



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:19 am BST

PDB ID : 5DM6  
Title : Crystal structure of the 50S ribosomal subunit from *Deinococcus radiodurans*  
Authors : Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.  
Deposited on : 2015-09-08  
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

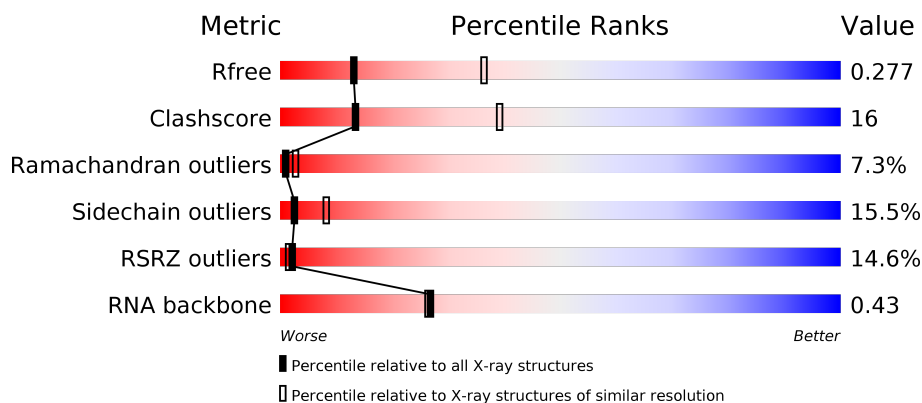
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	224	<div> <div>89%</div> <div> <div>54%</div> <div>38%</div> <div>8%</div> </div> </div>
2	A	274	<div> <div>11%</div> <div>58%</div> <div>37%</div> <div>5%</div> </div>
3	B	205	<div> <div>3%</div> <div>53%</div> <div>40%</div> <div>7%</div> </div>
4	C	197	<div> <div>8%</div> <div>44%</div> <div>46%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	171	
7	F	144	
8	G	142	
9	H	134	
10	I	141	
11	J	136	
12	K	113	
13	L	104	
14	M	109	
15	N	117	
16	O	94	
17	P	127	
18	Q	93	
19	R	110	
20	S	175	
21	T	84	
22	U	72	
23	V	66	
24	W	55	
25	Z	57	
26	1	54	
27	2	47	
28	3	65	
29	X	2881	

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Mol	Chain	Length	Quality of chain
30	Y	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6014	-	-	-	X
31	MG	X	6038	-	-	-	X
31	MG	X	6046	-	-	-	X
31	MG	X	6048	-	-	-	X
31	MG	X	6058	-	-	-	X
31	MG	X	6093	-	-	-	X
31	MG	X	6098	-	-	-	X
31	MG	X	6099	-	-	-	X
31	MG	X	6107	-	-	-	X
31	MG	X	6108	-	-	-	X
31	MG	X	6111	-	-	-	X
31	MG	X	6113	-	-	-	X
31	MG	X	6119	-	-	-	X
31	MG	X	6121	-	-	-	X
31	MG	X	6133	-	-	-	X
31	MG	X	6138	-	-	-	X
31	MG	X	6141	-	-	-	X
31	MG	X	6146	-	-	-	X
31	MG	X	6156	-	-	-	X
31	MG	X	6159	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6167	-	-	-	X
31	MG	X	6170	-	-	-	X
31	MG	X	6175	-	-	-	X
31	MG	X	6177	-	-	-	X
31	MG	X	6179	-	-	-	X
31	MG	X	6180	-	-	-	X
31	MG	X	6183	-	-	-	X
31	MG	X	6186	-	-	-	X
31	MG	X	6187	-	-	-	X
31	MG	X	6191	-	-	-	X
31	MG	X	6192	-	-	-	X

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 89337 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 L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	expression tag	UNP Q9RSS7
F	2	ARG	-	expression tag	UNP Q9RSS7
F	3	ARG	-	expression tag	UNP Q9RSS7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1115	704	209	199	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	141	Total	C	N	O		0	0	0
			1068	655	216	197				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1091	696	202	186	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			879	541	178	158	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	107	GLY	-	expression tag	UNP Q9RWB4
M	108	LYS	-	expression tag	UNP Q9RWB4
M	109	ALA	-	expression tag	UNP Q9RWB4
M	110	ALA	-	expression tag	UNP Q9RWB4

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			742	465	139	138			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			826	513	160	152	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1346	849	236	255	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			453	278	93	77	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1510	U	UNK	conflict	GB 11612676

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

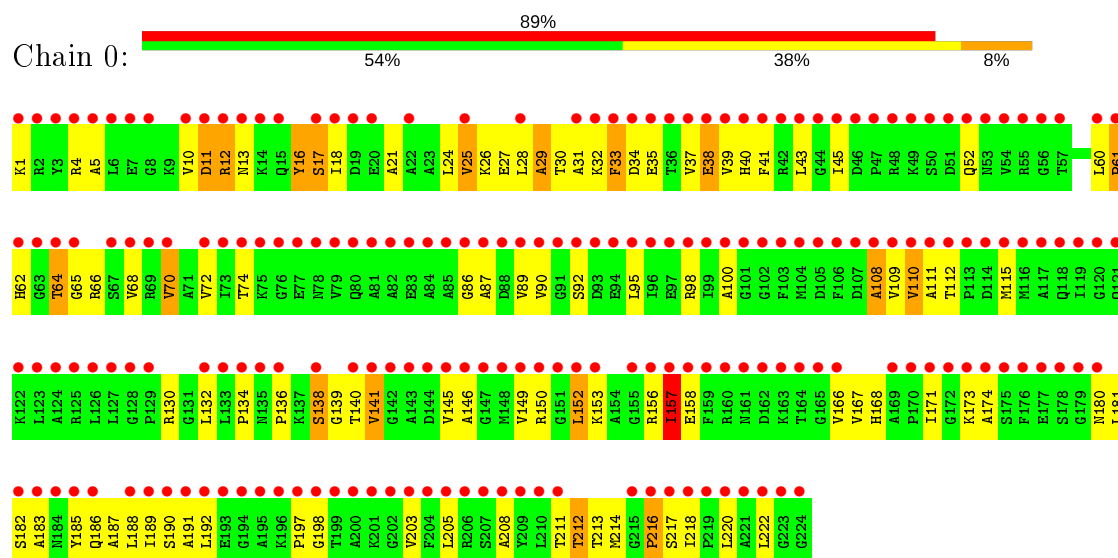
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	192	Total	Mg	0	0
			192	192		
31	Y	5	Total	Mg	0	0
			5	5		
31	M	1	Total	Mg	0	0
			1	1		

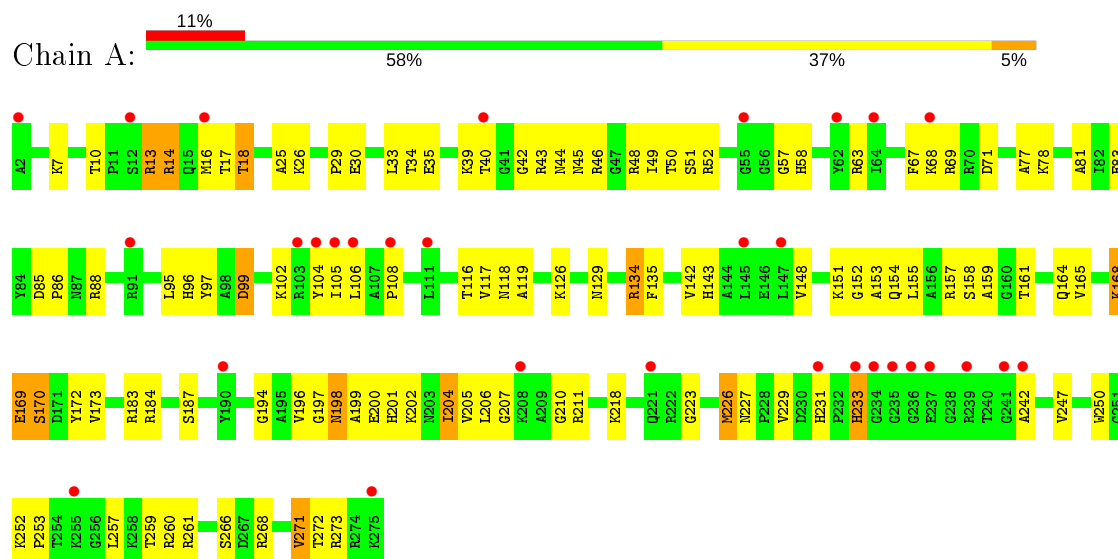
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: 50S ribosomal protein L1

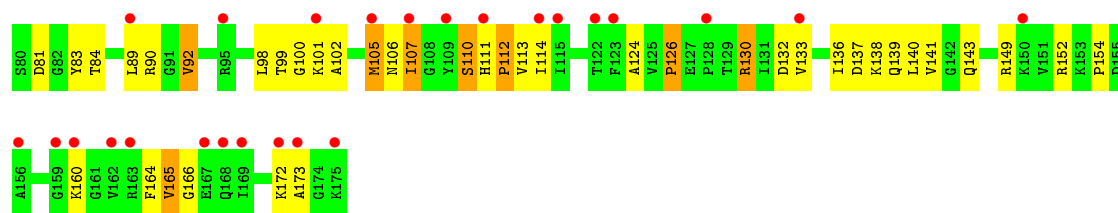


#### • Molecule 2: 50S ribosomal protein L2



#### • Molecule 3: 50S ribosomal protein L3

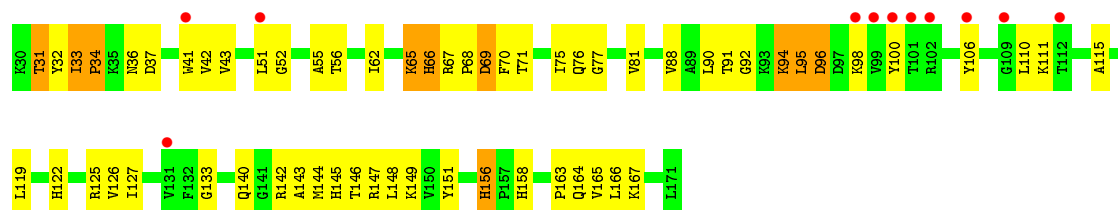




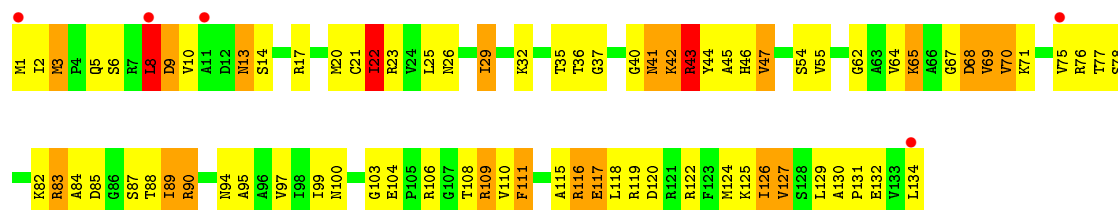
• Molecule 7: 50S ribosomal protein L11



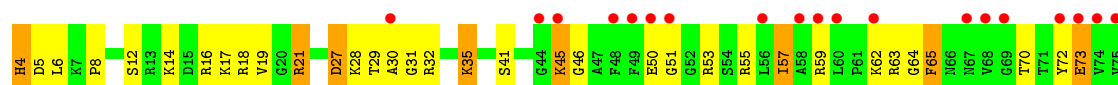
• Molecule 8: 50S ribosomal protein L13

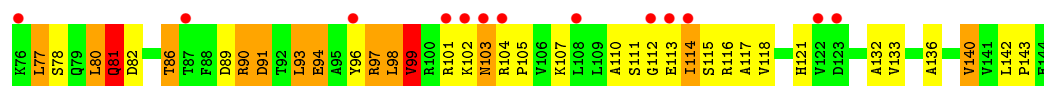


• Molecule 9: 50S ribosomal protein L14

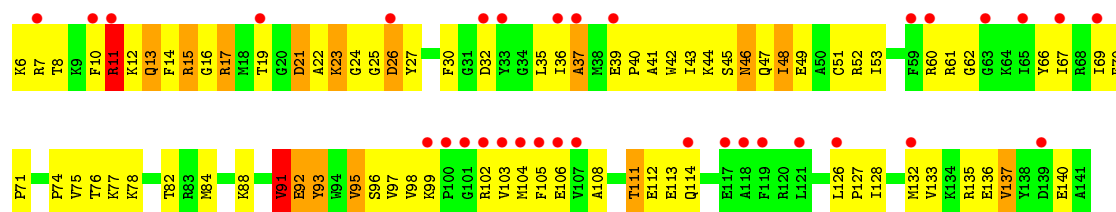


• Molecule 10: 50S ribosomal protein L15

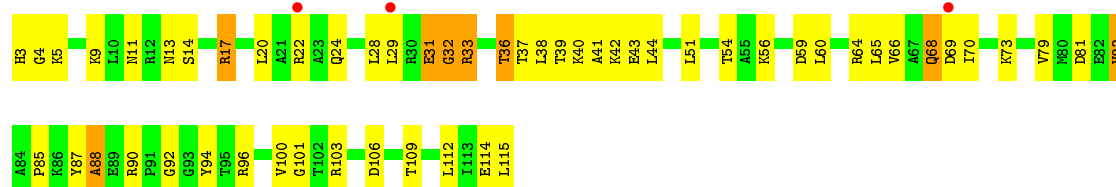




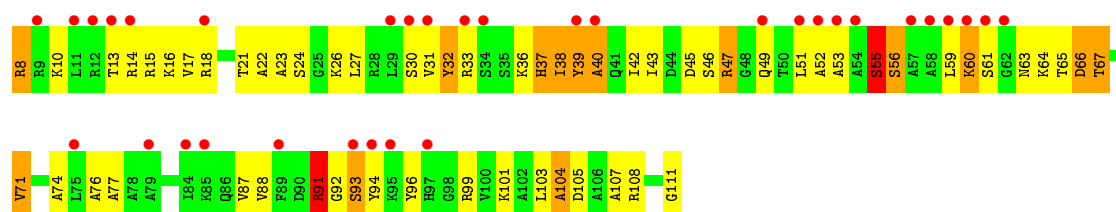
- Molecule 11: 50S ribosomal protein L16



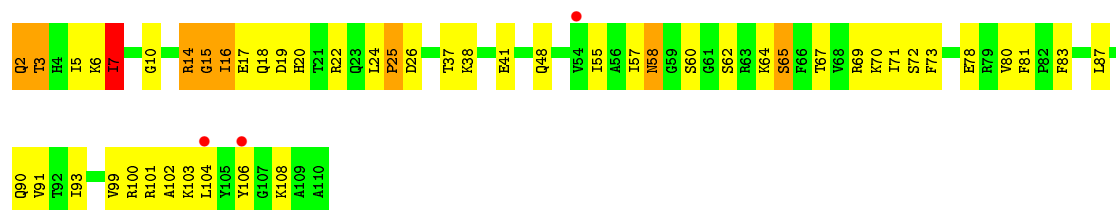
- Molecule 12: 50S ribosomal protein L17



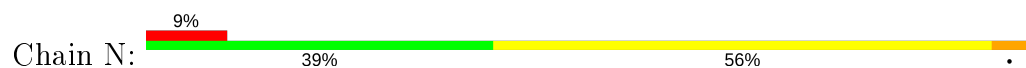
- Molecule 13: 50S ribosomal protein L18

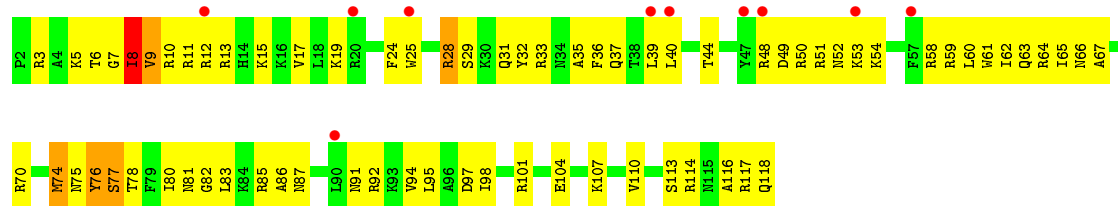


- Molecule 14: 50S ribosomal protein L19

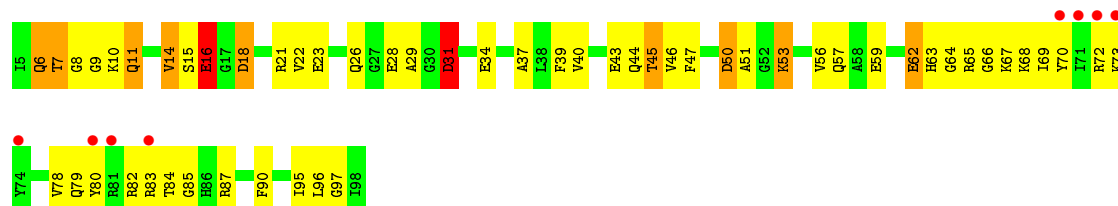


- Molecule 15: 50S ribosomal protein L20

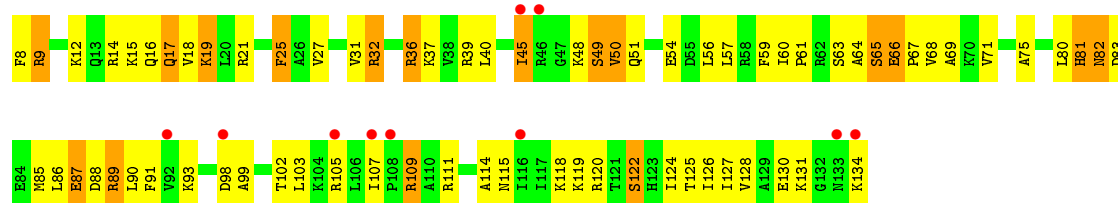
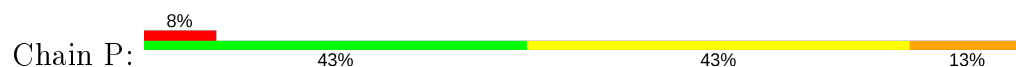




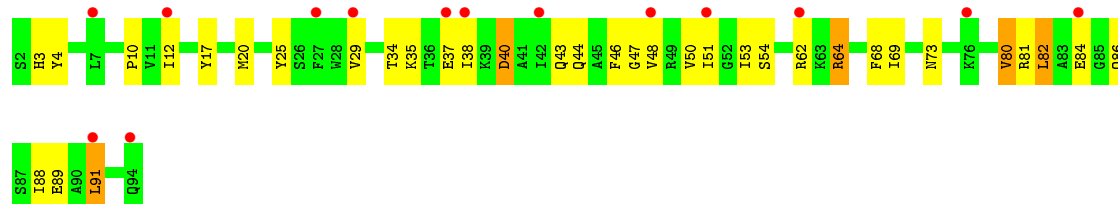
• Molecule 16: 50S ribosomal protein L21



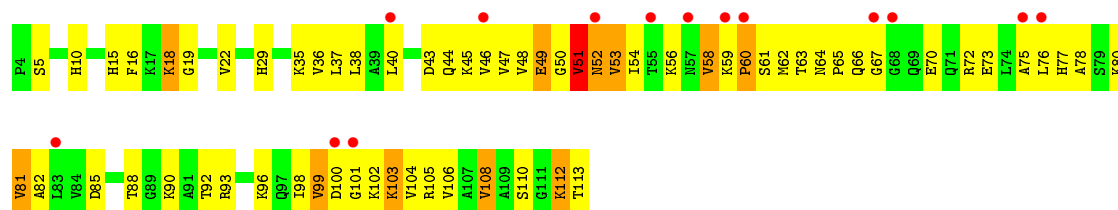
• Molecule 17: 50S ribosomal protein L22



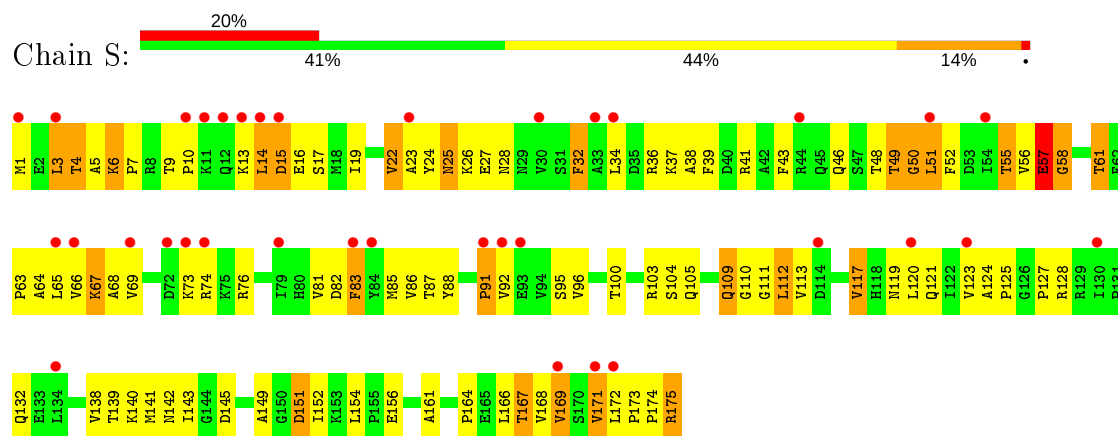
• Molecule 18: 50S ribosomal protein L23



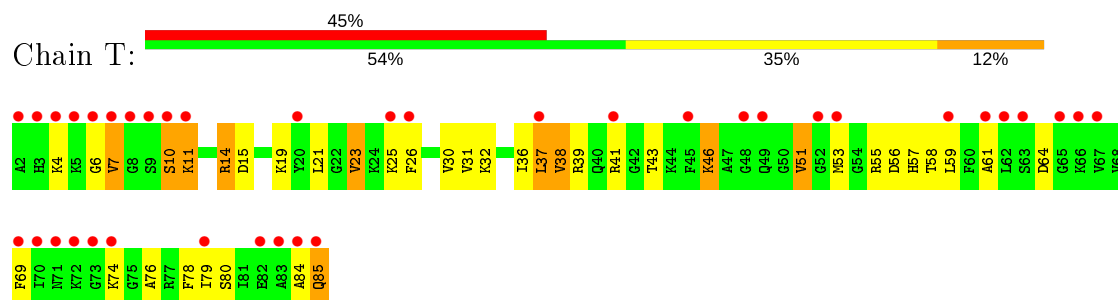
• Molecule 19: 50S ribosomal protein L24



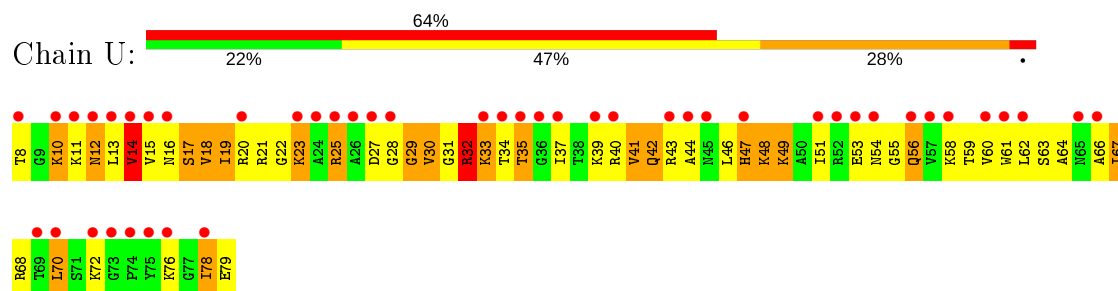
- Molecule 20: 50S ribosomal protein L25



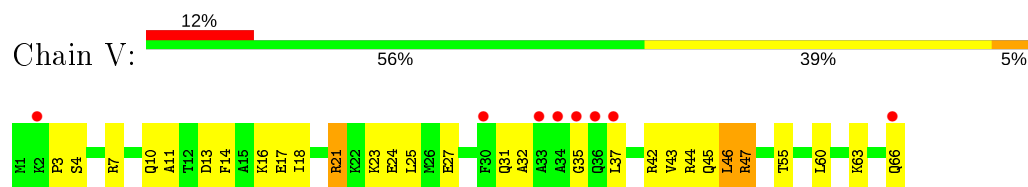
- Molecule 21: 50S ribosomal protein L27



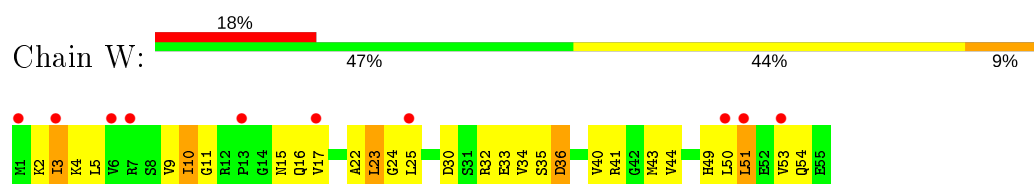
- Molecule 22: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L29

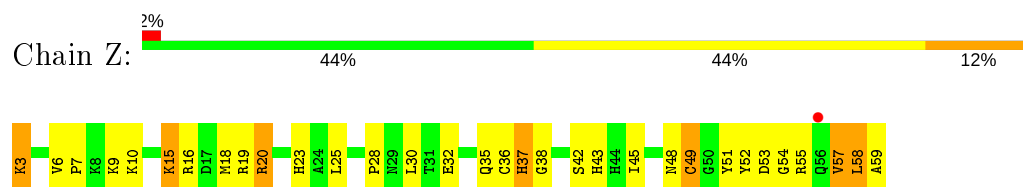


- Molecule 24: 50S ribosomal protein L30

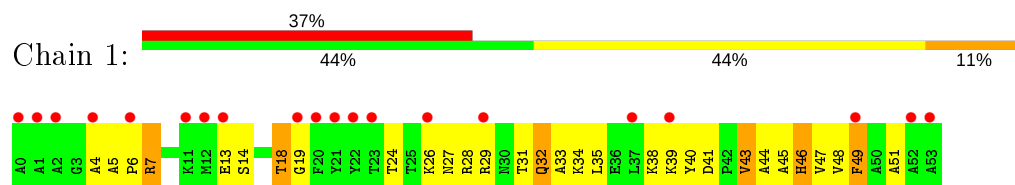




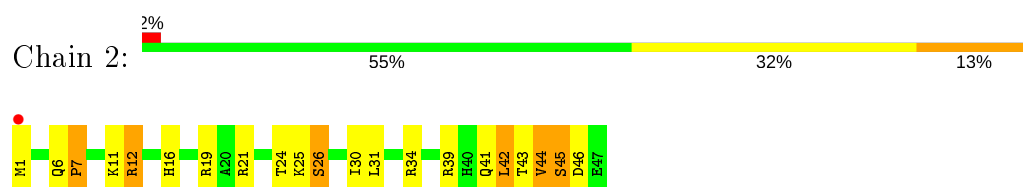
- Molecule 25: 50S ribosomal protein L32



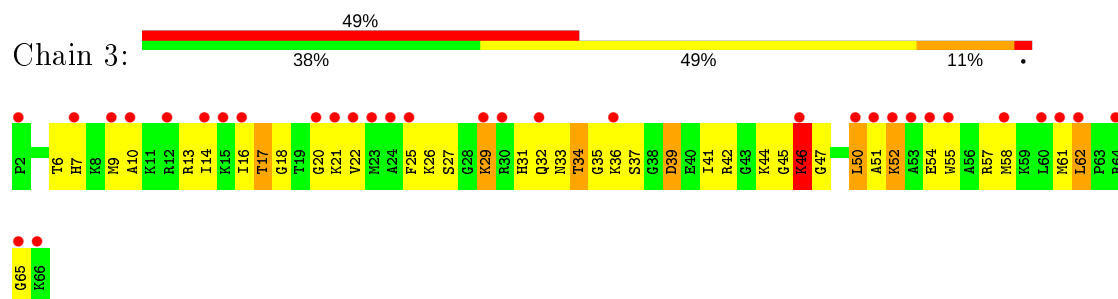
- Molecule 26: 50S ribosomal protein L33



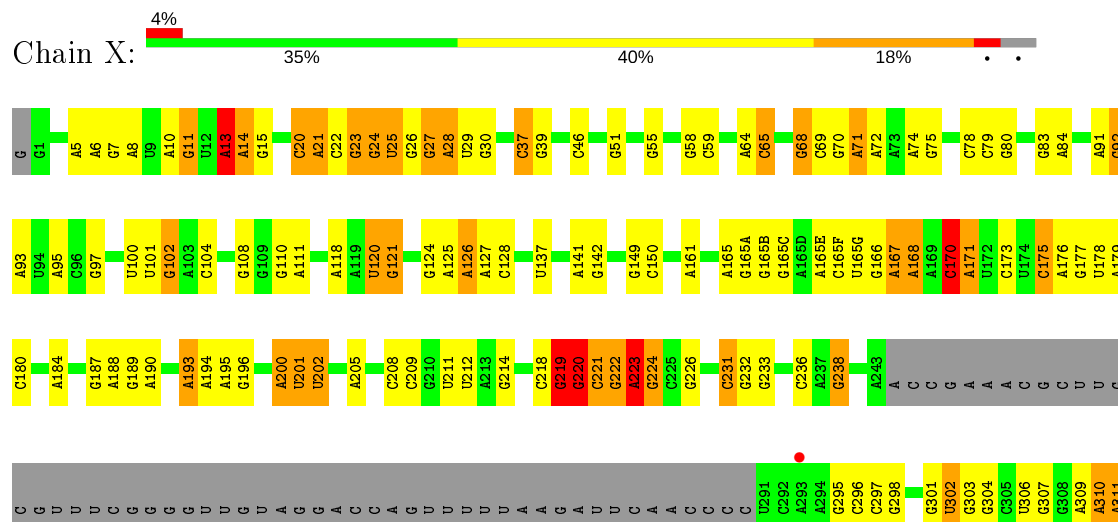
- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



