0.45
27:X:699:G:H5''	27:X:699:G:H8	1.82	0.45
2:B:115:GLY:O	2:B:119:ARG:HB2	2.17	0.44
8:I:22:GLY:HA3	27:X:674:U:O2'	2.17	0.44
27:X:649:G:C8	27:X:650:U:H5	2.35	0.44
27:X:613:A:N7	27:X:668:A:H1'	2.31	0.44
2:B:152:LYS:CB	6:G:106:TYR:HB2	2.45	0.44
27:X:577:U:O2'	27:X:579:G:N7	2.42	0.44
27:X:1468:A:OP2	27:X:1468:A:C8	2.69	0.44
27:X:2495:G:C6	27:X:2548:G:C2	3.05	0.44
13:N:93:LYS:H	13:N:93:LYS:HG3	1.49	0.44
28:Y:80:A:H2'	28:Y:81:C:O4'	2.17	0.44
27:X:2864:C:H2'	27:X:2865:G:C8	2.52	0.44
28:Y:56:G:O5'	28:Y:56:G:H8	2.00	0.44
20:U:49:LYS:HB2	20:U:61:TRP:HA	1.99	0.44
25:2:36:ALA:C	25:2:38:GLY:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2053:G:C2	27:X:2054:A:C4	3.05	0.44
27:X:2269:G:N2	27:X:2322:U:H1'	2.32	0.44
22:W:12:ARG:HA	22:W:13:PRO:HD3	1.83	0.44
6:G:94:LYS:HE2	6:G:94:LYS:HB3	1.48	0.44
20:U:37:ILE:HD12	27:X:177:U:O2'	2.17	0.44
27:X:1121:G:H2'	27:X:1122:A:C8	2.52	0.44
2:B:134:TRP:HB2	2:B:135:HIS:CD2	2.52	0.44
27:X:1329:U:O2'	27:X:1330:G:H5'	2.17	0.44
27:X:495:C:H2'	27:X:496:C:C6	2.52	0.44
17:R:105:ARG:NH2	17:R:112:LYS:HA	2.32	0.44
4:D:115:ARG:HH22	4:D:178:ARG:NH1	2.12	0.44
27:X:205:A:H2'	27:X:206:U:H5'	1.99	0.44
15:P:11:LYS:HD2	27:X:1225:G:N7	2.32	0.44
27:X:1210:C:C2	27:X:1211:G:C8	3.05	0.44
17:R:14:LEU:HD21	17:R:41:PRO:HA	1.99	0.44
7:H:116:ARG:CZ	12:M:38:LYS:HD2	2.47	0.44
27:X:2451:G:H22	27:X:2456:U:H5''	1.81	0.44
27:X:2058:U:C4	27:X:2217:G:C6	3.05	0.44
16:Q:10:PRO:HD3	21:V:30:PHE:CD2	2.52	0.44
8:I:100:ARG:NH1	27:X:614:G:N7	2.64	0.44
1:A:142:VAL:HG12	1:A:193:ILE:HA	1.98	0.44
17:R:23:ILE:HG22	17:R:33:THR:HB	1.98	0.44
27:X:2728:A:H2'	27:X:2729:A:C8	2.51	0.44
1:A:32:ALA:HB3	1:A:83:GLU:CD	2.38	0.44
27:X:588:G:C2	27:X:1275:A:C4	3.05	0.44
27:X:2044:G:N2	27:X:2046:C:C2	2.85	0.44
27:X:2372:A:H62	27:X:2401:A:H61	1.65	0.44
1:A:24:LEU:HB3	1:A:25:THR:H	1.61	0.44
11:L:88:VAL:HG12	11:L:89:PHE:H	1.82	0.44
11:L:91:ARG:HH22	27:X:2355:A:H61	1.66	0.44
28:Y:39:C:H5''	28:Y:40:C:C5	2.53	0.44
8:I:54:SER:HB3	8:I:55:ARG:HE	1.82	0.44
27:X:2406:C:H5'	27:X:2408:G:H5'	1.99	0.44
20:U:46:LEU:C	20:U:47:HIS:CG	2.90	0.44
13:N:60:LEU:O	13:N:64:ARG:HG3	2.17	0.44
27:X:748:A:H5''	27:X:749:C:C5	2.52	0.44
13:N:75:ASN:H	13:N:78:THR:HB	1.83	0.44
1:A:99:ASP:HB3	27:X:1507:A:O4'	2.17	0.44
27:X:354:C:H2'	27:X:355:G:H8	1.82	0.44
1:A:246:PRO:HG2	1:A:248:THR:O	2.18	0.44
1:A:16:MET:HE1	1:A:24:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:THR:N	3:C:51:VAL:HG21	2.32	0.44
27:X:1482:U:OP2	27:X:1562:G:O2'	2.35	0.44
5:E:160:LYS:NZ	27:X:2637:C:H5'	2.32	0.44
23:Z:51:TYR:CD1	23:Z:55:ARG:HD3	2.53	0.44
8:I:73:GLU:OE2	8:I:73:GLU:N	2.50	0.44
18:S:3:LEU:HD11	18:S:33:ALA:H	1.81	0.44
27:X:1686:A:O3'	27:X:2528:G:H5'	2.17	0.44
3:C:39:ARG:HE	3:C:91:TYR:HD2	1.65	0.44
27:X:2510:A:C2'	27:X:2511:G:H5'	2.48	0.44
16:Q:72:ARG:NH2	27:X:1324:G:O2'	2.51	0.44
5:E:156:ALA:O	5:E:172:LYS:N	2.43	0.44
15:P:39:ARG:NH2	27:X:527:C:O2'	2.47	0.44
27:X:1816:G:H2'	27:X:1817:U:H6	1.83	0.44
27:X:1882:G:N2	27:X:1885:C:N4	2.60	0.44
7:H:8:LEU:HD22	7:H:94:ASN:HB3	2.00	0.44
27:X:1329:U:C2	27:X:1330:G:N7	2.85	0.44
27:X:494:A:N7	27:X:507:A:H2	2.16	0.44
23:Z:4:HIS:HB3	27:X:2039:G:H22	1.83	0.44
27:X:2495:G:O2'	27:X:2496:C:H5'	2.18	0.44
6:G:134:MET:HG3	27:X:1148:G:O2'	2.17	0.44
6:G:151:TYR:HB2	6:G:157:PRO:HB3	1.99	0.44
5:E:88:GLU:HG3	5:E:130:ARG:HG2	1.99	0.44
12:M:22:ARG:NH1	12:M:22:ARG:HB3	2.32	0.44
1:A:208:LYS:O	1:A:211:ARG:HB2	2.18	0.44
27:X:763:A:H2'	27:X:764:A:H5''	1.98	0.44
27:X:98:U:H4'	27:X:99:U:H5''	1.99	0.44
2:B:116:VAL:CG2	2:B:136:ARG:HG3	2.23	0.44
27:X:245:C:H42	27:X:437:G:H1	1.64	0.44
19:T:20:TYR:CD2	27:X:2335:U:H4'	2.52	0.44
2:B:61:LYS:HB3	2:B:62:PRO:HD3	1.99	0.44
27:X:748:A:H3'	27:X:749:C:C6	2.52	0.44
2:B:105:THR:CG2	2:B:197:VAL:HB	2.48	0.44
6:G:62:ILE:HG13	6:G:80:VAL:HG23	2.00	0.44
19:T:26:PHE:CD1	27:X:934:G:H1'	2.53	0.44
26:3:57:ARG:O	26:3:61:MET:N	2.50	0.44
27:X:2251:U:H5''	27:X:2252:A:OP1	2.18	0.44
27:X:2058:U:H1'	27:X:2576:G:H21	1.81	0.44
27:X:1065:A:H2'	27:X:1066:G:H8	1.83	0.44
27:X:2351:G:C2	27:X:2352:A:C5	3.06	0.44
27:X:580:A:H4'	27:X:581:A:OP1	2.17	0.44
8:I:38:LYS:HG2	8:I:40:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:840:U:H4'	27:X:841:G:N2	2.32	0.44
27:X:2578:G:N2	27:X:2579:A:C4	2.86	0.44
6:G:35:LYS:HA	6:G:35:LYS:HD3	1.44	0.44
16:Q:35:LYS:HB2	27:X:1614:C:H5''	2.00	0.44
23:Z:16:ARG:HD3	23:Z:20:ARG:CZ	2.48	0.44
27:X:836:G:N2	27:X:847:C:O2	2.51	0.44
7:H:17:ARG:H	7:H:58:ALA:HA	1.82	0.44
27:X:2528:G:C2	27:X:2529:G:N7	2.85	0.44
27:X:1296:G:N2	27:X:1299:A:C8	2.85	0.44
3:C:112:GLN:NE2	3:C:116:LYS:HD2	2.33	0.44
10:K:49:GLU:O	10:K:52:ILE:HG12	2.18	0.44
27:X:448:C:H2'	27:X:449:C:O4'	2.18	0.44
7:H:83:ARG:HD2	7:H:89:ILE:HD11	2.00	0.44
27:X:1935:A:C6	27:X:1936:A:N1	2.85	0.44
12:M:78:GLU:OE2	12:M:108:ARG:NE	2.48	0.44
27:X:2474:G:H2'	27:X:2475:C:O4'	2.18	0.44
27:X:1810:U:HO2'	27:X:1811:A:P	2.40	0.44
15:P:44:VAL:O	15:P:48:LYS:HD3	2.18	0.44
27:X:2493:U:H2'	27:X:2494:C:H6	1.81	0.44
27:X:616:U:O2'	27:X:671:A:H4'	2.18	0.44
27:X:1777:A:C4	27:X:1921:A:C6	3.06	0.44
3:C:176:ASN:ND2	3:C:178:TYR:HB3	2.32	0.44
27:X:1773:C:H1'	27:X:2588:U:C5'	2.48	0.44
27:X:1795:C:H2'	27:X:1796:A:C8	2.52	0.44
27:X:586:G:C6	27:X:587:A:N6	2.86	0.44
3:C:112:GLN:HE22	3:C:116:LYS:HD2	1.83	0.44
27:X:753:U:H2'	27:X:754:G:C8	2.52	0.44
22:W:18:LYS:HB2	27:X:863:C:H4'	1.99	0.44
27:X:2634:G:O2'	27:X:2643:G:O6	2.28	0.44
27:X:1679:U:O2	27:X:2666:U:H5''	2.18	0.44
18:S:66:VAL:HG22	18:S:83:PHE:CE2	2.53	0.44
1:A:59:LYS:O	1:A:59:LYS:HG3	2.18	0.44
15:P:29:LYS:HB3	15:P:30:TYR:CD2	2.52	0.44
27:X:796:A:H8	27:X:797:A:H4'	1.82	0.44
27:X:226:C:H4'	27:X:227:G:O5'	2.18	0.44
27:X:2198:U:N3	27:X:2199:C:H1'	2.32	0.44
27:X:2201:G:H2'	27:X:2202:G:C8	2.51	0.44
6:G:158:HIS:HA	6:G:161:GLN:HE22	1.83	0.44
27:X:1597:A:H2'	27:X:1598:C:C6	2.52	0.44
27:X:14:A:N6	27:X:15:G:C2	2.86	0.44
15:P:27:VAL:CG1	27:X:504:G:H4'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1359:G:C6	27:X:1617:G:C6	3.06	0.44
5:E:55:PRO:HD2	5:E:61:HIS:CD2	2.53	0.44
27:X:1698:C:O2'	27:X:1753:A:N3	2.42	0.44
5:E:17:VAL:HG13	5:E:26:VAL:HG22	1.98	0.44
9:J:54:VAL:O	9:J:57:ARG:HB2	2.18	0.43
27:X:1670:G:H5'	27:X:2797:G:N2	2.33	0.43
27:X:1098:G:H22	27:X:1114:A:H1'	1.82	0.43
11:L:32:TYR:CZ	28:Y:9:G:H5'	2.53	0.43
27:X:1835:C:H2'	27:X:1836:C:C6	2.52	0.43
27:X:748:A:H3'	27:X:749:C:H6	1.83	0.43
27:X:500:G:H2'	27:X:501:G:O4'	2.18	0.43
1:A:133:LEU:HB2	1:A:187:SER:HA	2.00	0.43
2:B:120:TRP:CE3	2:B:155:ARG:HD2	2.53	0.43
27:X:957:G:H2'	27:X:958:G:H8	1.83	0.43
1:A:222:ARG:HG3	27:X:1780:A:OP1	2.17	0.43
27:X:2670:C:H2'	27:X:2671:C:H6	1.83	0.43
17:R:97:GLN:NE2	17:R:101:GLY:HA2	2.33	0.43
27:X:1026:U:H2'	27:X:1027:C:C6	2.53	0.43
27:X:1580:C:H2'	27:X:1581:C:C6	2.53	0.43
27:X:1043:A:H2	27:X:1133:G:H22	1.65	0.43
9:J:35:LEU:HD11	9:J:130:THR:HB	2.00	0.43
27:X:1141:U:HO2'	27:X:1142:G:P	2.39	0.43
8:I:56:LEU:HD22	26:3:52:LYS:HZ1	1.83	0.43
27:X:649:G:H2'	27:X:650:U:H6	1.84	0.43
27:X:2307:A:H2'	27:X:2308:A:C8	2.53	0.43
27:X:2041:A:H61	30:X:2902:ERY:H282	1.83	0.43
27:X:1399:C:H2'	27:X:1400:A:C8	2.53	0.43
2:B:95:ILE:HG22	2:B:96:PHE:CD1	2.53	0.43
27:X:773:G:C2'	27:X:774:A:H5'	2.48	0.43
2:B:122:PHE:CE1	27:X:2491:C:H4'	2.53	0.43
27:X:2310:G:N2	27:X:2364:C:C4	2.86	0.43
8:I:80:LEU:HD21	8:I:89:ASP:OD2	2.18	0.43
28:Y:64:C:H2'	28:Y:65:A:C8	2.52	0.43
4:D:12:VAL:HG22	4:D:172:SER:HB2	2.00	0.43
27:X:1219:C:H2'	27:X:1220:G:O4'	2.18	0.43
8:I:63:ARG:HD3	26:3:30:ARG:HH22	1.82	0.43
1:A:108:PRO:HG2	1:A:111:LEU:HD12	2.00	0.43
27:X:1336:G:O6	27:X:1337:G:C6	2.72	0.43
27:X:1573:G:H3'	27:X:1574:A:H5''	2.00	0.43
12:M:103:LYS:O	12:M:104:LEU:HB2	2.18	0.43
1:A:254:THR:O	27:X:1836:C:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:81:ASN:ND2	27:X:1162:A:H4'	2.33	0.43
11:L:8:ARG:HB2	11:L:8:ARG:CZ	2.48	0.43
27:X:2555:G:OP1	27:X:2555:G:H3'	2.19	0.43
17:R:48:VAL:HG13	17:R:50:GLY:H	1.83	0.43
27:X:1880:G:C6	27:X:1881:U:C4	3.06	0.43
14:O:39:PHE:CE2	14:O:46:VAL:HB	2.53	0.43
14:O:32:LYS:HD3	14:O:32:LYS:HA	1.77	0.43
27:X:2017:U:H2'	27:X:2018:G:H5''	2.00	0.43
26:3:15:LYS:HZ3	26:3:60:LEU:HD21	1.84	0.43
27:X:1398:G:N2	27:X:1415:C:O2	2.51	0.43
27:X:2048:C:H1'	27:X:2428:U:N3	2.33	0.43
2:B:34:VAL:HG11	2:B:78:LEU:HD21	2.00	0.43
28:Y:27:A:N6	28:Y:55:C:H5''	2.34	0.43
27:X:1255:A:H2'	27:X:1256:C:H6	1.82	0.43
28:Y:30:C:H2'	28:Y:31:A:C8	2.53	0.43
10:K:107:GLY:HA3	27:X:1992:G:H1'	2.00	0.43
27:X:1974:U:H6	27:X:1974:U:O5'	2.01	0.43
27:X:2511:G:C6	27:X:2512:A:C5	3.07	0.43
21:V:41:HIS:CD2	27:X:95:G:H4'	2.52	0.43
27:X:485:G:C6	27:X:520:C:N4	2.86	0.43
27:X:1712:G:N3	27:X:1712:G:H3'	2.34	0.43
27:X:2470:U:O2	27:X:2470:U:H2'	2.17	0.43
27:X:2027:C:C2'	27:X:2028:C:H5'	2.48	0.43
8:I:59:ARG:HA	27:X:2371:A:H8	1.81	0.43
18:S:125:PRO:HA	18:S:158:CYS:SG	2.58	0.43
27:X:956:A:C4	27:X:2427:A:C2	3.06	0.43
27:X:529:U:H2'	27:X:530:G:H8	1.83	0.43
27:X:859:U:H3	27:X:944:A:H61	1.66	0.43
27:X:754:G:H2'	27:X:755:C:C6	2.53	0.43
27:X:2451:G:H2'	27:X:2454:C:H42	1.83	0.43
27:X:611:C:N4	27:X:612:G:C5	2.86	0.43
22:W:39:ALA:O	27:X:864:C:O2'	2.37	0.43
23:Z:10:LYS:HG3	27:X:1276:U:O4'	2.18	0.43
27:X:1493:A:H2'	27:X:1494:G:O4'	2.19	0.43
24:1:3:LYS:HB3	24:1:3:LYS:HE2	1.83	0.43
27:X:2224:U:H5''	27:X:2225:G:H5'	2.00	0.43
1:A:258:LYS:HG3	27:X:1790:G:OP1	2.18	0.43
27:X:617:U:C5	27:X:632:A:N1	2.87	0.43
27:X:632:A:C2	27:X:633:G:C4	3.07	0.43
1:A:63:ARG:HH22	27:X:1584:G:P	2.42	0.43
4:D:66:ILE:HD12	28:Y:44:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1574:A:H2'	27:X:1575:C:H5''	2.00	0.43
12:M:101:ARG:HH21	12:M:101:ARG:HG2	1.84	0.43
11:L:32:TYR:CG	28:Y:9:G:H4'	2.54	0.43
7:H:104:GLU:HB3	7:H:125:LYS:HD2	1.99	0.43
5:E:103:LEU:HD21	5:E:105:MET:HG3	1.99	0.43
2:B:54:LYS:HB3	2:B:74:PRO:HB2	2.00	0.43
20:U:48:LYS:HE2	20:U:48:LYS:HB2	1.76	0.43
14:O:15:SER:OG	14:O:96:LEU:HD13	2.18	0.43
4:D:52:LYS:HE3	4:D:147:ASP:HB2	2.01	0.43
25:2:8:ASN:HB3	25:2:11:LYS:HB3	2.00	0.43
6:G:46:ALA:HB2	6:G:54:LEU:HD22	2.00	0.43
27:X:240:U:H2'	27:X:241:C:O4'	2.19	0.43
14:O:48:GLY:C	14:O:50:ASP:H	2.22	0.43
18:S:130:ILE:HD12	18:S:130:ILE:H	1.84	0.43
25:2:42:LEU:H	25:2:42:LEU:HD12	1.83	0.43
26:3:25:PHE:CG	26:3:46:LYS:HA	2.54	0.43
27:X:1949:A:O2'	27:X:2572:U:H5'	2.18	0.43
27:X:1398:G:O2'	27:X:1399:C:O5'	2.36	0.43
19:T:57:HIS:N	19:T:57:HIS:CD2	2.87	0.43
1:A:188:GLU:H	1:A:188:GLU:HG2	1.46	0.43
27:X:2234:G:C6	27:X:2235:G:C4	3.06	0.43
27:X:2367:A:N7	27:X:2368:G:C5	2.87	0.43
15:P:60:ILE:HA	15:P:61:PRO:HD3	1.67	0.43
27:X:734:G:C2	27:X:735:G:C8	3.07	0.43
24:1:54:LYS:HB2	24:1:54:LYS:HE2	1.76	0.43
1:A:248:THR:HG22	1:A:249:PRO:HD2	2.01	0.43
1:A:91:ARG:NH1	1:A:109:GLU:HA	2.34	0.43
12:M:104:LEU:HD23	12:M:106:TYR:CE2	2.54	0.43
27:X:187:U:H2'	27:X:188:G:C8	2.54	0.43
27:X:2262:C:C2	27:X:2368:G:C2	3.06	0.43
27:X:1429:A:N6	27:X:1600:U:H4'	2.33	0.43
27:X:1769:U:H2'	27:X:1775:A:H62	1.83	0.43
27:X:1408:A:C6	27:X:1411:C:C2	3.07	0.43
11:L:33:ARG:HH11	11:L:99:ARG:HD2	1.84	0.43
7:H:7:ARG:HB3	7:H:18:GLU:OE2	2.18	0.43
27:X:883:A:H2'	27:X:884:C:O4'	2.19	0.43
15:P:109:ARG:O	15:P:109:ARG:HD2	2.19	0.43
18:S:49:THR:O	18:S:49:THR:OG1	2.37	0.43
15:P:99:ALA:O	15:P:124:THR:HG22	2.19	0.43
1:A:24:LEU:HD22	1:A:205:VAL:HG13	2.00	0.43
24:1:9:ILE:O	24:1:10:VAL:HB	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2574:G:N1	27:X:2578:G:C6	2.86	0.43
27:X:1845:A:N1	27:X:2070:G:H1'	2.34	0.43
8:I:17:LYS:HE2	8:I:17:LYS:HB3	1.81	0.43
27:X:78:C:H2'	27:X:79:G:H8	1.84	0.43
27:X:17:G:H1	27:X:533:C:H42	1.66	0.43
27:X:1154:A:OP1	27:X:1154:A:H8	2.01	0.43
23:Z:6:VAL:HG13	23:Z:7:PRO:O	2.19	0.43
15:P:9:ARG:HB3	15:P:10:ASN:H	1.46	0.43
27:X:172:A:H61	27:X:175:C:H3'	1.84	0.43
8:I:42:GLY:H	8:I:45:LYS:HE3	1.84	0.43
8:I:77:LEU:HB2	8:I:110:ALA:HA	2.01	0.43
27:X:1370:U:H2'	27:X:1371:G:C8	2.53	0.43
27:X:194:G:H3'	27:X:195:A:H8	1.84	0.43
9:J:136:GLU:OE1	9:J:137:VAL:HB	2.19	0.43