- Molecule 29: 23S ribosomal RNA



G1296	C1297	G1235	A1168	G1102	G1030	A955	U	C817	C742	C662	A532	A466	U	G312
G1297	C1298	G1236	A1169	A1103	U1033	G956	A	G818	C743	G663	G533	G467	A374	C313
G1298	G1237	A1238	C1104	C1104	G1034	G957	C	A819	U744	G664	A536	G468	G382	U314
G1299	G1238	G1239	G1172B	G1107	G1035	U958	C	A820	G745			G469		A315
U1300	A1301	G1240	A1173	G1108	U1036	A959	A	A821	C746	G669	U537	A470	G386	C316
G1241	G1242	G1243	U1037	G1109	U1037	A960	G	U822	U747	A670	G538	A471	U387	A317
G1309	A1174	C1175	U1037	C1109	U1037	G961	C	G823	G748	C671	C539	A472	G387	C318
	G1175	C1176	U1038	G1110	U1038	U962	U	U824	A749	U672	C540	G473	G388	C319
	G1176		C1038	G964		G963	A	A825	A750	C673		G474	A389	U320
U1312	G1179	G1244	C1041	G969		G969	C	G828	C752		C544	U475	C392	C321
U1313	U1180	G1245	G1042	G970		G970	C	U827	A753	A676	U545	A479	G393	A391
C1314	A1181	A1246	C1043	C971		C971		G829	G754	C678	U547	A480	G394	G323
U1315	G1182	G1248	A1045	C972		C972	A899	A829		C679	U548	G481	A394	A324
U1249	G1187	G1249	A1046	C973		C973			U761	A680	G549	A482	U395	G327
G1318	U1188	G1250	G1047	C974		C974	C902	A833	A762	G681	C550	A483	G396	U328
G1319	A1189	C1251	A1048	C974		C974	C903	C834	U763	G682		C484	A397	G329
G1320	G1190	G1252	C1049	A906		A906		A835	G765	G683		C485	C398	A330
A1321	G1191	G1253	A1054	U907		U907			A774	G684		C486	U399	G331
A1322	G1192	A1254	G1055	G908		G908		U839	G775	A685		C487	A401	A332
G1323	G1193	G1255	G1056	C982		C982	A909	C840	G776	G686		C488	G400	G333
G1324	A1194	C1256	A1057	C983		C983	A910	G841	A777			G489	A402	U334
G1325	G1195	C1257	A1057	A984		A984	A911		G778			G490	U403	C335
U1326	A1196	G1260	U1060	G989		G989	C912	U844	G778	A690		C492	C404	C336
C1327	G1197	C1261	U1061	A990		A990	U913	G845	U779	G691		G493	C405	U337
G1328	U1198	A1262	G1062	C991		C991	C914	U846	G780	G692		G494	G406	G338
U1329	U1199	G1263	A1129	C992		C992	C915	U847	A782	A694		G495	C407	U339
C1330	G1199	G1264	G1056	C993		C993		U848	G783	G695		G496	G408	A340
C1331	A1201	G1265	A1057	C994		C994	A918	G849	A784	G696		G497	C409	
G1332	G1202	G1266	U1066	U994		U994	G920	C950	G785	G697		G498	G410	G344
C1333	U1203	U1267	G1068	C995		C995	G921	C951	G786	G700		G499	G411	A345
	U1268	A1269	A1069	A996		A996		A852	U787	G701		G500	A412	A346
	C1204	G1270	A1070	C997		C997	A925	U853	A788			A501	C413	C347
G1338	G1205	G1271	C1072	C998		C998	C926			A637		A502	G442	
A1341	G1206	A1272	A1073	G1003		G1003	C928	C856	G704	G570		A503	C438	G348
A1342	G1207	G1273	G1074	U1004		U1004	G929	C857	A705	A571		A504	A439	A349
G1343	A1211	A1274	C1075	C1005		C1005	U930	U858	A706	G573		A505	G440	G350
U1344	G1212	A1275	C1076	C1006		C1006	U931	G859		C574		A506	U441	
C1345	A1213	A1276	A1077	G1007		G1007	U932		U713	A575		A507	G442	G
G1346	A1214	A1277	C1078	U1008		U1008	A933	G862	U714	U576		A508	U443	U
	G1215	G1278	C1079	A1009		A1009	G934	A863	G715	C509		C510	C444	G
	C1216	A1279	U1080	U935		U935	U935	G864	A716	A578		U511	G445	A
A1353	G1217	A1280	C1080	C936		C936		C965	C717	G579		G512	A446	C
A1354	A1218	G1281	C1083	C937		C937		A866	A718	C580		G513	A447	U
G1355	G1221	A1282	G1087	G940		G940		C871	G601	G648		A514	U448	U
U1356	A1222	G1283	A1088	G942		G942		A872	A802	G649		A515	A449	G
G1358	A1223	A1284	G1089	G944		G944		A873	U803	G582		C516	G450	U
A1359	G1224	G1285	U1090	U943		U943		G874	G804	G651		C517	C451	A
G1360	A1225	A1286	G1091	G944		G944		G875	C806	G585		G518	G452	C
	G1226	U1287	C1092	G945		G945		C876	U807	A586		U519	C453	U
A1361	A1227	G1288	G1093	G946		G946		U877	C731	C587		G520	A454	G
A1365	G1228	A1289	U1094	G947		G947		A878	G809	U588		G521	U456	C
A1366	G1229	A1290	A1095	C948		C948		G	U810	A590		A522	G458	A
C1367	A1230	U1291	G1024	U949		U949		G	G811	G656		C523	U459	C
G1368	G1231	G1292	G1025	G950		G950		G	A734	A592			A460	C
G1369	U1293	U1294	U1026	C951		C951		G	G738	C592A		A526	C461	U
G1370	U1294	C1295	A1027	C951		C951		G	G739	U598		G530	C462	G
G1371	U1234		A1028	G954		G954		C	G741	G599		G531	G465	G

C1372	C1373	C1378	C1379	C1380	C1384	C1390	C1391	C1392	C1393	C1394	C1395	C1405	C1406	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1422	C1423	C1424	C1427	C1428	C1429	C1430	C1435	C1436	C1437	C1440	C1440A	C1444	C1445	C1450	C1451	C1452	C1453	C1454	C1455	C1458	C1459	C1460	C1461	C1464	C1465																																																																																																																																							
U1466	U1467	U1468	U1474	U1477	U1478	U1479	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1525	U1526	U1529	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1546	U1547																																																																																																																																	
G1557	G1558	G1559	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1578	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590	G1591	G1592	G1593	G1594	G1597	G1598	G1599	G1602	G1606	G1607	G1608	G1609	G1610	G1611	G1612	G1613	G1614	G1615	G1616	G1619	G1620	G1621	G1622	G1625A	G1626	G1627	G1628	G1629	G1630	G1634	G1635	G1636	G1637																																																																																																																																		
C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1684	C1685	C1686	C1687	C1688	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1726	C1728	C1729																																																																																																																												
C1730	C1731	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	G1745	C1746	G1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	G1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1794	C1795	C1796	C1797	C1798	C1799																																																																																																																							
C1800	C1801	C1805	C1808	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1838	C1839	C1840	C1841	C1842	C1843	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1858	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880																																																																																																																							
G1881	G1882	G1883	G1884	G1885	G1886	G1887	C1892	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1926	C1927	C1928	C1929	C1930	C1931	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1949	C1950	C1951	C1952	C1953	C1954	C1955	C1956																																																																																																																															
C1957	C1958	U1963	U1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1977	C1978	C1979	C1980	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026																																																																																																																												
G2027	U2028	C2029	C2030	C2031	C2032	G2035	C2036	C2037	C2038	A2042	C2043	C2044	C2045	C2046	U2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	U2075	U2076	C2077	C2080	C2081	C2090	C2091	C2092	C2093	C2094	C2098	C2099	C2100																																																																																																																																
G2101	G2102	U2103	U2104	U2107	C2108	U2109	C2110	C2111	C2112	U2113	U2114	C2115	C2116	C2117	U2118	C2119	G2120	G2121	U2122	C2123	C2124	C2125	C2126	C2127	C2128	C2129	U2130	G2131	C2132	C2133	C2134	C2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	C2144	C2145	C2146	C2147	C2148	C2149	C2150	C2151	C2152	C2153	C2154	C2157	C2158	C2164	C2167																																																																																																																														
G2168	A2169	A2170	A2171	A2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	C2181	A2182	C2183	A2186	C2187	U2188	U2189	C2190	C2191	U2194	U2195	C2196	U2197	C2198	A2198	G2203	C2204	A2205	C2206	A2210	A2211	A2212	U2213	U2217	U2218	U2219	C2220	C2221	C2222	C2223	C2224	A2225	U2229	C2230	U2233	C2234	U2235	U2236	C2237	C2238	C2239	C2242	C2243	C2244	C2245	C2246	C2247																																																																																																																										
C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2287	C2288	C2289	C2290	C2291	C2292	C2293	C2294	C2295	C2296	C2299	C2300	C2302	C2303	C2304	C2305	C2306	C2307	C2308	C2309	C2310	C2311	C2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	C2320	C2321	C2322	C2323	C2324	C2325	C2326	C2327	C2328	C2329	C2330	C2331	C2332	C2333	C2334	C2335	C2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	C2344	C2345	C2346	C2347	C2348	C2349	C2350	C2351	C2352	C2355	C2356	C2357	C2358	C2359	C2360	C2361	C2362	C2363	C2364	C2365	C2366	C2367	C2368	C2369	C2370	C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2386	C2387	C2388	C2389	C2390	C2391	C2392	C2393	C2394	C2395	C2396	C2400	C2401	C2402	C2403	C2404	C2405	C2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	U2423	U2424	C2425	C2426	C2427	C2428	C2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.90Å 410.76Å 696.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.96 – 2.90 58.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.96-2.90) 81.6 (58.96-2.90)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.61 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.235 , 0.270 0.243 , 0.277	Depositor DCC
$R_{free}$ test set	24732 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 65.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	89337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0	0.30	0/1674	0.49	0/2257
2	A	0.39	0/2149	0.59	0/2890
3	B	0.69	1/1568 (0.1%)	0.86	1/2105 (0.0%)
4	C	0.51	0/1530	0.73	1/2070 (0.0%)
5	D	0.36	0/1420	0.56	0/1903
6	E	0.39	0/1309	0.55	0/1771
7	F	0.33	0/1067	0.52	1/1446 (0.1%)
8	G	0.47	0/1139	0.67	0/1539
9	H	0.76	0/1007	0.91	2/1352 (0.1%)
10	I	0.52	0/1082	0.76	1/1448 (0.1%)
11	J	0.65	0/1114	0.78	0/1486
12	K	0.83	0/887	1.04	0/1188
13	L	0.52	0/784	0.73	0/1045
14	M	0.77	0/880	0.83	0/1179
15	N	0.64	0/994	0.80	1/1323 (0.1%)
16	O	0.53	0/751	0.73	0/1000
17	P	0.69	0/1027	0.83	0/1373
18	Q	0.45	0/738	0.59	0/988
19	R	0.54	0/836	0.72	0/1121
20	S	0.41	0/1371	0.67	0/1862
21	T	0.54	0/634	0.69	0/838
22	U	0.61	0/557	0.88	1/741 (0.1%)
23	V	0.41	0/538	0.57	0/714
24	W	0.51	0/426	0.68	0/568
25	Z	0.71	0/465	0.90	0/622
26	1	0.49	0/411	0.73	0/554
27	2	0.48	0/397	0.65	0/521
28	3	0.54	0/516	0.70	0/673
29	X	0.78	37/66826 (0.1%)	1.44	971/104247 (0.9%)
30	Y	0.64	0/2907	1.20	8/4529 (0.2%)
All	All	0.72	38/97004 (0.0%)	1.29	987/145353 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	3
4	C	0	1
8	G	0	1
25	Z	0	2
All	All	0	7

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	761	A	C6-N1	8.06	1.41	1.35
29	X	1999	C	N3-C4	-7.01	1.29	1.33
29	X	1638	C	N1-C6	-6.80	1.33	1.37
29	X	1661	G	C6-N1	-6.69	1.34	1.39
29	X	1661	G	C5-C4	-6.50	1.33	1.38
29	X	2879	G	N9-C8	6.44	1.42	1.37
29	X	492	A	N3-C4	-6.41	1.31	1.34
29	X	761	A	C5-C4	6.30	1.43	1.38
29	X	2879	G	C5-C4	6.25	1.42	1.38
29	X	2509	G	C6-N1	-6.18	1.35	1.39
29	X	1660	C	N3-C4	-6.06	1.29	1.33
29	X	761	A	N3-C4	6.03	1.38	1.34
29	X	2012	G	N9-C8	-6.03	1.33	1.37
29	X	2510	C	N3-C4	-6.02	1.29	1.33
29	X	1665	A	N9-C4	5.84	1.41	1.37
29	X	761	A	N9-C8	5.77	1.42	1.37
29	X	2001	A	N9-C4	-5.77	1.34	1.37
29	X	2510	C	N1-C6	-5.74	1.33	1.37
29	X	1753	A	N3-C4	-5.73	1.31	1.34
29	X	2430	A	N9-C4	5.61	1.41	1.37
29	X	1652	A	N7-C5	-5.60	1.35	1.39
29	X	2848	G	N9-C8	-5.60	1.33	1.37
29	X	1997	A	C6-N1	5.56	1.39	1.35
29	X	2574	G	C2-N3	-5.56	1.28	1.32
29	X	2580	U	C4-C5	-5.51	1.38	1.43
29	X	2510	C	C4-C5	-5.37	1.38	1.43
29	X	1637	A	N7-C5	-5.30	1.36	1.39
29	X	2008	C	C2-O2	-5.27	1.19	1.24
29	X	1992	G	N3-C4	-5.27	1.31	1.35
29	X	1998	A	N9-C4	-5.25	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	127	ALA	CA-CB	-5.23	1.41	1.52
29	X	2009	G	C5-C4	-5.21	1.34	1.38
29	X	2015	A	N3-C4	-5.19	1.31	1.34
29	X	2879	G	C8-N7	5.18	1.34	1.30
29	X	1262	A	C5-C6	-5.16	1.36	1.41
29	X	2632	A	N3-C4	-5.05	1.31	1.34
29	X	2551	C	N1-C6	-5.04	1.34	1.37
29	X	1614	A	N9-C4	-5.01	1.34	1.37