1:A:124:GLU:HA	1:A:125:PRO:HD3	1.80	0.43
26:3:13:ARG:HD2	26:3:24:ALA:HA	2.01	0.43
6:G:71:THR:HG22	6:G:76:GLN:OE1	2.17	0.43
13:N:20:ARG:HH22	14:O:72:ARG:HD3	1.83	0.43
26:3:9:MET:N	26:3:9:MET:SD	2.92	0.43
19:T:40:GLN:HE21	19:T:57:HIS:HB3	1.84	0.43
9:J:15:ARG:HE	9:J:73:LYS:NZ	2.17	0.43
12:M:38:LYS:HE2	12:M:38:LYS:HB3	1.78	0.43
1:A:39:LYS:HE2	1:A:87:ASN:HD21	1.84	0.43
1:A:87:ASN:O	27:X:1809:G:H5''	2.19	0.43
4:D:51:ASP:O	4:D:55:LYS:HG2	2.18	0.43
27:X:1196:G:H2'	27:X:1197:U:O4'	2.19	0.43
9:J:126:LEU:HA	9:J:127:PRO:HD3	1.86	0.43
23:Z:40:LYS:HD3	23:Z:46:CYS:HB2	1.99	0.43
13:N:101:ARG:O	13:N:103:PRO:HD3	2.18	0.43
1:A:218:LYS:HD2	1:A:219:PRO:HD2	2.00	0.42
27:X:2044:G:H2'	27:X:2480:C:O2'	2.19	0.42
26:3:23:MET:HB3	26:3:25:PHE:HE2	1.82	0.42
27:X:2331:A:C4	27:X:2345:A:C2	3.06	0.42
7:H:3:MET:O	7:H:6:SER:HB3	2.19	0.42
9:J:61:ARG:NH1	18:S:175:ARG:HD3	2.34	0.42
3:C:46:ARG:HD2	3:C:51:VAL:HG11	2.01	0.42
22:W:46:THR:HG22	22:W:47:VAL:HG13	2.01	0.42
18:S:141:MET:SD	18:S:147:ILE:HG12	2.59	0.42
4:D:104:ILE:HD13	4:D:173:MET:HB3	2.01	0.42
27:X:1281:A:H2'	27:X:1282:A:O4'	2.19	0.42
4:D:65:PRO:HA	4:D:89:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:69:G:H5''	27:X:111:G:H1'	2.01	0.42
20:U:17:SER:CB	20:U:44:ALA:HA	2.49	0.42
27:X:149:A:H2'	27:X:150:A:C8	2.54	0.42
5:E:175:LYS:HD3	5:E:175:LYS:HA	1.74	0.42
13:N:24:PHE:O	13:N:29:SER:HB3	2.19	0.42
27:X:820:U:H1'	27:X:2424:G:OP1	2.19	0.42
9:J:40:PRO:HB3	9:J:99:LYS:HD2	2.00	0.42
27:X:1330:G:H2'	27:X:1331:G:O4'	2.19	0.42
14:O:72:ARG:HA	14:O:82:ARG:O	2.18	0.42
12:M:104:LEU:HD22	12:M:107:LEU:HD11	2.01	0.42
27:X:745:C:H2'	27:X:746:G:O4'	2.19	0.42
13:N:81:ASN:CG	27:X:1162:A:H4'	2.39	0.42
5:E:157:TYR:CZ	27:X:2510:A:H5'	2.53	0.42
20:U:20:ARG:HD3	20:U:43:ARG:HD2	2.01	0.42
14:O:39:PHE:HE2	14:O:46:VAL:HB	1.84	0.42
27:X:2559:U:C2'	27:X:2560:G:H5'	2.49	0.42
10:K:20:LEU:HD23	10:K:21:ALA:N	2.35	0.42
27:X:1260:A:C6	27:X:1262:U:C2	3.07	0.42
13:N:65:ILE:HD13	13:N:95:LEU:HD22	2.01	0.42
27:X:565:A:O5'	27:X:565:A:H8	2.02	0.42
3:C:97:ARG:HA	3:C:100:ARG:HB2	2.00	0.42
20:U:15:VAL:HG23	20:U:16:ASN:H	1.83	0.42
27:X:1832:G:H1	27:X:1885:C:H42	1.65	0.42
1:A:183:ARG:NH2	1:A:263:ARG:HB3	2.34	0.42
1:A:210:GLY:HA2	1:A:213:ARG:CG	2.45	0.42
24:1:8:ILE:HD13	24:1:8:ILE:H	1.85	0.42
14:O:85:GLY:H	27:X:1238:A:H5'	1.84	0.42
27:X:1032:A:O2'	27:X:1134:C:H5''	2.19	0.42
27:X:1466:C:N4	27:X:1476:G:H1	2.16	0.42
27:X:105:G:C2	27:X:106:G:C8	3.07	0.42
11:L:39:TYR:OH	28:Y:117:G:N2	2.52	0.42
7:H:109:ARG:HA	7:H:129:LEU:HD22	2.00	0.42
7:H:129:LEU:HA	7:H:129:LEU:HD23	1.74	0.42
27:X:1742:G:C2	27:X:1743:C:C4	3.07	0.42
27:X:475:U:C2	27:X:801:A:C6	3.07	0.42
27:X:2328:G:H1	27:X:2347:C:H42	1.66	0.42
27:X:725:C:H2'	27:X:726:G:H8	1.84	0.42
1:A:133:LEU:HA	1:A:133:LEU:HD23	1.91	0.42
17:R:25:LEU:H	17:R:80:LYS:HA	1.83	0.42
27:X:764:A:C2	27:X:802:A:C4	3.07	0.42
27:X:2221:G:H22	27:X:2413:A:H2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:877:G:H1	27:X:924:C:H42	1.67	0.42
20:U:68:ARG:O	20:U:72:LYS:HG2	2.19	0.42
27:X:2011:U:H2'	27:X:2012:A:C8	2.54	0.42
27:X:1603:A:H2'	27:X:1604:A:H8	1.84	0.42
5:E:106:ASN:HD22	5:E:112:PRO:HB3	1.84	0.42
27:X:488:A:H8	27:X:488:A:OP1	2.02	0.42
14:O:26:GLN:HG2	14:O:27:GLY:N	2.34	0.42
27:X:795:A:OP2	27:X:1768:U:O2'	2.26	0.42
15:P:119:ILE:HG13	15:P:120:ILE:N	2.35	0.42
2:B:147:PRO:HD3	27:X:1141:U:C5	2.54	0.42
1:A:16:MET:HE1	1:A:23:GLY:HA2	2.01	0.42
28:Y:39:C:N4	28:Y:50:U:O2'	2.53	0.42
28:Y:42:U:O2'	28:Y:45:C:N4	2.53	0.42
4:D:90:THR:OG1	28:Y:44:C:N3	2.42	0.42
25:2:44:VAL:HG11	27:X:124:A:OP1	2.19	0.42
4:D:4:LEU:CG	4:D:5:LYS:H	2.27	0.42
27:X:1227:A:H4'	27:X:1252:C:H4'	2.02	0.42
15:P:73:ASN:O	15:P:77:ALA:N	2.42	0.42
27:X:1469:U:H5'	27:X:1470:G:OP2	2.20	0.42
27:X:930:A:C2	28:Y:82:U:H4'	2.55	0.42
27:X:2780:A:N3	27:X:2780:A:H2'	2.35	0.42
2:B:131:SER:C	2:B:134:TRP:HE1	2.19	0.42
9:J:53:ILE:O	9:J:57:ARG:HG2	2.20	0.42
10:K:60:LEU:CG	10:K:64:ARG:HD2	2.36	0.42
15:P:64:ALA:O	15:P:67:PRO:HD2	2.20	0.42
6:G:119:LEU:HA	6:G:119:LEU:HD13	1.64	0.42
27:X:54:G:H2'	27:X:55:A:H8	1.83	0.42
14:O:6:GLN:HB2	14:O:7:THR:H	1.66	0.42
27:X:2284:U:H5'	27:X:2286:G:N1	2.32	0.42
27:X:2432:A:O2'	27:X:2551:A:H1'	2.19	0.42
16:Q:43:GLN:HG2	16:Q:48:VAL:O	2.20	0.42
27:X:748:A:H5''	27:X:749:C:H5	1.84	0.42
27:X:1086:C:H2'	27:X:1087:C:H5''	2.01	0.42
27:X:14:A:C5	27:X:536:A:C2	3.07	0.42
4:D:118:ASN:HB3	4:D:122:PHE:HZ	1.85	0.42
17:R:52:ASN:HB2	17:R:73:GLU:HA	2.01	0.42
8:I:90:ARG:HA	8:I:121:HIS:CG	2.54	0.42
27:X:564:U:H2'	27:X:565:A:C8	2.54	0.42
27:X:2817:A:H2'	27:X:2818:G:O4'	2.19	0.42
27:X:398:C:N4	27:X:424:G:H1	2.18	0.42
3:C:156:ASN:HA	3:C:159:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:103:TYR:CD2	27:X:1142:G:O4'	2.73	0.42
27:X:2424:G:O2'	27:X:2425:G:H5'	2.19	0.42
8:I:17:LYS:HG3	8:I:19:VAL:N	2.31	0.42
3:C:48:ARG:H	3:C:48:ARG:HG3	1.45	0.42
2:B:5:LEU:CD2	2:B:195:LEU:HD11	2.49	0.42
27:X:1016:C:C2	27:X:1154:A:C5	3.07	0.42
27:X:1562:G:H8	27:X:1562:G:OP2	2.03	0.42
17:R:52:ASN:HB2	17:R:72:ARG:O	2.20	0.42
3:C:128:ALA:O	3:C:130:THR:N	2.51	0.42
27:X:1437:A:H2'	27:X:1438:G:H8	1.85	0.42
27:X:802:A:OP2	27:X:802:A:H8	2.02	0.42
15:P:109:ARG:HG3	15:P:109:ARG:H	1.64	0.42
9:J:123:GLY:HA2	9:J:126:LEU:HD12	2.01	0.42
20:U:68:ARG:NH1	27:X:413:G:N7	2.67	0.42
27:X:340:G:O4'	27:X:488:A:H1'	2.20	0.42
14:O:26:GLN:HG3	14:O:63:HIS:HD2	1.85	0.42
4:D:105:ASN:O	4:D:109:PRO:HG2	2.19	0.42
27:X:427:C:H2'	27:X:428:A:C8	2.54	0.42
22:W:38:PRO:HB2	27:X:865:A:O2'	2.20	0.42
27:X:788:G:C4	27:X:807:A:C8	3.08	0.42
4:D:161:LYS:HG3	4:D:162:THR:HG23	2.02	0.42
27:X:964:A:H2'	27:X:965:G:O4'	2.19	0.42
27:X:590:C:H2'	27:X:591:G:H8	1.84	0.42
14:O:82:ARG:HD3	14:O:82:ARG:HA	1.56	0.42
1:A:96:HIS:HE1	1:A:100:GLY:HA2	1.84	0.42
14:O:10:LYS:HE3	14:O:13:ARG:NH2	2.35	0.42
14:O:6:GLN:HG2	27:X:1007:A:O2'	2.19	0.42
27:X:2327:U:H6	27:X:2327:U:O5'	2.03	0.42
27:X:1454:U:H2'	27:X:1455:C:H6	1.83	0.42
1:A:94:LEU:HD12	1:A:95:LEU:N	2.35	0.42
17:R:15:HIS:HE1	17:R:80:LYS:HE2	1.84	0.42
10:K:39:THR:OG1	27:X:1668:G:H5'	2.20	0.42
1:A:207:GLY:O	27:X:1782:A:O2'	2.35	0.42
13:N:89:ASP:HB3	13:N:91:ASN:HB2	2.02	0.42
27:X:102:C:C4	27:X:103:U:C4	3.08	0.42
24:1:17:GLY:O	24:1:19:GLY:N	2.51	0.42
12:M:19:ASP:OD2	12:M:19:ASP:N	2.33	0.42
24:1:8:ILE:O	24:1:9:ILE:HG12	2.20	0.42
27:X:591:G:H3'	27:X:592:G:C8	2.42	0.42
27:X:1812:U:H2'	27:X:1812:U:O2	2.20	0.42
6:G:43:VAL:HG21	6:G:158:HIS:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:130:ARG:CZ	5:E:130:ARG:HB3	2.49	0.42
25:2:3:ARG:HD3	25:2:3:ARG:HA	1.51	0.42
27:X:2263:C:O2'	27:X:2267:A:N6	2.53	0.42
27:X:459:A:N1	27:X:466:A:O2'	2.45	0.42
14:O:64:GLY:HA3	14:O:90:PHE:CE1	2.54	0.42
13:N:72:HIS:CD2	13:N:110:VAL:HG21	2.55	0.42
27:X:2696:A:H2'	27:X:2697:G:H8	1.84	0.42
27:X:1730:G:N2	27:X:1736:C:O2	2.51	0.42
2:B:103:ASP:O	2:B:199:ARG:HG3	2.20	0.42
27:X:2043:A:O4'	27:X:2481:G:H1'	2.20	0.42
11:L:97:HIS:CG	11:L:98:GLY:N	2.85	0.42
3:C:45:THR:HG21	3:C:85:GLY:HA3	2.00	0.42
16:Q:4:TYR:HB3	21:V:26:MET:HE2	2.02	0.42
2:B:133:LYS:C	2:B:134:TRP:CD1	2.93	0.42
14:O:78:VAL:HG22	27:X:1202:U:H5'	2.02	0.42
27:X:1810:U:O2'	27:X:1811:A:O5'	2.36	0.42
16:Q:64:ARG:HH21	27:X:1349:A:H5'	1.84	0.42
27:X:797:A:N7	27:X:805:G:C4	2.88	0.42
27:X:79:G:N2	27:X:104:C:O2	2.52	0.42
2:B:195:LEU:HB3	12:M:2:GLN:HE21	1.84	0.42
27:X:762:A:H4'	27:X:1284:G:N3	2.34	0.42
27:X:615:C:H1'	27:X:670:U:H1'	2.00	0.42
28:Y:58:G:H5''	28:Y:59:A:OP1	2.20	0.42
27:X:1484:G:H2'	27:X:1485:U:H6	1.85	0.42
27:X:459:A:O4'	27:X:461:A:N6	2.53	0.42
27:X:485:G:C5	27:X:520:C:N4	2.88	0.42
9:J:64:LYS:O	9:J:107:VAL:HA	2.19	0.42
1:A:67:PHE:CE2	1:A:106:LEU:HD11	2.54	0.42
27:X:1505:U:H1'	27:X:1506:C:C5	2.55	0.42
27:X:48:A:H61	27:X:154:U:H2'	1.85	0.42
6:G:116:ARG:HE	6:G:126:VAL:HG13	1.85	0.42
13:N:10:ARG:HG3	27:X:1264:C:OP1	2.19	0.42
3:C:176:ASN:HD22	3:C:178:TYR:HB3	1.85	0.42
5:E:44:ARG:HH22	5:E:51:LEU:HD23	1.85	0.42
25:2:4:THR:O	27:X:700:C:H5'	2.19	0.42
27:X:2321:C:O2'	27:X:2353:G:H5''	2.20	0.42
8:I:84:GLU:OE2	8:I:87:THR:OG1	2.30	0.42
9:J:119:PHE:CD1	9:J:132:MET:HB2	2.55	0.42
27:X:1212:U:H2'	27:X:1213:U:C6	2.55	0.42
27:X:1788:C:C4	27:X:1789:U:C4	3.07	0.41
27:X:2048:C:H1'	27:X:2428:U:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2338:C:H2'	27:X:2339:A:C8	2.55	0.41
27:X:2553:G:C2	27:X:2554:C:O2	2.73	0.41
18:S:79:ILE:HD11	28:Y:78:A:O2'	2.19	0.41
20:U:49:LYS:HB3	20:U:61:TRP:CE3	2.55	0.41
1:A:118:ASN:HD22	1:A:119:ALA:H	1.68	0.41
27:X:502:A:H2'	27:X:503:G:O4'	2.19	0.41
27:X:753:U:H2'	27:X:754:G:H8	1.85	0.41
27:X:2189:A:H61	27:X:2190:A:N6	2.18	0.41
27:X:742:G:C2	27:X:1766:U:C6	3.08	0.41
25:2:24:THR:OG1	25:2:25:LYS:N	2.53	0.41
25:2:25:LYS:O	25:2:29:ASN:HB2	2.20	0.41
2:B:17:ASN:HB3	2:B:18:ASP:H	1.57	0.41
12:M:44:ARG:NH2	12:M:46:ARG:HE	2.18	0.41
1:A:69:ARG:NH1	1:A:128:GLY:O	2.40	0.41
2:B:48:GLN:NE2	27:X:2614:A:O2'	2.53	0.41
28:Y:75:A:H4'	28:Y:75:A:OP1	2.19	0.41
13:N:66:ASN:HB2	13:N:70:ARG:HH11	1.85	0.41
15:P:35:PRO:O	15:P:39:ARG:HD3	2.20	0.41
27:X:1793:A:N1	27:X:1814:G:H1'	2.35	0.41
27:X:1615:C:H2'	27:X:1616:C:C6	2.55	0.41
6:G:116:ARG:HD2	6:G:119:LEU:HG	2.02	0.41
27:X:837:U:H2'	27:X:838:A:C8	2.54	0.41
3:C:10:ASN:OD1	3:C:13:ARG:NH1	2.53	0.41
1:A:133:LEU:HD23	1:A:136:VAL:HG21	2.01	0.41
27:X:627:A:C6	27:X:628:A:C6	3.08	0.41
27:X:2188:A:H2'	27:X:2189:A:N7	2.36	0.41
22:W:22:ALA:HA	27:X:942:U:O2'	2.20	0.41
26:3:50:LEU:HD23	26:3:53:ALA:CB	2.50	0.41
17:R:96:LYS:O	17:R:104:VAL:HA	2.20	0.41
9:J:75:VAL:HG21	9:J:93:TYR:HE1	1.86	0.41
9:J:12:LYS:HD3	27:X:923:A:N7	2.34	0.41
27:X:1137:A:H4'	27:X:1138:A:O5'	2.19	0.41
7:H:101:ASN:N	7:H:101:ASN:HD22	2.18	0.41
2:B:136:ARG:O	2:B:137:ARG:C	2.59	0.41
3:C:162:ARG:NH2	27:X:331:U:O2'	2.54	0.41
24:1:28:ARG:O	24:1:33:ALA:HB2	2.20	0.41
27:X:2578:G:C2	27:X:2579:A:C4	3.08	0.41
27:X:1030:U:C4	27:X:1031:C:H5	2.38	0.41
3:C:180:ILE:HG22	3:C:186:LEU:HD13	2.03	0.41
27:X:1447:U:HO2'	27:X:1448:A:H8	1.69	0.41
27:X:2499:C:N3	27:X:2546:G:C8	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:84:VAL:HB	17:R:88:THR:O	2.20	0.41
4:D:102:LYS:O	4:D:106:ILE:HB	2.21	0.41
3:C:178:TYR:OH	27:X:1216:G:O2'	2.32	0.41
12:M:8:ASN:HA	27:X:2851:G:O5'	2.21	0.41
8:I:44:GLY:HA2	27:X:684:C:H5	1.84	0.41
27:X:2705:A:H8	27:X:2706:U:O2'	2.03	0.41
28:Y:53:G:H2'	28:Y:54:U:H5''	2.02	0.41
14:O:93:ILE:HG13	14:O:95:ILE:HD11	2.02	0.41
27:X:182:G:HO2'	27:X:183:U:P	2.44	0.41
8:I:86:THR:HG21	8:I:117:ALA:O	2.20	0.41
5:E:11:VAL:HA	5:E:12:PRO:HD2	1.95	0.41
27:X:2447:G:O2'	27:X:2448:A:H8	1.85	0.41
27:X:2046:C:O2	27:X:2430:A:C2	2.74	0.41
1:A:257:LEU:HB3	27:X:1794:A:O3'	2.21	0.41
1:A:49:ILE:HG22	27:X:792:U:OP1	2.20	0.41
27:X:640:C:H5''	27:X:660:G:O2'	2.20	0.41
23:Z:36:CYS:HB3	23:Z:49:CYS:HB3	1.94	0.41
10:K:28:LEU:CD2	10:K:115:LEU:HG	2.49	0.41
27:X:671:A:H2'	27:X:672:C:O4'	2.20	0.41
27:X:2283:G:N3	27:X:2283:G:H2'	2.35	0.41
10:K:73:LYS:HA	10:K:76:VAL:HG12	2.03	0.41
17:R:40:LEU:HA	17:R:41:PRO:HD2	1.95	0.41
4:D:79:LEU:HA	4:D:79:LEU:HD23	1.92	0.41
27:X:2705:A:O2'	27:X:2706:U:O5'	2.33	0.41
27:X:1841:G:H1	27:X:1876:C:H42	1.68	0.41
9:J:49:GLU:OE2	9:J:52:ARG:NH2	2.54	0.41
27:X:1228:G:C6	27:X:1229:C:C4	3.08	0.41
27:X:1278:A:H2	27:X:1997:A:N6	2.09	0.41
8:I:62:LYS:HB3	26:3:13:ARG:N	2.35	0.41
8:I:62:LYS:HG3	8:I:63:ARG:N	2.35	0.41
27:X:525:A:C8	27:X:526:C:C6	3.09	0.41
1:A:157:ARG:HH11	1:A:157:ARG:HB2	1.85	0.41
27:X:1462:C:C2	27:X:1480:G:N2	2.89	0.41
6:G:67:ARG:HB2	6:G:67:ARG:HH11	1.86	0.41
27:X:726:G:H1'	27:X:731:A:H61	1.86	0.41
5:E:86:ASN:O	5:E:165:VAL:HG22	2.20	0.41
8:I:74:VAL:HG11	27:X:638:A:C8	2.56	0.41
19:T:23:VAL:HB	19:T:26:PHE:CE2	2.54	0.41
27:X:1010:U:O2'	27:X:1011:A:H5'	2.20	0.41
7:H:37:GLY:O	27:X:2542:U:H5''	2.20	0.41
9:J:14:PHE:HE1	9:J:90:ALA:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:99:ALA:HB2	13:N:106:PHE:CE1	2.56	0.41
23:Z:15:LYS:O	23:Z:18:MET:HB3	2.19	0.41
27:X:1024:G:H2'	27:X:1025:A:C8	2.55	0.41
19:T:37:LEU:HD11	19:T:61:ALA:HB2	2.03	0.41
27:X:2667:C:N4	27:X:2700:U:OP2	2.41	0.41
5:E:95:ARG:HH22	5:E:97:LYS:HD3	1.86	0.41
11:L:14:ARG:HB2	11:L:14:ARG:HE	1.50	0.41
27:X:1642:G:H8	27:X:1642:G:O5'	2.03	0.41
27:X:645:G:H2'	27:X:646:C:C6	2.55	0.41
30:X:2902:ERY:H71	30:X:2902:ERY:H4	1.92	0.41
27:X:1031:C:OP1	27:X:1045:G:N2	2.30	0.41
16:Q:64:ARG:NH1	27:X:1348:C:H4'	2.35	0.41
2:B:5:LEU:HD21	2:B:79:ARG:CG	2.50	0.41
6:G:134:MET:HE3	6:G:134:MET:HB3	1.58	0.41
2:B:62:PRO:HG3	27:X:2767:C:H1'	2.01	0.41
27:X:828:C:C2	27:X:1207:G:C2	3.08	0.41
15:P:72:LEU:HA	15:P:129:ILE:HD12	2.01	0.41
3:C:152:THR:OG1	3:C:153:ASP:N	2.53	0.41
15:P:27:VAL:HG23	15:P:128:THR:HG22	2.02	0.41
21:V:41:HIS:ND1	27:X:94:C:O2'	2.33	0.41
27:X:2557:G:OP1	27:X:2593:A:N6	2.53	0.41
8:I:33:GLY:CA	14:O:79:GLN:HG3	2.49	0.41
1:A:124:GLU:O	1:A:126:LYS:N	2.52	0.41
27:X:2733:A:H2'	27:X:2734:U:O4'	2.20	0.41
11:L:12:ARG:HG3	11:L:13:THR:N	2.35	0.41
27:X:176:A:H2	27:X:2061:C:HO2'	1.65	0.41
4:D:132:ILE:HG13	4:D:154:ILE:HD13	2.03	0.41
15:P:119:ILE:O	15:P:120:ILE:HG12	2.21	0.41
27:X:2042:A:C6	27:X:2482:A:C2	3.08	0.41
8:I:58:ALA:HA	26:3:12:ARG:NH1	2.35	0.41
1:A:44:ASN:CB	1:A:49:ILE:HA	2.51	0.41
9:J:39:GLU:HA	9:J:40:PRO:HD3	1.79	0.41
27:X:1398:G:O2'	27:X:1399:C:O4'	2.25	0.41
3:C:48:ARG:C	3:C:50:GLN:N	2.74	0.41
27:X:2679:G:H1	27:X:2686:C:N4	2.16	0.41
1:A:89:SER:O	1:A:198:ASN:ND2	2.46	0.41
8:I:30:ALA:N	27:X:824:U:H2'	2.35	0.41
27:X:2522:G:H2'	27:X:2523:G:O4'	2.21	0.41
27:X:944:A:C2	27:X:945:G:C8	3.09	0.41
27:X:2510:A:H2'	27:X:2511:G:H5'	2.02	0.41
27:X:754:G:C2	27:X:755:C:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ALA:HB2	1:A:97:TYR:CD1	2.56	0.41
27:X:665:A:N7	27:X:666:U:H1'	2.36	0.41
27:X:922:A:N7	27:X:923:A:C6	2.89	0.41
27:X:2751:C:H2'	27:X:2752:C:C6	2.55	0.41
6:G:41:TRP:CZ3	6:G:79:PHE:CG	3.09	0.41
12:M:9:ARG:O	12:M:13:LEU:HB2	2.21	0.41
3:C:98:GLN:HE21	3:C:98:GLN:HB3	1.56	0.41
7:H:2:ILE:HG12	7:H:45:ALA:O	2.21	0.41
15:P:41:VAL:O	15:P:44:VAL:HG22	2.21	0.41
14:O:65:ARG:NH2	27:X:1237:G:OP2	2.53	0.41
14:O:23:GLU:CB	14:O:91:THR:HG21	2.48	0.41
11:L:39:TYR:HD2	11:L:41:GLN:HG3	1.86	0.41
19:T:45:PHE:HE2	19:T:77:ARG:CZ	2.33	0.41
3:C:68:ARG:HH12	27:X:687:G:H1'	1.83	0.41
27:X:2050:G:C6	27:X:2423:G:C6	3.09	0.41
8:I:99:VAL:O	8:I:101:ARG:HG2	2.21	0.41
1:A:27:LYS:HZ3	1:A:29:PRO:CB	2.33	0.41
27:X:2663:U:H3	27:X:2705:A:H62	1.66	0.41
11:L:15:ARG:HA	11:L:15:ARG:HD3	1.57	0.41
27:X:2394:G:C2	27:X:2395:C:C2	3.08	0.41
27:X:998:C:O2	27:X:1011:A:H2	2.04	0.41
21:V:43:VAL:O	21:V:47:ARG:HG2	2.21	0.41
27:X:1533:G:H2'	27:X:1534:A:H8	1.85	0.41
27:X:457:C:O2'	27:X:458:G:H5'	2.21	0.41
17:R:85:ASP:O	17:R:87:GLU:N	2.46	0.41
7:H:100:ASN:C	7:H:100:ASN:OD1	2.59	0.41
21:V:2:LYS:HE3	21:V:2:LYS:HB2	1.90	0.41
6:G:111:LYS:HG2	27:X:1142:G:H5''	2.01	0.41
8:I:41:SER:HB2	27:X:844:G:O3'	2.21	0.41
27:X:1816:G:H2'	27:X:1817:U:C6	2.56	0.41
27:X:2501:U:O2'	27:X:2626:U:OP1	2.32	0.41
17:R:56:LYS:HD3	17:R:69:GLN:NE2	2.35	0.41
27:X:2355:A:OP1	27:X:2355:A:H8	2.04	0.41
27:X:2579:A:O2'	27:X:2580:C:H5'	2.21	0.41
27:X:481:A:H3'	27:X:482:A:C8	2.56	0.41
2:B:9:ILE:HG13	2:B:25:VAL:O	2.21	0.41
27:X:1365:U:O2'	27:X:1586:A:N3	2.43	0.41
1:A:36:ALA:CB	1:A:63:ARG:HA	2.50	0.41
27:X:224:G:H4'	27:X:399:G:C6	2.56	0.41
27:X:2702:G:H2'	27:X:2703:C:O4'	2.21	0.41
27:X:474:G:C6	27:X:478:G:O6	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:12:ARG:HG2	10:K:12:ARG:NH1	2.36	0.41
27:X:1250:A:H5'	27:X:1250:A:C8	2.54	0.41
27:X:2432:A:N6	27:X:2479:U:H3	2.15	0.41
20:U:51:ILE:HG23	20:U:59:THR:HG22	2.03	0.41
6:G:62:ILE:HG22	6:G:135:LEU:HD21	2.02	0.41
27:X:242:A:N6	27:X:441:A:C8	2.89	0.41
2:B:59:VAL:CG1	2:B:64:GLN:HG3	2.51	0.41
27:X:2838:U:H2'	27:X:2839:G:H8	1.86	0.41
27:X:1991:C:H2'	27:X:1992:G:C8	2.53	0.41
27:X:1869:A:H2'	27:X:1870:U:O4'	2.21	0.41
27:X:1779:C:H2'	27:X:1780:A:C8	2.56	0.41
13:N:72:HIS:HD2	13:N:110:VAL:HG21	1.86	0.41
19:T:56:ASP:OD1	19:T:58:THR:OG1	2.34	0.41
27:X:2185:U:H2'	27:X:2186:G:C8	2.56	0.41
7:H:113:PRO:HD3	12:M:73:PHE:HB2	2.03	0.41
1:A:69:ARG:NH2	1:A:192:THR:OG1	2.54	0.41
4:D:77:PHE:HB2	27:X:2289:A:N1	2.36	0.41
13:N:86:ALA:C	13:N:88:ILE:N	2.73	0.41
27:X:534:U:P	27:X:549:G:H21	2.43	0.41
27:X:717:G:N3	27:X:739:G:C2	2.89	0.41
27:X:1609:G:H2'	27:X:1610:A:O4'	2.21	0.41
27:X:487:G:N2	27:X:489:A:H3'	2.35	0.41
27:X:216:U:H2'	27:X:217:U:C6	2.56	0.41
11:L:42:ILE:HD13	11:L:42:ILE:HA	1.90	0.41
15:P:113:ALA:HB1	15:P:114:ARG:HD2	2.02	0.41
27:X:2772:U:H2'	27:X:2773:G:C8	2.56	0.41
9:J:55:MET:HG3	9:J:122:ALA:HB2	2.03	0.41
27:X:1385:C:H2'	27:X:1386:A:O4'	2.21	0.41
27:X:2443:C:H2'	27:X:2444:C:H6	1.86	0.41
13:N:33:ARG:HG2	13:N:33:ARG:H	1.46	0.41
3:C:65:GLY:CA	27:X:2042:A:H5''	2.50	0.41
27:X:617:U:H5	27:X:632:A:N1	2.19	0.41
27:X:215:G:H1'	27:X:619:A:H1'	2.03	0.41
24:1:10:VAL:HG22	24:1:11:LYS:N	2.36	0.41
6:G:56:THR:HG21	27:X:1016:C:O2'	2.21	0.41
27:X:2712:G:H3'	27:X:2713:A:O4'	2.21	0.41
7:H:116:ARG:HD3	12:M:40:ARG:HB2	2.03	0.41
27:X:1123:G:C6	27:X:1124:U:N3	2.89	0.41
27:X:830:C:H3'	27:X:831:G:H8	1.86	0.41
27:X:1417:C:H2'	27:X:1418:C:C6	2.56	0.41
27:X:923:A:N3	27:X:2243:C:H1'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:127:VAL:HG22	7:H:133:VAL:HG21	2.03	0.41
27:X:1717:A:H5'	27:X:1718:A:OP2	2.20	0.41
9:J:24:GLY:HA3	27:X:920:G:P	2.61	0.41
28:Y:32:C:O5'	28:Y:32:C:H6	2.03	0.41
27:X:2616:U:H5''	27:X:2617:G:OP2	2.21	0.40
27:X:1671:A:O4'	27:X:2798:A:H5'	2.21	0.40
3:C:165:SER:HB3	3:C:166:TRP:CE3	2.56	0.40
23:Z:52:TYR:CE1	27:X:2859:U:N3	2.88	0.40
12:M:101:ARG:HH22	27:X:1745:C:P	2.43	0.40
25:2:35:ARG:NH1	27:X:53:G:H1'	2.36	0.40
17:R:14:LEU:HD23	17:R:14:LEU:HA	1.85	0.40
10:K:96:ARG:HB2	27:X:2857:C:H5'	2.03	0.40
27:X:2220:A:H2'	27:X:2221:G:C8	2.56	0.40
3:C:17:LEU:HD12	3:C:17:LEU:HA	1.78	0.40
27:X:877:G:C6	27:X:878:C:N4	2.89	0.40
27:X:2288:A:C5	27:X:2289:A:N7	2.89	0.40
2:B:148:GLY:HA3	27:X:2036:G:C4'	2.51	0.40
20:U:28:GLY:HA3	20:U:32:ARG:HG2	2.03	0.40
27:X:1754:G:H4'	27:X:1754:G:OP1	2.21	0.40
26:3:15:LYS:HD3	26:3:15:LYS:HA	1.70	0.40
8:I:56:LEU:HD22	26:3:52:LYS:NZ	2.37	0.40
15:P:125:SER:OG	15:P:126:HIS:N	2.53	0.40
27:X:1882:G:N2	27:X:1886:G:C6	2.89	0.40
3:C:163:ASN:ND2	3:C:166:TRP:HB2	2.36	0.40
6:G:52:GLY:HA3	27:X:1150:C:H5'	2.04	0.40
9:J:26:ASP:OD1	9:J:28:VAL:N	2.52	0.40
27:X:951:G:N3	27:X:1205:G:H4'	2.35	0.40
18:S:152:ILE:HD11	18:S:168:VAL:HB	2.03	0.40
27:X:825:C:C6	27:X:1263:G:C5	3.10	0.40
13:N:52:ASN:O	13:N:55:ARG:N	2.55	0.40
28:Y:31:A:N3	28:Y:58:G:N2	2.69	0.40
3:C:189:ASP:HB3	3:C:190:ALA:H	1.65	0.40
22:W:47:VAL:HG23	22:W:51:LEU:HD21	2.03	0.40
18:S:1:MET:HB3	18:S:2:GLU:H	1.70	0.40
27:X:1251:G:O2'	27:X:1252:C:H5'	2.21	0.40
27:X:1531:C:H5'	27:X:1532:A:OP1	2.21	0.40
7:H:88:THR:O	12:M:79:ARG:HG2	2.22	0.40
13:N:2:PRO:HD3	27:X:456:C:O5'	2.22	0.40
6:G:139:ARG:HB2	27:X:567:G:OP1	2.21	0.40
20:U:10:LYS:HD3	20:U:11:LYS:N	2.37	0.40
27:X:2609:G:H21	27:X:2866:A:H1'	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:VAL:HB	4:D:155:THR:OG1	2.21	0.40
27:X:350:U:H6	27:X:350:U:O5'	2.04	0.40
20:U:33:LYS:HD3	20:U:33:LYS:HA	1.72	0.40
27:X:538:A:N3	27:X:2025:A:C6	2.89	0.40
15:P:30:TYR:HB3	15:P:123:ARG:CZ	2.51	0.40
27:X:494:A:C8	27:X:495:C:C5	3.09	0.40
26:3:32:GLN:H	26:3:32:GLN:HG3	1.67	0.40
28:Y:36:A:N6	28:Y:46:G:H2'	2.36	0.40
27:X:312:G:O2'	27:X:313:U:H6	2.03	0.40
27:X:1850:G:C1'	27:X:1867:A:H62	2.35	0.40
27:X:1742:G:H2'	27:X:1743:C:C6	2.56	0.40
27:X:676:G:C6	27:X:677:G:C5	3.10	0.40
3:C:84:PHE:CD2	27:X:597:U:H1'	2.57	0.40
8:I:43:ALA:HB1	27:X:684:C:H41	1.85	0.40
27:X:2262:C:H2'	27:X:2263:C:O4'	2.21	0.40
27:X:2013:A:H4'	27:X:2014:A:H8	1.87	0.40
3:C:147:LYS:O	3:C:185:ARG:N	2.50	0.40
2:B:37:LYS:HD2	2:B:42:ASP:OD1	2.22	0.40
27:X:1080:A:N7	27:X:1084:A:N6	2.69	0.40
27:X:1026:U:H2'	27:X:1027:C:H6	1.86	0.40
3:C:86:PRO:C	3:C:87:LYS:HD2	2.42	0.40
27:X:45:C:OP2	27:X:192:G:H2'	2.21	0.40
27:X:2455:A:N3	27:X:2460:G:N1	2.62	0.40
2:B:136:ARG:CZ	2:B:157:ALA:HB2	2.51	0.40
6:G:111:LYS:HE2	27:X:1142:G:H5"	2.03	0.40
27:X:2281:C:N4	27:X:2293:G:H1	2.04	0.40
26:3:25:PHE:CD2	26:3:25:PHE:N	2.88	0.40
8:I:56:LEU:HD21	8:I:59:ARG:NH2	2.35	0.40
7:H:3:MET:HG2	7:H:44:TYR:CE1	2.57	0.40
24:1:11:LYS:HE3	24:1:26:LYS:HD3	2.03	0.40
25:2:19:ARG:O	25:2:22:MET:HB3	2.22	0.40
27:X:836:G:C4	27:X:837:U:C5	3.10	0.40
2:B:109:LYS:HE2	2:B:191:ALA:HB2	2.02	0.40
12:M:103:LYS:N	12:M:103:LYS:HD2	2.36	0.40
20:U:53:GLU:HB2	20:U:56:GLN:O	2.21	0.40
27:X:692:C:H2'	27:X:693:A:C8	2.56	0.40
13:N:13:ARG:NH2	27:X:1264:C:OP1	2.53	0.40
10:K:36:THR:OG1	27:X:1291:G:OP1	2.16	0.40
27:X:1773:C:H2'	27:X:2587:G:O2'	2.22	0.40
27:X:2827:G:C6	27:X:2828:C:N3	2.90	0.40
27:X:573:C:H2'	27:X:574:C:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:67:LEU:O	5:E:71:LEU:HG	2.22	0.40
16:Q:20:MET:HG3	16:Q:25:TYR:CD1	2.57	0.40
27:X:1354:A:H2'	27:X:1410:U:O2	2.21	0.40
1:A:222:ARG:NH2	27:X:1819:U:OP2	2.53	0.40
27:X:2533:U:H2'	27:X:2534:U:C6	2.56	0.40
5:E:143:GLN:HE21	27:X:2724:G:H21	1.69	0.40
27:X:2030:U:H2'	27:X:2031:A:C8	2.57	0.40
27:X:2609:G:N3	27:X:2866:A:O2'	2.53	0.40
27:X:192:G:H4'	27:X:193:A:H4'	2.04	0.40
27:X:600:G:C6	27:X:602:C:C4	3.09	0.40
27:X:1473:U:O2	27:X:1474:A:N6	2.55	0.40
15:P:51:GLN:HE22	23:Z:39:LYS:NZ	2.20	0.40
28:Y:119:G:C6	28:Y:120:G:C5	3.10	0.40
2:B:114:GLN:C	27:X:1672:A:H4'	2.42	0.40
2:B:147:PRO:HB2	2:B:149:ARG:HG2	2.03	0.40
15:P:31:VAL:O	15:P:125:SER:HB3	2.21	0.40
27:X:1174:G:N2	27:X:1175:A:C5	2.89	0.40
27:X:2821:G:H2'	27:X:2822:U:O4'	2.20	0.40
27:X:759:C:C2	30:X:2902:ERY:H371	2.56	0.40
27:X:2212:U:H2'	27:X:2213:G:C8	2.56	0.40
6:G:131:VAL:O	6:G:134:MET:N	2.41	0.40
27:X:1413:U:H2'	27:X:1414:G:H8	1.87	0.40
27:X:2698:G:H2'	27:X:2699:G:O4'	2.21	0.40
21:V:18:ILE:HG23	21:V:22:LYS:HE2	2.04	0.40
18:S:116:VAL:N	18:S:168:VAL:O	2.49	0.40
9:J:6:LYS:HB2	9:J:7:ARG:H	1.68	0.40
27:X:2528:G:C2	27:X:2529:G:C5	3.09	0.40
27:X:2763:U:H2'	27:X:2764:U:C6	2.51	0.40
17:R:14:LEU:HD13	17:R:16:PHE:CZ	2.57	0.40
27:X:2662:C:C4	27:X:2663:U:C5	3.10	0.40
10:K:45:ARG:O	10:K:49:GLU:HG3	2.21	0.40
27:X:1662:G:H8	27:X:1662:G:O5'	2.04	0.40
27:X:2825:A:H2'	27:X:2825:A:N3	2.35	0.40
27:X:354:C:H2'	27:X:355:G:C8	2.55	0.40
10:K:9:LYS:HE2	27:X:1669:A:OP1	2.22	0.40
15:P:12:LYS:HA	15:P:15:LYS:HB2	2.04	0.40
23:Z:8:LYS:O	27:X:2000:U:H4'	2.21	0.40
27:X:1695:U:H2'	27:X:1696:C:O4'	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	Percentiles	
1	A	258/275 (94%)	221 (86%)	34 (13%)	3 (1%)	16	61
2	B	203/211 (96%)	178 (88%)	24 (12%)	1 (0%)	34	77
3	C	192/205 (94%)	164 (85%)	26 (14%)	2 (1%)	19	65
4	D	175/180 (97%)	155 (89%)	19 (11%)	1 (1%)	30	74
5	E	169/185 (91%)	157 (93%)	11 (6%)	1 (1%)	30	74
6	G	140/174 (80%)	127 (91%)	13 (9%)	0	100	100
7	H	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	24	69
8	I	132/156 (85%)	102 (77%)	26 (20%)	4 (3%)	5	41
9	J	134/141 (95%)	113 (84%)	21 (16%)	0	100	100
10	K	111/116 (96%)	102 (92%)	8 (7%)	1 (1%)	21	67
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100	100
12	M	106/165 (64%)	99 (93%)	6 (6%)	1 (1%)	21	67
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	11	53
14	O	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
15	P	128/137 (93%)	109 (85%)	15 (12%)	4 (3%)	5	41
16	Q	91/95 (96%)	76 (84%)	12 (13%)	3 (3%)	5	39
17	R	108/115 (94%)	91 (84%)	16 (15%)	1 (1%)	21	67
18	S	173/237 (73%)	154 (89%)	19 (11%)	0	100	100
19	T	72/91 (79%)	62 (86%)	9 (12%)	1 (1%)	14	57
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	2	24
21	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
22	W	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	38 (74%)	10 (20%)	3 (6%)	2	23
25	2	44/47 (94%)	41 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	3	57/65 (88%)	46 (81%)	10 (18%)	1 (2%)	11	52
All	All	3025/3379 (90%)	2632 (87%)	359 (12%)	34 (1%)	17	63