All (987) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	761	A	N1-C6-N6	22.08	131.85	118.60
29	X	761	A	C5-N7-C8	-17.56	95.12	103.90
29	X	2713	U	O5'-P-OP2	-17.29	89.95	110.70
29	X	761	A	C4-C5-N7	16.33	118.87	110.70
29	X	761	A	C5-C6-N6	-14.62	112.00	123.70
29	X	2879	G	C5-N7-C8	-14.56	97.02	104.30
29	X	2840	C	C6-N1-C2	14.18	125.97	120.30
29	X	2879	G	N7-C8-N9	13.73	119.97	113.10
29	X	761	A	N7-C8-N9	13.73	120.66	113.80
29	X	2879	G	C4-C5-N7	12.72	115.89	110.80
29	X	761	A	C6-C5-N7	-12.49	123.56	132.30
29	X	2616	C	O5'-P-OP1	-12.20	94.72	105.70
29	X	1779	U	C5-C6-N1	-12.03	116.69	122.70
29	X	2689	U	O5'-P-OP1	-11.60	95.26	105.70
29	X	1262	A	N1-C6-N6	11.30	125.38	118.60
29	X	568	U	O5'-P-OP2	-11.10	95.71	105.70
29	X	1660	C	O5'-P-OP2	-10.96	95.83	105.70
29	X	1999	C	C2-N3-C4	-10.94	114.43	119.90
29	X	1665	A	C8-N9-C4	-10.93	101.43	105.80
29	X	2713	U	O5'-P-OP1	10.82	123.69	110.70
29	X	2879	G	C8-N9-C4	-10.73	102.11	106.40
29	X	1999	C	C5-C6-N1	-10.56	115.72	121.00
29	X	2883	A	O5'-P-OP2	-10.45	96.30	105.70
29	X	1490	C	C6-N1-C2	-10.31	116.18	120.30
29	X	2712(A)	A	O5'-P-OP2	-10.29	96.44	105.70
29	X	1490	C	N3-C2-O2	-10.23	114.74	121.90
29	X	1286	A	O5'-P-OP2	-10.18	96.54	105.70
29	X	2060	A	O5'-P-OP2	-10.17	96.54	105.70
29	X	2874	C	O5'-P-OP2	-10.15	96.56	105.70
29	X	2879	G	C6-C5-N7	-10.14	124.32	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2840	C	C5-C6-N1	-10.13	115.93	121.00
29	X	2710	C	O5'-P-OP2	10.02	122.72	110.70
29	X	1273	U	O5'-P-OP1	-10.00	96.70	105.70
29	X	659	C	C6-N1-C2	9.99	124.30	120.30
29	X	573	G	O5'-P-OP1	-9.97	96.73	105.70
29	X	2824	C	O5'-P-OP2	-9.87	96.82	105.70
29	X	1490	C	N1-C2-O2	9.86	124.81	118.90
29	X	761	A	N9-C4-C5	-9.81	101.87	105.80
29	X	498	G	N1-C6-O6	9.81	125.79	119.90
29	X	2035	G	O5'-P-OP1	9.69	122.32	110.70
29	X	2707	C	O5'-P-OP2	-9.66	97.01	105.70
29	X	2261	C	C6-N1-C2	-9.64	116.44	120.30
29	X	1661	G	O5'-P-OP1	9.53	122.14	110.70
29	X	660	G	C8-N9-C4	9.53	110.21	106.40
29	X	2501	C	C2-N1-C1'	-9.50	108.35	118.80
29	X	2713	U	C5-C6-N1	-9.41	118.00	122.70
29	X	1668	A	C8-N9-C4	9.24	109.50	105.80
29	X	1264	G	N1-C6-O6	-9.23	114.36	119.90
29	X	2676	C	C5-C6-N1	-9.23	116.39	121.00
29	X	2892	G	N3-C4-C5	9.20	133.20	128.60
29	X	1754	A	N7-C8-N9	-9.17	109.21	113.80
29	X	2066	C	C6-N1-C2	-9.16	116.64	120.30
29	X	2571	C	C6-N1-C2	-9.12	116.65	120.30
29	X	1661	G	C5-C6-N1	9.11	116.06	111.50
29	X	2879	G	C5-C6-O6	-9.09	123.15	128.60
29	X	2508	G	N1-C6-O6	-9.08	114.45	119.90
29	X	2509	G	C5-C6-N1	9.07	116.03	111.50
29	X	2885	C	O5'-P-OP2	-9.05	97.56	105.70
29	X	2689	U	C5-C6-N1	-9.02	118.19	122.70
29	X	2519	U	O5'-P-OP1	-9.02	97.59	105.70
29	X	1264	G	O5'-P-OP2	-8.92	97.68	105.70
29	X	650	C	C2-N1-C1'	8.90	128.59	118.80
29	X	2692	C	C6-N1-C2	-8.85	116.76	120.30
29	X	1660	C	C2-N3-C4	-8.82	115.49	119.90
29	X	1659	U	OP1-P-OP2	8.80	132.79	119.60
29	X	1990	C	N1-C2-O2	8.78	124.17	118.90
29	X	2514	U	N3-C2-O2	8.71	128.30	122.20
29	X	1330	C	O5'-P-OP2	-8.71	97.86	105.70
29	X	650	C	C6-N1-C2	-8.71	116.82	120.30
29	X	2501	C	C6-N1-C1'	8.71	131.25	120.80
29	X	1261	C	C6-N1-C2	8.70	123.78	120.30
29	X	1262	A	C4-C5-N7	8.64	115.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2847	U	N3-C4-O4	8.63	125.44	119.40
29	X	2645	G	C8-N9-C4	-8.62	102.95	106.40
30	Y	32	C	C6-N1-C2	-8.61	116.85	120.30
29	X	2036	C	C6-N1-C2	-8.61	116.86	120.30
29	X	1999	C	N1-C2-N3	8.60	125.22	119.20
29	X	1754	A	C5-N7-C8	8.58	108.19	103.90
29	X	1997	A	N1-C6-N6	8.55	123.73	118.60
29	X	586	A	O5'-P-OP2	-8.54	98.02	105.70
29	X	2826	A	O5'-P-OP1	-8.53	98.02	105.70
29	X	2032	G	C5-C6-O6	-8.53	123.48	128.60
29	X	1279	A	O5'-P-OP1	8.52	120.92	110.70
29	X	2583	G	C5-C6-O6	-8.51	123.49	128.60
29	X	2032	G	N1-C6-O6	8.47	124.98	119.90
29	X	1998	A	C8-N9-C4	8.47	109.19	105.80
29	X	1656	C	O5'-P-OP2	-8.47	98.08	105.70
29	X	2001	A	O5'-P-OP2	8.38	120.76	110.70
29	X	1267	U	O5'-P-OP2	-8.35	98.19	105.70
29	X	2499	C	C6-N1-C2	-8.34	116.96	120.30
29	X	1999	C	N1-C2-O2	-8.34	113.90	118.90
29	X	2619	C	N3-C2-O2	-8.32	116.08	121.90
29	X	2580	U	C5-C4-O4	-8.31	120.91	125.90
29	X	2574	G	C8-N9-C4	-8.31	103.08	106.40
29	X	744	U	O5'-P-OP1	8.30	120.66	110.70
29	X	2676	C	C6-N1-C2	8.27	123.61	120.30
29	X	1152	C	C6-N1-C2	-8.26	117.00	120.30
29	X	27	G	O5'-P-OP1	-8.24	98.28	105.70
29	X	1490	C	C2-N1-C1'	8.21	127.83	118.80
29	X	1661	G	N7-C8-N9	-8.17	109.02	113.10
29	X	1322	A	C8-N9-C4	8.16	109.07	105.80
29	X	513	A	O5'-P-OP2	8.16	120.49	110.70
29	X	498	G	C5-C6-O6	-8.15	123.71	128.60
29	X	943	U	O5'-P-OP1	-8.14	98.37	105.70
29	X	1784	A	C8-N9-C4	8.11	109.04	105.80
29	X	1668	A	N7-C8-N9	-8.10	109.75	113.80
29	X	2619	C	N1-C2-O2	8.09	123.75	118.90
29	X	738	G	N1-C6-O6	-8.07	115.06	119.90
29	X	1668	A	O5'-P-OP2	-8.06	98.45	105.70
29	X	946	G	N1-C6-O6	-8.05	115.07	119.90
29	X	659	C	C5-C6-N1	-8.04	116.98	121.00
29	X	2501	C	N3-C4-N4	-8.02	112.38	118.00
29	X	2574	G	N3-C4-N9	-8.02	121.19	126.00
29	X	2717	G	C2-N3-C4	8.02	115.91	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1262	A	C5-C6-N6	-8.02	117.28	123.70
29	X	1673	U	C5-C4-O4	-8.02	121.09	125.90
29	X	1661	G	C6-N1-C2	-7.95	120.33	125.10
29	X	2050	C	C6-N1-C2	-7.94	117.12	120.30
29	X	962	U	O5'-P-OP1	-7.92	98.57	105.70
29	X	1277	A	O5'-P-OP2	-7.92	98.57	105.70
29	X	660	G	N7-C8-N9	-7.89	109.16	113.10
29	X	1998	A	C6-N1-C2	-7.88	113.87	118.60
29	X	1262	A	C6-C5-N7	-7.86	126.80	132.30
29	X	2659	G	N1-C6-O6	7.84	124.61	119.90
29	X	2618	G	C8-N9-C4	-7.82	103.27	106.40
29	X	2561	A	O5'-P-OP2	-7.80	98.68	105.70
29	X	1951	U	N3-C4-O4	7.79	124.86	119.40
29	X	472	A	C2-N3-C4	-7.77	106.71	110.60
29	X	645	U	N3-C2-O2	-7.77	116.76	122.20
29	X	1279	A	C8-N9-C4	7.77	108.91	105.80
29	X	2820	A	N1-C6-N6	-7.75	113.95	118.60
29	X	2600	A	O5'-P-OP1	-7.75	98.73	105.70
29	X	1777	U	N1-C2-O2	7.72	128.21	122.80
29	X	2729	C	O5'-P-OP1	-7.72	98.75	105.70
29	X	492	A	N1-C2-N3	7.72	133.16	129.30
29	X	2708	G	C8-N9-C4	7.72	109.49	106.40
29	X	1990	C	N3-C2-O2	-7.70	116.51	121.90
29	X	1646	C	N1-C2-O2	7.68	123.51	118.90
29	X	2032	G	C4-C5-N7	7.68	113.87	110.80
29	X	2546	U	N3-C2-O2	-7.68	116.82	122.20
29	X	650	C	C5-C6-N1	7.68	124.84	121.00
29	X	25	U	OP1-P-O3'	7.67	122.08	105.20
29	X	2825	C	N3-C4-N4	7.67	123.36	118.00
29	X	2551	C	N1-C2-O2	-7.66	114.31	118.90
29	X	676	A	N7-C8-N9	7.65	117.63	113.80
29	X	2443	C	N3-C2-O2	-7.64	116.55	121.90
29	X	1991	U	O5'-P-OP2	-7.63	98.83	105.70
29	X	1951	U	N3-C4-C5	-7.63	110.02	114.60
29	X	1660	C	OP1-P-OP2	7.63	131.04	119.60
29	X	1663	U	C5-C6-N1	7.62	126.51	122.70
29	X	2575	C	C6-N1-C2	-7.62	117.25	120.30
29	X	2581	G	C8-N9-C4	-7.62	103.35	106.40
29	X	2499	C	C5-C6-N1	7.62	124.81	121.00
29	X	472	A	O4'-C1'-N9	7.61	114.29	108.20
29	X	2712	C	O5'-P-OP2	-7.59	98.87	105.70
29	X	1749	A	C8-N9-C4	-7.58	102.77	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2063	C	N1-C2-O2	-7.58	114.35	118.90
29	X	2549	G	O5'-P-OP1	-7.57	98.89	105.70
29	X	2869	G	OP2-P-O3'	7.57	121.85	105.20
29	X	2695	C	N3-C2-O2	7.56	127.19	121.90
29	X	445	C	O5'-P-OP2	-7.56	98.89	105.70
29	X	1647	G	O5'-P-OP1	-7.54	98.91	105.70
29	X	782	A	N1-C6-N6	7.53	123.12	118.60
29	X	2843	G	C8-N9-C4	-7.52	103.39	106.40
29	X	30	G	C8-N9-C4	-7.52	103.39	106.40
29	X	1673	U	N3-C4-C5	7.52	119.11	114.60
29	X	531	C	C5-C6-N1	-7.50	117.25	121.00
30	Y	32	C	C5-C6-N1	7.49	124.74	121.00
29	X	1665	A	N9-C4-C5	7.48	108.79	105.80
29	X	2569	G	C5-C6-N1	-7.47	107.77	111.50
29	X	1999	C	C4-C5-C6	7.46	121.13	117.40
29	X	1630	U	N3-C4-C5	-7.44	110.13	114.60
29	X	1997	A	O5'-P-OP1	-7.44	99.00	105.70
29	X	2500	U	C5-C6-N1	7.44	126.42	122.70
29	X	676	A	C5-N7-C8	-7.42	100.19	103.90
29	X	1461	G	O5'-P-OP2	7.41	119.59	110.70
29	X	866	A	N9-C4-C5	-7.39	102.84	105.80
29	X	1616	A	C8-N9-C4	-7.39	102.84	105.80
29	X	2001	A	C2-N3-C4	-7.38	106.91	110.60
29	X	2712(A)	A	N1-C6-N6	7.36	123.02	118.60
29	X	2712(A)	A	OP2-P-O3'	7.36	121.39	105.20
29	X	2032	G	C5-N7-C8	-7.36	100.62	104.30
29	X	1652	A	N1-C6-N6	7.35	123.01	118.60
29	X	1990	C	C6-N1-C2	-7.35	117.36	120.30
29	X	2060	A	OP2-P-O3'	7.34	121.34	105.20
29	X	1662	U	C2-N3-C4	-7.32	122.61	127.00
29	X	1779	U	C4-C5-C6	7.32	124.09	119.70
29	X	2613	U	O5'-P-OP1	-7.32	99.11	105.70
29	X	1950	G	C8-N9-C4	-7.29	103.48	106.40
29	X	1660	C	N1-C2-N3	7.29	124.30	119.20
29	X	2645	G	N7-C8-N9	7.27	116.74	113.10
29	X	1653	G	N3-C2-N2	7.27	124.99	119.90
29	X	2892	G	N3-C4-N9	-7.23	121.66	126.00
29	X	327	G	C8-N9-C4	-7.22	103.51	106.40
29	X	2765	A	O4'-C1'-N9	7.21	113.97	108.20
29	X	2515	C	N3-C2-O2	-7.18	116.87	121.90
29	X	2556	C	C6-N1-C2	7.18	123.17	120.30
29	X	2021	U	O5'-P-OP2	7.17	119.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1661	G	N1-C6-O6	-7.16	115.60	119.90
29	X	2870	C	C6-N1-C2	-7.13	117.45	120.30
29	X	1996	C	OP1-P-OP2	-7.12	108.91	119.60
29	X	2027	G	O5'-P-OP2	-7.10	99.31	105.70
29	X	2613	U	O5'-P-OP2	7.07	119.19	110.70
29	X	1236	G	O5'-P-OP1	-7.07	99.34	105.70
29	X	2046	G	O5'-P-OP2	-7.07	99.34	105.70
29	X	598	U	C5-C6-N1	-7.06	119.17	122.70
29	X	1227	G	O5'-P-OP1	-7.06	99.35	105.70
29	X	841	G	N1-C6-O6	7.06	124.14	119.90
29	X	750	A	O5'-P-OP2	7.05	119.16	110.70
29	X	1998	A	N1-C6-N6	7.02	122.81	118.60
29	X	1206	G	C6-C5-N7	7.00	134.60	130.40
29	X	1328	G	C5-C6-N1	6.98	114.99	111.50
29	X	1285	G	N3-C2-N2	6.98	124.79	119.90
29	X	1278	G	C8-N9-C4	6.98	109.19	106.40
29	X	2392	A	C8-N9-C4	-6.97	103.01	105.80
29	X	1727	C	C6-N1-C2	6.96	123.09	120.30
29	X	1264	G	C5-C6-O6	6.96	132.78	128.60
29	X	2580	U	N3-C2-O2	6.95	127.07	122.20
29	X	25	U	C6-N1-C2	-6.94	116.84	121.00
29	X	2419	U	N3-C4-C5	-6.94	110.44	114.60
29	X	1266	G	N3-C2-N2	6.92	124.75	119.90
29	X	734	A	O4'-C1'-N9	6.90	113.72	108.20
29	X	649	G	N3-C4-C5	6.89	132.04	128.60
29	X	2684	U	OP1-P-O3'	6.88	120.33	105.20
29	X	1277	A	OP1-P-OP2	6.88	129.91	119.60
29	X	802	A	O5'-P-OP1	-6.87	99.51	105.70
29	X	2673	G	O5'-P-OP2	-6.86	99.52	105.70
29	X	2712	C	C2-N3-C4	-6.85	116.47	119.90
29	X	2451	A	N1-C2-N3	6.85	132.72	129.30
29	X	1262	A	C5-N7-C8	-6.84	100.48	103.90
29	X	788	A	N1-C6-N6	6.83	122.70	118.60
29	X	1695	G	C4-N9-C1'	6.83	135.37	126.50
29	X	1278	G	N7-C8-N9	-6.81	109.69	113.10
29	X	2488	A	N1-C6-N6	-6.81	114.51	118.60
29	X	1779	U	C2-N1-C1'	-6.81	109.53	117.70
29	X	1652	A	C6-C5-N7	-6.81	127.53	132.30
29	X	1208	C	C6-N1-C2	-6.80	117.58	120.30
29	X	1758	G	O5'-P-OP2	-6.79	99.59	105.70
29	X	673	C	C6-N1-C2	6.77	123.01	120.30
29	X	649	G	N3-C4-N9	-6.77	121.94	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1754	A	C8-N9-C4	6.77	108.51	105.80
29	X	2513	G	C8-N9-C4	-6.76	103.69	106.40
29	X	2496	C	C6-N1-C2	-6.76	117.60	120.30
29	X	2512	C	C6-N1-C2	-6.76	117.60	120.30
29	X	995	C	C5-C6-N1	-6.75	117.62	121.00
29	X	2699	C	C5-C6-N1	-6.75	117.63	121.00
29	X	1652	A	C2-N3-C4	-6.74	107.23	110.60
29	X	588	U	C6-N1-C2	6.73	125.04	121.00
29	X	2713	U	C4-C5-C6	6.73	123.74	119.70
29	X	746	C	N3-C4-C5	-6.73	119.21	121.90
29	X	2454	G	N9-C4-C5	6.72	108.09	105.40
29	X	2678	G	OP2-P-O3'	6.72	119.99	105.20
29	X	1461	G	O5'-P-OP1	-6.72	99.65	105.70
30	Y	29	C	C6-N1-C2	-6.72	117.61	120.30
29	X	1200	C	N1-C2-O2	-6.71	114.87	118.90
29	X	774	A	C2-N3-C4	-6.71	107.24	110.60
29	X	983	A	N1-C6-N6	-6.70	114.58	118.60
29	X	1210	G	C4-N9-C1'	6.70	135.21	126.50
29	X	2612	C	C2-N1-C1'	6.70	126.17	118.80
29	X	2430	A	C8-N9-C4	-6.69	103.12	105.80
29	X	1977	A	C8-N9-C4	6.69	108.48	105.80
29	X	995	C	C6-N1-C2	6.68	122.97	120.30
29	X	1156	A	N1-C6-N6	6.67	122.60	118.60
29	X	2715	C	C6-N1-C2	-6.66	117.64	120.30
29	X	1665	A	C6-N1-C2	-6.65	114.61	118.60
29	X	650	C	N3-C4-N4	6.64	122.65	118.00
29	X	1206	G	C4-N9-C1'	-6.64	117.86	126.50
29	X	1206	G	C8-N9-C1'	6.64	135.63	127.00
29	X	1262	A	N9-C4-C5	-6.64	103.15	105.80
29	X	676	A	C6-C5-N7	-6.63	127.66	132.30
29	X	1659	U	O5'-P-OP1	-6.63	99.73	105.70
29	X	492	A	C6-N1-C2	-6.63	114.62	118.60
29	X	2873	A	O5'-P-OP1	-6.62	99.74	105.70
29	X	1322	A	N7-C8-N9	-6.62	110.49	113.80
29	X	1641	A	C8-N9-C4	6.61	108.44	105.80
29	X	1003	G	C8-N9-C4	-6.61	103.76	106.40
29	X	1663	U	C4-C5-C6	-6.60	115.74	119.70
29	X	2446	G	N9-C4-C5	-6.60	102.76	105.40
29	X	1747	G	N3-C4-C5	-6.60	125.30	128.60
29	X	645	U	C6-N1-C2	-6.59	117.04	121.00
29	X	2025	C	C6-N1-C2	-6.58	117.67	120.30
29	X	1327	C	N1-C2-O2	-6.57	114.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	513	A	O5'-P-OP1	-6.57	99.79	105.70
29	X	1236	G	O5'-P-OP2	6.56	118.57	110.70
29	X	2001	A	OP1-P-OP2	-6.55	109.78	119.60
29	X	2511	U	O5'-P-OP2	-6.55	99.81	105.70
29	X	2454	G	C8-N9-C4	-6.54	103.78	106.40
15	N	28	ARG	NE-CZ-NH1	6.54	123.57	120.30
29	X	170	C	C5-C6-N1	6.54	124.27	121.00
29	X	1660	C	C5-C6-N1	-6.53	117.73	121.00
29	X	2712(A)	A	C5-C6-N6	-6.53	118.47	123.70
29	X	2036	C	C5-C6-N1	6.51	124.25	121.00
29	X	23	G	O5'-P-OP1	-6.51	99.84	105.70
29	X	1627	G	C8-N9-C4	6.51	109.00	106.40
29	X	2443	C	C6-N1-C2	-6.50	117.70	120.30
29	X	2879	G	C4-N9-C1'	6.49	134.94	126.50
29	X	571	A	N1-C6-N6	6.49	122.49	118.60
29	X	1998	A	C5-C6-N6	-6.48	118.52	123.70
29	X	1320	G	O5'-P-OP1	-6.48	99.87	105.70
29	X	531	C	C4-C5-C6	6.48	120.64	117.40
29	X	170	C	C2-N1-C1'	6.47	125.92	118.80
29	X	1673	U	N3-C2-O2	6.47	126.73	122.20
29	X	2689	U	C5-C4-O4	6.46	129.78	125.90
29	X	486	C	N3-C2-O2	6.46	126.42	121.90
29	X	1156	A	N9-C4-C5	-6.46	103.22	105.80
29	X	1654	A	OP2-P-O3'	6.46	119.41	105.20
29	X	957	C	N1-C2-O2	6.45	122.77	118.90
29	X	1255	U	OP1-P-O3'	6.45	119.39	105.20
29	X	845	G	N3-C4-C5	6.44	131.82	128.60
29	X	1786	A	O4'-C1'-N9	6.44	113.35	108.20
29	X	1392	A	C8-N9-C4	-6.43	103.23	105.80
29	X	2709	G	O5'-P-OP1	6.43	118.41	110.70
29	X	2731	G	O5'-P-OP2	-6.43	99.92	105.70
29	X	2271	G	C4-N9-C1'	6.42	134.85	126.50
29	X	20	C	N3-C4-N4	6.42	122.50	118.00
29	X	2009	G	N7-C8-N9	-6.42	109.89	113.10
29	X	1629	G	N3-C4-N9	-6.42	122.15	126.00
29	X	2508	G	C8-N9-C4	-6.42	103.83	106.40
29	X	2250	G	N3-C4-N9	-6.41	122.16	126.00
29	X	2822	G	N3-C4-N9	6.41	129.84	126.00
29	X	2347	C	O4'-C1'-N1	6.41	113.33	108.20
29	X	2060	A	C8-N9-C4	-6.40	103.24	105.80
29	X	2508	G	C5-C6-O6	6.40	132.44	128.60
29	X	940	G	C8-N9-C4	6.40	108.96	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1395	A	O4'-C1'-N9	6.40	113.32	108.20
29	X	1662	U	C5-C6-N1	-6.40	119.50	122.70
29	X	474	G	OP2-P-O3'	6.39	119.25	105.20
29	X	2883	A	OP1-P-O3'	6.38	119.25	105.20
29	X	2050	C	N1-C2-N3	6.38	123.67	119.20
29	X	673	C	C2-N1-C1'	-6.38	111.78	118.80
29	X	2714	G	C8-N9-C4	-6.38	103.85	106.40
29	X	2038	G	N1-C6-O6	6.37	123.72	119.90
29	X	2516	G	N3-C4-C5	-6.37	125.41	128.60
29	X	957	C	C2-N1-C1'	6.37	125.81	118.80
29	X	1616	A	O5'-P-OP1	-6.37	99.97	105.70
29	X	1779	U	N1-C2-N3	6.37	118.72	114.90
29	X	2824	C	O5'-P-OP1	6.37	118.35	110.70
29	X	516	C	C6-N1-C2	-6.37	117.75	120.30
29	X	1695	G	N3-C4-N9	6.37	129.82	126.00
29	X	1997	A	OP1-P-OP2	6.37	129.15	119.60
29	X	2583	G	N3-C2-N2	-6.37	115.44	119.90
29	X	1666	G	O4'-C1'-N9	6.36	113.28	108.20
29	X	734	A	O5'-P-OP1	6.35	118.32	110.70
29	X	2723	C	C4-C5-C6	6.34	120.57	117.40
29	X	650	C	N1-C2-O2	6.33	122.70	118.90
29	X	1661	G	C5-N7-C8	6.33	107.47	104.30
29	X	1695	G	C8-N9-C1'	-6.33	118.77	127.00
29	X	957	C	C6-N1-C1'	-6.32	113.21	120.80
29	X	2643	G	C8-N9-C4	6.32	108.93	106.40
29	X	1394	G	C6-C5-N7	-6.32	126.61	130.40
29	X	2020	A	N1-C6-N6	6.32	122.39	118.60
29	X	1027	U	C2-N1-C1'	-6.31	110.13	117.70
29	X	1665	A	N1-C2-N3	6.31	132.45	129.30
29	X	2720	U	O5'-P-OP1	-6.30	100.03	105.70
29	X	649	G	C2-N3-C4	-6.30	108.75	111.90
29	X	915	C	C6-N1-C2	-6.30	117.78	120.30
29	X	635	C	C6-N1-C2	-6.28	117.79	120.30
29	X	2045	C	C5-C4-N4	-6.28	115.81	120.20
29	X	1685	C	C6-N1-C2	6.27	122.81	120.30
29	X	2612	C	N1-C2-O2	6.27	122.66	118.90
29	X	2844	G	N3-C4-C5	-6.25	125.48	128.60
29	X	734	A	C5'-C4'-O4'	6.25	116.59	109.10
29	X	1777	U	N3-C2-O2	-6.25	117.83	122.20
29	X	2052	G	N3-C4-C5	-6.24	125.48	128.60
29	X	2271	G	N3-C4-N9	6.24	129.75	126.00
29	X	2052	G	C5-C6-O6	-6.24	124.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2509	G	N1-C6-O6	-6.24	116.16	119.90
29	X	2871	G	O5'-P-OP2	-6.24	100.08	105.70
29	X	2777	G	O5'-P-OP2	-6.24	100.09	105.70
29	X	2000	G	OP1-P-O3'	-6.24	91.48	105.20
29	X	2044	C	OP1-P-O3'	6.23	118.90	105.20
29	X	948	C	O5'-P-OP2	6.22	118.17	110.70
29	X	1761	C	C6-N1-C2	-6.21	117.81	120.30
29	X	1144	G	C8-N9-C4	6.21	108.89	106.40
29	X	1998	A	N7-C8-N9	-6.21	110.70	113.80
29	X	2871	G	OP1-P-OP2	6.21	128.91	119.60
29	X	1280	A	C2-N3-C4	-6.20	107.50	110.60
29	X	2572	A	N7-C8-N9	-6.18	110.71	113.80
29	X	1256	G	C5-C6-O6	-6.18	124.89	128.60
29	X	841	G	C5-C6-N1	-6.18	108.41	111.50
29	X	1264	G	N3-C4-C5	-6.18	125.51	128.60
29	X	2577	A	OP1-P-OP2	6.18	128.86	119.60
29	X	2712(A)	A	C5-N7-C8	-6.17	100.82	103.90
29	X	2271	G	N3-C4-C5	-6.17	125.52	128.60
29	X	1291	U	C5-C6-N1	-6.16	119.62	122.70
29	X	2533	A	C8-N9-C4	6.16	108.26	105.80
29	X	672	U	N1-C2-N3	6.16	118.59	114.90
29	X	338	G	N3-C4-C5	-6.15	125.53	128.60
29	X	2582	G	O5'-P-OP1	6.14	118.07	110.70
29	X	2718	G	N3-C4-C5	-6.14	125.53	128.60
29	X	1265	A	C4-C5-C6	6.14	120.07	117.00
29	X	2869	G	N3-C4-N9	-6.14	122.32	126.00
29	X	2010	G	O5'-P-OP2	6.13	118.06	110.70
29	X	2576	G	C5-C6-O6	-6.13	124.92	128.60
29	X	1675	C	N3-C4-C5	-6.12	119.45	121.90
29	X	2553	G	C2'-C3'-O3'	6.12	123.49	113.70
29	X	2049	G	C4-C5-N7	6.12	113.25	110.80
29	X	452	G	N3-C4-N9	6.11	129.67	126.00
29	X	1394	G	C4-N9-C1'	6.11	134.44	126.50
29	X	2732	G	N1-C2-N2	-6.11	110.70	116.20
29	X	2052	G	C6-N1-C2	-6.10	121.44	125.10
29	X	486	C	N1-C2-O2	-6.10	115.24	118.90
29	X	2821	A	O5'-P-OP2	-6.10	100.21	105.70
29	X	1629	G	N3-C4-C5	6.09	131.65	128.60
29	X	2723	C	N3-C4-C5	-6.09	119.46	121.90
29	X	1655	A	OP1-P-OP2	-6.09	110.47	119.60
29	X	2294	C	C6-N1-C2	-6.09	117.86	120.30
29	X	1006	C	N3-C2-O2	-6.08	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	964	C	N1-C2-O2	-6.08	115.25	118.90
29	X	2726	U	N1-C2-O2	-6.08	118.54	122.80
29	X	2574	G	N9-C4-C5	6.08	107.83	105.40
29	X	2688	C	OP1-P-O3'	6.07	118.55	105.20
29	X	2002	G	OP2-P-O3'	6.07	118.55	105.20
29	X	2038	G	C5-C6-O6	-6.07	124.96	128.60
29	X	2869	G	N3-C4-C5	6.06	131.63	128.60
29	X	2843	G	OP2-P-O3'	6.06	118.53	105.20
29	X	30	G	N9-C4-C5	6.06	107.82	105.40
29	X	1206	G	C4-C5-N7	-6.06	108.38	110.80
29	X	2684	U	C6-N1-C2	-6.06	117.36	121.00
29	X	851	C	O5'-P-OP1	-6.05	100.25	105.70
29	X	2612	C	N3-C4-C5	-6.05	119.48	121.90
29	X	2612	C	N3-C4-N4	6.05	122.24	118.00
29	X	1252	G	O5'-P-OP2	-6.05	100.25	105.70
29	X	2789	C	O5'-P-OP2	-6.04	100.26	105.70
29	X	582	G	OP2-P-O3'	6.04	118.48	105.20
29	X	1205	C	N1-C2-O2	6.04	122.52	118.90
29	X	2513	G	C5-C6-O6	6.03	132.22	128.60
29	X	220	G	O5'-P-OP1	-6.03	100.28	105.70
29	X	1394	G	C8-N9-C1'	-6.03	119.17	127.00
29	X	1784	A	N7-C8-N9	-6.02	110.79	113.80
29	X	991	C	C6-N1-C2	-6.02	117.89	120.30
29	X	2847	U	C4-C5-C6	6.02	123.31	119.70
29	X	944	G	C2-N3-C4	-6.01	108.89	111.90
29	X	1292	C	C6-N1-C2	6.01	122.70	120.30
29	X	1635	G	N9-C4-C5	-6.01	103.00	105.40
29	X	761	A	C8-N9-C4	-6.00	103.40	105.80
29	X	944	G	C5-N7-C8	-6.00	101.30	104.30
29	X	1239	C	O5'-P-OP2	6.00	117.91	110.70
29	X	744	U	O5'-P-OP2	-6.00	100.30	105.70
29	X	1652	A	N1-C2-N3	6.00	132.30	129.30
29	X	2269	A	C8-N9-C4	6.00	108.20	105.80
29	X	2768	C	C6-N1-C2	5.99	122.70	120.30
29	X	498	G	C6-C5-N7	-5.99	126.81	130.40
29	X	2443	C	C2-N1-C1'	5.99	125.39	118.80
29	X	2509	G	C2-N3-C4	5.99	114.89	111.90
29	X	2000	G	OP2-P-O3'	5.97	118.35	105.20
29	X	2572	A	C8-N9-C4	5.97	108.19	105.80
29	X	1951	U	C4-C5-C6	5.97	123.28	119.70
29	X	13	A	C8-N9-C4	-5.96	103.42	105.80
29	X	1455	G	N3-C4-C5	-5.96	125.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2712(A)	A	C4-C5-N7	5.96	113.68	110.70
29	X	676	A	O4'-C1'-N9	5.96	112.97	108.20
29	X	732	C	C5-C4-N4	5.96	124.37	120.20
29	X	487	C	OP2-P-O3'	5.95	118.29	105.20
29	X	799	G	C8-N9-C4	-5.95	104.02	106.40
29	X	957	C	C2-N3-C4	5.95	122.88	119.90
29	X	517	C	C2-N1-C1'	5.94	125.33	118.80
29	X	732	C	N1-C2-N3	5.94	123.36	119.20
29	X	1998	A	OP1-P-OP2	5.94	128.51	119.60
29	X	1665	A	N3-C4-C5	-5.94	122.64	126.80
29	X	512	G	O4'-C1'-N9	5.94	112.95	108.20
29	X	974	G	C8-N9-C4	-5.93	104.03	106.40
29	X	1753	A	N1-C2-N3	5.93	132.26	129.30
29	X	486	C	C6-N1-C2	5.92	122.67	120.30
29	X	1668	A	C5-N7-C8	5.92	106.86	103.90
29	X	2501	C	O4'-C1'-N1	5.92	112.93	108.20
29	X	2517	C	O5'-P-OP1	-5.92	100.38	105.70
29	X	2547	U	N1-C2-N3	5.91	118.45	114.90
29	X	2833	U	O4'-C1'-N1	5.91	112.93	108.20
29	X	1230	G	OP1-P-OP2	-5.91	110.74	119.60
29	X	2271	G	C8-N9-C1'	-5.91	119.32	127.00
29	X	2419	U	N3-C4-O4	5.91	123.54	119.40
29	X	2260	C	N3-C4-N4	-5.91	113.86	118.00
29	X	1999	C	O5'-P-OP1	5.90	117.78	110.70
29	X	475	U	C2-N1-C1'	5.90	124.78	117.70
29	X	1629	G	C2-N3-C4	-5.90	108.95	111.90
29	X	1751	U	C5-C4-O4	-5.89	122.37	125.90
29	X	2842	A	OP2-P-O3'	5.89	118.15	105.20
29	X	504	G	O4'-C1'-N9	-5.88	103.49	108.20
29	X	907	U	O4'-C1'-N1	5.88	112.90	108.20
29	X	1206	G	O4'-C1'-N9	5.88	112.90	108.20
29	X	1998	A	N1-C2-N3	5.88	132.24	129.30
29	X	1998	A	C8-N9-C1'	-5.88	117.13	127.70
29	X	2576	G	C8-N9-C4	5.88	108.75	106.40
29	X	942	G	OP2-P-O3'	5.87	118.12	105.20
29	X	516	C	N3-C2-O2	-5.87	117.79	121.90
29	X	1936	A	C2-N3-C4	-5.87	107.66	110.60
29	X	2007	U	OP2-P-O3'	5.87	118.11	105.20
29	X	2843	G	N7-C8-N9	5.87	116.03	113.10
29	X	2820	A	C5-C6-N6	5.87	128.39	123.70
29	X	1967	C	C6-N1-C2	-5.86	117.95	120.30
29	X	1649	G	C8-N9-C4	5.86	108.74	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2555	U	N3-C2-O2	5.86	126.30	122.20