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	120	ILE
16	Q	6	ILE
16	Q	69	ILE
1	A	24	LEU
1	A	25	THR
13	N	94	VAL
16	Q	59	PRO
24	1	9	ILE
24	1	10	VAL
15	P	125	SER
20	U	60	VAL
5	E	165	VAL
7	H	42	LYS
8	I	39	SER
8	I	103	ASN
15	P	119	ILE
20	U	15	VAL
20	U	39	LYS
10	K	18	VAL
15	P	99	ALA
19	T	19	LYS
24	1	18	THR
2	B	121	ASN
4	D	8	TYR
13	N	8	ILE
17	R	80	LYS
26	3	37	SER
1	A	219	PRO
3	C	15	ILE
12	M	29	PRO
20	U	30	VAL
3	C	22	VAL
8	I	61	PRO
8	I	68	VAL



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
1	A	202/216 (94%)	163 (81%)	39 (19%)	2	11
2	B	155/157 (99%)	127 (82%)	28 (18%)	2	13
3	C	154/163 (94%)	131 (85%)	23 (15%)	4	22
4	D	153/156 (98%)	140 (92%)	13 (8%)	13	50
5	E	136/144 (94%)	115 (85%)	21 (15%)	3	21
6	G	118/146 (81%)	93 (79%)	25 (21%)	1	8
7	H	103/103 (100%)	88 (85%)	15 (15%)	4	23
8	I	101/121 (84%)	82 (81%)	19 (19%)	2	11
9	J	110/115 (96%)	87 (79%)	23 (21%)	1	9
10	K	90/93 (97%)	70 (78%)	20 (22%)	1	7
11	L	74/82 (90%)	57 (77%)	17 (23%)	1	6
12	M	94/133 (71%)	71 (76%)	23 (24%)	1	5
13	N	96/97 (99%)	81 (84%)	15 (16%)	3	20
14	O	75/79 (95%)	61 (81%)	14 (19%)	2	11
15	P	112/118 (95%)	87 (78%)	25 (22%)	1	7
16	Q	75/76 (99%)	61 (81%)	14 (19%)	2	11
17	R	91/96 (95%)	72 (79%)	19 (21%)	1	9
18	S	149/192 (78%)	135 (91%)	14 (9%)	11	45
19	T	55/67 (82%)	44 (80%)	11 (20%)	1	10
20	U	57/66 (86%)	45 (79%)	12 (21%)	1	9
21	V	53/55 (96%)	46 (87%)	7 (13%)	5	27
22	W	48/48 (100%)	39 (81%)	9 (19%)	2	11
23	Z	50/53 (94%)	44 (88%)	6 (12%)	6	31
24	1	46/48 (96%)	32 (70%)	14 (30%)	0	3
25	2	39/40 (98%)	28 (72%)	11 (28%)	0	3
26	3	46/51 (90%)	36 (78%)	10 (22%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2482/2715 (91%)	2035 (82%)	447 (18%)	<b>2</b> <b>13</b>

All (447) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	ARG
1	A	16	MET
1	A	26	LYS
1	A	34	THR
1	A	40	THR
1	A	43	ARG
1	A	48	ARG
1	A	49	ILE
1	A	53	PHE
1	A	65	ILE
1	A	68	LYS
1	A	84	TYR
1	A	104	TYR
1	A	111	LEU
1	A	118	ASN
1	A	122	GLU
1	A	151	LYS
1	A	157	ARG
1	A	161	THR
1	A	164	GLN
1	A	165	VAL
1	A	186	HIS
1	A	188	GLU
1	A	198	ASN
1	A	201	HIS
1	A	206	LEU
1	A	211	ARG
1	A	214	TRP
1	A	215	LEU
1	A	218	LYS
1	A	220	HIS
1	A	229	VAL
1	A	240	THR
1	A	244	ARG
1	A	247	VAL
1	A	248	THR

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Mol	Chain	Res	Type
1	A	252	LYS
1	A	269	PHE
2	B	9	ILE
2	B	12	THR
2	B	19	ARG
2	B	56	GLU
2	B	66	HIS
2	B	69	LYS
2	B	72	VAL
2	B	79	ARG
2	B	82	ARG
2	B	84	PHE
2	B	87	ASP
2	B	92	ASN
2	B	107	THR
2	B	118	LYS
2	B	119	ARG
2	B	128	SER
2	B	137	ARG
2	B	140	SER
2	B	143	GLN
2	B	150	VAL
2	B	155	ARG
2	B	156	MET
2	B	162	MET
2	B	164	ARG
2	B	173	VAL
2	B	188	ILE
2	B	198	LEU
2	B	199	ARG
3	C	5	ASN
3	C	14	THR
3	C	17	LEU
3	C	24	SER
3	C	31	VAL
3	C	45	THR
3	C	48	ARG
3	C	51	VAL
3	C	52	SER
3	C	62	LYS
3	C	64	THR
3	C	74	VAL

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Mol	Chain	Res	Type
3	C	76	THR
3	C	98	GLN
3	C	116	LYS
3	C	120	VAL
3	C	143	ASP
3	C	150	LEU
3	C	152	THR
3	C	155	GLU
3	C	157	THR
3	C	165	SER
3	C	188	ILE
4	D	46	ASP
4	D	62	LEU
4	D	66	ILE
4	D	67	ILE
4	D	74	ILE
4	D	80	ARG
4	D	90	THR
4	D	112	ARG
4	D	128	TYR
4	D	130	LEU
4	D	143	TYR
4	D	146	VAL
4	D	150	ARG
5	E	20	GLN
5	E	32	GLU
5	E	43	VAL
5	E	44	ARG
5	E	57	ASP
5	E	61	HIS
5	E	70	THR
5	E	86	ASN
5	E	90	ARG
5	E	105	MET
5	E	113	VAL
5	E	116	GLU
5	E	129	THR
5	E	130	ARG
5	E	136	ILE
5	E	155	ASP
5	E	164	PHE
5	E	165	VAL