29	X	2866	U	N3-C2-O2	-5.86	118.10	122.20
29	X	2273	A	N9-C4-C5	5.84	108.14	105.80
29	X	1700	A	O5'-P-OP2	5.84	117.71	110.70
29	X	948	C	C5-C6-N1	5.84	123.92	121.00
29	X	1320	G	C5-C6-O6	5.83	132.10	128.60
29	X	823	G	O5'-P-OP2	-5.83	100.46	105.70
29	X	1995	U	C5-C4-O4	-5.83	122.40	125.90
29	X	577	G	OP1-P-OP2	5.82	128.34	119.60
29	X	2680	C	C6-N1-C2	-5.82	117.97	120.30
29	X	168	A	C6-C5-N7	-5.82	128.22	132.30
29	X	1629	G	N1-C6-O6	5.82	123.39	119.90
29	X	554	U	C5-C6-N1	-5.82	119.79	122.70
29	X	1155	A	O4'-C1'-N9	5.82	112.86	108.20
29	X	635	C	N3-C2-O2	-5.82	117.83	121.90
29	X	2709	G	N3-C4-N9	5.82	129.49	126.00
29	X	1208	C	N3-C4-C5	-5.81	119.58	121.90
29	X	1673	U	C6-N1-C2	5.81	124.49	121.00
29	X	673	C	N3-C2-O2	5.81	125.97	121.90
29	X	957	C	N1-C2-N3	-5.80	115.14	119.20
29	X	1453	A	O4'-C1'-N9	-5.80	103.56	108.20
29	X	2715	C	N1-C2-O2	5.79	122.38	118.90
29	X	2012	G	N3-C4-N9	5.79	129.48	126.00
29	X	1995	U	OP2-P-O3'	5.79	117.94	105.20
29	X	488	G	O5'-P-OP2	-5.79	100.49	105.70
29	X	2690	C	N3-C4-C5	-5.79	119.58	121.90
29	X	1630	U	N3-C4-O4	5.79	123.45	119.40
29	X	1274	A	OP1-P-O3'	5.79	117.93	105.20
29	X	2261	C	C5-C6-N1	5.79	123.89	121.00
29	X	866	A	C8-N9-C4	5.78	108.11	105.80
29	X	2050	C	O5'-P-OP1	-5.78	100.50	105.70
29	X	2048	A	O5'-P-OP1	5.78	117.63	110.70
29	X	2618	G	N7-C8-N9	5.78	115.99	113.10
29	X	2266	A	N1-C6-N6	-5.77	115.14	118.60
29	X	2722	G	OP1-P-O3'	5.77	117.90	105.20
29	X	1771	C	O5'-P-OP2	-5.77	100.50	105.70
29	X	2348	U	C5-C6-N1	5.77	125.59	122.70
29	X	232	G	C8-N9-C4	-5.77	104.09	106.40
29	X	2584	U	O5'-P-OP1	-5.77	100.51	105.70
29	X	580	C	OP2-P-O3'	5.77	117.89	105.20
29	X	37	C	N1-C2-O2	5.77	122.36	118.90
29	X	744	U	C4-C5-C6	5.77	123.16	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2839	G	OP1-P-OP2	5.77	128.25	119.60
29	X	651(B)	C	C5-C6-N1	5.76	123.88	121.00
29	X	1995	U	N3-C4-O4	5.76	123.43	119.40
29	X	2272	U	C5-C6-N1	-5.76	119.82	122.70
29	X	2352	A	C8-N9-C4	5.76	108.10	105.80
29	X	951	C	C5-C6-N1	-5.76	118.12	121.00
29	X	2438	U	N3-C2-O2	-5.75	118.17	122.20
29	X	2567	G	N3-C4-C5	-5.75	125.72	128.60
29	X	2512	C	C5-C6-N1	5.75	123.87	121.00
29	X	2050	C	C2-N3-C4	-5.74	117.03	119.90
29	X	2424	C	C6-N1-C2	-5.74	118.00	120.30
29	X	2879	G	N1-C6-O6	5.74	123.34	119.90
29	X	472	A	C5-C6-N1	-5.73	114.83	117.70
29	X	2002	G	O5'-P-OP1	5.73	117.58	110.70
29	X	2549	G	OP1-P-O3'	5.73	117.81	105.20
29	X	1130	U	C5-C6-N1	-5.73	119.84	122.70
29	X	2294	C	O5'-P-OP1	-5.73	100.54	105.70
29	X	2695	C	C5-C6-N1	5.73	123.86	121.00
29	X	1292	C	C5-C6-N1	-5.73	118.14	121.00
29	X	974	G	N7-C8-N9	5.72	115.96	113.10
29	X	2544	G	C8-N9-C4	-5.72	104.11	106.40
29	X	1260	G	OP1-P-O3'	5.72	117.79	105.20
29	X	2571	C	C5-C4-N4	5.72	124.20	120.20
29	X	1217	C	C6-N1-C2	-5.72	118.01	120.30
29	X	1647	G	O5'-P-OP2	5.71	117.56	110.70
29	X	1674	G	OP1-P-OP2	5.71	128.16	119.60
29	X	1674	G	N1-C6-O6	-5.71	116.48	119.90
29	X	2611	U	OP2-P-O3'	5.71	117.75	105.20
29	X	515	A	N1-C6-N6	-5.70	115.18	118.60
29	X	2052	G	N3-C4-N9	5.69	129.41	126.00
29	X	1210	G	N3-C4-C5	-5.69	125.76	128.60
29	X	2488	A	N9-C4-C5	5.68	108.07	105.80
29	X	1326	U	C5-C4-O4	-5.68	122.49	125.90
29	X	2050	C	P-O3'-C3'	5.68	126.52	119.70
29	X	2611	U	C2-N1-C1'	5.68	124.52	117.70
29	X	2371	G	C5-C6-O6	5.68	132.01	128.60
29	X	1282	U	N3-C4-O4	5.67	123.37	119.40
29	X	2832	U	C6-N1-C2	5.67	124.40	121.00
29	X	777	A	O5'-P-OP1	-5.67	100.60	105.70
29	X	2514	U	O5'-P-OP1	-5.67	100.60	105.70
29	X	2514	U	N1-C2-O2	-5.67	118.83	122.80
29	X	1132	A	O5'-P-OP1	-5.67	100.60	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	748	G	O5'-P-OP2	-5.66	100.60	105.70
29	X	2049	G	OP1-P-O3'	5.66	117.65	105.20
29	X	1779	U	O4'-C1'-N1	5.66	112.72	108.20
29	X	1289	C	O5'-P-OP2	-5.65	100.61	105.70
29	X	2604	U	C5-C6-N1	-5.64	119.88	122.70
29	X	746	C	OP1-P-O3'	5.64	117.61	105.20
29	X	1292	C	N1-C2-O2	-5.64	115.52	118.90
29	X	2273	A	C8-N9-C4	-5.63	103.55	105.80
29	X	2067	G	C8-N9-C4	-5.62	104.15	106.40
29	X	2882	C	OP1-P-OP2	5.62	128.03	119.60
29	X	1240	C	N1-C2-O2	5.62	122.27	118.90
29	X	2001	A	N1-C2-N3	5.62	132.11	129.30
29	X	223	A	OP1-P-O3'	5.62	117.56	105.20
29	X	1754	A	O5'-P-OP2	-5.62	100.64	105.70
29	X	2006	C	C5-C6-N1	5.62	123.81	121.00
29	X	2777	G	C8-N9-C4	5.62	108.65	106.40
29	X	1264	G	C5-N7-C8	5.61	107.11	104.30
29	X	2822	G	OP1-P-OP2	5.61	128.01	119.60
29	X	2686	G	OP1-P-O3'	5.61	117.54	105.20
29	X	2732	G	N3-C2-N2	5.61	123.83	119.90
29	X	1978	A	OP2-P-O3'	5.61	117.53	105.20
29	X	2689	U	N3-C4-O4	-5.61	115.48	119.40
29	X	1662	U	N1-C2-O2	-5.60	118.88	122.80
29	X	1163	G	C5-C6-O6	5.60	131.96	128.60
29	X	1785	A	OP2-P-O3'	5.60	117.52	105.20
29	X	2419	U	C6-N1-C2	-5.60	117.64	121.00
29	X	945	A	N1-C6-N6	5.60	121.96	118.60
29	X	1511	G	C8-N9-C4	-5.60	104.16	106.40
29	X	2451	A	N9-C4-C5	5.59	108.04	105.80
29	X	2825	C	C5-C4-N4	-5.59	116.28	120.20
29	X	2035	G	P-O3'-C3'	5.59	126.41	119.70
29	X	2558	C	C5-C6-N1	5.59	123.80	121.00
29	X	2392	A	N7-C8-N9	5.58	116.59	113.80
29	X	479	A	O4'-C1'-N9	5.58	112.67	108.20
29	X	2036	C	N1-C2-O2	5.58	122.25	118.90
29	X	2250	G	N3-C2-N2	-5.58	115.99	119.90
29	X	1753	A	C6-N1-C2	-5.58	115.25	118.60
29	X	2005	A	C8-N9-C4	5.58	108.03	105.80
29	X	754	G	N7-C8-N9	-5.57	110.31	113.10
29	X	2565	A	C8-N9-C4	-5.57	103.57	105.80
30	Y	39	C	C2-N1-C1'	5.57	124.93	118.80
29	X	1755	U	C5-C6-N1	-5.56	119.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	673	C	N1-C2-O2	-5.56	115.56	118.90
29	X	1995	U	C5-C6-N1	5.56	125.48	122.70
29	X	2035	G	OP1-P-OP2	-5.56	111.26	119.60
29	X	1674	G	O5'-P-OP1	-5.56	100.70	105.70
29	X	2719	G	C8-N9-C4	5.56	108.62	106.40
29	X	2698	U	C5-C4-O4	5.56	129.23	125.90
29	X	2684	U	O5'-P-OP2	-5.55	100.70	105.70
29	X	1650	A	N7-C8-N9	-5.55	111.03	113.80
29	X	2514	U	OP1-P-O3'	5.55	117.41	105.20
29	X	2641	G	C8-N9-C4	5.55	108.62	106.40
29	X	2278	A	O5'-P-OP2	-5.54	100.71	105.70
29	X	753	A	N7-C8-N9	-5.54	111.03	113.80
29	X	809	G	N1-C6-O6	-5.54	116.58	119.90
29	X	2053	G	C2-N3-C4	-5.54	109.13	111.90
3	B	137	ARG	NE-CZ-NH1	-5.54	117.53	120.30
29	X	1653	G	N1-C2-N2	-5.54	111.22	116.20
29	X	2676	C	O5'-P-OP1	5.54	117.34	110.70
29	X	517	C	N3-C2-O2	-5.53	118.03	121.90
29	X	1684	C	O5'-P-OP1	5.53	117.34	110.70
29	X	2553	G	P-O3'-C3'	5.53	126.34	119.70
29	X	516	C	N1-C2-O2	5.53	122.22	118.90
29	X	2049	G	N3-C4-N9	5.52	129.31	126.00
29	X	319	C	C6-N1-C2	-5.52	118.09	120.30
29	X	1993	U	N3-C2-O2	-5.52	118.33	122.20
29	X	670	A	O4'-C1'-N9	-5.52	103.79	108.20
29	X	918	A	N1-C6-N6	-5.52	115.29	118.60
29	X	2877	G	C8-N9-C4	5.52	108.61	106.40
29	X	2566	A	OP1-P-O3'	5.51	117.33	105.20
29	X	2833	U	C6-N1-C1'	5.51	128.92	121.20
29	X	983	A	C4-C5-N7	-5.50	107.95	110.70
29	X	1653	G	N3-C4-N9	5.50	129.30	126.00
29	X	2042	A	C8-N9-C4	-5.50	103.60	105.80
29	X	1695	G	C6-C5-N7	-5.50	127.10	130.40
29	X	1266	G	N1-C2-N2	-5.50	111.25	116.20
29	X	2551	C	C2-N3-C4	-5.50	117.15	119.90
29	X	2058	A	C5-N7-C8	-5.50	101.15	103.90
29	X	957	C	C5-C4-N4	-5.49	116.36	120.20
29	X	2043	C	C6-N1-C2	-5.49	118.10	120.30
29	X	2049	G	N3-C2-N2	5.49	123.74	119.90
29	X	1157	G	OP2-P-O3'	5.49	117.28	105.20
29	X	2689	U	C2-N1-C1'	-5.49	111.11	117.70
29	X	2717	G	C8-N9-C4	-5.49	104.21	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	581	C	O5'-P-OP2	-5.48	100.77	105.70
29	X	1257	C	N3-C4-C5	-5.48	119.71	121.90
29	X	845	G	C2-N3-C4	-5.48	109.16	111.90
29	X	1998	A	C4-C5-C6	5.48	119.74	117.00
29	X	2032	G	C6-C5-N7	-5.48	127.11	130.40
29	X	1688	U	N1-C2-O2	-5.48	118.97	122.80
29	X	645	U	C5-C4-O4	5.47	129.18	125.90
29	X	2840	C	N3-C4-C5	5.47	124.09	121.90
29	X	2872	G	O5'-P-OP2	-5.47	100.78	105.70
29	X	748	G	O4'-C1'-N9	5.47	112.57	108.20
29	X	2711	A	C2-N3-C4	-5.47	107.87	110.60
29	X	2715	C	N3-C2-O2	-5.47	118.07	121.90
29	X	1256	G	N1-C6-O6	5.46	123.18	119.90
29	X	517	C	C6-N1-C2	-5.46	118.11	120.30
29	X	1297	C	N3-C4-C5	5.46	124.08	121.90
22	U	17	SER	C-N-CA	5.46	135.34	121.70
29	X	841	G	OP2-P-O3'	5.46	117.21	105.20
29	X	2500	U	N1-C2-O2	5.46	126.62	122.80
29	X	2836	G	C8-N9-C4	5.46	108.58	106.40
29	X	972	G	C8-N9-C4	-5.46	104.22	106.40
29	X	2692	C	N3-C4-C5	-5.46	119.72	121.90
29	X	1701	A	N1-C6-N6	5.45	121.87	118.60
29	X	1777	U	C2-N3-C4	5.45	130.27	127.00
29	X	1978	A	O5'-P-OP2	5.45	117.25	110.70
29	X	676	A	C4-C5-N7	5.45	113.43	110.70
29	X	2582	G	OP1-P-OP2	-5.45	111.42	119.60
29	X	1997	A	C5-C6-N6	-5.45	119.34	123.70
29	X	1261	C	N3-C2-O2	5.45	125.71	121.90
29	X	1656	C	C5-C4-N4	-5.45	116.39	120.20
29	X	2590	A	C8-N9-C4	5.45	107.98	105.80
29	X	1455	G	C8-N9-C4	-5.45	104.22	106.40
29	X	585	G	C4-C5-N7	-5.44	108.62	110.80
29	X	2593	U	C6-N1-C2	-5.44	117.73	121.00
29	X	24	G	OP1-P-OP2	5.44	127.76	119.60
29	X	1327	C	OP2-P-O3'	5.44	117.17	105.20
29	X	1627	G	N7-C8-N9	-5.43	110.38	113.10
29	X	2717	G	N9-C4-C5	5.43	107.57	105.40
29	X	2512	C	O5'-P-OP2	-5.43	100.81	105.70
29	X	1951	U	C6-N1-C2	-5.43	117.74	121.00
29	X	11	G	N1-C6-O6	5.43	123.16	119.90
29	X	472	A	N1-C2-N3	5.43	132.01	129.30
29	X	2332	U	N3-C2-O2	-5.43	118.40	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2618	G	N3-C2-N2	-5.43	116.10	119.90
29	X	1652	A	C4-C5-N7	5.42	113.41	110.70
29	X	1149	C	C6-N1-C2	-5.42	118.13	120.30
29	X	1204	C	C6-N1-C2	-5.42	118.13	120.30
29	X	2064	C	O5'-P-OP2	5.42	117.21	110.70
9	H	8	LEU	CA-CB-CG	5.42	127.75	115.30
29	X	2048	A	O5'-P-OP2	-5.42	100.83	105.70
29	X	1295	C	OP2-P-O3'	5.41	117.11	105.20
29	X	1656	C	C6-N1-C1'	-5.41	114.31	120.80
29	X	1314	C	C2-N1-C1'	5.41	124.75	118.80
29	X	2833	U	C5-C4-O4	5.41	129.15	125.90
29	X	1950	G	C2-N3-C4	5.41	114.60	111.90
29	X	329	G	OP2-P-O3'	5.40	117.09	105.20
29	X	2002	G	N1-C6-O6	5.40	123.14	119.90
29	X	2003	G	C6-N1-C2	-5.40	121.86	125.10
29	X	2581	G	N7-C8-N9	5.40	115.80	113.10
29	X	26	G	OP1-P-OP2	-5.40	111.50	119.60
29	X	706	A	C8-N9-C4	5.40	107.96	105.80
29	X	732	C	N3-C2-O2	-5.40	118.12	121.90
29	X	1955	U	O5'-P-OP2	-5.40	100.84	105.70
29	X	1980	G	C8-N9-C4	-5.40	104.24	106.40
30	Y	12	C	C6-N1-C2	5.40	122.46	120.30
29	X	2875	U	N3-C4-O4	5.39	123.18	119.40
29	X	2555	U	N1-C2-O2	-5.39	119.03	122.80
29	X	2852	G	OP1-P-OP2	-5.39	111.51	119.60
29	X	2853	C	O5'-P-OP1	5.39	117.17	110.70
29	X	1650	A	C5-N7-C8	5.39	106.59	103.90
29	X	2371	G	C4-C5-N7	-5.39	108.64	110.80
29	X	1005	C	C5-C6-N1	5.39	123.69	121.00
29	X	2576	G	C4-C5-N7	5.39	112.95	110.80
29	X	782	A	C6-C5-N7	-5.38	128.53	132.30
29	X	462	C	OP2-P-O3'	5.38	117.03	105.20
29	X	911	A	N1-C6-N6	5.38	121.83	118.60
29	X	2711	A	N1-C2-N3	5.38	131.99	129.30
29	X	2823	A	C2-N3-C4	-5.37	107.91	110.60
29	X	2690	C	N3-C2-O2	-5.37	118.14	121.90
29	X	2715	C	C5-C6-N1	5.37	123.68	121.00
29	X	1779	U	C2-N3-C4	-5.37	123.78	127.00
29	X	2881	U	C6-N1-C2	-5.36	117.78	121.00
29	X	1264	G	C4-C5-N7	-5.36	108.66	110.80
29	X	1256	G	O5'-P-OP1	-5.36	100.88	105.70
29	X	1272	A	OP1-P-OP2	5.36	127.64	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2529	G	N1-C6-O6	5.36	123.12	119.90
29	X	2714	G	P-O3'-C3'	5.36	126.13	119.70
29	X	803	U	N3-C2-O2	-5.35	118.45	122.20
29	X	676	A	N1-C6-N6	5.35	121.81	118.60
29	X	1755	U	C2-N1-C1'	-5.35	111.28	117.70
29	X	2359	C	C6-N1-C2	-5.35	118.16	120.30
29	X	2722	G	O5'-P-OP2	-5.35	100.89	105.70
29	X	2561	A	OP1-P-OP2	5.34	127.61	119.60
29	X	1779	U	C5-C4-O4	5.34	129.10	125.90
29	X	1216	C	C6-N1-C2	-5.33	118.17	120.30
29	X	2446	G	N3-C4-N9	5.33	129.20	126.00
29	X	822	U	N3-C2-O2	-5.33	118.47	122.20
29	X	231	C	C6-N1-C2	-5.33	118.17	120.30
29	X	2849	C	N1-C2-O2	-5.32	115.70	118.90
29	X	582	G	C8-N9-C4	5.32	108.53	106.40
29	X	651(B)	C	N1-C2-O2	5.32	122.09	118.90
29	X	2722	G	C8-N9-C4	-5.32	104.27	106.40
29	X	1608	A	C4-C5-C6	5.31	119.66	117.00
29	X	170	C	C6-N1-C2	-5.31	118.17	120.30
29	X	2676	C	C4-C5-C6	5.31	120.06	117.40
29	X	1663	U	O4'-C1'-N1	5.31	112.45	108.20
29	X	845	G	C5-N7-C8	-5.31	101.65	104.30
29	X	1653	G	C8-N9-C4	5.31	108.52	106.40
29	X	1695	G	N3-C4-C5	-5.31	125.95	128.60
29	X	2892	G	C2-N3-C4	-5.30	109.25	111.90
29	X	2571	C	C2-N3-C4	5.30	122.55	119.90
29	X	2879	G	C2-N3-C4	-5.30	109.25	111.90
29	X	782	A	C5-C6-N6	-5.30	119.46	123.70
29	X	2680	C	O5'-P-OP1	-5.30	100.93	105.70
29	X	2709	G	N3-C4-C5	-5.30	125.95	128.60
29	X	2684	U	C5-C6-N1	5.30	125.35	122.70
29	X	2382	G	N1-C6-O6	5.29	123.08	119.90
29	X	948	C	OP1-P-O3'	5.29	116.84	105.20
29	X	957	C	C5-C6-N1	5.29	123.65	121.00
29	X	2619	C	OP1-P-O3'	5.29	116.84	105.20
29	X	2847	U	C5-C4-O4	-5.29	122.73	125.90
29	X	1949	G	C4-C5-N7	-5.29	108.68	110.80
29	X	1980	G	O5'-P-OP2	-5.29	100.94	105.70
29	X	2618	G	N1-C6-O6	5.29	123.07	119.90
30	Y	81	C	C6-N1-C2	-5.29	118.18	120.30
29	X	944	G	N1-C6-O6	5.29	123.07	119.90
29	X	1629	G	C5-C6-N1	-5.29	108.86	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1985	G	C8-N9-C4	5.28	108.51	106.40
29	X	2680	C	N1-C2-N3	5.28	122.90	119.20
29	X	2646	U	C5-C6-N1	5.28	125.34	122.70
29	X	1536	C	N1-C2-O2	5.28	122.07	118.90
29	X	1137	G	C6-C5-N7	-5.28	127.23	130.40
29	X	907	U	C5-C6-N1	-5.28	120.06	122.70
29	X	1660	C	P-O3'-C3'	-5.28	113.37	119.70
29	X	1943	U	C6-N1-C2	5.28	124.17	121.00
29	X	1993	U	N1-C2-N3	5.28	118.06	114.90
29	X	2721	A	O5'-P-OP2	-5.27	100.95	105.70
29	X	649	G	N1-C6-O6	5.27	123.06	119.90
30	Y	84	G	C8-N9-C4	5.27	108.51	106.40
29	X	983	A	N9-C4-C5	5.27	107.91	105.80
29	X	2611	U	N1-C2-O2	5.27	126.49	122.80
29	X	20	C	C6-N1-C2	-5.27	118.19	120.30
29	X	791	C	C6-N1-C2	5.27	122.41	120.30
29	X	1394	G	C4-C5-N7	5.27	112.91	110.80
29	X	2025	C	C5-C6-N1	5.27	123.63	121.00
29	X	2500	U	C6-N1-C2	-5.26	117.84	121.00
29	X	2712(A)	A	C6-C5-N7	-5.26	128.62	132.30
29	X	1231	U	C5-C6-N1	5.26	125.33	122.70
29	X	808	A	C4-C5-C6	5.25	119.62	117.00
29	X	1265	A	O5'-P-OP2	-5.25	100.98	105.70
29	X	1137	G	N1-C6-O6	5.25	123.05	119.90
29	X	911	A	C5-C6-N6	-5.24	119.50	123.70
29	X	1394	G	N3-C4-N9	5.24	129.15	126.00
29	X	2461	C	O5'-P-OP2	-5.24	100.98	105.70
29	X	2446	G	C6-C5-N7	-5.24	127.26	130.40
29	X	2008	C	O5'-P-OP1	5.23	116.98	110.70
29	X	1252	G	C4-C5-N7	-5.23	108.71	110.80
29	X	949	U	O5'-P-OP2	5.23	116.97	110.70
29	X	2832	U	C5-C6-N1	-5.23	120.08	122.70
29	X	1165	U	C5-C6-N1	-5.23	120.09	122.70
29	X	2250	G	N7-C8-N9	5.23	115.71	113.10
29	X	850	C	C6-N1-C2	-5.23	118.21	120.30
29	X	2006	C	C6-N1-C2	-5.23	118.21	120.30
29	X	2335	A	C8-N9-C4	-5.22	103.71	105.80
29	X	650	C	C6-N1-C1'	-5.22	114.53	120.80
29	X	2250	G	N1-C2-N2	5.22	120.90	116.20
29	X	1163	G	C4-C5-N7	-5.22	108.71	110.80
29	X	2013	A	OP2-P-O3'	5.22	116.68	105.20
29	X	318	C	C6-N1-C2	-5.22	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2864	G	OP1-P-O3'	5.22	116.68	105.20
29	X	409	C	C6-N1-C2	-5.22	118.21	120.30
29	X	600	C	N1-C2-O2	5.22	122.03	118.90
29	X	1747	G	N3-C4-N9	5.22	129.13	126.00
29	X	2544	G	N3-C4-C5	-5.21	125.99	128.60
29	X	974	G	C5-N7-C8	-5.21	101.69	104.30
29	X	1675	C	C4-C5-C6	5.21	120.01	117.40
29	X	1660	C	N3-C2-O2	-5.21	118.25	121.90
29	X	1977	A	N7-C8-N9	-5.21	111.19	113.80
29	X	649	G	N3-C2-N2	-5.21	116.25	119.90
29	X	2818	G	C8-N9-C4	5.21	108.48	106.40
29	X	2683	C	N3-C4-C5	-5.21	119.82	121.90
29	X	1154	G	N1-C6-O6	5.21	123.02	119.90
29	X	218	C	C6-N1-C2	-5.21	118.22	120.30
29	X	747	U	N1-C2-O2	-5.21	119.16	122.80
30	Y	91	A	C8-N9-C4	5.20	107.88	105.80
29	X	2430	A	C2-N3-C4	5.20	113.20	110.60
29	X	1322	A	OP2-P-O3'	5.20	116.64	105.20
29	X	565	C	O5'-P-OP2	5.20	116.94	110.70
29	X	1653	G	O4'-C1'-N9	5.20	112.36	108.20
29	X	2562	U	N3-C2-O2	-5.20	118.56	122.20
29	X	2824	C	C6-N1-C2	-5.19	118.22	120.30
29	X	1652	A	C5-N7-C8	-5.19	101.31	103.90
29	X	676	A	C8-N9-C4	-5.19	103.72	105.80
29	X	2250	G	C5-N7-C8	-5.19	101.71	104.30
29	X	2709	G	O5'-P-OP2	-5.18	101.03	105.70
29	X	931	U	N3-C2-O2	-5.18	118.57	122.20
29	X	1154	G	C5-C6-O6	-5.18	125.49	128.60
29	X	2037	G	O5'-P-OP2	5.18	116.92	110.70
29	X	810	U	OP1-P-O3'	5.18	116.59	105.20
29	X	2695	C	N1-C2-O2	-5.18	115.79	118.90
7	F	99	LEU	CA-CB-CG	5.18	127.21	115.30
29	X	1616	A	N9-C4-C5	5.18	107.87	105.80
29	X	2045	C	N3-C4-N4	5.18	121.62	118.00
29	X	2272	U	N3-C4-O4	-5.17	115.78	119.40
29	X	168	A	N1-C6-N6	5.17	121.70	118.60
29	X	825	A	N1-C6-N6	5.17	121.70	118.60
29	X	1156	A	C5-C6-N6	-5.17	119.56	123.70
29	X	1027	U	O4'-C1'-N1	5.17	112.33	108.20
29	X	2572	A	C5-N7-C8	5.17	106.48	103.90
29	X	1263	U	OP2-P-O3'	5.17	116.56	105.20
29	X	983	A	C5-N7-C8	5.16	106.48	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2501	C	N3-C4-C5	5.16	123.97	121.90
29	X	2060	A	O5'-P-OP1	5.16	116.89	110.70
29	X	2271	G	C6-C5-N7	-5.15	127.31	130.40
29	X	1299	G	C2-N3-C4	-5.15	109.33	111.90
29	X	2708	G	O5'-P-OP2	-5.15	101.07	105.70
29	X	496	G	OP2-P-O3'	5.14	116.52	105.20
29	X	951	C	N3-C4-N4	-5.14	114.40	118.00
29	X	1451	C	C2-N1-C1'	5.14	124.45	118.80
29	X	2883	A	OP1-P-OP2	5.14	127.31	119.60
29	X	1613	G	N3-C4-N9	5.14	129.08	126.00
29	X	2273	A	N1-C6-N6	-5.14	115.52	118.60
29	X	732	C	N3-C4-N4	-5.14	114.40	118.00
29	X	2332	U	C4-C5-C6	5.13	122.78	119.70
29	X	2830	G	C5-N7-C8	5.13	106.87	104.30
29	X	2036	C	C2-N1-C1'	5.12	124.44	118.80
29	X	1673	U	C2-N3-C4	-5.12	123.93	127.00
29	X	491	G	C5-C6-O6	5.12	131.67	128.60
29	X	2254	C	N3-C4-N4	-5.12	114.42	118.00
29	X	2576	G	N9-C4-C5	-5.12	103.35	105.40
29	X	2728	U	N3-C2-O2	-5.12	118.62	122.20
29	X	447	A	C2-N3-C4	-5.11	108.04	110.60
29	X	1490	C	C5-C6-N1	5.11	123.56	121.00
29	X	2036	C	N3-C2-O2	-5.11	118.32	121.90
29	X	2703	C	C6-N1-C2	-5.11	118.25	120.30
29	X	2488	A	OP2-P-O3'	5.11	116.44	105.20
29	X	2721	A	N1-C2-N3	5.11	131.85	129.30
29	X	2722	G	N3-C2-N2	5.11	123.48	119.90
29	X	1027	U	C6-N1-C1'	5.11	128.35	121.20
29	X	1210	G	C8-N9-C4	-5.11	104.36	106.40
29	X	2571	C	C5-C6-N1	5.11	123.55	121.00
29	X	1664	A	O4'-C1'-N9	-5.11	104.12	108.20
29	X	2003	G	C5-C6-N1	5.11	114.05	111.50
29	X	2060	A	P-O3'-C3'	5.10	125.82	119.70
29	X	2822	G	N3-C4-C5	-5.10	126.05	128.60
29	X	824	U	C2-N3-C4	-5.10	123.94	127.00
29	X	1649	G	N7-C8-N9	-5.10	110.55	113.10
29	X	2627	G	N3-C2-N2	-5.10	116.33	119.90
29	X	2574	G	C8-N9-C1'	5.10	133.63	127.00
29	X	338	G	C4-N9-C1'	5.10	133.13	126.50
29	X	992	C	C6-N1-C2	-5.10	118.26	120.30
29	X	1606	G	N1-C6-O6	-5.10	116.84	119.90
29	X	1753	A	C4-C5-C6	5.10	119.55	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	576	U	N1-C2-O2	-5.10	119.23	122.80
29	X	1006	C	O5'-P-OP1	-5.10	101.11	105.70
29	X	1759	C	C6-N1-C2	5.10	122.34	120.30
29	X	1210	G	C8-N9-C1'	-5.09	120.38	127.00
29	X	1289	C	N3-C4-C5	5.09	123.94	121.90
29	X	2773	C	OP2-P-O3'	5.09	116.40	105.20
29	X	236	C	C6-N1-C2	5.09	122.33	120.30
29	X	2841	C	O5'-P-OP1	5.09	116.81	110.70
29	X	588	U	C5-C6-N1	-5.09	120.16	122.70
29	X	2025	C	N3-C4-N4	5.09	121.56	118.00
29	X	1992	G	O5'-P-OP1	-5.08	101.12	105.70
29	X	2617	C	C6-N1-C2	5.08	122.33	120.30
29	X	2259	G	OP2-P-O3'	5.08	116.38	105.20
29	X	2685	G	O5'-P-OP2	5.08	116.79	110.70
29	X	2516	G	N1-C6-O6	-5.08	116.86	119.90
29	X	1678	U	O5'-P-OP2	5.07	116.79	110.70
29	X	1749	A	N7-C8-N9	5.07	116.33	113.80
29	X	1929	G	O4'-C1'-N9	5.07	112.25	108.20
29	X	219	G	P-O3'-C3'	5.06	125.78	119.70
29	X	1165	U	C6-N1-C2	5.06	124.04	121.00
29	X	1320	G	N1-C6-O6	-5.06	116.86	119.90
10	I	21	ARG	NE-CZ-NH2	-5.06	117.77	120.30
29	X	2551	C	N1-C2-N3	5.06	122.74	119.20
29	X	1652	A	C5-C6-N6	-5.06	119.66	123.70
29	X	2488	A	C5-C6-N6	5.06	127.75	123.70
29	X	2447	G	O4'-C1'-N9	5.06	112.25	108.20
29	X	2453	A	N1-C2-N3	-5.06	126.77	129.30
9	H	43	ARG	NE-CZ-NH2	-5.05	117.77	120.30
29	X	669	G	C2-N3-C4	5.05	114.43	111.90
29	X	1240	C	C6-N1-C2	-5.05	118.28	120.30
29	X	1279	A	N7-C8-N9	-5.05	111.27	113.80
29	X	1613	G	N3-C2-N2	5.05	123.44	119.90
29	X	1661	G	O5'-P-OP2	-5.05	101.16	105.70
29	X	2848	G	C4-C5-C6	5.05	121.83	118.80
29	X	168	A	C4-C5-C6	5.05	119.52	117.00
29	X	574	C	O5'-P-OP1	-5.05	101.16	105.70
29	X	774	A	N3-C4-C5	5.05	130.33	126.80
29	X	956	G	O5'-P-OP2	-5.05	101.16	105.70
29	X	2046	G	OP1-P-O3'	5.05	116.30	105.20
29	X	565	C	C5-C6-N1	5.04	123.52	121.00
29	X	1726	U	C5-C6-N1	-5.04	120.18	122.70
29	X	1753	A	C8-N9-C4	-5.04	103.78	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	302	U	N3-C2-O2	-5.04	118.67	122.20
29	X	1660	C	C4-C5-C6	5.04	119.92	117.40
29	X	580	C	N1-C2-O2	-5.04	115.88	118.90
29	X	669	G	N1-C2-N2	5.04	120.73	116.20
29	X	2612	C	C2-N3-C4	5.04	122.42	119.90
29	X	2724	U	C6-N1-C2	-5.04	117.98	121.00
29	X	940	G	N3-C4-C5	5.03	131.12	128.60
29	X	599	G	OP2-P-O3'	5.03	116.27	105.20
29	X	944	G	N7-C8-N9	5.03	115.61	113.10
29	X	1005	C	C6-N1-C2	-5.03	118.29	120.30
29	X	946	G	N3-C4-C5	-5.03	126.09	128.60
29	X	1253	G	OP2-P-O3'	5.03	116.26	105.20
29	X	1319	G	C8-N9-C1'	-5.03	120.46	127.00
29	X	2881	U	N3-C4-C5	-5.03	111.58	114.60
29	X	998	C	C5-C6-N1	-5.03	118.49	121.00
29	X	540	C	C6-N1-C2	5.02	122.31	120.30
29	X	2250	G	O5'-P-OP2	-5.02	101.18	105.70
29	X	2558	C	C6-N1-C2	-5.02	118.29	120.30
29	X	21	A	C8-N9-C4	-5.02	103.79	105.80
29	X	2053	G	N1-C2-N3	5.02	126.91	123.90
29	X	2067	G	C6-C5-N7	-5.02	127.39	130.40
29	X	997	G	N9-C4-C5	-5.01	103.39	105.40
29	X	2844	G	N3-C4-N9	5.01	129.01	126.00
29	X	2722	G	C4-N9-C1'	5.01	133.02	126.50
29	X	738	G	O4'-C1'-N9	5.01	112.21	108.20
29	X	783	A	C8-N9-C4	-5.01	103.80	105.80
29	X	844	U	O5'-P-OP2	-5.01	101.19	105.70
29	X	866	A	O4'-C1'-N9	-5.01	104.19	108.20
4	C	35	LEU	CA-CB-CG	-5.00	103.79	115.30
29	X	1291	U	C6-N1-C2	5.00	124.00	121.00
29	X	486	C	C2-N1-C1'	-5.00	113.30	118.80
29	X	1606	G	N7-C8-N9	-5.00	110.60	113.10
29	X	2690	C	C4-C5-C6	5.00	119.90	117.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	178	GLY	Peptide
3	B	73	ALA	Peptide
3	B	85	ALA	Peptide
4	C	187	VAL	Peptide