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Mol	Chain	Res	Type
5	E	167	GLU
5	E	168	GLN
5	E	169	ILE
6	G	31	THR
6	G	32	TYR
6	G	39	GLN
6	G	41	TRP
6	G	56	THR
6	G	61	ARG
6	G	62	ILE
6	G	63	ARG
6	G	67	ARG
6	G	69	ASP
6	G	76	GLN
6	G	83	ILE
6	G	90	LEU
6	G	91	THR
6	G	93	LYS
6	G	99	VAL
6	G	101	THR
6	G	102	ARG
6	G	111	LYS
6	G	116	ARG
6	G	132	PHE
6	G	145	HIS
6	G	150	VAL
6	G	161	GLN
6	G	171	LEU
7	H	23	ARG
7	H	25	LEU
7	H	41	ASN
7	H	47	VAL
7	H	78	SER
7	H	93	ARG
7	H	102	GLN
7	H	104	GLU
7	H	108	THR
7	H	114	VAL
7	H	117	GLU
7	H	119	ARG
7	H	120	ASP
7	H	126	ILE

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Mol	Chain	Res	Type
7	H	127	VAL
8	I	13	ARG
8	I	18	ARG
8	I	21	ARG
8	I	32	ARG
8	I	39	SER
8	I	49	PHE
8	I	50	GLU
8	I	53	ARG
8	I	59	ARG
8	I	60	LEU
8	I	73	GLU
8	I	78	SER
8	I	80	LEU
8	I	88	PHE
8	I	89	ASP
8	I	96	TYR
8	I	103	ASN
8	I	114	ILE
8	I	141	VAL
9	J	6	LYS
9	J	7	ARG
9	J	8	THR
9	J	10	PHE
9	J	11	ARG
9	J	17	ARG
9	J	21	ASP
9	J	27	TYR
9	J	28	VAL
9	J	44	LYS
9	J	54	VAL
9	J	60	ARG
9	J	64	LYS
9	J	68	ARG
9	J	69	ILE
9	J	88	LYS
9	J	93	TYR
9	J	103	VAL
9	J	111	THR
9	J	130	THR
9	J	132	MET
9	J	133	VAL

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Mol	Chain	Res	Type
9	J	135	ARG
10	K	5	LYS
10	K	8	ARG
10	K	9	LYS
10	K	11	ASN
10	K	12	ARG
10	K	14	SER
10	K	17	ARG
10	K	33	ARG
10	K	35	GLN
10	K	48	VAL
10	K	51	LEU
10	K	59	ASP
10	K	64	ARG
10	K	94	TYR
10	K	95	THR
10	K	98	LEU
10	K	99	ARG
10	K	109	THR
10	K	110	MET
10	K	112	LEU
11	L	8	ARG
11	L	11	LEU
11	L	17	VAL
11	L	31	VAL
11	L	33	ARG
11	L	37	HIS
11	L	38	ILE
11	L	39	TYR
11	L	43	ILE
11	L	45	ASP
11	L	59	LEU
11	L	67	THR
11	L	87	VAL
11	L	88	VAL
11	L	91	ARG
11	L	93	SER
11	L	100	VAL
12	M	2	GLN
12	M	5	ILE
12	M	16	ILE
12	M	19	ASP

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Mol	Chain	Res	Type
12	M	21	THR
12	M	22	ARG
12	M	24	LEU
12	M	29	PRO
12	M	31	ASP
12	M	33	VAL
12	M	34	ARG
12	M	37	THR
12	M	39	VAL
12	M	40	ARG
12	M	45	THR
12	M	50	PHE
12	M	72	SER
12	M	79	ARG
12	M	87	LEU
12	M	88	VAL
12	M	91	VAL
12	M	101	ARG
12	M	103	LYS
13	N	3	ARG
13	N	5	LYS
13	N	8	ILE
13	N	11	ARG
13	N	18	LEU
13	N	22	LYS
13	N	28	ARG
13	N	30	LYS
13	N	33	ARG
13	N	37	GLN
13	N	84	LYS
13	N	90	LEU
13	N	93	LYS
13	N	102	GLU
13	N	117	ARG
14	O	12	TYR
14	O	13	ARG
14	O	14	VAL
14	O	21	ARG
14	O	34	GLU
14	O	47	PHE
14	O	67	LYS
14	O	69	ILE

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Mol	Chain	Res	Type
14	O	72	ARG
14	O	76	SER
14	O	81	ARG
14	O	82	ARG
14	O	88	GLN
14	O	91	THR
15	P	9	ARG
15	P	12	LYS
15	P	20	LEU
15	P	21	ARG
15	P	32	ARG
15	P	39	ARG
15	P	43	ASP
15	P	48	LYS
15	P	86	LEU
15	P	88	ASP
15	P	91	PHE
15	P	92	VAL
15	P	93	LYS
15	P	96	TYR
15	P	98	ASP
15	P	102	THR
15	P	103	LEU
15	P	104	LYS
15	P	105	ARG
15	P	106	LEU
15	P	109	ARG
15	P	114	ARG
15	P	122	LYS
15	P	128	THR
15	P	131	VAL
16	Q	5	ASP
16	Q	6	ILE
16	Q	7	LEU
16	Q	12	ILE
16	Q	26	SER
16	Q	27	PHE
16	Q	56	MET
16	Q	58	VAL
16	Q	62	ARG
16	Q	63	LYS
16	Q	67	ARG

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Mol	Chain	Res	Type
16	Q	73	ASN
16	Q	80	VAL
16	Q	84	GLU
17	R	5	SER
17	R	10	HIS
17	R	11	ASN
17	R	18	LYS
17	R	38	LEU
17	R	52	ASN
17	R	53	VAL
17	R	54	ILE
17	R	55	THR
17	R	56	LYS
17	R	62	MET
17	R	64	ASN
17	R	83	LEU
17	R	88	THR
17	R	92	THR
17	R	95	ARG
17	R	97	GLN
17	R	106	VAL
17	R	112	LYS
18	S	25	ASN
18	S	26	LYS
18	S	28	ASN
18	S	34	LEU
18	S	49	THR
18	S	52	PHE
18	S	53	ASP
18	S	71	MET
18	S	79	ILE
18	S	83	PHE
18	S	99	HIS
18	S	120	LEU
18	S	130	ILE
18	S	168	VAL
19	T	14	ARG
19	T	19	LYS
19	T	25	LYS
19	T	41	ARG
19	T	46	LYS
19	T	49	GLN

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Mol	Chain	Res	Type
19	T	55	ARG
19	T	56	ASP
19	T	62	LEU
19	T	64	ASP
19	T	71	ASN
20	U	8	THR
20	U	13	LEU
20	U	19	ILE
20	U	21	ARG
20	U	23	LYS
20	U	32	ARG
20	U	34	THR
20	U	35	THR
20	U	37	ILE
20	U	47	HIS
20	U	63	SER
20	U	70	LEU
21	V	7	ARG
21	V	19	ASP
21	V	25	LEU
21	V	26	MET
21	V	29	ARG
21	V	37	LEU
21	V	42	ARG
22	W	4	LYS
22	W	6	VAL
22	W	9	VAL
22	W	23	LEU
22	W	31	SER
22	W	34	VAL
22	W	37	THR
22	W	45	LYS
22	W	51	LEU
23	Z	6	VAL
23	Z	11	THR
23	Z	25	LEU
23	Z	29	ASN
23	Z	41	LEU
23	Z	44	HIS
24	1	4	ASP
24	1	8	ILE
24	1	20	PHE

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Mol	Chain	Res	Type
24	1	21	TYR
24	1	22	TYR
24	1	26	LYS
24	1	27	ASN
24	1	28	ARG
24	1	36	GLU
24	1	41	ASP
24	1	43	VAL
24	1	47	HIS
24	1	48	VAL
24	1	54	LYS
25	2	3	ARG
25	2	4	THR
25	2	10	ARG
25	2	14	LYS
25	2	19	ARG
25	2	22	MET
25	2	28	ARG
25	2	29	ASN
25	2	40	HIS
25	2	42	LEU
25	2	44	VAL
26	3	6	THR
26	3	11	LYS
26	3	19	THR
26	3	31	HIS
26	3	32	GLN
26	3	36	LYS
26	3	39	ASP
26	3	46	LYS
26	3	55	TRP
26	3	57	ARG

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

Mol	Chain	Res	Type
1	A	87	ASN
1	A	198	ASN
2	B	35	GLN
2	B	48	GLN
2	B	135	HIS
2	B	169	ASN

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Mol	Chain	Res	Type
3	C	34	GLN
3	C	98	GLN
3	C	112	GLN
3	C	163	ASN
4	D	37	ASN
4	D	129	ASN
4	D	135	GLN
4	D	171	GLN
5	E	61	HIS
5	E	65	HIS
5	E	74	ASN
5	E	106	ASN
5	E	168	GLN
6	G	39	GLN
6	G	76	GLN
6	G	84	ASN
6	G	158	HIS
6	G	161	GLN
7	H	101	ASN
8	I	66	ASN
8	I	79	GLN
8	I	103	ASN
9	J	58	HIS
10	K	3	HIS
10	K	11	ASN
11	L	37	HIS
11	L	86	GLN
12	M	2	GLN
12	M	20	HIS
13	N	37	GLN
13	N	41	ASN
13	N	52	ASN
13	N	63	GLN
13	N	72	HIS
13	N	81	ASN
14	O	88	GLN
15	P	16	GLN
15	P	51	GLN
15	P	78	ASN
15	P	81	HIS
15	P	118	ASN
16	Q	44	GLN

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Mol	Chain	Res	Type
16	Q	57	ASN
16	Q	71	GLN
16	Q	73	ASN
16	Q	94	GLN
17	R	10	HIS
17	R	15	HIS
17	R	32	GLN
17	R	69	GLN
17	R	71	GLN
17	R	97	GLN
18	S	118	HIS
19	T	71	ASN
19	T	85	GLN
21	V	10	GLN
22	W	15	ASN
22	W	49	HIS
23	Z	44	HIS
24	1	32	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2673/2880 (92%)	638 (23%)	40 (1%)
28	Y	121/124 (97%)	29 (23%)	1 (0%)
All	All	2794/3004 (93%)	667 (23%)	41 (1%)

All (667) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	3	U
27	X	4	C
27	X	13	A
27	X	14	A
27	X	17	G
27	X	34	U
27	X	37	C
27	X	39	C
27	X	45	C
27	X	49	U
27	X	50	G
27	X	51	A

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Mol	Chain	Res	Type
27	X	59	G
27	X	60	A
27	X	63	A
27	X	69	G
27	X	70	A
27	X	73	A
27	X	74	G
27	X	83	A
27	X	88	G
27	X	89	A
27	X	90	G
27	X	91	A
27	X	98	U
27	X	100	G
27	X	107	G
27	X	108	G
27	X	116	A
27	X	118	U
27	X	123	A
27	X	124	A
27	X	129	A
27	X	135	U
27	X	136	A
27	X	143	A
27	X	146	C
27	X	151	G
27	X	173	A
27	X	176	A
27	X	178	C
27	X	181	A
27	X	192	G
27	X	193	A
27	X	199	A
27	X	205	A
27	X	206	U
27	X	207	U
27	X	209	G
27	X	210	A
27	X	220	U
27	X	221	A
27	X	222	G
27	X	225	G

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Mol	Chain	Res	Type
27	X	227	G
27	X	229	G
27	X	238	G
27	X	242	A
27	X	243	G
27	X	246	C
27	X	248	A
27	X	304	A
27	X	305	A
27	X	310	A
27	X	312	G
27	X	319	G
27	X	321	A
27	X	322	A
27	X	323	G
27	X	335	A
27	X	340	G
27	X	341	A
27	X	342	G
27	X	343	A
27	X	360	A
27	X	393	U
27	X	399	G
27	X	400	U
27	X	408	U
27	X	409	G
27	X	414	A
27	X	419	G
27	X	421	G
27	X	424	G
27	X	425	A
27	X	429	C
27	X	433	G
27	X	441	A
27	X	453	U
27	X	456	C
27	X	459	A
27	X	463	C
27	X	467	U
27	X	469	G
27	X	490	A
27	X	491	A

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Mol	Chain	Res	Type
27	X	492	G
27	X	493	A
27	X	494	A
27	X	504	G
27	X	514	G
27	X	515	A
27	X	518	A
27	X	519	C
27	X	520	C
27	X	537	C
27	X	538	A
27	X	539	A
27	X	540	G
27	X	541	C
27	X	542	A
27	X	543	G
27	X	554	U
27	X	555	U
27	X	556	A
27	X	557	U
27	X	559	C
27	X	560	G
27	X	564	U
27	X	572	G
27	X	582	G
27	X	584	A
27	X	587	A
27	X	591	G
27	X	595	A
27	X	596	C
27	X	613	A
27	X	614	G
27	X	616	U
27	X	624	A
27	X	625	A
27	X	626	A
27	X	627	A
27	X	628	A
27	X	631	G
27	X	632	A
27	X	633	G
27	X	642	A

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Mol	Chain	Res	Type
27	X	645	G
27	X	648	A
27	X	649	G
27	X	651	C
27	X	654	A
27	X	655	A
27	X	656	U
27	X	657	A
27	X	658	G
27	X	664	C
27	X	665	A
27	X	666	U
27	X	667	U
27	X	668	A
27	X	677	G
27	X	682	G
27	X	690	A
27	X	695	G
27	X	697	G
27	X	699	G
27	X	703	A
27	X	725	C
27	X	729	A
27	X	731	A
27	X	732	G
27	X	743	A
27	X	749	C
27	X	753	U
27	X	759	C
27	X	760	U
27	X	761	G
27	X	766	A
27	X	774	A
27	X	784	U
27	X	789	G
27	X	790	A
27	X	795	A
27	X	797	A
27	X	798	G
27	X	801	A
27	X	802	A
27	X	803	C

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Mol	Chain	Res	Type
27	X	804	C
27	X	805	G
27	X	806	A
27	X	814	G
27	X	818	G
27	X	824	U
27	X	825	C
27	X	830	C
27	X	832	A
27	X	840	U
27	X	841	G
27	X	843	G
27	X	859	U
27	X	872	G
27	X	879	A
27	X	891	A
27	X	914	C
27	X	922	A
27	X	931	G
27	X	938	G
27	X	939	C
27	X	940	G
27	X	943	U
27	X	944	A
27	X	952	A
27	X	956	A
27	X	957	G
27	X	966	A
27	X	967	G
27	X	969	U
27	X	972	C
27	X	973	U
27	X	976	C
27	X	979	A
27	X	985	G
27	X	992	A
27	X	999	A
27	X	1000	G
27	X	1006	C
27	X	1007	A
27	X	1016	C
27	X	1018	C

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Mol	Chain	Res	Type
27	X	1019	U
27	X	1020	A
27	X	1022	A
27	X	1023	U
27	X	1024	G
27	X	1033	G
27	X	1034	U
27	X	1035	G
27	X	1037	U
27	X	1044	U
27	X	1046	U
27	X	1051	U
27	X	1054	C
27	X	1055	A
27	X	1056	U
27	X	1058	G
27	X	1060	C
27	X	1071	U
27	X	1073	G
27	X	1081	A
27	X	1082	G
27	X	1083	C
27	X	1086	C
27	X	1087	C
27	X	1096	A
27	X	1097	A
27	X	1099	A
27	X	1101	U
27	X	1105	U
27	X	1108	U
27	X	1109	A
27	X	1113	C
27	X	1120	C
27	X	1121	G
27	X	1123	G
27	X	1127	C
27	X	1128	G
27	X	1140	A
27	X	1142	G
27	X	1145	C
27	X	1146	G
27	X	1149	G

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Mol	Chain	Res	Type
27	X	1152	C
27	X	1153	A
27	X	1183	C
27	X	1185	C
27	X	1187	A
27	X	1189	G
27	X	1194	U
27	X	1195	U
27	X	1200	G
27	X	1203	A
27	X	1208	A
27	X	1209	G
27	X	1217	U
27	X	1223	G
27	X	1225	G
27	X	1240	G
27	X	1249	G
27	X	1250	A
27	X	1251	G
27	X	1260	A
27	X	1261	G
27	X	1262	U
27	X	1263	G
27	X	1266	G
27	X	1269	G
27	X	1278	A
27	X	1279	G
27	X	1284	G
27	X	1285	A
27	X	1286	U
27	X	1288	A
27	X	1289	A
27	X	1301	U
27	X	1302	C
27	X	1313	U
27	X	1314	A
27	X	1315	A
27	X	1321	A
27	X	1325	U
27	X	1332	G
27	X	1334	A
27	X	1341	G

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Mol	Chain	Res	Type
27	X	1342	U
27	X	1347	C
27	X	1349	A
27	X	1354	A
27	X	1358	C
27	X	1365	U
27	X	1378	A
27	X	1379	A
27	X	1381	G
27	X	1391	A
27	X	1392	U
27	X	1393	G
27	X	1397	A
27	X	1398	G
27	X	1404	C
27	X	1408	A
27	X	1409	U
27	X	1413	U
27	X	1428	G
27	X	1429	A
27	X	1430	G
27	X	1432	G
27	X	1433	A
27	X	1434	U
27	X	1435	G
27	X	1441	A
27	X	1442	C
27	X	1443	G
27	X	1459	U
27	X	1460	G
27	X	1465	G
27	X	1467	U
27	X	1468	A
27	X	1469	U
27	X	1470	G
27	X	1475	U
27	X	1482	U
27	X	1490	U
27	X	1497	C
27	X	1498	G
27	X	1508	G
27	X	1517	C

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Mol	Chain	Res	Type
27	X	1518	C
27	X	1524	C
27	X	1525	A
27	X	1527	G
27	X	1528	C
27	X	1541	G
27	X	1551	U
27	X	1552	C
27	X	1553	G
27	X	1554	G
27	X	1562	G
27	X	1571	G
27	X	1574	A
27	X	1575	C
27	X	1582	A
27	X	1585	A
27	X	1600	U
27	X	1601	U
27	X	1602	G
27	X	1603	A
27	X	1608	U
27	X	1624	A
27	X	1625	A
27	X	1626	A
27	X	1629	G
27	X	1631	C
27	X	1632	A
27	X	1634	A
27	X	1641	C
27	X	1648	C
27	X	1651	U
27	X	1656	U
27	X	1661	C
27	X	1664	G
27	X	1665	C
27	X	1666	G
27	X	1667	A
27	X	1668	G
27	X	1682	A
27	X	1688	U
27	X	1691	G
27	X	1710	U

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Mol	Chain	Res	Type
27	X	1711	C
27	X	1713	G
27	X	1719	G
27	X	1732	U
27	X	1735	G
27	X	1747	G
27	X	1754	G
27	X	1755	G
27	X	1760	G
27	X	1764	A
27	X	1771	A
27	X	1775	A
27	X	1776	A
27	X	1782	A
27	X	1790	G
27	X	1791	C
27	X	1792	C
27	X	1793	A
27	X	1799	A
27	X	1801	C
27	X	1807	A
27	X	1808	C
27	X	1811	A
27	X	1812	U
27	X	1813	A
27	X	1819	U
27	X	1821	A
27	X	1830	C
27	X	1831	G
27	X	1859	A
27	X	1861	G
27	X	1867	A
27	X	1868	A
27	X	1882	G
27	X	1884	A
27	X	1910	A
27	X	1912	G
27	X	1919	A
27	X	1920	A
27	X	1921	A
27	X	1922	U
27	X	1923	U

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Mol	Chain	Res	Type
27	X	1924	C
27	X	1930	C
27	X	1938	U
27	X	1946	U
27	X	1947	G
27	X	1948	C
27	X	1949	A
27	X	1950	C
27	X	1951	G
27	X	1953	A
27	X	1954	A
27	X	1955	G
27	X	1958	G
27	X	1965	U
27	X	1974	U
27	X	1976	U
27	X	1980	A
27	X	2001	G
27	X	2003	A
27	X	2004	U
27	X	2006	G
27	X	2014	A
27	X	2015	G
27	X	2016	A
27	X	2018	G
27	X	2023	C
27	X	2025	A
27	X	2026	C
27	X	2028	C
27	X	2032	G
27	X	2035	G
27	X	2038	C
27	X	2039	G
27	X	2043	A
27	X	2044	G
27	X	2045	A
27	X	2052	G
27	X	2059	U
27	X	2075	U
27	X	2083	G
27	X	2089	C
27	X	2171	U

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Mol	Chain	Res	Type
27	X	2172	U
27	X	2182	A
27	X	2189	A
27	X	2190	A
27	X	2191	A
27	X	2192	U
27	X	2193	C
27	X	2196	U
27	X	2197	U
27	X	2198	U
27	X	2199	C
27	X	2200	G
27	X	2204	A
27	X	2205	C
27	X	2217	G
27	X	2218	G
27	X	2247	A
27	X	2252	A
27	X	2259	G
27	X	2262	C
27	X	2265	A
27	X	2266	A
27	X	2267	A
27	X	2272	A
27	X	2284	U
27	X	2285	U
27	X	2286	G
27	X	2287	G
27	X	2290	A
27	X	2291	U
27	X	2298	U
27	X	2299	A
27	X	2300	G
27	X	2301	A
27	X	2306	A
27	X	2307	A
27	X	2311	U
27	X	2312	A
27	X	2313	G
27	X	2315	A
27	X	2324	G
27	X	2326	C

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Mol	Chain	Res	Type
27	X	2327	U
27	X	2330	G
27	X	2333	A
27	X	2351	G
27	X	2358	C
27	X	2362	G
27	X	2364	C
27	X	2367	A
27	X	2368	G
27	X	2369	U
27	X	2375	G
27	X	2381	A
27	X	2385	U
27	X	2386	G
27	X	2397	A
27	X	2398	U
27	X	2401	A
27	X	2402	U
27	X	2404	A
27	X	2405	A
27	X	2406	C
27	X	2407	G
27	X	2408	G
27	X	2410	U
27	X	2413	A
27	X	2420	C
27	X	2424	G
27	X	2426	G
27	X	2427	A
27	X	2429	A
27	X	2441	U
27	X	2449	G
27	X	2452	U
27	X	2453	C
27	X	2455	A
27	X	2460	G
27	X	2463	G
27	X	2470	U
27	X	2471	U
27	X	2477	C
27	X	2480	C
27	X	2481	G

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Mol	Chain	Res	Type
27	X	2482	A
27	X	2484	G
27	X	2485	U
27	X	2497	A
27	X	2498	U
27	X	2504	G
27	X	2508	G
27	X	2511	G
27	X	2521	A
27	X	2545	A
27	X	2546	G
27	X	2552	C
27	X	2553	G
27	X	2557	G
27	X	2564	U
27	X	2581	A
27	X	2582	G
27	X	2588	U
27	X	2591	C
27	X	2593	A
27	X	2594	U
27	X	2600	A
27	X	2601	C
27	X	2608	A
27	X	2617	G
27	X	2624	G
27	X	2625	U
27	X	2633	A
27	X	2639	A
27	X	2642	G
27	X	2650	G
27	X	2664	G
27	X	2666	U
27	X	2668	U
27	X	2670	C
27	X	2677	U
27	X	2688	G
27	X	2691	C
27	X	2692	A
27	X	2693	U
27	X	2694	G
27	X	2698	G

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Mol	Chain	Res	Type
27	X	2706	U
27	X	2707	G
27	X	2711	G
27	X	2713	A
27	X	2724	G
27	X	2728	A
27	X	2732	C
27	X	2737	A
27	X	2738	A
27	X	2744	A
27	X	2745	A
27	X	2757	G
27	X	2758	A
27	X	2759	U
27	X	2760	G
27	X	2761	A
27	X	2769	C
27	X	2771	C
27	X	2782	G
27	X	2793	G
27	X	2795	A
27	X	2796	A
27	X	2798	A
27	X	2807	U
27	X	2808	U
27	X	2809	A
27	X	2811	G
27	X	2814	G
27	X	2825	A
27	X	2832	G
27	X	2847	G
27	X	2849	C
27	X	2851	G
27	X	2855	C
27	X	2858	A
27	X	2861	A
27	X	2866	A
27	X	2868	G
28	Y	14	C
28	Y	15	A
28	Y	17	A
28	Y	22	U

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Mol	Chain	Res	Type
28	Y	26	G
28	Y	28	A
28	Y	29	C
28	Y	37	C
28	Y	39	C
28	Y	40	C
28	Y	43	G
28	Y	44	C
28	Y	46	G
28	Y	47	A
28	Y	49	C
28	Y	52	G
28	Y	54	U
28	Y	56	G
28	Y	59	A
28	Y	69	G
28	Y	75	A
28	Y	86	A
28	Y	99	G
28	Y	102	A
28	Y	108	G
28	Y	111	C
28	Y	112	A
28	Y	115	G
28	Y	123	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	38	G
27	X	50	G
27	X	537	C
27	X	538	A
27	X	542	A
27	X	557	U
27	X	760	U
27	X	788	G
27	X	789	G
27	X	956	A
27	X	1019	U
27	X	1053	G
27	X	1059	A

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Mol	Chain	Res	Type
27	X	1096	A
27	X	1141	U
27	X	1182	U
27	X	1250	A
27	X	1313	U
27	X	1391	A
27	X	1441	A
27	X	1496	G
27	X	1607	A
27	X	1625	A
27	X	1664	G
27	X	1810	U
27	X	1919	A
27	X	1923	U
27	X	1975	G
27	X	2204	A
27	X	2299	A
27	X	2312	A
27	X	2363	G
27	X	2404	A
27	X	2409	A
27	X	2452	U
27	X	2705	A
27	X	2736	U
27	X	2756	A
27	X	2824	C
27	X	2846	G
28	Y	58	G

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 70 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	ERY	X	2902	-	53,53,53	0.85	1 (1%)	82,82,82	1.29	10 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	ERY	X	2902	-	-	0/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2902	ERY	C4-C3	-2.20	1.49	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2902	ERY	O8-C23-C22	-2.72	103.96	110.01
30	X	2902	ERY	C2-C3-C4	-2.41	105.94	112.77
30	X	2902	ERY	C30-C2-C1	-2.26	103.83	109.19
30	X	2902	ERY	C13-O2-C1	-2.23	114.36	118.10
30	X	2902	ERY	C16-C15-C14	-2.17	111.25	115.04
30	X	2902	ERY	O1-C1-C2	-2.13	119.02	124.27
30	X	2902	ERY	C34-C10-C11	-2.04	111.69	114.44
30	X	2902	ERY	O10-C6-C7	2.05	113.80	108.49
30	X	2902	ERY	C6-C7-C8	2.06	119.47	114.98
30	X	2902	ERY	O2-C1-C2	2.09	115.75	111.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	2902	ERY	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	260/275 (94%)	0.07	7 (2%) 58 48	48, 104, 163, 221	0
2	B	205/211 (97%)	-0.28	5 (2%) 62 52	27, 50, 107, 233	0
3	C	194/205 (94%)	0.12	14 (7%) 18 14	39, 102, 180, 292	0
4	D	177/180 (98%)	0.28	15 (8%) 13 11	114, 175, 232, 282	0
5	E	171/185 (92%)	-0.18	6 (3%) 48 37	57, 131, 192, 243	0
6	G	142/174 (81%)	0.03	10 (7%) 19 15	38, 77, 160, 339	0
7	H	134/134 (100%)	-0.35	2 (1%) 76 68	33, 45, 87, 135	0
8	I	134/156 (85%)	0.27	5 (3%) 45 36	55, 126, 192, 315	0
9	J	136/141 (96%)	0.05	4 (2%) 55 45	56, 94, 163, 214	0
10	K	113/116 (97%)	-0.46	0 100 100	27, 32, 67, 100	0
11	L	104/114 (91%)	0.15	10 (9%) 10 9	130, 161, 200, 243	0
12	M	108/165 (65%)	-0.43	0 100 100	30, 43, 95, 242	0
13	N	117/118 (99%)	-0.15	2 (1%) 73 64	41, 76, 133, 232	0
14	O	94/100 (94%)	-0.21	4 (4%) 39 30	52, 94, 178, 204	0
15	P	130/137 (94%)	-0.37	0 100 100	33, 51, 147, 188	0
16	Q	93/95 (97%)	-0.35	1 (1%) 82 74	49, 94, 162, 192	0
17	R	110/115 (95%)	0.06	4 (3%) 46 37	65, 100, 189, 259	0
18	S	175/237 (73%)	0.55	24 (13%) 4 4	93, 144, 224, 285	0
19	T	74/91 (81%)	0.21	7 (9%) 10 9	72, 112, 158, 228	0
20	U	72/81 (88%)	0.49	5 (6%) 20 15	75, 119, 185, 238	0
21	V	65/67 (97%)	-0.19	2 (3%) 52 43	76, 115, 164, 208	0
22	W	55/55 (100%)	0.32	4 (7%) 18 14	72, 91, 128, 190	0
23	Z	56/60 (93%)	-0.39	0 100 100	32, 40, 80, 152	0
24	1	53/55 (96%)	0.59	7 (13%) 4 5	102, 129, 217, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	2	46/47 (97%)	0.18	1 (2%) 65 55	38, 67, 122, 169	0
26	3	59/65 (90%)	0.45	5 (8%) 13 11	81, 100, 172, 278	0
27	X	2680/2880 (93%)	-0.14	88 (3%) 50 40	26, 76, 186, 299	0
28	Y	122/124 (98%)	-0.10	4 (3%) 50 40	74, 153, 190, 332	0
All	All	5879/6383 (92%)	-0.06	236 (4%) 42 33	26, 89, 188, 339	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	S	23	ALA	8.1
18	S	22	VAL	8.0
18	S	15	ASP	7.6
27	X	1072	U	7.4
27	X	731	A	6.9
28	Y	123	U	6.5
4	D	153	ASP	6.4
27	X	1071	U	6.1
27	X	1913	G	6.1
20	U	28	GLY	5.9
3	C	44	SER	5.6
27	X	1073	G	5.4
27	X	1099	A	5.4
27	X	1060	C	5.2
4	D	43	SER	5.2
27	X	1086	C	5.2
27	X	1070	G	5.0
27	X	1115	C	4.9
20	U	27	ASP	4.9
4	D	134	GLU	4.8
8	I	75	VAL	4.8
11	L	52	ALA	4.7
20	U	26	ALA	4.7
18	S	14	LEU	4.6
3	C	19	LEU	4.4
27	X	1069	G	4.4
9	J	84	MET	4.4
4	D	23	SER	4.4
24	1	35	LEU	4.3
8	I	74	VAL	4.3
25	2	1	MET	4.2
27	X	1188	A	4.1