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Mol	Chain	Res	Type	Group
8	G	37	ASP	Peptide
25	Z	37	HIS	Peptide
25	Z	52	TYR	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	0	1651	0	1693	59	0
2	A	2107	0	2190	82	0
3	B	1540	0	1600	75	0
4	C	1507	0	1525	80	0
5	D	1401	0	1481	64	0
6	E	1287	0	1336	49	0
7	F	1048	0	1088	23	0
8	G	1115	0	1144	47	0
9	H	997	0	1046	67	0
10	I	1068	0	1103	60	0
11	J	1091	0	1125	64	0
12	K	879	0	930	43	0
13	L	778	0	820	38	0
14	M	867	0	890	43	0
15	N	978	0	1020	72	0
16	O	742	0	756	37	0
17	P	1014	0	1096	60	0
18	Q	727	0	753	25	0
19	R	826	0	881	54	0
20	S	1346	0	1372	65	0
21	T	626	0	655	33	0
22	U	553	0	604	59	0
23	V	534	0	558	16	0
24	W	424	0	470	20	0
25	Z	453	0	455	38	0
26	1	404	0	416	21	0
27	2	393	0	420	19	0
28	3	509	0	565	40	0
29	X	59673	0	30060	1282	0
30	Y	2601	0	1327	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	M	1	0	0	0	0
31	X	192	0	0	0	0
31	Y	5	0	0	0	0
All	All	89337	0	59379	2369	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 16.

All (2369) 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)
12:K:103:ARG:HD2	29:X:1287:A:H5'	1.33	1.04
9:H:41:ASN:ND2	29:X:2674:A:O2'	1.91	1.04
15:N:48:ARG:HD2	29:X:1156:A:H61	1.20	1.03
8:G:31:THR:HG21	15:N:61:TRP:HE1	1.26	1.00
29:X:500:G:H22	29:X:503:A:H5''	1.26	0.97
3:B:75:THR:HG22	3:B:77:ILE:H	1.34	0.93
17:P:85:MET:HE3	17:P:130:GLU:HG3	1.50	0.93
28:3:29:LYS:NZ	29:X:2419:U:OP2	2.03	0.92
12:K:9:LYS:NZ	29:X:2002:G:OP2	2.04	0.91
19:R:100:ASP:HB3	19:R:101:GLY:HA3	1.52	0.91
26:1:39:LYS:HB2	26:1:49:PHE:HE2	1.35	0.89
11:J:66:TYR:HB2	11:J:106:GLU:HB2	1.56	0.87
29:X:2345:G:H4'	29:X:2346:A:H5''	1.56	0.87
22:U:20:ARG:HB3	22:U:43:ARG:HH21	1.40	0.87
15:N:91:ASN:HD21	29:X:996:A:H4'	1.40	0.87
12:K:79:VAL:HA	12:K:83:VAL:HG13	1.58	0.86
19:R:96:LYS:NZ	29:X:297:C:OP1	2.08	0.86
29:X:1212:G:H1'	29:X:1237:A:H61	1.41	0.85
29:X:1526:G:H22	29:X:1546:G:H1	1.22	0.85
10:I:21:ARG:HA	29:X:811:U:H2'	1.60	0.84
14:M:2:GLN:N	29:X:2820:A:N1	2.26	0.84
29:X:2836:G:H2'	29:X:2837:A:C8	2.13	0.84
29:X:612:G:O2'	29:X:615:A:N6	2.11	0.84
18:Q:51:ILE:HD11	18:Q:81:ARG:HE	1.44	0.83
28:3:13:ARG:NH2	29:X:222:G:OP2	2.11	0.82
22:U:27:ASP:HA	22:U:32:ARG:HH21	1.43	0.82
29:X:1360:G:H22	29:X:2213:U:H3	1.25	0.82
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.59	0.82
22:U:20:ARG:HB3	22:U:43:ARG:HD2	1.61	0.82
4:C:95:LEU:HD12	4:C:96:PRO:HD2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:34:THR:OG1	29:X:2420:C:OP1	1.98	0.81
29:X:2689:U:O2	29:X:2713:U:H5''	1.81	0.81
13:L:37:HIS:ND1	30:Y:30:C:OP1	2.12	0.81
20:S:149:ALA:HB3	20:S:164:PRO:HA	1.62	0.81
20:S:105:GLN:O	20:S:109:GLN:NE2	2.12	0.81
30:Y:17:A:OP1	30:Y:110:U:O2'	1.98	0.80
29:X:309:A:N3	29:X:329:G:O2'	2.15	0.79
17:P:60:ILE:HD11	25:Z:28:PRO:HD3	1.63	0.79
27:2:43:THR:O	27:2:45:SER:N	2.16	0.79
17:P:86:LEU:HD12	17:P:89:ARG:HH21	1.45	0.79
5:D:75:SER:H	5:D:79:LEU:HD22	1.47	0.79
28:3:33:ASN:O	28:3:35:GLY:N	2.15	0.78
8:G:33:ILE:HG21	29:X:538:G:H5'	1.64	0.78
25:Z:19:ARG:NH2	29:X:1264:G:OP1	2.16	0.78
29:X:1019:U:H3	29:X:1142:A:H62	1.32	0.78
29:X:2601:C:H3'	29:X:2602:A:H5''	1.65	0.78
29:X:578:A:OP1	29:X:1255:U:O2'	2.01	0.78
28:3:17:THR:HG22	28:3:20:GLY:H	1.49	0.77
16:O:7:THR:HB	16:O:22:VAL:HG11	1.66	0.77
29:X:2693:U:H2'	29:X:2694:G:H8	1.48	0.77
29:X:679:C:H2'	29:X:680:A:H8	1.49	0.77
10:I:94:GLU:HA	10:I:97:ARG:HH11	1.50	0.77
20:S:168:VAL:HG12	20:S:169:VAL:H	1.48	0.77
11:J:15:ARG:HG3	11:J:74:PRO:HD2	1.66	0.77
11:J:42:TRP:HB3	11:J:95:VAL:HG21	1.66	0.77
29:X:844:U:H3'	29:X:845:G:C8	2.20	0.77
19:R:22:VAL:HG11	19:R:81:VAL:HG22	1.65	0.77
29:X:2320:A:N6	29:X:2333:A:O2'	2.17	0.76
22:U:23:LYS:HB3	22:U:37:ILE:HG22	1.67	0.76
30:Y:16:U:H1'	30:Y:109:G:H21	1.48	0.76
9:H:69:VAL:HG12	9:H:70:VAL:H	1.50	0.76
19:R:52:ASN:HA	19:R:73:GLU:HA	1.67	0.76
10:I:21:ARG:HH22	29:X:587:C:P	2.09	0.76
15:N:37:GLN:HG3	29:X:1252:G:H1	1.51	0.76
19:R:58:VAL:HG13	19:R:60:PRO:HD2	1.67	0.76
29:X:165(E):A:H2'	29:X:165(F):C:C6	2.21	0.76
5:D:150:ARG:HH21	29:X:2305:U:H3	1.30	0.76
25:Z:35:GLN:O	25:Z:37:HIS:N	2.18	0.76
29:X:1042:G:N2	29:X:1113:U:O2	2.18	0.75
29:X:500:G:N2	29:X:503:A:H5''	2.00	0.75
4:C:136:TRP:O	4:C:140:ASN:ND2	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:12:LYS:O	11:J:13:GLN:HB2	1.87	0.75
25:Z:19:ARG:HA	29:X:2046:G:H5'	1.67	0.75
29:X:2323:G:H1	29:X:2332:U:H5	1.34	0.75
13:L:65:THR:OG1	30:Y:52:G:OP1	2.04	0.75
14:M:57:ILE:O	14:M:58:ASN:ND2	2.20	0.75
29:X:2262:U:H2'	29:X:2263:C:H6	1.52	0.75
6:E:89:LEU:HD21	6:E:105:MET:HE1	1.69	0.75
24:W:23:LEU:HD21	24:W:43:MET:HB3	1.67	0.75
29:X:1626:A:H61	29:X:1639:U:H3	1.32	0.75
1:O:150:ARG:HA	1:O:153:LYS:HB2	1.68	0.74
22:U:32:ARG:H	22:U:32:ARG:NE	1.84	0.74
4:C:68:ARG:HH21	29:X:2060:A:H62	1.34	0.74
23:V:63:LYS:HA	23:V:66:GLN:HG3	1.67	0.74
5:D:108:LEU:HD23	5:D:111:ILE:HD12	1.69	0.74
29:X:10:A:H2'	29:X:11:G:C8	2.22	0.74
3:B:134:TRP:CD1	3:B:137:ARG:HB2	2.22	0.74
17:P:80:LEU:HD11	17:P:87:GLU:HG3	1.69	0.74
22:U:30:VAL:O	22:U:32:ARG:NH1	2.20	0.74
29:X:1926:U:OP2	29:X:1929:G:N1	2.17	0.74
20:S:25:ASN:HB3	20:S:28:ASN:H	1.51	0.74
29:X:1049:C:H42	29:X:2751:G:H1	1.33	0.74
15:N:54:LYS:NZ	29:X:995:C:OP2	2.20	0.73
29:X:1212:G:H1'	29:X:1237:A:N6	2.02	0.73
29:X:1905:C:H5''	29:X:1906:G:H5'	1.70	0.73
10:I:17:LYS:HD2	29:X:663:G:H5''	1.68	0.73
1:O:182:SER:HA	1:O:185:TYR:HB3	1.69	0.73
29:X:1283:G:H22	29:X:1286:A:H5'	1.54	0.73
29:X:1418:G:O2'	29:X:1578:U:O4	2.05	0.73
13:L:55:SER:OG	13:L:56:SER:N	2.20	0.73
29:X:1019:U:H3	29:X:1142:A:N6	1.86	0.73
4:C:68:ARG:NH2	29:X:2060:A:H62	1.85	0.73
4:C:67:ALA:HA	29:X:1255:U:C5	2.24	0.73
3:B:169:ASN:ND2	29:X:2731:G:OP1	2.21	0.73
12:K:90:ARG:NH1	29:X:2880:C:O2'	2.22	0.73
3:B:109:LYS:NZ	29:X:2723:C:OP1	2.19	0.73
29:X:828:G:H2'	29:X:829:A:C8	2.23	0.73
8:G:81:VAL:HG11	8:G:156:HIS:HD2	1.53	0.73
12:K:92:GLY:HA2	12:K:94:TYR:CZ	2.23	0.72
19:R:99:VAL:HG12	19:R:103:LYS:HG3	1.71	0.72
29:X:221:C:H4'	29:X:222:G:H5''	1.71	0.72
5:D:90:THR:OG1	30:Y:44:C:N3	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:122:PHE:HD2	5:D:129:ASN:H	1.34	0.72
12:K:33:ARG:HB2	12:K:114:GLU:HB3	1.71	0.72
20:S:117:VAL:HG23	20:S:168:VAL:HG13	1.71	0.72
3:B:93:VAL:O	3:B:95:ILE:N	2.20	0.72
25:Z:45:ILE:HG21	25:Z:57:VAL:HG23	1.69	0.72
29:X:2683:C:H2'	29:X:2684:U:H6	1.55	0.72
22:U:53:GLU:OE1	22:U:58:LYS:N	2.21	0.72
3:B:92:ASN:HD22	3:B:182:ILE:HG13	1.54	0.72
11:J:17:ARG:NH2	29:X:956:G:O6	2.22	0.72
25:Z:51:TYR:CE1	25:Z:55:ARG:HG3	2.25	0.72
3:B:189:PRO:HA	29:X:2680:C:H5'	1.70	0.72
4:C:193:LEU:HA	4:C:196:VAL:HG22	1.72	0.72
11:J:21:ASP:OD2	11:J:22:ALA:N	2.23	0.72
19:R:100:ASP:HB3	19:R:101:GLY:CA	2.20	0.72
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.23	0.72
10:I:111:SER:OG	10:I:112:GLY:N	2.23	0.71
13:L:33:ARG:HH22	13:L:103:LEU:HD12	1.55	0.71
15:N:37:GLN:HA	15:N:40:LEU:HD12	1.71	0.71
29:X:483:A:H3'	29:X:484:C:H6	1.54	0.71
29:X:635:C:O2'	29:X:639:U:OP1	2.03	0.71
12:K:3:HIS:O	12:K:5:LYS:N	2.22	0.71
20:S:4:THR:OG1	20:S:5:ALA:N	2.22	0.71
3:B:147:PRO:HG2	3:B:149:ARG:HG2	1.73	0.71
10:I:32:ARG:NH2	29:X:671:C:OP2	2.23	0.71
22:U:51:ILE:HG23	22:U:59:THR:HA	1.73	0.71
29:X:2373:A:H2'	29:X:2374:G:C8	2.25	0.71
29:X:678:C:H2'	29:X:679:C:H6	1.54	0.71
10:I:86:THR:OG1	10:I:116:ARG:NH1	2.24	0.71
29:X:1242:A:H2'	29:X:1243:C:C6	2.25	0.71
12:K:92:GLY:HA2	12:K:94:TYR:CE2	2.25	0.71
29:X:2304:G:H22	29:X:2312:U:H3	1.37	0.70
5:D:35:VAL:HG11	29:X:2314:G:H5'	1.72	0.70
2:A:134:ARG:HB3	2:A:187:SER:HB2	1.72	0.70
8:G:31:THR:HG21	15:N:61:TRP:NE1	2.06	0.70
29:X:2291:U:O2'	29:X:2374:G:N3	2.24	0.70
3:B:62:PRO:O	29:X:2786:U:O2'	2.08	0.70
29:X:303:G:H2'	29:X:304:G:C8	2.26	0.70
29:X:547:A:OP1	29:X:1221:C:H5'	1.92	0.70
29:X:1414:G:N2	29:X:1585:U:O4'	2.25	0.70
9:H:1:MET:HE2	29:X:1665:A:H1'	1.74	0.70
11:J:78:LYS:HD3	29:X:956:G:H5''	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2218:U:H2'	29:X:2219:U:C6	2.27	0.70
17:P:57:LEU:HD13	17:P:69:ALA:HA	1.74	0.70
29:X:1242:A:H2'	29:X:1243:C:H6	1.56	0.70
16:O:7:THR:O	16:O:9:GLY:N	2.25	0.69
12:K:36:THR:OG1	29:X:1278:G:OP1	2.09	0.69
1:O:130:ARG:HD2	29:X:2169:A:H5'	1.74	0.69
6:E:172:LYS:NZ	29:X:2529:G:OP2	2.17	0.69
3:B:60:ASN:HB3	3:B:62:PRO:HD2	1.74	0.69
12:K:11:ASN:OD1	29:X:1652:A:N6	2.25	0.69
29:X:1645:G:H5''	29:X:1646:C:H5'	1.73	0.69
13:L:64:LYS:HG3	30:Y:53:G:H5''	1.73	0.69
27:2:21:ARG:HD2	27:2:30:ILE:HD12	1.75	0.69
2:A:268:ARG:HH21	29:X:2224:G:H5''	1.56	0.69
12:K:31:GLU:O	12:K:33:ARG:N	2.21	0.69
4:C:22:VAL:HG13	4:C:106:MET:HG2	1.74	0.69
29:X:83:G:N2	29:X:102:G:H1'	2.08	0.69
20:S:3:LEU:HG	20:S:32:PHE:CD1	2.28	0.69
9:H:9:ASP:N	9:H:9:ASP:OD2	2.26	0.69
24:W:22:ALA:O	24:W:24:GLY:N	2.26	0.69
22:U:29:GLY:O	22:U:31:GLY:N	2.26	0.69
22:U:20:ARG:HB3	22:U:43:ARG:NH2	2.07	0.69
29:X:1607:C:N4	29:X:1622:G:OP2	2.24	0.69
29:X:165(E):A:H2'	29:X:165(F):C:H6	1.58	0.69
28:3:36:LYS:HD3	28:3:41:ILE:HD12	1.75	0.69
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.75	0.69
18:Q:64:ARG:HB2	18:Q:69:ILE:HD13	1.73	0.69
29:X:1876:A:H2'	29:X:1877:A:H8	1.58	0.69
29:X:507:A:C5'	29:X:508:A:H5'	2.23	0.69
5:D:131:GLY:HA2	5:D:154:ILE:H	1.58	0.68
29:X:1796:U:H2'	29:X:1797:C:C6	2.27	0.68
29:X:1936:A:H2	29:X:1943:U:H3	1.41	0.68
22:U:48:LYS:HG2	22:U:49:LYS:H	1.59	0.68
1:O:149:VAL:HA	1:O:152:LEU:HD12	1.75	0.68
1:O:40:HIS:HA	1:O:168:HIS:HB3	1.74	0.68
29:X:1054:A:H2'	29:X:1055:G:C8	2.29	0.68
29:X:521:G:H2'	29:X:522:A:H8	1.58	0.68
29:X:1163:G:H2'	29:X:1164:A:H8	1.58	0.68
1:O:174:ALA:HA	1:O:181:LEU:HD21	1.76	0.68
29:X:2373:A:H2'	29:X:2374:G:H8	1.57	0.68
29:X:544:C:H1'	29:X:547:A:H8	1.58	0.68
9:H:26:ASN:HB2	9:H:42:LYS:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:9:ILE:HD11	3:B:27:LEU:HB2	1.75	0.68
6:E:107:ILE:O	6:E:152:ARG:NH1	2.22	0.67
29:X:2357:G:N2	29:X:2360:A:OP2	2.26	0.67
26:1:39:LYS:HB2	26:1:49:PHE:CE2	2.24	0.67
7:F:96:VAL:HB	7:F:136:VAL:HG12	1.74	0.67
29:X:507:A:H5''	29:X:508:A:H5'	1.76	0.67
9:H:22:ILE:HD11	29:X:1952:A:N3	2.09	0.67
17:P:36:ARG:HA	17:P:39:ARG:HD2	1.77	0.67
29:X:2323:G:N1	29:X:2332:U:H5	1.92	0.67
17:P:49:SER:O	17:P:51:GLN:N	2.28	0.67
15:N:13:ARG:NH1	29:X:1251:C:OP1	2.20	0.67
2:A:161:THR:HG21	29:X:1819:A:H5''	1.75	0.67
29:X:2661:G:H2'	29:X:2662:A:C8	2.30	0.67
29:X:445:C:H2'	29:X:446:G:H5''	1.77	0.67
29:X:680:A:H2'	29:X:681:G:C8	2.30	0.67
29:X:569:U:O2'	29:X:983:A:N1	2.26	0.67
28:3:33:ASN:C	28:3:35:GLY:H	1.97	0.67
21:T:10:SER:OG	29:X:2277:G:OP2	2.13	0.67
29:X:678:C:H2'	29:X:679:C:C6	2.29	0.67
29:X:1526:G:N2	29:X:1546:G:H1	1.92	0.67
22:U:54:ASN:O	22:U:56:GLN:N	2.21	0.66
10:I:18:ARG:NH2	29:X:1250:G:N7	2.43	0.66
20:S:46:GLN:HB3	20:S:50:GLY:HA2	1.76	0.66
17:P:82:ASN:ND2	29:X:495:G:N3	2.41	0.66
9:H:109:ARG:HA	9:H:129:LEU:HD13	1.76	0.66
25:Z:51:TYR:CD1	25:Z:55:ARG:HG3	2.30	0.66
29:X:1557:G:H3'	29:X:1558:A:H5''	1.77	0.66
29:X:458:G:N2	29:X:470:A:OP2	2.26	0.66
29:X:562:U:HO2'	29:X:572:A:H8	1.44	0.66
29:X:650:C:H2'	29:X:651:G:H8	1.60	0.66
29:X:845:G:H8	29:X:845:G:OP2	1.78	0.66
9:H:124:MET:O	9:H:127:VAL:HG12	1.94	0.66
14:M:14:ARG:HB3	14:M:14:ARG:HH21	1.61	0.66
18:Q:10:PRO:HB3	18:Q:91:LEU:HD21	1.77	0.66
29:X:1124:C:H2'	29:X:1125:G:H8	1.60	0.66
29:X:920:G:N2	29:X:2269:A:OP2	2.28	0.66
2:A:142:VAL:HA	2:A:194:GLY:H	1.59	0.66
1:O:138:SER:OG	1:O:139:GLY:N	2.28	0.65
3:B:183:LEU:HD21	14:M:16:ILE:HD13	1.77	0.65
24:W:9:VAL:HG22	24:W:17:VAL:HG22	1.76	0.65
29:X:641:C:H42	29:X:646:A:H61	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:23:LYS:O	23:V:27:GLU:HG2	1.95	0.65
29:X:2461:C:H2'	29:X:2462:U:H6	1.61	0.65
4:C:154:ASP:OD1	4:C:157:THR:OG1	2.14	0.65
29:X:2319:U:H4'	29:X:2320:A:H5'	1.77	0.65
29:X:699:A:H2'	29:X:700:G:O4'	1.97	0.65
29:X:1779:U:O2	29:X:1783:A:N6	2.30	0.65
16:O:6:GLN:HB2	16:O:11:GLN:HA	1.77	0.65
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.78	0.65
8:G:34:PRO:HG3	8:G:69:ASP:OD2	1.97	0.65
4:C:27:LEU:O	4:C:31:VAL:HG23	1.96	0.65
26:1:26:LYS:HB2	26:1:31:THR:HG21	1.79	0.65
26:1:35:LEU:HB3	26:1:51:ALA:HB2	1.77	0.65
4:C:28:HIS:CD2	10:I:8:PRO:HB3	2.32	0.64
13:L:8:ARG:HH11	13:L:8:ARG:HB2	1.61	0.64
29:X:1198:U:H2'	29:X:1199:U:C6	2.32	0.64
2:A:211:ARG:NH1	29:X:1566:A:OP1	2.27	0.64
29:X:2626:C:H2'	29:X:2627:G:H8	1.62	0.64
29:X:2035:G:OP1	29:X:2035:G:H4'	1.96	0.64
4:C:7:ILE:HB	4:C:121:ASP:O	1.97	0.64
6:E:9:ILE:HG22	6:E:11:VAL:HG13	1.80	0.64
29:X:2294:C:H2'	29:X:2295:C:H6	1.63	0.64
16:O:39:PHE:HD1	16:O:47:PHE:HB3	1.62	0.64
29:X:1876:A:H2'	29:X:1877:A:C8	2.33	0.64
19:R:77:HIS:HD2	29:X:328:U:H5'	1.63	0.64
29:X:823:G:H2'	29:X:824:U:H6	1.63	0.64
9:H:22:ILE:HD11	29:X:1952:A:C4	2.32	0.64
29:X:2101:G:H2'	29:X:2102:G:C8	2.32	0.64
1:O:11:ASP:OD1	1:O:13:ASN:ND2	2.29	0.64
4:C:117:LEU:HD13	4:C:188:ILE:HD12	1.80	0.64
10:I:14:LYS:NZ	29:X:1193:G:OP1	2.27	0.64
24:W:15:ASN:OD1	24:W:16:GLN:N	2.29	0.64
29:X:1071:G:O2'	29:X:1089:G:OP2	2.15	0.64
29:X:616:A:H2'	29:X:617:A:C8	2.32	0.64
29:X:643:A:H2'	29:X:644:A:C8	2.33	0.64
1:O:16:TYR:HB3	1:O:21:ALA:HB2	1.80	0.64
16:O:21:ARG:HD3	16:O:90:PHE:CE1	2.33	0.64
29:X:1784:A:H4'	29:X:1785:A:O5'	1.98	0.64
22:U:25:ARG:NH2	29:X:2432:A:O2'	2.31	0.64
22:U:28:GLY:O	22:U:30:VAL:N	2.30	0.63
29:X:2688:C:N4	29:X:2720:U:OP2	2.30	0.63
29:X:648:G:H2'	29:X:649:G:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:78:LYS:HB3	2:A:116:THR:HG22	1.79	0.63
6:E:28:GLY:HA3	6:E:79:VAL:HB	1.78	0.63
10:I:35:LYS:NZ	29:X:568:U:OP1	2.30	0.63
11:J:36:ILE:HG12	11:J:103:VAL:HG22	1.77	0.63
29:X:2439:A:H4'	29:X:2440:C:H5''	1.79	0.63
2:A:30:GLU:HB3	2:A:33:LEU:HB2	1.79	0.63
29:X:1664:A:C2	29:X:2726:U:C2	2.86	0.63
29:X:521:G:H2'	29:X:522:A:C8	2.33	0.63
29:X:698:C:O2'	29:X:734:A:N6	2.30	0.63
29:X:823:G:H2'	29:X:824:U:C6	2.33	0.63
17:P:109:ARG:HG3	17:P:109:ARG:HH11	1.62	0.63
29:X:1429:G:H2'	29:X:1430:C:C6	2.34	0.63
29:X:395:U:H2'	29:X:396:G:C8	2.34	0.63
8:G:42:VAL:HG11	8:G:166:LEU:HB2	1.79	0.63
9:H:110:VAL:HG23	9:H:129:LEU:HB2	1.81	0.63
29:X:547:A:H5''	29:X:547:A:N3	2.14	0.63
10:I:133:VAL:HG11	10:I:140:VAL:HG23	1.79	0.63
29:X:2695:C:H2'	29:X:2696:U:H6	1.64	0.63
29:X:634:G:H2'	29:X:635:C:H6	1.64	0.63
4:C:9:GLN:O	4:C:10:ASN:ND2	2.32	0.63
8:G:151:TYR:OH	8:G:158:HIS:NE2	2.32	0.63
18:Q:35:LYS:HD2	18:Q:53:ILE:HG23	1.80	0.63
29:X:1289:C:H2'	29:X:1290:U:H6	1.64	0.63
2:A:157:ARG:NH1	29:X:1818:U:OP2	2.31	0.63
15:N:58:ARG:O	15:N:62:ILE:HG13	1.98	0.62
29:X:2845:C:H2'	29:X:2846:G:H8	1.64	0.62
9:H:83:ARG:HD3	9:H:89:ILE:HD11	1.81	0.62
11:J:52:ARG:NH1	11:J:53:ILE:HG12	2.14	0.62
2:A:223:GLY:HA2	2:A:226:MET:HG3	1.81	0.62
10:I:63:ARG:NH1	29:X:2417:C:OP1	2.33	0.62
15:N:50:ARG:HA	15:N:53:LYS:HE2	1.82	0.62
17:P:15:LYS:NZ	29:X:502:A:O2'	2.17	0.62
2:A:259:THR:HG1	29:X:1797:C:HO2'	1.45	0.62
15:N:92:ARG:HG2	29:X:997:G:OP1	2.00	0.62
16:O:18:ASP:N	16:O:18:ASP:OD1	2.33	0.62
4:C:46:ARG:HB3	4:C:50:GLN:HB2	1.80	0.62
29:X:776:G:N1	29:X:2072:G:OP1	2.24	0.62
29:X:1783:A:HO2'	29:X:2607:G:HO2'	1.47	0.62
9:H:69:VAL:HG12	9:H:70:VAL:N	2.14	0.62
16:O:62:GLU:HG3	16:O:63:HIS:N	2.14	0.62
19:R:48:VAL:O	19:R:50:GLY:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:56:VAL:O	20:S:58:GLY:N	2.33	0.62
6:E:99:THR:HB	6:E:102:ALA:HB3	1.81	0.62
29:X:2693:U:H2'	29:X:2694:G:C8	2.34	0.62
29:X:2849:C:H4'	29:X:2850:A:H5'	1.81	0.62
29:X:1848:A:H2'	29:X:1849:G:O4'	2.00	0.62
29:X:27:G:O2'	29:X:28:A:OP2	2.16	0.62
29:X:657:U:H2'	29:X:658:A:C8	2.35	0.62
29:X:2219:U:H3'	29:X:2220:C:H4'	1.80	0.62
14:M:55:ILE:HA	14:M:104:LEU:HD12	1.82	0.61
20:S:74:ARG:HH22	30:Y:94:G:H5''	1.64	0.61
29:X:1495:A:N1	29:X:1496:A:N6	2.47	0.61
29:X:2168:G:N2	29:X:2171:A:O4'	2.32	0.61
14:M:104:LEU:HA	14:M:106:TYR:CE2	2.35	0.61
16:O:78:VAL:HG12	16:O:80:TYR:HB2	1.82	0.61
17:P:114:ALA:HB2	29:X:1614:A:N1	2.15	0.61
29:X:2218:U:H2'	29:X:2219:U:C5	2.35	0.61
29:X:2060:A:H1'	29:X:2502:G:C1'	2.30	0.61
29:X:634:G:H2'	29:X:635:C:C6	2.35	0.61
22:U:49:LYS:HB2	22:U:61:TRP:CE3	2.35	0.61
10:I:16:ARG:HH22	29:X:589:U:P	2.23	0.61
2:A:271:VAL:HG22	2:A:272:THR:HG23	1.82	0.61
5:D:103:LEU:HD12	5:D:107:GLY:HA3	1.82	0.61
9:H:99:ILE:HD12	9:H:103:GLY:HA2	1.81	0.61
19:R:76:LEU:HD22	19:R:80:LYS:HD3	1.81	0.61
20:S:39:PHE:CE1	20:S:43:PHE:HB2	2.36	0.61
29:X:1450:G:H2'	29:X:1451:C:H6	1.65	0.61
29:X:2448:A:HO2'	29:X:2449:U:H5	1.45	0.61
29:X:2845:C:H2'	29:X:2846:G:C8	2.36	0.61
29:X:807:U:H2'	29:X:808:A:H8	1.64	0.61
29:X:960:A:H5''	29:X:961:C:OP2	2.00	0.61
3:B:119:ARG:HG2	3:B:120:TRP:CD1	2.35	0.61
19:R:51:VAL:HG13	19:R:52:ASN:H	1.65	0.61
29:X:744:U:H2'	29:X:745:G:O4'	2.00	0.61
6:E:92:VAL:HG23	6:E:160:LYS:HE2	1.83	0.61
10:I:94:GLU:HA	10:I:97:ARG:NH1	2.15	0.61
19:R:22:VAL:HG13	19:R:82:ALA:H	1.65	0.61
29:X:2057:A:H2'	29:X:2058:A:C8	2.35	0.61
29:X:443:A:H2	29:X:1245:G:N3	1.97	0.61
9:H:88:THR:HB	14:M:80:VAL:HB	1.82	0.61
12:K:28:LEU:HD21	12:K:115:LEU:HD11	1.81	0.61
29:X:1188:U:H2'	29:X:1189:A:H8	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:39:ARG:NH2	29:X:468:G:N7	2.48	0.61
29:X:1124:C:H2'	29:X:1125:G:C8	2.35	0.61
29:X:2874:C:H2'	29:X:2875:U:H6	1.66	0.61
29:X:733:G:N7	29:X:761:A:C6	2.69	0.61
1:0:112:THR:HB	1:0:115:MET:HB2	1.83	0.61
16:O:80:TYR:CE2	29:X:1187:G:H5''	2.36	0.60
29:X:2347:C:H2'	29:X:2348:U:C6	2.36	0.60
1:0:205:LEU:HB3	1:0:222:LEU:HD13	1.83	0.60
12:K:87:TYR:CD1	12:K:90:ARG:HD2	2.36	0.60
15:N:48:ARG:HD2	29:X:1156:A:N6	2.03	0.60
29:X:1423:A:H2'	29:X:1424:G:H8	1.65	0.60
29:X:323:G:OP1	29:X:338:G:N2	2.33	0.60
5:D:66:ILE:HD11	30:Y:43:G:H2'	1.82	0.60
16:O:14:VAL:HG11	16:O:95:ILE:HG13	1.82	0.60
20:S:151:ASP:N	20:S:151:ASP:OD2	2.33	0.60
29:X:536:A:H2'	29:X:537:U:C6	2.36	0.60
5:D:150:ARG:NH2	29:X:2305:U:H3	1.98	0.60
3:B:111:LYS:NZ	29:X:2724:U:OP1	2.24	0.60
25:Z:15:LYS:O	25:Z:18:MET:N	2.33	0.60
5:D:166:ALA:O	5:D:170:LEU:HG	2.02	0.60
6:E:130:ARG:NH1	6:E:132:ASP:OD2	2.35	0.60
15:N:74:MET:HE2	15:N:110:VAL:HG13	1.83	0.60
1:0:72:VAL:HB	1:0:90:VAL:HG13	1.83	0.60
15:N:17:VAL:HG21	15:N:32:TYR:HE1	1.65	0.60
15:N:81:ASN:HD22	29:X:1151:A:H4'	1.66	0.60
29:X:439:A:H2'	29:X:440:G:C8	2.36	0.60
29:X:79:C:H2'	29:X:80:G:H8	1.66	0.60
28:3:54:GLU:O	28:3:58:MET:HG2	2.01	0.60
3:B:51:TYR:N	3:B:75:THR:HG21	2.16	0.60
4:C:53:LYS:HB2	4:C:73:SER:HB3	1.84	0.60
20:S:138:VAL:HA	20:S:141:MET:HE3	1.84	0.60
22:U:20:ARG:CB	22:U:43:ARG:HD2	2.31	0.60
29:X:1423:A:H2'	29:X:1424:G:C8	2.37	0.60
29:X:2267:A:H5''	29:X:2268:A:H5'	1.83	0.60
12:K:79:VAL:HA	12:K:83:VAL:CG1	2.30	0.60
29:X:2100:G:H1	29:X:2189:U:H3	1.49	0.60
29:X:2262:U:H2'	29:X:2263:C:C6	2.35	0.60
29:X:2532:G:O2'	29:X:2657:A:N1	2.34	0.60
1:0:29:ALA:HB1	1:0:35:GLU:HB3	1.82	0.59
6:E:124:ALA:HB3	6:E:132:ASP:HB2	1.83	0.59
20:S:3:LEU:HD21	20:S:56:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:171:ILE:HD12	1:0:181:LEU:HD22	1.84	0.59
4:C:164:VAL:HB	4:C:167:VAL:HG22	1.82	0.59
11:J:69:ILE:HG23	11:J:104:MET:HA	1.84	0.59
29:X:120:U:H4'	29:X:121:G:H5''	1.84	0.59
29:X:303:G:H2'	29:X:304:G:H8	1.66	0.59
27:2:34:ARG:HD3	29:X:467:G:OP2	2.01	0.59
29:X:650:C:H2'	29:X:651:G:C8	2.37	0.59
2:A:13:ARG:NH2	29:X:729:G:OP2	2.25	0.59
11:J:35:LEU:HD23	11:J:105:PHE:HD2	1.67	0.59
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.83	0.59
21:T:26:PHE:HE1	29:X:857:C:H1'	1.67	0.59
22:U:20:ARG:HD3	22:U:43:ARG:CZ	2.32	0.59
29:X:1323:G:H2'	29:X:1324:G:H5'	1.85	0.59
29:X:676:A:C8	29:X:2443:C:H1'	2.37	0.59
25:Z:16:ARG:HD2	25:Z:20:ARG:NH1	2.17	0.59
28:3:17:THR:HG22	28:3:21:LYS:H	1.67	0.59
2:A:260:ARG:HH22	2:A:266:SER:HB2	1.67	0.59
5:D:74:ILE:HA	5:D:79:LEU:HB2	1.83	0.59
29:X:2307:G:H3'	29:X:2308:G:H8	1.68	0.59
25:Z:3:LYS:HD3	29:X:2611:U:H3'	1.83	0.59
30:Y:15:A:N1	30:Y:71:G:O2'	2.27	0.59
1:0:18:ILE:HG12	1:0:185:TYR:HE1	1.67	0.59
29:X:2626:C:H2'	29:X:2627:G:C8	2.38	0.59
12:K:13:ASN:C	12:K:17:ARG:HH21	2.05	0.59
13:L:63:ASN:HB2	13:L:67:THR:HG23	1.83	0.59
17:P:86:LEU:N	17:P:130:GLU:OE2	2.34	0.59
30:Y:64:C:H2'	30:Y:65:A:H8	1.67	0.59
20:S:4:THR:HA	20:S:57:GLU:HB2	1.83	0.59
22:U:21:ARG:HH21	22:U:23:LYS:HG2	1.67	0.59
15:N:44:THR:O	15:N:48:ARG:HG2	2.03	0.59
29:X:100:U:O2	29:X:102:G:N1	2.36	0.59
14:M:60:SER:HA	14:M:64:LYS:HB2	1.84	0.59
29:X:2522:U:O2'	29:X:2647:U:OP1	2.17	0.59
15:N:13:ARG:NH1	29:X:1251:C:H5''	2.17	0.59
29:X:2091:U:H5''	29:X:2092:U:H2'	1.85	0.59
29:X:680:A:H2'	29:X:681:G:H8	1.67	0.59
1:0:68:VAL:HG21	1:0:153:LYS:HG2	1.85	0.58
27:2:34:ARG:NH2	27:2:41:GLN:O	2.36	0.58
13:L:15:ARG:NH2	29:X:2293:A:O5'	2.36	0.58
11:J:23:LYS:O	20:S:73:LYS:NZ	2.36	0.58
29:X:1450:G:H2'	29:X:1451:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2308:G:OP1	29:X:2310:A:N6	2.31	0.58
28:3:58:MET:HA	28:3:61:MET:HG3	1.86	0.58
2:A:39:LYS:NZ	2:A:57:GLY:O	2.36	0.58
2:A:7:LYS:NZ	29:X:706:A:OP1	2.35	0.58
29:X:1047:G:O2'	29:X:1109:C:N4	2.36	0.58
29:X:1405:C:H2'	29:X:1406:G:C8	2.38	0.58
6:E:160:LYS:NZ	29:X:2658:C:OP1	2.32	0.58
4:C:189:ASP:OD1	4:C:190:ALA:N	2.29	0.58
29:X:1412:U:H3'	29:X:1413:G:H5''	1.85	0.58
29:X:1657:C:H2'	29:X:1658:C:H6	1.67	0.58
29:X:1827:U:H5'	29:X:1971:A:H5'	1.86	0.58
28:3:10:ALA:HB1	28:3:14:ILE:HD12	1.84	0.58
8:G:62:ILE:O	8:G:77:GLY:HA3	2.04	0.58
8:G:91:THR:O	8:G:94:LYS:HB2	2.03	0.58
15:N:92:ARG:HA	15:N:95:LEU:HB2	1.86	0.58
29:X:2438:U:O2'	29:X:2440:C:OP1	2.20	0.58
29:X:642:G:H21	29:X:645:U:H3	1.50	0.58
30:Y:27:A:H8	30:Y:27:A:OP2	1.86	0.58
29:X:2233:U:H2'	29:X:2234:G:C8	2.39	0.58
29:X:493:G:H2'	29:X:494:G:O4'	2.04	0.58
2:A:108:PRO:HB3	2:A:143:HIS:HE1	1.69	0.58
12:K:85:PRO:O	12:K:88:ALA:HB2	2.04	0.58
15:N:83:LEU:HD23	15:N:113:SER:HB2	1.84	0.58
29:X:2521:C:H2'	29:X:2522:U:C6	2.38	0.58
4:C:119:ALA:HA	4:C:189:ASP:O	2.03	0.58
10:I:19:VAL:HB	10:I:30:ALA:HB1	1.84	0.58
15:N:75:ASN:OD1	15:N:77:SER:N	2.37	0.58
25:Z:16:ARG:NH1	29:X:1263:U:OP1	2.36	0.58
29:X:1676:A:C2	29:X:1993:U:H5'	2.39	0.58
29:X:820:A:N3	29:X:943:U:O2'	2.31	0.58
4:C:179:ASP:OD1	4:C:182:ARG:NH2	2.37	0.58
10:I:41:SER:HB2	29:X:671:C:C6	2.39	0.58
11:J:41:ALA:HB2	11:J:128:ILE:HG21	1.85	0.58
17:P:91:PHE:CD2	17:P:131:LYS:HB2	2.38	0.58
22:U:17:SER:HA	22:U:18:VAL:HB	1.86	0.58
22:U:51:ILE:HG12	22:U:59:THR:HB	1.86	0.58
29:X:24:G:H2'	29:X:25:U:H6	1.68	0.58
29:X:302:U:H2'	29:X:303:G:H8	1.69	0.58
29:X:740:U:H2'	29:X:741:G:C8	2.39	0.58
6:E:24:PHE:HB2	6:E:37:TYR:CD1	2.39	0.58