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Mol	Chain	Res	Type	RSRZ
17	R	83	LEU	4.1
18	S	83	PHE	4.1
27	X	1954	A	4.1
27	X	1055	A	4.1
3	C	47	THR	4.0
27	X	728	G	4.0
18	S	68	ALA	4.0
11	L	53	ALA	4.0
24	1	27	ASN	3.8
14	O	47	PHE	3.8
1	A	236	GLY	3.8
4	D	75	SER	3.8
6	G	97	ASP	3.8
27	X	1068	A	3.8
18	S	21	ALA	3.7
4	D	22	TYR	3.6
14	O	23	GLU	3.6
27	X	727	U	3.6
11	L	40	ALA	3.6
18	S	171	VAL	3.6
27	X	200	A	3.6
6	G	129	HIS	3.5
27	X	730	C	3.5
27	X	1912	G	3.5
4	D	42	SER	3.5
26	3	38	GLY	3.5
27	X	424	G	3.4
27	X	1090	C	3.4
27	X	2444	C	3.4
27	X	1098	G	3.4
27	X	1114	A	3.3
18	S	32	PHE	3.3
27	X	75	C	3.3
18	S	91	PRO	3.2
17	R	102	LYS	3.2
19	T	15	ASP	3.2
27	X	1085	G	3.2
4	D	25	VAL	3.2
27	X	2082	C	3.2
19	T	73	GLY	3.2
18	S	30	VAL	3.2
19	T	16	SER	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
27	X	2171	U	3.1
5	E	175	LYS	3.1
11	L	33	ARG	3.1
18	S	124	ALA	3.1
18	S	92	VAL	3.1
28	Y	68	A	3.1
9	J	79	PRO	3.1
27	X	2090	U	3.0
18	S	86	VAL	3.0
27	X	1059	A	3.0
3	C	91	TYR	3.0
27	X	1951	G	3.0
18	S	114	ASP	3.0
5	E	174	GLY	3.0
4	D	132	ILE	3.0
27	X	1091	C	3.0
18	S	82	ASP	2.9
8	I	54	SER	2.9
27	X	426	C	2.9
4	D	152	MET	2.9
27	X	1104	G	2.9
24	1	40	TYR	2.9
27	X	425	A	2.9
2	B	136	ARG	2.9
27	X	1190	C	2.9
6	G	159	SER	2.8
19	T	14	ARG	2.8
11	L	39	TYR	2.8
13	N	91	ASN	2.8
27	X	2287	G	2.8
1	A	237	GLU	2.8
20	U	29	GLY	2.8
2	B	205	SER	2.8
27	X	2089	C	2.8
27	X	1524	C	2.8
27	X	2731	G	2.7
27	X	420	C	2.7
27	X	1950	C	2.7
27	X	248	A	2.7
14	O	11	GLN	2.7
18	S	54	ILE	2.7
3	C	81	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
27	X	1067	G	2.7
27	X	1432	G	2.7
24	1	14	SER	2.6
6	G	168	THR	2.6
3	C	166	TRP	2.6
27	X	1087	C	2.6
27	X	1186	G	2.6
27	X	2083	G	2.6
27	X	435	A	2.6
27	X	74	G	2.6
28	Y	6	C	2.5
26	3	55	TRP	2.5
8	I	76	LYS	2.5
27	X	1187	A	2.5
3	C	45	THR	2.5
9	J	77	LYS	2.5
28	Y	2	C	2.5
27	X	434	C	2.5
27	X	2381	A	2.5
21	V	48	ARG	2.5
2	B	203	LYS	2.5
27	X	2173	G	2.5
6	G	44	VAL	2.5
13	N	92	ARG	2.5
26	3	37	SER	2.4
24	1	4	ASP	2.4
27	X	361	G	2.4
27	X	2289	A	2.4
9	J	78	LYS	2.4
2	B	34	VAL	2.4
7	H	19	ILE	2.4
11	L	54	ALA	2.4
18	S	69	VAL	2.4
6	G	156	HIS	2.4
27	X	1888	C	2.4
27	X	2290	A	2.4
27	X	1846	A	2.4
4	D	154	ILE	2.4
5	E	64	LEU	2.4
21	V	52	GLN	2.4
3	C	20	PRO	2.3
27	X	1191	G	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	80	GLY	2.3
4	D	36	VAL	2.3
26	3	63	PRO	2.3
27	X	729	A	2.3
3	C	193	LEU	2.3
22	W	50	LEU	2.3
27	X	1515	U	2.3
1	A	69	ARG	2.3
4	D	76	ASN	2.3
27	X	1089	C	2.3
18	S	31	SER	2.3
19	T	17	ASN	2.3
17	R	55	THR	2.3
8	I	108	LEU	2.3
27	X	2037	A	2.3
27	X	2170	C	2.3
1	A	220	HIS	2.3
11	L	38	ILE	2.2
24	1	23	THR	2.2
27	X	1097	A	2.2
27	X	1593	C	2.2
18	S	81	VAL	2.2
1	A	249	PRO	2.2
3	C	83	ALA	2.2
27	X	199	A	2.2
7	H	8	LEU	2.2
4	D	138	PHE	2.2
14	O	46	VAL	2.2
3	C	189	ASP	2.2
4	D	29	PRO	2.2
27	X	1847	G	2.2
18	S	65	LEU	2.2
24	1	2	ALA	2.2
18	S	143	ILE	2.2
27	X	2270	U	2.2
27	X	225	G	2.2
5	E	173	ALA	2.2
22	W	6	VAL	2.2
3	C	66	ASN	2.2
27	X	2340	C	2.2
6	G	105	GLY	2.1
27	X	2359	U	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	135	HIS	2.1
27	X	1062	G	2.1
11	L	96	TYR	2.1
27	X	2390	A	2.1
11	L	51	LEU	2.1
27	X	1887	G	2.1
27	X	1390	G	2.1
18	S	29	ASN	2.1
26	3	39	ASP	2.1
17	R	82	ALA	2.1
27	X	1074	G	2.1
20	U	61	TRP	2.1
11	L	97	HIS	2.1
27	X	1801	C	2.1
27	X	1057	A	2.1
27	X	1919	A	2.1
19	T	59	LEU	2.1
27	X	2088	U	2.1
3	C	73	SER	2.1
27	X	1483	G	2.1
27	X	1056	U	2.1
18	S	125	PRO	2.1
6	G	66	HIS	2.0
19	T	71	ASN	2.0
1	A	55	GLY	2.0
1	A	241	GLY	2.0
6	G	103	TYR	2.0
27	X	1588	A	2.0
27	X	1884	A	2.0
5	E	123	PHE	2.0
16	Q	15	LYS	2.0
22	W	7	ARG	2.0
22	W	23	LEU	2.0
5	E	37	TYR	2.0
6	G	158	HIS	2.0
27	X	1872	A	2.0

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

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



## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
29	MG	X	2957	1/1	0.94	0.82	88.73	52,52,52,52	0
29	MG	X	2903	1/1	0.95	0.67	34.47	30,30,30,30	0
29	MG	X	2961	1/1	0.93	1.06	30.91	56,56,56,56	0
29	MG	X	2916	1/1	0.93	0.88	29.58	41,41,41,41	0
29	MG	X	2965	1/1	0.91	0.91	24.90	43,43,43,43	0
29	MG	X	2926	1/1	0.93	0.91	20.54	44,44,44,44	0
29	MG	X	2914	1/1	0.99	0.57	18.26	27,27,27,27	0
29	MG	X	2909	1/1	0.97	0.46	16.41	28,28,28,28	0
29	MG	X	2942	1/1	0.97	0.67	15.69	46,46,46,46	0
29	MG	K	202	1/1	0.76	0.82	10.86	27,27,27,27	0
29	MG	X	2910	1/1	0.96	0.62	10.67	56,56,56,56	0
29	MG	X	2922	1/1	0.97	0.35	10.03	29,29,29,29	0
29	MG	X	2944	1/1	0.97	0.40	8.85	35,35,35,35	0
29	MG	X	2939	1/1	0.93	0.62	8.75	50,50,50,50	0
29	MG	X	2959	1/1	0.97	0.66	8.48	41,41,41,41	0
29	MG	X	2954	1/1	0.97	0.45	8.37	45,45,45,45	0
29	MG	X	2913	1/1	0.96	0.47	6.57	43,43,43,43	0
29	MG	X	2923	1/1	0.94	0.39	6.22	40,40,40,40	0
29	MG	X	2947	1/1	0.96	0.26	2.58	34,34,34,34	0
29	MG	X	2948	1/1	0.96	0.29	2.26	34,34,34,34	0
29	MG	K	201	1/1	0.86	0.46	2.24	27,27,27,27	0
30	ERY	X	2902	51/51	0.94	0.24	0.92	31,34,36,36	0
29	MG	A	301	1/1	0.93	0.39	0.54	54,54,54,54	0
29	MG	X	2915	1/1	0.83	0.18	-0.69	63,63,63,63	0
29	MG	X	2929	1/1	0.98	0.13	-1.42	30,30,30,30	0
29	MG	X	2931	1/1	0.87	0.56	-	46,46,46,46	0
29	MG	X	2937	1/1	0.95	0.70	-	44,44,44,44	0
29	MG	X	2952	1/1	0.91	0.43	-	29,29,29,29	0
29	MG	X	2956	1/1	0.93	0.52	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MG	X	2921	1/1	0.95	0.33	-	28,28,28,28	0
29	MG	B	301	1/1	0.80	0.77	-	34,34,34,34	0
29	MG	X	2960	1/1	0.92	0.32	-	61,61,61,61	0
29	MG	X	2949	1/1	0.98	0.44	-	42,42,42,42	0
29	MG	X	2924	1/1	0.99	0.23	-	38,38,38,38	0
29	MG	X	2936	1/1	0.96	0.65	-	45,45,45,45	0
29	MG	X	2911	1/1	0.91	0.53	-	56,56,56,56	0
29	MG	X	2938	1/1	0.98	0.79	-	31,31,31,31	0
29	MG	X	2927	1/1	0.95	0.35	-	29,29,29,29	0
29	MG	X	2904	1/1	0.95	0.55	-	32,32,32,32	0
29	MG	X	2920	1/1	0.96	0.45	-	52,52,52,52	0
29	MG	X	2932	1/1	0.98	0.40	-	37,37,37,37	0
29	MG	X	2901	1/1	0.94	0.39	-	69,69,69,69	0
29	MG	X	2946	1/1	0.91	0.19	-	46,46,46,46	0
29	MG	X	2943	1/1	0.93	0.97	-	42,42,42,42	0
29	MG	X	2906	1/1	0.85	0.85	-	28,28,28,28	0
29	MG	X	2962	1/1	0.94	0.13	-	69,69,69,69	0
29	MG	X	2945	1/1	0.97	0.14	-	38,38,38,38	0
29	MG	X	2958	1/1	0.82	0.49	-	44,44,44,44	0
29	MG	X	2917	1/1	0.91	0.86	-	40,40,40,40	0
29	MG	X	2930	1/1	0.80	1.01	-	29,29,29,29	0
29	MG	X	2919	1/1	0.82	0.10	-	62,62,62,62	0
29	MG	X	2925	1/1	0.91	1.08	-	31,31,31,31	0
29	MG	X	2953	1/1	0.99	0.38	-	56,56,56,56	0
29	MG	M	201	1/1	0.97	0.36	-	35,35,35,35	0
29	MG	X	2912	1/1	0.96	0.14	-	27,27,27,27	0
29	MG	X	2940	1/1	0.98	0.37	-	36,36,36,36	0
29	MG	X	2934	1/1	0.95	0.26	-	29,29,29,29	0
29	MG	X	2907	1/1	0.90	0.78	-	28,28,28,28	0
29	MG	M	202	1/1	0.97	0.36	-	35,35,35,35	0
29	MG	X	2955	1/1	0.97	0.47	-	30,30,30,30	0
29	MG	X	2935	1/1	0.97	0.49	-	34,34,34,34	0
29	MG	X	2950	1/1	0.95	0.40	-	32,32,32,32	0
29	MG	X	2905	1/1	0.95	0.50	-	31,31,31,31	0
29	MG	X	2941	1/1	0.97	0.46	-	38,38,38,38	0
29	MG	X	2908	1/1	0.94	0.60	-	32,32,32,32	0
29	MG	X	2918	1/1	0.98	0.82	-	43,43,43,43	0
29	MG	X	2951	1/1	0.92	0.75	-	32,32,32,32	0
29	MG	X	2964	1/1	0.93	0.88	-	28,28,28,28	0
29	MG	X	2933	1/1	0.86	0.65	-	36,36,36,36	0
29	MG	X	2963	1/1	0.90	0.31	-	56,56,56,56	0
29	MG	X	2928	1/1	0.98	0.39	-	55,55,55,55	0

## 6.5 Other polymers

There are no such residues in this entry.