14:M:102:ALA:O	14:M:103:LYS:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:81:ASN:OD1	15:N:82:GLY:N	2.37	0.58
21:T:84:ALA:O	21:T:85:GLN:HB3	2.03	0.58
29:X:1283:G:N2	29:X:1286:A:H5'	2.17	0.58
29:X:576:U:H2'	29:X:577:G:C8	2.39	0.58
6:E:37:TYR:HD2	6:E:68:THR:HG23	1.69	0.58
7:F:115:LEU:HD22	7:F:126:THR:HG21	1.86	0.58
8:G:146:THR:O	8:G:149:LYS:NZ	2.37	0.58
11:J:32:ASP:H	11:J:108:ALA:HB2	1.68	0.58
21:T:21:LEU:HD11	21:T:41:ARG:HE	1.69	0.58
8:G:110:LEU:HD13	29:X:1131:G:O4'	2.03	0.58
29:X:1217:C:H2'	29:X:1218:A:H8	1.69	0.58
29:X:127:A:H5''	29:X:128:C:C6	2.39	0.58
29:X:2221:G:H2'	29:X:2222:G:C8	2.39	0.58
29:X:544:C:H1'	29:X:547:A:C8	2.38	0.58
19:R:19:GLY:H	19:R:36:VAL:HB	1.69	0.57
4:C:22:VAL:HG11	4:C:110:SER:HB3	1.86	0.57
5:D:60:ILE:HG22	5:D:140:GLU:HB2	1.86	0.57
13:L:33:ARG:HD2	13:L:99:ARG:HB2	1.86	0.57
21:T:39:ARG:HH21	29:X:2355:C:H1'	1.68	0.57
24:W:10:ILE:HD13	29:X:989:G:C8	2.39	0.57
16:O:70:TYR:OH	29:X:1223:G:O6	2.22	0.57
29:X:1657:C:H2'	29:X:1658:C:C6	2.39	0.57
29:X:2060:A:H1'	29:X:2502:G:O4'	2.04	0.57
29:X:2438:U:O2'	29:X:2439:A:H5''	2.04	0.57
29:X:2650:U:H2'	29:X:2651:C:H6	1.69	0.57
29:X:483:A:H3'	29:X:484:C:C6	2.39	0.57
29:X:14:A:C6	29:X:526:A:C2	2.92	0.57
4:C:106:MET:O	4:C:110:SER:OG	2.18	0.57
4:C:186:LEU:HG	4:C:188:ILE:HD13	1.86	0.57
20:S:68:ALA:HB3	20:S:82:ASP:HB2	1.86	0.57
29:X:1841:U:H2'	29:X:1842:G:H8	1.69	0.57
2:A:25:ALA:HB3	2:A:81:ALA:HB1	1.87	0.57
4:C:15:ILE:HG12	4:C:197:GLU:HB2	1.86	0.57
29:X:1087:G:N2	29:X:1089:G:O2'	2.38	0.57
29:X:1353:A:H2'	29:X:1354:A:C8	2.39	0.57
29:X:1783:A:O2'	29:X:2607:G:O2'	2.21	0.57
29:X:2219:U:C3'	29:X:2220:C:H4'	2.35	0.57
29:X:2801:G:H2'	29:X:2802:G:C8	2.39	0.57
19:R:77:HIS:HD2	29:X:328:U:H4'	1.70	0.57
11:J:111:THR:HG23	11:J:114:GLN:HG3	1.85	0.57
29:X:165:A:H2'	29:X:165(A):G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2063:C:O2	29:X:2451:A:C2	2.58	0.57
29:X:2751:G:N2	29:X:2751:G:OP1	2.32	0.57
29:X:465:G:C6	29:X:466:A:N6	2.73	0.57
29:X:588:U:H2'	29:X:589:U:C6	2.40	0.57
30:Y:67:C:N4	30:Y:111:C:O2'	2.32	0.57
5:D:108:LEU:HA	5:D:111:ILE:HG13	1.86	0.57
5:D:60:ILE:HG13	5:D:61:THR:HG23	1.85	0.57
9:H:62:GLY:O	9:H:65:LYS:HE3	2.05	0.57
9:H:119:ARG:NE	14:M:41:GLU:OE1	2.38	0.57
17:P:87:GLU:O	17:P:89:ARG:N	2.33	0.57
20:S:10:PRO:HB2	20:S:14:LEU:HD21	1.86	0.57
29:X:1936:A:H2	29:X:1943:U:N3	2.02	0.57
1:O:136:PRO:HA	1:O:141:VAL:HG11	1.86	0.57
6:E:37:TYR:CD2	6:E:68:THR:HG23	2.39	0.57
27:2:7:PRO:HB2	29:X:1309:G:H4'	1.87	0.57
29:X:322:A:H5'	29:X:340:A:H1'	1.87	0.57
29:X:651(A):G:H2'	29:X:651(B):C:H4'	1.86	0.57
2:A:143:HIS:ND1	2:A:194:GLY:O	2.35	0.57
14:M:57:ILE:C	14:M:58:ASN:HD22	2.08	0.57
29:X:640:C:H2'	29:X:641:C:C6	2.40	0.57
29:X:679:C:H2'	29:X:680:A:C8	2.35	0.57
30:Y:6:C:H2'	30:Y:7:C:C6	2.40	0.57
26:1:31:THR:O	26:1:33:ALA:N	2.38	0.57
8:G:31:THR:OG1	29:X:995:C:N3	2.38	0.57
10:I:90:ARG:HD2	10:I:93:LEU:HG	1.87	0.57
11:J:42:TRP:HB3	11:J:95:VAL:CG2	2.34	0.57
19:R:58:VAL:HG22	19:R:59:LYS:H	1.70	0.57
22:U:27:ASP:C	22:U:32:ARG:HD3	2.24	0.57
7:F:133:SER:HB3	29:X:1062:G:H21	1.70	0.57
14:M:100:ARG:HG3	29:X:1747:G:H5''	1.87	0.57
5:D:41:GLY:O	5:D:43:SER:N	2.38	0.57
17:P:50:VAL:HG21	17:P:90:LEU:HB3	1.86	0.57
22:U:14:VAL:O	22:U:16:ASN:N	2.37	0.57
29:X:1153:C:H2'	29:X:1154:G:C8	2.39	0.57
29:X:474:G:C6	29:X:510:C:N4	2.73	0.57
29:X:920:G:C2	29:X:921:G:H1'	2.40	0.57
20:S:15:ASP:O	20:S:17:SER:N	2.38	0.56
25:Z:55:ARG:NH2	25:Z:59:ALA:H	2.03	0.56
10:I:115:SER:O	10:I:136:ALA:HB1	2.04	0.56
22:U:48:LYS:HG2	22:U:49:LYS:N	2.19	0.56
19:R:77:HIS:CD2	29:X:328:U:H5'	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:8:LEU:N	9:H:8:LEU:HD23	2.21	0.56
19:R:15:HIS:ND1	29:X:336:C:H4'	2.20	0.56
29:X:1224:G:O2'	29:X:1225:A:H5'	2.04	0.56
29:X:214:G:N2	29:X:226:G:H2'	2.20	0.56
29:X:536:A:H2'	29:X:537:U:H6	1.70	0.56
11:J:77:LYS:HG2	29:X:957:C:H5'	1.86	0.56
4:C:47:THR:H	4:C:50:GLN:HG3	1.70	0.56
29:X:2168:G:N1	29:X:2171:A:OP2	2.37	0.56
3:B:91:VAL:HB	3:B:93:VAL:HG12	1.87	0.56
11:J:75:VAL:HB	11:J:93:TYR:CE2	2.41	0.56
29:X:2256:G:N2	29:X:2275:C:C4	2.73	0.56
29:X:2408:U:H2'	29:X:2409:G:H8	1.71	0.56
29:X:1939:U:OP1	29:X:2604:U:O2'	2.23	0.56
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.21	0.56
29:X:413:C:O2'	29:X:1880:U:O2'	2.17	0.56
29:X:2345:G:N3	29:X:2381:C:H2'	2.21	0.56
29:X:392:C:H2'	29:X:393:G:H8	1.70	0.56
29:X:676:A:H8	29:X:2443:C:H1'	1.68	0.56
1:O:29:ALA:O	1:O:31:ALA:N	2.38	0.56
2:A:78:LYS:NZ	29:X:1502:C:OP1	2.37	0.56
5:D:127:ASN:ND2	5:D:158:THR:O	2.39	0.56
19:R:105:ARG:HD3	19:R:112:LYS:HD3	1.87	0.56
22:U:13:LEU:HD12	22:U:14:VAL:H	1.70	0.56
29:X:2182:A:H2'	29:X:2183:G:H8	1.71	0.56
3:B:120:TRP:CE3	3:B:155:ARG:HD2	2.41	0.56
21:T:15:ASP:OD1	29:X:2264:C:N4	2.38	0.56
6:E:67:LEU:HD11	29:X:2758:A:C5	2.41	0.56
27:2:12:ARG:HG3	29:X:686:G:O6	2.06	0.56
29:X:981:A:H2	29:X:2027:G:N3	2.03	0.56
30:Y:62:C:H2'	30:Y:63:A:H8	1.70	0.56
1:O:10:VAL:HG11	1:O:216:PRO:HG2	1.87	0.56
18:Q:84:GLU:HB2	18:Q:86:GLN:HG3	1.88	0.56
16:O:83:ARG:HG2	29:X:1225:A:H4'	1.88	0.56
29:X:1676:A:N6	29:X:1677:A:N1	2.53	0.56
3:B:48:GLN:NE2	29:X:2635:A:O2'	2.37	0.56
29:X:2691:C:H5'	29:X:2872:G:H5'	1.87	0.56
26:I:45:ALA:HB1	29:X:2371:G:H4'	1.88	0.56
13:L:47:ARG:NH1	13:L:49:GLN:OE1	2.38	0.56
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.87	0.56
29:X:2564:A:C6	29:X:2565:A:N1	2.74	0.56
29:X:2729:C:H2'	29:X:2730:C:H6	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:546:U:H5'	29:X:547:A:C2	2.41	0.56
17:P:18:VAL:O	17:P:19:LYS:HB2	2.05	0.56
29:X:1373:A:H5''	29:X:2212:A:N6	2.21	0.56
29:X:1787:U:H2'	29:X:1788:C:H6	1.71	0.56
29:X:1906:G:O2'	29:X:1907:G:H5''	2.06	0.56
29:X:2289:G:N2	29:X:2344:U:O2	2.39	0.56
21:T:53:MET:HG3	21:T:59:LEU:HD23	1.88	0.55
2:A:168:LYS:HG3	2:A:173:VAL:HG22	1.87	0.55
3:B:105:THR:HB	3:B:197:VAL:CG1	2.36	0.55
15:N:75:ASN:HD21	29:X:1011:A:P	2.28	0.55
29:X:515:A:H2	29:X:1260:G:N3	2.04	0.55
3:B:136:ARG:HB2	29:X:1657:C:P	2.46	0.55
29:X:2229:U:H2'	29:X:2230:G:H8	1.70	0.55
8:G:110:LEU:HD22	29:X:1131:G:H4'	1.88	0.55
17:P:114:ALA:O	17:P:115:ASN:ND2	2.39	0.55
19:R:18:LYS:NZ	19:R:37:LEU:O	2.39	0.55
29:X:2018:G:H2'	29:X:2019:A:C8	2.41	0.55
6:E:143:GLN:HG3	29:X:2745:C:O2'	2.07	0.55
26:I:19:GLY:HA3	29:X:2400:G:H4'	1.89	0.55
5:D:83:MET:HG2	5:D:84:PRO:HD2	1.87	0.55
8:G:142:ARG:HA	8:G:145:HIS:CD2	2.42	0.55
8:G:151:TYR:HH	8:G:158:HIS:CD2	2.24	0.55
13:L:33:ARG:HE	13:L:38:ILE:HG21	1.70	0.55
29:X:2376:A:H8	29:X:2376:A:OP1	1.89	0.55
29:X:24:G:H2'	29:X:25:U:C6	2.41	0.55
29:X:2652:C:H2'	29:X:2653:U:O4'	2.06	0.55
15:N:91:ASN:ND2	29:X:996:A:H4'	2.15	0.55
11:J:12:LYS:HD3	29:X:911:A:C6	2.41	0.55
11:J:49:GLU:O	11:J:53:ILE:HG13	2.07	0.55
15:N:37:GLN:HG3	29:X:1252:G:N1	2.21	0.55
29:X:1270:C:H5''	29:X:1271:G:O5'	2.07	0.55
29:X:2168:G:N2	29:X:2171:A:O5'	2.39	0.55
15:N:31:GLN:NE2	29:X:580:C:H4'	2.21	0.55
4:C:22:VAL:HG21	4:C:110:SER:HA	1.88	0.55
9:H:21:CYS:SG	9:H:22:ILE:N	2.80	0.55
12:K:106:ASP:HB3	29:X:1287:A:N7	2.22	0.55
15:N:33:ARG:HD2	29:X:1252:G:N3	2.22	0.55
8:G:32:TYR:O	15:N:64:ARG:NH1	2.37	0.55
29:X:1024:G:C6	29:X:1025:G:C6	2.95	0.55
29:X:1060:U:H4'	29:X:1061:U:H5'	1.88	0.55
29:X:1678:U:O2'	29:X:1679:C:H5'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:864:G:H1'	29:X:914:C:N4	2.22	0.55
29:X:989:G:OP1	29:X:1157:G:O2'	2.22	0.55
30:Y:34:C:H2'	30:Y:35:C:C6	2.42	0.55
28:3:33:ASN:O	28:3:36:LYS:HA	2.07	0.55
22:U:64:ALA:O	22:U:67:ILE:HG22	2.07	0.55
29:X:1055:G:H1	29:X:1104:C:H42	1.54	0.55
29:X:1268:A:H2'	29:X:1269:A:O4'	2.07	0.55
29:X:1427:A:H4'	29:X:1428:C:O5'	2.05	0.55
29:X:1653:G:H8	29:X:1653:G:OP2	1.90	0.55
29:X:2280:G:H1'	29:X:2327:A:H1'	1.88	0.55
29:X:588:U:O4	29:X:670:A:H1'	2.07	0.55
1:0:10:VAL:HG22	1:0:218:ILE:HD11	1.88	0.55
4:C:192:ALA:HA	4:C:195:ILE:HD11	1.88	0.55
5:D:9:ASN:O	5:D:13:ARG:HG3	2.07	0.55
6:E:37:TYR:CE2	6:E:72:VAL:HG22	2.42	0.55
17:P:59:PHE:HD1	25:Z:30:LEU:HD11	1.72	0.55
29:X:2318:G:O2'	29:X:2321:G:O6	2.24	0.55
29:X:2330:G:H2'	29:X:2331:G:O4'	2.06	0.55
29:X:2619:C:O2'	29:X:2620:U:H5'	2.07	0.55
29:X:2716:A:O2'	29:X:2717:G:H5'	2.07	0.55
29:X:936:C:H2'	29:X:937:C:H6	1.72	0.55
9:H:13:ASN:OD1	9:H:108:THR:N	2.40	0.55
12:K:87:TYR:OH	12:K:115:LEU:HB3	2.07	0.55
29:X:2756:U:H4'	29:X:2757:A:OP1	2.07	0.55
29:X:345:A:H2'	29:X:346:A:N7	2.22	0.55
29:X:733:G:N7	29:X:761:A:N6	2.54	0.55
29:X:740:U:H2'	29:X:741:G:H8	1.72	0.55
13:L:22:ALA:O	13:L:24:SER:N	2.40	0.55
17:P:32:ARG:HH21	17:P:119:LYS:HG2	1.71	0.55
29:X:2328:A:H2'	29:X:2329:A:C8	2.42	0.55
3:B:14:ILE:HD11	3:B:173:VAL:HG11	1.88	0.54
11:J:44:LYS:HB2	11:J:47:GLN:HG3	1.88	0.54
13:L:26:LYS:HD3	13:L:87:VAL:O	2.07	0.54
14:M:104:LEU:HD23	14:M:106:TYR:HE2	1.72	0.54
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.89	0.54
20:S:91:PRO:HD3	20:S:127:PRO:HD3	1.88	0.54
21:T:51:VAL:HG11	21:T:79:ILE:O	2.06	0.54
4:C:39:ARG:HG2	29:X:443:A:N7	2.21	0.54
5:D:14:PRO:HA	5:D:17:MET:HB2	1.89	0.54
8:G:92:GLY:HA2	8:G:94:LYS:H	1.71	0.54
14:M:69:ARG:HB2	14:M:78:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1151:A:H2'	29:X:1152:C:H6	1.73	0.54
29:X:1172(B):C:H2'	29:X:1172(C):G:H2'	1.88	0.54
29:X:1429:G:H2'	29:X:1430:C:H6	1.71	0.54
29:X:20:C:H2'	29:X:21:A:H8	1.73	0.54
29:X:695:G:OP1	29:X:1380:G:O2'	2.23	0.54
28:3:25:PHE:HA	28:3:47:GLY:HA2	1.89	0.54
28:3:21:LYS:HB3	28:3:55:TRP:CH2	2.42	0.54
29:X:1203:U:H2'	29:X:1204:C:C6	2.42	0.54
29:X:733:G:C8	29:X:761:A:N6	2.76	0.54
4:C:56:ARG:HB2	29:X:797:U:OP2	2.07	0.54
30:Y:64:C:H2'	30:Y:65:A:C8	2.42	0.54
1:0:152:LEU:HD23	1:0:157:ILE:HD12	1.89	0.54
1:0:157:ILE:HD13	1:0:157:ILE:H	1.72	0.54
28:3:29:LYS:NZ	28:3:41:ILE:HG23	2.22	0.54
5:D:106:ILE:HB	5:D:139:PRO:HB3	1.89	0.54
9:H:13:ASN:HD21	9:H:109:ARG:H	1.55	0.54
29:X:2314:G:H2'	29:X:2315:U:C6	2.43	0.54
29:X:2519:U:C5	29:X:2541:A:C6	2.95	0.54
29:X:936:C:H2'	29:X:937:C:C6	2.43	0.54
2:A:151:LYS:HD3	29:X:2203:G:H4'	1.88	0.54
7:F:30:TYR:HB2	7:F:59:ILE:HD12	1.89	0.54
17:P:109:ARG:HG3	17:P:109:ARG:NH1	2.21	0.54
29:X:83:G:H1	29:X:102:G:HO2'	1.55	0.54
29:X:2028:U:H2'	29:X:2029:A:C8	2.43	0.54
29:X:2203:G:H2'	29:X:2204:A:H8	1.71	0.54
29:X:1127:A:C8	29:X:2518:A:H5''	2.43	0.54
1:0:180:ASN:HA	1:0:183:ALA:HB3	1.88	0.54
5:D:111:ILE:HG12	5:D:137:ILE:HD12	1.90	0.54
5:D:135:GLN:HG3	5:D:151:GLY:HA2	1.89	0.54
13:L:38:ILE:HD12	13:L:40:ALA:H	1.73	0.54
22:U:78:ILE:HG12	22:U:79:GLU:H	1.72	0.54
24:W:25:LEU:HD22	24:W:30:ASP:HB3	1.90	0.54
2:A:50:THR:HG22	29:X:1813:G:H21	1.72	0.54
5:D:116:GLY:HA2	5:D:176:PRO:HB2	1.90	0.54
8:G:43:VAL:HG23	8:G:163:PRO:HB2	1.90	0.54
2:A:44:ASN:O	2:A:46:ARG:N	2.41	0.54
3:B:144:ARG:NH1	29:X:2572:A:C4	2.75	0.54
4:C:4:ILE:HG22	4:C:13:ARG:HH12	1.73	0.54
29:X:1668:A:O4'	29:X:1669:A:C2	2.61	0.54
29:X:821:A:H5''	29:X:822:U:H6	1.73	0.54
2:A:126:LYS:HG3	2:A:129:ASN:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:52:ARG:HG3	11:J:67:ILE:HD11	1.90	0.54
3:B:141:ILE:HD11	29:X:2052:G:C8	2.42	0.54
29:X:296:C:H2'	29:X:297:C:H6	1.72	0.54
1:O:27:GLU:O	1:O:29:ALA:N	2.41	0.54
1:O:43:LEU:HD12	1:O:167:VAL:HG11	1.88	0.54
1:O:65:GLY:HA3	1:O:173:LYS:HD2	1.90	0.54
7:F:78:ILE:HG12	7:F:99:LEU:HD23	1.89	0.54
29:X:1787:U:H2'	29:X:1788:C:C6	2.42	0.54
29:X:220:G:OP2	29:X:221:C:H5'	2.08	0.54
29:X:2695:C:H2'	29:X:2696:U:C6	2.42	0.54
2:A:88:ARG:HD2	2:A:106:LEU:HD21	1.89	0.53
9:H:104:GLU:HG2	9:H:125:LYS:HD2	1.90	0.53
15:N:94:VAL:O	15:N:98:ILE:HG12	2.07	0.53
29:X:297:C:H2'	29:X:298:G:O4'	2.07	0.53
19:R:67:GLY:HA3	29:X:483:A:O3'	2.08	0.53
3:B:4:ILE:HG12	3:B:5:LEU:H	1.73	0.53
4:C:35:LEU:HD23	4:C:38:ARG:HD2	1.90	0.53
29:X:1316:U:H2'	29:X:1317:G:H8	1.73	0.53
29:X:335:C:H2'	29:X:336:C:H6	1.72	0.53
29:X:5:A:H2'	29:X:6:A:C8	2.43	0.53
1:O:212:THR:HG22	1:O:213:THR:H	1.74	0.53
17:P:27:VAL:HG22	17:P:125:THR:OG1	2.09	0.53
20:S:55:THR:HG22	20:S:61:THR:HB	1.89	0.53
22:U:17:SER:CA	22:U:18:VAL:HB	2.38	0.53
29:X:2153:G:H2'	29:X:2154:G:C8	2.44	0.53
29:X:2461:C:H2'	29:X:2462:U:C6	2.43	0.53
1:O:25:VAL:HG13	1:O:37:VAL:HG21	1.91	0.53
28:3:16:ILE:HG21	28:3:65:GLY:HA2	1.91	0.53
29:X:2221:G:H2'	29:X:2222:G:H8	1.72	0.53
29:X:2600:A:H2'	29:X:2601:C:C6	2.44	0.53
29:X:438:C:H2'	29:X:439:A:H8	1.74	0.53
26:1:18:THR:HG21	26:1:43:VAL:HB	1.90	0.53
19:R:58:VAL:HA	29:X:483:A:H4'	1.91	0.53
10:I:16:ARG:NH2	29:X:589:U:OP2	2.40	0.53
29:X:629:C:H4'	29:X:649:G:H21	1.73	0.53
29:X:799:G:OP2	29:X:800:A:O2'	2.17	0.53
25:Z:42:SER:HB3	29:X:2885:C:H42	1.74	0.53
8:G:91:THR:HG21	29:X:1140:U:H6	1.74	0.53
9:H:47:VAL:HG23	9:H:77:THR:HG23	1.91	0.53
10:I:101:ARG:HE	29:X:626:G:H1	1.56	0.53
18:Q:46:PHE:O	18:Q:48:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1661:G:H2'	29:X:1662:U:O4'	2.08	0.53
29:X:2567:G:H2'	29:X:2568:C:C6	2.44	0.53
29:X:2885:C:H2'	29:X:2886:A:O4'	2.07	0.53
29:X:819:A:OP2	29:X:1187:G:N2	2.31	0.53
29:X:991:C:H2'	29:X:992:C:H6	1.73	0.53
17:P:60:ILE:CD1	25:Z:28:PRO:HD3	2.35	0.53
3:B:9:ILE:HD11	3:B:27:LEU:CB	2.38	0.53
8:G:33:ILE:HD11	29:X:537:U:H4'	1.91	0.53
16:O:43:GLU:C	16:O:45:THR:H	2.12	0.53
16:O:50:ASP:O	16:O:53:LYS:HG2	2.09	0.53
20:S:6:LYS:HB3	20:S:32:PHE:HA	1.91	0.53
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.89	0.53
25:Z:15:LYS:HA	25:Z:18:MET:HG3	1.90	0.53
3:B:135:HIS:NE2	29:X:1658:C:OP1	2.42	0.53
29:X:1066:U:H2'	29:X:1068:G:OP2	2.08	0.53
29:X:2299:A:H61	29:X:2317:U:H3	1.56	0.53
29:X:971:C:H2'	29:X:972:G:O4'	2.09	0.53
15:N:6:THR:O	15:N:9:VAL:HG23	2.09	0.53
19:R:85:ASP:HB3	19:R:88:THR:OG1	2.08	0.53
22:U:19:ILE:HA	22:U:42:GLN:HA	1.91	0.53
29:X:2243:U:H2'	29:X:2244:U:C6	2.44	0.53
29:X:438:C:H2'	29:X:439:A:C8	2.43	0.53
29:X:445:C:C2'	29:X:446:G:H5''	2.38	0.53
4:C:8:GLY:H	4:C:121:ASP:HB3	1.72	0.52
18:Q:53:ILE:HG12	18:Q:54:SER:N	2.24	0.52
21:T:21:LEU:HD11	21:T:41:ARG:NE	2.24	0.52
29:X:1440:U:H2'	29:X:1440(A):C:C6	2.45	0.52
29:X:165(G):U:N3	29:X:175:C:O2	2.42	0.52
29:X:2219:U:H3'	29:X:2220:C:C4'	2.38	0.52
29:X:2898:G:H2'	29:X:2899:A:C8	2.44	0.52
29:X:1029:A:C8	29:X:1030:G:C8	2.97	0.52
29:X:1864:U:OP1	29:X:2410:G:O2'	2.22	0.52
9:H:82:LYS:HB3	9:H:82:LYS:NZ	2.24	0.52
12:K:38:LEU:O	12:K:41:ALA:HB3	2.10	0.52
16:O:66:GLY:O	16:O:87:ARG:NH1	2.39	0.52
29:X:1222:C:H2'	29:X:1223:G:H8	1.73	0.52
29:X:1222:C:H2'	29:X:1223:G:C8	2.44	0.52
29:X:1320:G:C2	29:X:1329:U:H5''	2.44	0.52
29:X:1858:G:H8	29:X:1884:A:N7	2.08	0.52
29:X:2261:C:O2'	29:X:2262:U:H5'	2.09	0.52
28:3:44:LYS:NZ	29:X:2362:G:OP1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2824:C:H2'	29:X:2825:C:O4'	2.09	0.52
19:R:93:ARG:NH2	29:X:301:G:OP2	2.39	0.52
30:Y:72:C:H2'	30:Y:73:C:H6	1.74	0.52
30:Y:80:A:H2'	30:Y:81:C:O4'	2.09	0.52
28:3:17:THR:HG21	28:3:21:LYS:HG3	1.90	0.52
2:A:39:LYS:HZ1	2:A:58:HIS:C	2.11	0.52
3:B:27:LEU:HD13	14:M:7:ILE:HD11	1.91	0.52
4:C:19:LEU:HB3	4:C:20:PRO:HA	1.90	0.52
4:C:93:TYR:CE1	29:X:660:G:H5'	2.45	0.52
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.91	0.52
14:M:24:LEU:HD13	14:M:91:VAL:HG21	1.90	0.52
15:N:6:THR:O	15:N:8:ILE:N	2.41	0.52
20:S:25:ASN:HA	20:S:85:MET:HB2	1.92	0.52
20:S:69:VAL:HG22	20:S:81:VAL:HG22	1.91	0.52
21:T:43:THR:H	29:X:2331:G:H4'	1.74	0.52
22:U:33:LYS:O	29:X:2395:C:O2'	2.19	0.52
29:X:1043:C:O2	29:X:1112:G:N2	2.30	0.52
29:X:1047:G:N3	29:X:1110:G:N2	2.54	0.52
29:X:1114:G:H2'	29:X:1115:A:H8	1.73	0.52
29:X:200:A:H2'	29:X:201:U:H5'	1.91	0.52
29:X:2272:U:H5''	29:X:2273:A:OP1	2.10	0.52
29:X:2695:C:O2'	29:X:2696:U:H5'	2.10	0.52
28:3:36:LYS:HB2	28:3:37:SER:CA	2.40	0.52
7:F:21:PRO:HG2	7:F:22:PRO:HD3	1.92	0.52
8:G:96:ASP:OD1	8:G:96:ASP:N	2.41	0.52
10:I:72:TYR:HB3	10:I:107:LYS:HB2	1.91	0.52
15:N:114:ARG:O	15:N:118:GLN:HG3	2.10	0.52
17:P:37:LYS:HA	17:P:40:LEU:HD12	1.92	0.52
20:S:109:GLN:NE2	20:S:142:ASN:OD1	2.42	0.52
24:W:4:LYS:O	24:W:51:LEU:HD12	2.10	0.52
29:X:1823:G:H2'	29:X:1824:G:H8	1.74	0.52
29:X:2101:G:H2'	29:X:2102:G:H8	1.75	0.52
29:X:2430:A:H2'	29:X:2430:A:N3	2.23	0.52
29:X:2599:G:C2	29:X:2600:A:C8	2.98	0.52
29:X:1998:A:H4'	29:X:2724:U:O2'	2.10	0.52
9:H:76:ARG:O	9:H:94:ASN:HA	2.09	0.52
15:N:3:ARG:HB3	29:X:1248:G:C5	2.42	0.52
29:X:1479:G:H2'	29:X:1480:G:H8	1.75	0.52
29:X:559:G:H2'	29:X:560:C:O4'	2.09	0.52
4:C:102:LEU:HD12	4:C:102:LEU:O	2.10	0.52
22:U:17:SER:CB	22:U:44:ALA:HA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:32:ARG:HE	22:U:32:ARG:H	1.56	0.52
29:X:1266:G:O2'	29:X:2012:G:O6	2.17	0.52
29:X:2729:C:H2'	29:X:2730:C:C6	2.45	0.52
29:X:624:C:O2'	29:X:657:U:OP1	2.26	0.52
29:X:946:G:H2'	29:X:947:G:H8	1.74	0.52
2:A:33:LEU:HD13	2:A:104:TYR:CD2	2.45	0.52
2:A:172:TYR:CD1	2:A:184:ARG:HG2	2.44	0.52
6:E:83:TYR:CD1	6:E:138:LYS:HB2	2.45	0.52
10:I:77:LEU:O	10:I:80:LEU:N	2.43	0.52
30:Y:27:A:N6	30:Y:56:G:OP2	2.39	0.52
2:A:77:ALA:HB2	2:A:97:TYR:CD1	2.44	0.52
9:H:40:GLY:HA2	29:X:2563:U:H4'	1.92	0.52
29:X:1289:C:H2'	29:X:1290:U:C6	2.45	0.52
29:X:1587:A:H2'	29:X:1588:A:C8	2.45	0.52
2:A:260:ARG:NH1	29:X:1799:G:OP1	2.37	0.52
17:P:109:ARG:NH2	29:X:2013:A:N3	2.57	0.52
29:X:2408:U:H2'	29:X:2409:G:C8	2.45	0.52
26:1:13:GLU:O	26:1:49:PHE:HB3	2.09	0.52
2:A:118:ASN:H	2:A:129:ASN:HD22	1.57	0.52
6:E:137:ASP:OD1	6:E:138:LYS:N	2.43	0.52
6:E:17:VAL:HG13	6:E:26:VAL:HG22	1.92	0.52
13:L:39:TYR:HE1	30:Y:8:C:H1'	1.75	0.52
15:N:91:ASN:N	16:O:11:GLN:OE1	2.41	0.52
16:O:39:PHE:CD1	16:O:47:PHE:HB3	2.43	0.52
20:S:25:ASN:HB2	20:S:28:ASN:HB3	1.91	0.52
29:X:460:A:C2	29:X:470:A:C4	2.98	0.52
29:X:555:U:H2'	29:X:556:A:C8	2.44	0.52
30:Y:7:C:O2'	30:Y:29:C:O2	2.25	0.52
25:Z:38:GLY:HA3	25:Z:48:ASN:ND2	2.25	0.52
2:A:95:LEU:HD11	2:A:105:ILE:HD13	1.92	0.51
8:G:75:ILE:HG13	8:G:147:ARG:HH12	1.75	0.51
29:X:2468:G:O2'	29:X:2469:A:H8	1.93	0.51
29:X:71:A:H5''	29:X:72:A:H3'	1.92	0.51
30:Y:59:A:H5'	30:Y:60:A:OP2	2.10	0.51
30:Y:22:U:H3	30:Y:65:A:H61	1.57	0.51
4:C:120:VAL:H	4:C:190:ALA:HB2	1.75	0.51
6:E:23:VAL:O	6:E:25:LYS:N	2.44	0.51
20:S:66:VAL:HG22	20:S:83:PHE:HE1	1.75	0.51
21:T:46:LYS:HZ1	21:T:76:ALA:HA	1.75	0.51
29:X:1698:A:C8	29:X:1700:A:O4'	2.63	0.51
29:X:2098:U:H3	29:X:2191:G:H1	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:141:A:H2'	29:X:142:G:C8	2.44	0.51
29:X:1360:G:N2	29:X:2213:U:H3	2.03	0.51
29:X:2356:U:H2'	29:X:2357:G:C8	2.45	0.51
29:X:630:G:N2	29:X:632:A:H3'	2.25	0.51
27:2:45:SER:HB3	29:X:126:A:OP1	2.11	0.51
28:3:36:LYS:HB2	28:3:37:SER:HA	1.91	0.51
5:D:129:ASN:HB3	5:D:155:THR:HG23	1.92	0.51
10:I:86:THR:HG23	10:I:118:VAL:HG13	1.92	0.51
11:J:75:VAL:HB	11:J:93:TYR:HE2	1.75	0.51
21:T:46:LYS:NZ	21:T:76:ALA:HA	2.25	0.51
3:B:149:ARG:O	29:X:2052:G:H1'	2.10	0.51
24:W:35:SER:O	24:W:35:SER:OG	2.29	0.51
29:X:1358:G:O2'	29:X:1373:A:N6	2.42	0.51
29:X:1779:U:C5	29:X:1784:A:N7	2.78	0.51
4:C:42:THR:OG1	29:X:39:G:N2	2.37	0.51
8:G:95:LEU:HA	8:G:115:ALA:HB3	1.93	0.51
29:X:101:U:H5''	29:X:102:G:C8	2.46	0.51
1:0:70:VAL:HG12	1:0:108:ALA:HB3	1.91	0.51
18:Q:40:ASP:O	18:Q:44:GLN:HG2	2.10	0.51
24:W:49:HIS:CD2	24:W:50:LEU:HG	2.46	0.51
29:X:1014:A:H2'	29:X:1015:U:C6	2.46	0.51
29:X:1415:A:C6	29:X:1584:U:H4'	2.45	0.51
29:X:1838:C:H4'	29:X:1839:G:C8	2.45	0.51
29:X:1991:U:H2'	29:X:1992:G:H5'	1.92	0.51
29:X:2341:G:H2'	29:X:2342:C:O4'	2.11	0.51
3:B:116:VAL:HG21	3:B:138:PRO:HB3	1.93	0.51
3:B:141:ILE:HD11	29:X:2052:G:N7	2.26	0.51
9:H:132:GLU:HB2	14:M:73:PHE:HE1	1.75	0.51
19:R:77:HIS:CD2	29:X:328:U:H4'	2.46	0.51
1:0:140:THR:HG22	1:0:145:VAL:HG22	1.92	0.51
28:3:51:ALA:O	28:3:52:LYS:HB2	2.11	0.51
2:A:197:GLY:O	2:A:199:ALA:N	2.44	0.51
29:X:2048:A:H2'	29:X:2049:G:O4'	2.10	0.51
29:X:700:G:H22	29:X:732:C:H5	1.57	0.51
29:X:7:G:H2'	29:X:8:A:H8	1.76	0.51
20:S:22:VAL:HG21	30:Y:77:G:H1'	1.93	0.51
3:B:16:LYS:HD3	3:B:173:VAL:HG13	1.92	0.51
5:D:5:LYS:HB2	5:D:101:GLU:OE1	2.10	0.51
17:P:81:HIS:O	17:P:83:ASP:N	2.44	0.51
19:R:51:VAL:HG13	19:R:73:GLU:HB3	1.93	0.51
29:X:1114:G:H2'	29:X:1115:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1337:G:H2'	29:X:1338:G:H8	1.76	0.51
3:B:135:HIS:CD2	29:X:1658:C:OP1	2.64	0.51
29:X:2468:G:H22	29:X:2481:G:H2'	1.75	0.51
29:X:638:G:C5	29:X:639:U:C5	2.98	0.51
29:X:797:U:H2'	29:X:798:G:C8	2.45	0.51
29:X:983:A:C2'	29:X:984:A:H5'	2.41	0.51
29:X:994:U:O2'	29:X:996:A:OP1	2.19	0.51
1:0:110:VAL:HG12	1:0:111:ALA:H	1.76	0.50
2:A:48:ARG:NH2	29:X:778:G:H5'	2.25	0.50
14:M:25:PRO:HB2	14:M:93:ILE:HD11	1.93	0.50
15:N:86:ALA:HB2	15:N:116:ALA:HB2	1.92	0.50
17:P:111:ARG:HH21	29:X:747:U:H5'	1.76	0.50
29:X:1607:C:H4'	29:X:1608:A:O5'	2.11	0.50
29:X:1779:U:H6	29:X:1784:A:H62	1.58	0.50
29:X:2057:A:H2'	29:X:2058:A:H8	1.75	0.50
29:X:2857:G:N2	29:X:2860:A:OP2	2.24	0.50
28:3:17:THR:HG21	28:3:21:LYS:CG	2.41	0.50
2:A:268:ARG:NH2	29:X:2225:A:OP1	2.45	0.50
10:I:41:SER:HB2	29:X:671:C:C5	2.46	0.50
11:J:61:ARG:HD3	20:S:174:PRO:HB2	1.93	0.50
29:X:1113:U:H2'	29:X:1114:G:H8	1.76	0.50
29:X:1810:A:H2'	29:X:1811:G:O4'	2.10	0.50
29:X:2266:A:H4'	29:X:2267:A:N3	2.26	0.50
29:X:407:C:H2'	29:X:408:G:H8	1.76	0.50
29:X:569:U:H1'	29:X:947:G:O4'	2.12	0.50
29:X:1087:G:O6	29:X:1089:G:N2	2.43	0.50
29:X:1203:U:H2'	29:X:1204:C:H6	1.74	0.50
29:X:1324:G:C4	29:X:1328:G:O6	2.64	0.50
29:X:1886:A:H2'	29:X:1887:U:O4'	2.12	0.50
29:X:2412:A:C8	29:X:2413:G:C8	2.99	0.50
29:X:472:A:H3'	29:X:473:G:H5'	1.94	0.50
3:B:110:GLY:HA2	3:B:161:GLY:HA3	1.93	0.50
4:C:133:PHE:CE1	4:C:161:ALA:HB2	2.45	0.50
8:G:42:VAL:HA	8:G:164:GLN:H	1.76	0.50
9:H:68:ASP:O	9:H:69:VAL:HB	2.11	0.50
29:X:1163:G:C2	29:X:1164:A:N7	2.80	0.50
15:N:33:ARG:HB3	29:X:1252:G:C2	2.46	0.50
12:K:9:LYS:HB3	29:X:1653:G:C6	2.47	0.50
29:X:2220:C:H2'	29:X:2221:G:C8	2.46	0.50
29:X:633:A:H4'	29:X:2404:C:H5''	1.92	0.50
29:X:2031:A:C6	29:X:2498:C:H1'	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:818:G:H5'	29:X:839:U:OP1	2.10	0.50
1:0:38:GLU:HB2	1:0:211:THR:HB	1.92	0.50
26:1:5:ALA:HB3	26:1:6:PRO:HD3	1.94	0.50
5:D:65:PRO:HA	5:D:89:VAL:HG13	1.93	0.50
29:X:1288:U:C2	29:X:1327:C:O2	2.65	0.50
29:X:1416:G:O2'	29:X:1587:A:H1'	2.10	0.50
29:X:1667:G:O2'	29:X:1991:U:O4	2.25	0.50
26:1:14:SER:CA	26:1:49:PHE:HD1	2.24	0.50
28:3:44:LYS:C	28:3:46:LYS:H	2.14	0.50
2:A:69:ARG:HD2	2:A:119:ALA:HB2	1.93	0.50
2:A:231:HIS:HD2	2:A:233:HIS:H	1.60	0.50
6:E:38:ASN:HB2	6:E:64:LEU:HD22	1.93	0.50
11:J:48:ILE:O	11:J:51:CYS:N	2.45	0.50
15:N:104:GLU:O	15:N:107:LYS:HB3	2.11	0.50
18:Q:17:TYR:O	18:Q:20:MET:HG2	2.11	0.50
19:R:70:GLU:OE1	19:R:72:ARG:NH1	2.45	0.50
29:X:2817:C:C2	29:X:2830:G:N2	2.80	0.50
18:Q:10:PRO:HG2	18:Q:12:ILE:HD11	1.92	0.50
21:T:39:ARG:NH2	29:X:2355:C:O2	2.44	0.50
22:U:48:LYS:HZ1	29:X:2090:A:H2	1.60	0.50
29:X:1570:A:H2'	29:X:1571:A:C8	2.46	0.50
29:X:200:A:N3	29:X:202:U:H1'	2.27	0.50
29:X:2842:A:C2	29:X:2876:G:C2	2.99	0.50
29:X:753:A:O2'	29:X:754:G:H5'	2.11	0.50
29:X:807:U:H2'	29:X:808:A:C8	2.47	0.50
15:N:28:ARG:HE	29:X:532:A:H2'	1.76	0.50
20:S:25:ASN:CB	20:S:28:ASN:HB3	2.42	0.50
29:X:1316:U:O2'	29:X:1317:G:H5'	2.11	0.50
25:Z:6:VAL:HG12	29:X:2015:A:C2	2.47	0.50
29:X:610:U:H2'	29:X:611:U:C6	2.47	0.50
20:S:26:LYS:HG3	30:Y:108:G:P	2.52	0.50
30:Y:122:U:O5'	30:Y:122:U:H6	1.95	0.50
27:2:11:LYS:HE2	29:X:686:G:H5''	1.93	0.50
10:I:55:ARG:O	10:I:59:ARG:HG3	2.12	0.50
20:S:19:ILE:HD11	20:S:36:ARG:HG3	1.93	0.50
24:W:3:ILE:HD11	24:W:44:VAL:HG22	1.92	0.50
29:X:2728:U:H2'	29:X:2729:C:C6	2.46	0.50
29:X:390:A:H4'	29:X:391:A:H5'	1.94	0.50
4:C:28:HIS:O	4:C:32:THR:HG23	2.12	0.49
4:C:57:LYS:NZ	4:C:69:HIS:O	2.45	0.49
5:D:117:ILE:HG22	5:D:118:ASN:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:38:GLU:HB3	5:D:87:ILE:HB	1.93	0.49
9:H:23:ARG:HE	29:X:2561:A:H2	1.59	0.49
15:N:10:ARG:NH1	29:X:583:G:O5'	2.45	0.49
20:S:55:THR:O	20:S:55:THR:OG1	2.26	0.49
29:X:443:A:C2	29:X:1245:G:N3	2.80	0.49
4:C:89:ARG:NH2	29:X:1247:A:OP1	2.33	0.49
29:X:1638:C:H4'	29:X:2710:C:O2	2.12	0.49
29:X:1626:A:N6	29:X:1639:U:H3	2.06	0.49
21:T:56:ASP:OD2	29:X:2364:C:H5'	2.11	0.49
29:X:320:U:H4'	29:X:322:A:C8	2.47	0.49
29:X:566:U:O2'	29:X:809:G:OP2	2.25	0.49
1:O:68:VAL:HG11	1:O:153:LYS:HG2	1.94	0.49
3:B:141:ILE:HG23	29:X:2051:A:H4'	1.93	0.49
4:C:118:VAL:H	4:C:188:ILE:HD11	1.77	0.49
5:D:108:LEU:HD22	5:D:114:PHE:CE1	2.47	0.49
6:E:43:VAL:HB	6:E:52:VAL:HG22	1.94	0.49
18:Q:43:GLN:HG2	18:Q:48:VAL:O	2.12	0.49
29:X:1285:G:N1	29:X:1329:U:OP1	2.36	0.49
29:X:1779:U:C2	29:X:1783:A:N7	2.80	0.49
10:I:64:GLY:HA2	29:X:2415:G:O3'	2.11	0.49
29:X:945:A:C4	29:X:2448:A:C2	3.00	0.49
29:X:2564:A:C2	29:X:2647:U:H4'	2.47	0.49
29:X:2712(A):A:H5'	29:X:2713:U:OP2	2.12	0.49
29:X:507:A:O5'	29:X:508:A:H5'	2.12	0.49
1:O:187:ALA:HA	1:O:190:SER:HB3	1.93	0.49
9:H:41:ASN:HD22	9:H:42:LYS:N	2.10	0.49
10:I:21:ARG:HG2	10:I:21:ARG:HH11	1.77	0.49
19:R:18:LYS:HA	19:R:36:VAL:CG1	2.43	0.49
19:R:88:THR:O	19:R:90:LYS:HE2	2.13	0.49
22:U:41:VAL:O	22:U:42:GLN:NE2	2.35	0.49
29:X:1163:G:C2	29:X:1164:A:C5	3.00	0.49
29:X:1841:U:H2'	29:X:1842:G:C8	2.46	0.49
29:X:2895:C:H2'	29:X:2896:U:H6	1.77	0.49
29:X:639:U:H2'	29:X:640:C:C6	2.46	0.49
11:J:25:GLY:HA3	29:X:907:U:OP1	2.12	0.49
1:O:29:ALA:HB1	1:O:35:GLU:CB	2.42	0.49
9:H:55:VAL:HB	9:H:67:GLY:H	1.77	0.49
15:N:10:ARG:HH11	29:X:583:G:P	2.36	0.49
21:T:46:LYS:O	21:T:78:PHE:HA	2.12	0.49
29:X:1070:A:H5'	29:X:1072:C:OP2	2.12	0.49
29:X:1240:C:C2	29:X:1241:G:C8	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1748:C:H2'	29:X:1749:A:C8	2.47	0.49
29:X:214:G:O2'	29:X:226:G:O6	2.27	0.49
8:G:125:ARG:NH1	29:X:2640:G:OP1	2.44	0.49
10:I:114:ILE:HG21	10:I:132:ALA:O	2.11	0.49
11:J:35:LEU:HD23	11:J:105:PHE:CD2	2.48	0.49
29:X:1464:G:H2'	29:X:1465:G:H8	1.77	0.49
29:X:2307:G:H3'	29:X:2308:G:C8	2.47	0.49
29:X:295:G:N2	29:X:344:G:H1'	2.27	0.49
29:X:700:G:H1	29:X:732:C:H5	1.60	0.49
2:A:97:TYR:HB3	2:A:99:ASP:HB3	1.93	0.49
5:D:26:MET:O	5:D:30:ARG:NH2	2.45	0.49
6:E:43:VAL:HB	6:E:52:VAL:HG13	1.95	0.49
9:H:6:SER:OG	29:X:1666:G:H4'	2.12	0.49
13:L:33:ARG:NE	13:L:38:ILE:HG21	2.28	0.49
20:S:15:ASP:C	20:S:17:SER:H	2.14	0.49
22:U:10:LYS:HD3	22:U:11:LYS:H	1.78	0.49
23:V:32:ALA:HB2	23:V:37:LEU:HD22	1.93	0.49
29:X:1864:U:H3	29:X:1878:G:H1	1.59	0.49
2:A:148:VAL:HG11	29:X:2221:G:H21	1.77	0.49
29:X:2836:G:H2'	29:X:2837:A:H8	1.71	0.49
2:A:17:THR:OG1	2:A:205:VAL:N	2.37	0.49
11:J:26:ASP:N	11:J:26:ASP:OD1	2.32	0.49
17:P:14:ARG:O	17:P:18:VAL:HG22	2.13	0.49
29:X:1832:C:N4	29:X:1833:C:C4	2.81	0.49
29:X:2070:G:C2	29:X:2071:A:C4	3.00	0.49
29:X:2080:A:H2'	29:X:2081:U:C6	2.47	0.49
6:E:17:VAL:HG22	6:E:26:VAL:HG22	1.95	0.49
11:J:43:ILE:N	11:J:95:VAL:HG22	2.28	0.49
15:N:11:ARG:HH22	29:X:29:U:H4'	1.77	0.49
22:U:48:LYS:HE3	29:X:2091:U:H1'	1.93	0.49
29:X:1668:A:H4'	29:X:1669:A:O5'	2.12	0.49
29:X:1739:C:H2'	29:X:1740:G:H8	1.77	0.49
29:X:1756:A:H8	29:X:1756:A:O5'	1.95	0.49
29:X:2205:A:H2'	29:X:2210:A:N7	2.27	0.49
29:X:653:U:H2'	29:X:654:U:O4'	2.13	0.49
29:X:996:A:H2'	29:X:997:G:H8	1.77	0.49
2:A:102:LYS:NZ	29:X:1500:A:O2'	2.46	0.49
2:A:118:ASN:H	2:A:129:ASN:ND2	2.11	0.49
3:B:112:GLY:O	3:B:159:HIS:HA	2.12	0.49
7:F:14:ALA:HB1	7:F:45:THR:HB	1.95	0.49
13:L:92:GLY:C	13:L:94:TYR:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:104:LEU:HA	14:M:106:TYR:HE2	1.76	0.49
19:R:43:ASP:HB3	19:R:45:LYS:HG3	1.94	0.49
19:R:56:LYS:HG3	29:X:481:G:OP2	2.12	0.49
29:X:1826:G:H2'	29:X:1827:U:H6	1.76	0.49
29:X:2837:A:H2'	29:X:2838:G:H8	1.78	0.49
29:X:301:G:C4	29:X:302:U:C5	3.01	0.49
28:3:57:ARG:NH2	29:X:833:A:O3'	2.39	0.49
9:H:10:VAL:HG23	9:H:17:ARG:O	2.13	0.49
9:H:9:ASP:O	9:H:95:ALA:HA	2.13	0.49
16:O:15:SER:O	16:O:16:GLU:HB2	2.13	0.49
17:P:87:GLU:HA	17:P:90:LEU:HD13	1.95	0.49
23:V:44:ARG:O	23:V:47:ARG:HB3	2.13	0.49
29:X:1211:A:H4'	29:X:1212:G:OP2	2.13	0.49
29:X:1525:G:H2'	29:X:1526:G:O4'	2.12	0.49
29:X:2203:G:H2'	29:X:2204:A:C8	2.48	0.49
29:X:2584:U:H2'	29:X:2585:U:H2'	1.95	0.49
19:R:80:LYS:NZ	29:X:329:G:N7	2.55	0.49
29:X:846:U:H4'	29:X:847:U:O5'	2.13	0.49
2:A:29:PRO:HB2	2:A:34:THR:CG2	2.43	0.48
12:K:3:HIS:O	12:K:3:HIS:CD2	2.65	0.48
13:L:76:ALA:HB1	13:L:111:GLY:HA2	1.94	0.48
14:M:14:ARG:HB3	14:M:14:ARG:NH2	2.28	0.48
20:S:121:GLN:O	20:S:161:ALA:HB3	2.13	0.48
20:S:41:ARG:NH2	29:X:1041:C:OP1	2.44	0.48
2:A:206:LEU:HB2	29:X:1791:A:O3'	2.12	0.48
29:X:2195:U:H2'	29:X:2196:C:H6	1.79	0.48
17:P:99:ALA:O	29:X:25:U:H5'	2.13	0.48
17:P:15:LYS:HB3	29:X:502:A:H4'	1.95	0.48
29:X:519:U:C2	29:X:520:G:C8	3.01	0.48
29:X:79:C:H2'	29:X:80:G:C8	2.48	0.48
29:X:944:G:H3'	29:X:944:G:H8	1.78	0.48
15:N:54:LYS:HZ1	29:X:994:U:P	2.36	0.48
6:E:59:GLN:NE2	29:X:1035:U:OP1	2.47	0.48
11:J:8:THR:HG22	11:J:70:PHE:HE2	1.78	0.48
15:N:61:TRP:O	15:N:65:ILE:HG13	2.13	0.48
17:P:66:GLU:HB3	17:P:67:PRO:HD3	1.95	0.48
20:S:63:PRO:O	20:S:86:VAL:HG22	2.13	0.48
29:X:1323:G:O6	29:X:1324:G:C6	2.66	0.48
29:X:1467:U:H1'	29:X:1468:G:C8	2.48	0.48
29:X:1477:A:H2'	29:X:1478:G:O4'	2.13	0.48
29:X:1309:G:H21	29:X:1611:C:H5'	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1727:C:N3	29:X:1750:G:C6	2.81	0.48
29:X:1826:G:O2'	29:X:1971:A:OP2	2.32	0.48
29:X:2055:C:H5'	29:X:2056:G:H5''	1.95	0.48
29:X:211:U:H2'	29:X:212:U:C6	2.47	0.48
29:X:2323:G:C6	29:X:2332:U:H5	2.30	0.48
29:X:2064:C:O2	29:X:2450:A:N6	2.46	0.48
30:Y:63:A:C2	30:Y:64:C:C2	3.01	0.48
4:C:68:ARG:NH2	29:X:2060:A:N6	2.59	0.48
16:O:37:ALA:HB3	16:O:51:ALA:O	2.13	0.48
17:P:25:PHE:C	17:P:25:PHE:CD2	2.87	0.48
19:R:45:LYS:HA	19:R:76:LEU:O	2.14	0.48
24:W:22:ALA:O	29:X:931:U:H4'	2.12	0.48
29:X:1753:A:H4'	29:X:2715:C:O4'	2.14	0.48
29:X:2218:U:H2'	29:X:2219:U:H6	1.77	0.48
29:X:2346:A:H4'	29:X:2347:C:OP2	2.12	0.48
29:X:545:U:H4'	29:X:546:U:OP2	2.13	0.48
29:X:672:U:C2	29:X:809:G:N2	2.81	0.48
29:X:822:U:H2'	29:X:822:U:O2	2.14	0.48
29:X:848:G:C4	29:X:849:A:C8	3.01	0.48
29:X:864:G:N2	29:X:913:U:C2	2.81	0.48
5:D:70:ALA:C	5:D:72:LYS:H	2.16	0.48
5:D:72:LYS:HG2	5:D:81:GLN:HG2	1.94	0.48
8:G:94:LYS:O	8:G:98:LYS:HB3	2.13	0.48
11:J:61:ARG:HG2	20:S:175:ARG:H	1.78	0.48
12:K:14:SER:N	12:K:17:ARG:HH21	2.11	0.48
14:M:55:ILE:O	14:M:103:LYS:O	2.31	0.48
29:X:1316:U:C2	29:X:1317:G:C8	3.01	0.48
29:X:1493:A:C8	29:X:1494:A:C8	3.02	0.48
29:X:1510:U:H2'	29:X:1511:G:C8	2.48	0.48
29:X:2347:C:C5	29:X:2382:G:H1'	2.48	0.48
29:X:2850:A:C2	29:X:2851:C:C2	3.02	0.48
29:X:553:G:H2'	29:X:554:U:O4'	2.13	0.48
29:X:638:G:H2'	29:X:639:U:H6	1.78	0.48
29:X:797:U:H2'	29:X:798:G:H8	1.77	0.48
3:B:116:VAL:HB	3:B:122:PHE:CG	2.49	0.48
5:D:8:TYR:O	5:D:12:VAL:HG23	2.14	0.48
17:P:102:THR:HB	17:P:120:ARG:HA	1.95	0.48
29:X:1655:A:H3'	29:X:1656:C:C6	2.49	0.48
29:X:1850:G:H2'	29:X:1851:U:H5'	1.95	0.48
25:Z:6:VAL:HG12	29:X:2015:A:N3	2.28	0.48
29:X:2537:U:H2'	29:X:2538:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:16:GLN:HG2	29:X:502:A:OP1	2.13	0.48
29:X:658:A:H2'	29:X:659:C:O4'	2.14	0.48
26:1:27:ASN:ND2	26:1:29:ARG:HB2	2.29	0.48
3:B:39:ALA:N	3:B:45:GLU:OE2	2.47	0.48
4:C:35:LEU:HD23	4:C:35:LEU:HA	1.66	0.48
4:C:44:SER:HB2	4:C:88:PRO:HD3	1.95	0.48
5:D:143:TYR:HA	5:D:146:VAL:HG22	1.95	0.48
6:E:98:LEU:HD12	6:E:102:ALA:O	2.14	0.48
6:E:105:MET:HE2	6:E:107:ILE:HD11	1.96	0.48
13:L:27:LEU:O	13:L:88:VAL:N	2.47	0.48
15:N:82:GLY:HA3	15:N:113:SER:OG	2.13	0.48
20:S:3:LEU:HB3	20:S:34:LEU:HD23	1.96	0.48
29:X:1163:G:H2'	29:X:1164:A:C8	2.44	0.48
29:X:1480:G:O6	29:X:1512:C:N4	2.45	0.48
29:X:2219:U:C2	29:X:2220:C:H1'	2.48	0.48
28:3:27:SER:OG	29:X:2361:C:OP1	2.21	0.48
29:X:2455:G:H2'	29:X:2456:C:C6	2.49	0.48
29:X:2874:C:H2'	29:X:2875:U:C6	2.48	0.48
29:X:295:G:H2'	29:X:296:C:C6	2.49	0.48
26:1:14:SER:HA	26:1:49:PHE:HD1	1.79	0.48
12:K:37:THR:HB	12:K:40:LYS:HG3	1.94	0.48
12:K:51:LEU:CD2	12:K:66:VAL:HG22	2.43	0.48
20:S:49:THR:OG1	20:S:132:GLN:OE1	2.32	0.48
29:X:295:G:H2'	29:X:296:C:H6	1.78	0.48
17:P:21:ARG:NH2	29:X:496:G:H4'	2.28	0.48
1:0:152:LEU:HD23	1:0:157:ILE:HG21	1.96	0.48
28:3:44:LYS:O	28:3:46:LYS:N	2.46	0.48
3:B:188:ILE:CG2	3:B:189:PRO:HD2	2.43	0.48
6:E:154:PRO:HA	6:E:160:LYS:O	2.13	0.48
29:X:1101:U:H2'	29:X:1102:C:C6	2.49	0.48
29:X:1510:U:H2'	29:X:1511:G:N9	2.29	0.48
29:X:165(B):G:H1	29:X:180:C:H42	1.60	0.48
29:X:2071:A:H2'	29:X:2072:G:H8	1.77	0.48
6:E:110:SER:OG	29:X:2667:C:N3	2.38	0.48
29:X:492:A:H2'	29:X:493:G:O4'	2.13	0.48
30:Y:3:A:H2'	30:Y:4:C:C6	2.49	0.48
3:B:44:TYR:CE1	29:X:2637:U:H5'	2.48	0.48
6:E:83:TYR:CE1	6:E:138:LYS:HB2	2.49	0.48
13:L:64:LYS:HG3	30:Y:53:G:C5'	2.42	0.48
20:S:123:VAL:HG23	20:S:161:ALA:HB2	1.95	0.48
20:S:167:THR:OG1	29:X:875:G:H4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:5:LEU:HB2	24:W:25:LEU:CD1	2.44	0.48
29:X:1606:G:H5''	29:X:1607:C:OP1	2.13	0.48
29:X:1853:A:H2'	29:X:1854:A:C8	2.49	0.48
10:I:55:ARG:NH1	29:X:223:A:OP1	2.33	0.48
29:X:2251:G:H5''	29:X:2252:G:OP2	2.13	0.48
29:X:2304:G:H1	29:X:2312:U:H3	1.61	0.48
29:X:2500:U:H5''	29:X:2501:C:OP2	2.14	0.48
29:X:2032:G:N2	29:X:2572:A:C8	2.82	0.48
29:X:523:C:H5''	29:X:540:C:O2'	2.14	0.48
29:X:741:G:H2'	29:X:742:C:H6	1.78	0.48
7:F:111:LYS:HB3	7:F:114:ASP:HB2	1.96	0.48
19:R:48:VAL:C	19:R:50:GLY:H	2.17	0.48
2:A:158:SER:OG	29:X:1820:U:O2'	2.31	0.48
29:X:1838:C:H4'	29:X:1839:G:H8	1.78	0.48
29:X:2684:U:C2	29:X:2685:G:C8	3.02	0.48
29:X:572:A:H5''	29:X:573:G:OP2	2.13	0.48
29:X:640:C:H2'	29:X:641:C:H6	1.79	0.48
27:2:12:ARG:HH11	27:2:44:VAL:HG13	1.79	0.47
27:2:12:ARG:NH1	27:2:44:VAL:HG22	2.29	0.47
9:H:132:GLU:OE1	14:M:72:SER:OG	2.27	0.47
10:I:110:ALA:HB3	29:X:637:A:C5'	2.44	0.47
12:K:81:ASP:O	12:K:85:PRO:HG3	2.14	0.47
16:O:67:LYS:HG3	16:O:68:LYS:N	2.28	0.47
17:P:18:VAL:HG23	17:P:19:LYS:N	2.29	0.47
22:U:28:GLY:HA3	22:U:32:ARG:HB3	1.96	0.47
29:X:1592:U:H2'	29:X:1593:G:H8	1.79	0.47
29:X:200:A:H3'	29:X:200:A:C8	2.50	0.47
29:X:2120:G:N2	29:X:2177:C:H42	2.12	0.47
29:X:2304:G:N2	29:X:2312:U:H3	2.08	0.47
29:X:2282:G:H4'	29:X:2389:G:O2'	2.13	0.47
29:X:193:A:C8	29:X:238:G:C5	3.02	0.47
29:X:2443:C:O2'	29:X:2444:G:H5'	2.14	0.47
29:X:2658:C:H2'	29:X:2659:G:O4'	2.13	0.47
5:D:51:ASP:O	5:D:55:LYS:HG2	2.15	0.47
5:D:5:LYS:HD2	5:D:101:GLU:HB2	1.97	0.47
9:H:111:PHE:CD1	9:H:111:PHE:N	2.82	0.47
9:H:83:ARG:NH2	9:H:89:ILE:HD11	2.28	0.47
10:I:4:HIS:CD2	10:I:4:HIS:C	2.87	0.47
14:M:17:GLU:HG3	14:M:62:SER:HB3	1.96	0.47
19:R:112:LYS:HB3	19:R:112:LYS:HE3	1.53	0.47
20:S:43:PHE:CE2	20:S:69:VAL:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:7:ARG:HA	23:V:60:LEU:HD11	1.96	0.47
24:W:3:ILE:HD11	24:W:44:VAL:CG2	2.45	0.47
29:X:165:A:H2'	29:X:165(A):G:H8	1.77	0.47
29:X:1882:C:H2'	29:X:1883:G:O4'	2.14	0.47
29:X:222:G:C6	29:X:223:A:C6	3.01	0.47
29:X:2564:A:OP1	29:X:2648:G:O2'	2.16	0.47
29:X:2740:A:C8	29:X:2763:G:N2	2.82	0.47
29:X:407:C:H2'	29:X:408:G:C8	2.49	0.47
29:X:616:A:H2'	29:X:617:A:H8	1.76	0.47
29:X:934:G:H2'	29:X:935:U:H6	1.78	0.47
2:A:253:PRO:HD2	2:A:257:LEU:HD22	1.96	0.47
3:B:26:VAL:HG11	3:B:198:LEU:HD11	1.96	0.47
3:B:98:GLU:OE2	3:B:175:ILE:N	2.43	0.47
9:H:64:VAL:HG22	9:H:106:ARG:HH21	1.79	0.47
11:J:35:LEU:HB3	11:J:105:PHE:HB2	1.96	0.47
19:R:99:VAL:HG11	19:R:105:ARG:CZ	2.44	0.47
22:U:10:LYS:HD3	22:U:11:LYS:N	2.28	0.47
23:V:21:ARG:HG3	23:V:46:LEU:HD23	1.96	0.47
29:X:1565:C:H42	29:X:1568:G:H1	1.61	0.47
29:X:167:A:H61	29:X:170:C:H3'	1.79	0.47
29:X:2037:G:H2'	29:X:2038:G:C8	2.49	0.47
29:X:2675:A:H2'	29:X:2676:C:O4'	2.14	0.47
26:I:38:LYS:HD2	29:X:2344:U:OP1	2.15	0.47
4:C:28:HIS:HB2	10:I:6:LEU:HD13	1.96	0.47
7:F:75:SER:O	7:F:79:ARG:NH1	2.48	0.47
10:I:117:ALA:HB2	10:I:136:ALA:O	2.14	0.47
18:Q:43:GLN:O	18:Q:47:GLY:N	2.47	0.47
19:R:38:LEU:HD21	19:R:40:LEU:HD13	1.96	0.47
23:V:11:ALA:HA	23:V:14:PHE:CD2	2.49	0.47
29:X:1952:A:C6	29:X:1953:A:N1	2.82	0.47
29:X:2080:A:H2'	29:X:2081:U:H6	1.79	0.47
29:X:2393:A:H2'	29:X:2394:C:O4'	2.14	0.47
29:X:2543:G:H2'	29:X:2544:G:C8	2.50	0.47
29:X:2870:C:N4	29:X:2871:G:O6	2.47	0.47
29:X:944:G:C8	29:X:944:G:H3'	2.49	0.47
30:Y:16:U:H2'	30:Y:110:U:O2'	2.15	0.47
25:Z:55:ARG:HH21	25:Z:58:LEU:HA	1.78	0.47
1:O:17:SER:OG	1:O:18:ILE:N	2.46	0.47
4:C:97:ARG:O	4:C:101:GLN:HG2	2.14	0.47
9:H:110:VAL:H	9:H:129:LEU:HB3	1.78	0.47
23:V:13:ASP:O	23:V:17:GLU:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1216:C:H6	29:X:1216:C:O5'	1.97	0.47
15:N:37:GLN:CG	29:X:1252:G:H1	2.24	0.47
29:X:1318:G:C2'	29:X:1319:G:H5'	2.44	0.47
29:X:1824:G:H2'	29:X:1825:U:H6	1.78	0.47
29:X:200:A:H3'	29:X:200:A:H8	1.80	0.47
29:X:526:A:O2'	29:X:2043:C:O2	2.32	0.47
29:X:2712:C:O2'	29:X:2712(A):A:H5''	2.14	0.47
29:X:2681:C:C2	29:X:2724:U:O4	2.67	0.47
29:X:2801:G:H2'	29:X:2802:G:H8	1.79	0.47
27:2:31:LEU:HD23	27:2:42:LEU:HD22	1.96	0.47
28:3:33:ASN:HB2	29:X:2420:C:OP2	2.15	0.47
28:3:50:LEU:HA	28:3:50:LEU:HD13	1.66	0.47
2:A:16:MET:HG3	2:A:207:GLY:HA3	1.95	0.47
5:D:118:ASN:HD21	5:D:120:ASN:HB2	1.80	0.47
10:I:80:LEU:HD11	10:I:89:ASP:OD2	2.15	0.47
12:K:43:GLU:HG3	12:K:43:GLU:O	2.15	0.47
13:L:104:ALA:O	13:L:107:ALA:N	2.47	0.47
22:U:23:LYS:HD2	22:U:35:THR:HG21	1.95	0.47
29:X:1113:U:H2'	29:X:1114:G:C8	2.49	0.47
29:X:1285:G:H2'	29:X:1286:A:H5''	1.95	0.47
29:X:2114:A:H61	29:X:2119:A:H62	1.63	0.47
26:1:38:LYS:O	29:X:2344:U:H3'	2.15	0.47
29:X:2458:G:C8	29:X:2490:G:C6	3.03	0.47
29:X:2549:G:C2	29:X:2550:G:N7	2.82	0.47
25:Z:3:LYS:HB2	29:X:2611:U:C2	2.49	0.47
11:J:12:LYS:HD3	29:X:911:A:C5	2.50	0.47
5:D:111:ILE:HG22	5:D:114:PHE:HB2	1.96	0.47
6:E:21:ASP:HB2	6:E:23:VAL:HG23	1.95	0.47
10:I:81:GLN:HG2	10:I:114:ILE:HD13	1.97	0.47
20:S:141:MET:HG3	20:S:145:ASP:HB3	1.97	0.47
29:X:1154:G:H5''	29:X:1155:A:OP2	2.14	0.47
29:X:2560:C:C4	29:X:2561:A:N7	2.82	0.47
5:D:138:PHE:HB2	5:D:141:ILE:HB	1.97	0.47
7:F:37:PHE:HA	7:F:40:ALA:HB3	1.97	0.47
13:L:74:ALA:O	13:L:77:ALA:HB3	2.15	0.47
29:X:1656:C:H2'	29:X:1657:C:H6	1.80	0.47
3:B:149:ARG:NH1	29:X:2024:G:O3'	2.48	0.47
29:X:2816:C:C2	29:X:2831:G:N2	2.83	0.47
29:X:532:A:P	29:X:561:G:H21	2.37	0.47
29:X:588:U:H2'	29:X:589:U:H6	1.80	0.47
29:X:627:A:H4'	29:X:628:G:H5'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:43:THR:O	27:2:46:ASP:N	2.42	0.47
2:A:231:HIS:CD2	2:A:233:HIS:H	2.32	0.47
4:C:114:GLY:N	4:C:115:GLY:HA2	2.30	0.47
12:K:32:GLY:O	12:K:115:LEU:HD13	2.14	0.47
9:H:85:ASP:HB3	14:M:87:LEU:HD12	1.97	0.47
16:O:22:VAL:HG12	16:O:23:GLU:N	2.29	0.47
29:X:1973:G:H2'	29:X:1974:C:C6	2.50	0.47
29:X:2615:U:H2'	29:X:2616:C:C6	2.49	0.47
29:X:812:C:H2'	29:X:813:U:H6	1.80	0.47
6:E:111:HIS:HA	6:E:112:PRO:HD2	1.63	0.47
12:K:51:LEU:HD13	12:K:70:ILE:HD11	1.95	0.47
15:N:12:ARG:HD3	15:N:12:ARG:HA	1.59	0.47
29:X:2544:G:H2'	29:X:2545:G:H8	1.80	0.47
29:X:2698:U:H2'	29:X:2699:C:C6	2.50	0.47
29:X:2711:A:OP1	29:X:2712(A):A:P	2.72	0.47
29:X:947:G:H2'	29:X:948:C:C6	2.50	0.47
6:E:22:GLY:HA2	6:E:24:PHE:CE1	2.50	0.47
10:I:102:LYS:O	10:I:104:ARG:N	2.47	0.47
17:P:68:VAL:HG22	17:P:124:ILE:HG21	1.96	0.47
29:X:1196:C:C2	29:X:1197:G:C8	3.03	0.47
29:X:1333:C:H6	29:X:1333:C:O5'	1.98	0.47
29:X:208:C:H2'	29:X:209:C:H6	1.79	0.47
29:X:2119:A:O4'	29:X:2172:U:O2'	2.33	0.47
29:X:2294:C:H2'	29:X:2295:C:C6	2.47	0.47
29:X:2511:U:H2'	29:X:2512:C:H6	1.79	0.47
3:B:47:VAL:HG12	3:B:84:PHE:HB3	1.97	0.46
4:C:111:ARG:NH1	4:C:183:HIS:O	2.47	0.46
5:D:117:ILE:HG21	5:D:130:LEU:HD11	1.96	0.46
6:E:164:PHE:O	6:E:166:GLY:N	2.48	0.46
13:L:32:TYR:CE2	30:Y:9:G:H5'	2.50	0.46
17:P:12:LYS:O	17:P:16:GLN:HG3	2.15	0.46
20:S:15:ASP:N	20:S:15:ASP:OD2	2.47	0.46
22:U:46:LEU:HB2	29:X:2230:G:H4'	1.97	0.46
29:X:1136:G:H2'	29:X:1137:G:H8	1.80	0.46
29:X:2070:G:H2'	29:X:2071:A:C8	2.50	0.46
29:X:2364:C:H2'	29:X:2365:G:O4'	2.15	0.46
29:X:1782:C:H1'	29:X:2609:U:H5'	1.97	0.46
29:X:1999:C:H5''	29:X:2723:C:O2'	2.15	0.46
29:X:531:C:H5''	29:X:532:A:C4	2.50	0.46
29:X:793:A:OP2	29:X:2071:A:O2'	2.32	0.46
5:D:34:ILE:N	5:D:91:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:44:LYS:HD2	11:J:47:GLN:NE2	2.30	0.46
13:L:63:ASN:HB3	13:L:66:ASP:HB2	1.97	0.46
29:X:1137:G:H5'	29:X:1138:G:OP2	2.15	0.46
29:X:1342:A:O2'	29:X:1344:U:OP2	2.30	0.46
29:X:2683:C:H2'	29:X:2684:U:C6	2.42	0.46
29:X:641:C:H42	29:X:646:A:N6	2.11	0.46
30:Y:34:C:H2'	30:Y:35:C:H6	1.80	0.46
5:D:39:GLY:HA2	5:D:86:GLY:HA2	1.97	0.46
6:E:8:PRO:HD2	6:E:69:ARG:HH11	1.80	0.46
8:G:67:ARG:HA	8:G:68:PRO:HD2	1.81	0.46
12:K:54:THR:HG22	12:K:66:VAL:HG23	1.97	0.46
19:R:29:HIS:CD2	19:R:51:VAL:HA	2.50	0.46
24:W:36:ASP:OD1	24:W:41:ARG:NH1	2.49	0.46
29:X:1336:A:H2'	29:X:1337:G:C8	2.51	0.46
29:X:1525:G:C2	29:X:1526:G:H1'	2.50	0.46
29:X:1796:U:H2'	29:X:1797:C:H6	1.78	0.46
22:U:48:LYS:NZ	29:X:2229:U:O2	2.43	0.46
29:X:330:A:N3	29:X:330:A:H2'	2.30	0.46
29:X:37:C:H4'	29:X:451:C:OP1	2.16	0.46
29:X:643:A:O2'	29:X:644:A:OP1	2.30	0.46
30:Y:63:A:O2'	30:Y:64:C:H5'	2.14	0.46
2:A:33:LEU:HD13	2:A:104:TYR:HD2	1.79	0.46
4:C:30:VAL:HG11	4:C:177:VAL:HG21	1.97	0.46
11:J:111:THR:HG23	11:J:114:GLN:CG	2.45	0.46
14:M:78:GLU:OE2	14:M:108:LYS:HE2	2.15	0.46
21:T:56:ASP:HB2	21:T:58:THR:OG1	2.16	0.46
29:X:83:G:H22	29:X:102:G:H1'	1.77	0.46
29:X:2060:A:H1'	29:X:2502:G:H1'	1.97	0.46
1:O:214:MET:HA	29:X:2175:C:O2'	2.16	0.46
29:X:2283:C:C6	29:X:2389:G:H2'	2.50	0.46
29:X:2396:G:C2	29:X:2421:G:C2	3.03	0.46
29:X:310:A:O2'	29:X:311:A:O5'	2.29	0.46
29:X:581:C:H2'	29:X:582:G:H8	1.79	0.46
30:Y:71:G:C6	30:Y:72:C:C4	3.03	0.46
1:O:188:LEU:O	1:O:192:LEU:HB2	2.16	0.46
2:A:201:HIS:O	2:A:204:ILE:HG13	2.15	0.46
11:J:7:ARG:HB2	11:J:7:ARG:HE	1.52	0.46
14:M:67:THR:OG1	14:M:80:VAL:HG22	2.16	0.46
18:Q:29:VAL:HG11	18:Q:38:ILE:HG12	1.97	0.46
20:S:51:LEU:HA	20:S:64:ALA:O	2.15	0.46
22:U:72:LYS:HA	22:U:72:LYS:HD3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1483:A:H2'	29:X:1484:U:O4'	2.16	0.46
29:X:1413:G:H22	29:X:1587:A:H3'	1.80	0.46
29:X:2210:A:N6	29:X:2211:A:N1	2.64	0.46
29:X:2242:G:H2'	29:X:2243:U:O4'	2.15	0.46
29:X:2686:G:C2	29:X:2724:U:O2	2.69	0.46
29:X:5:A:H2'	29:X:6:A:H8	1.79	0.46
29:X:848:G:N3	29:X:933:A:H1'	2.31	0.46
30:Y:122:U:H5''	30:Y:123:U:OP2	2.16	0.46
4:C:5:ASN:HA	4:C:119:ALA:HB3	1.98	0.46
4:C:96:PRO:HB2	4:C:99:VAL:HG23	1.97	0.46
10:I:51:GLY:HA2	29:X:832:U:O2	2.16	0.46
15:N:10:ARG:NH1	29:X:583:G:P	2.89	0.46
17:P:32:ARG:NH2	17:P:119:LYS:HG2	2.31	0.46
20:S:91:PRO:HB3	20:S:127:PRO:HB3	1.96	0.46
24:W:40:VAL:HA	24:W:43:MET:HE3	1.98	0.46
29:X:1217:C:H2'	29:X:1218:A:C8	2.49	0.46
29:X:1956:U:H1'	29:X:2552:U:OP1	2.15	0.46
29:X:20:C:H2'	29:X:21:A:C8	2.50	0.46
29:X:2212:A:H5''	29:X:2213:U:H5	1.81	0.46
29:X:214:G:H22	29:X:226:G:H2'	1.80	0.46
29:X:2898:G:H2'	29:X:2899:A:H8	1.80	0.46
22:U:68:ARG:NH2	29:X:400:G:N7	2.57	0.46
29:X:799:G:H3'	29:X:800:A:H2'	1.97	0.46
29:X:852:A:C5	29:X:853:U:C5	3.04	0.46
30:Y:59:A:H2'	30:Y:59:A:N3	2.31	0.46
21:T:38:VAL:HG23	21:T:59:LEU:HB2	1.97	0.46
20:S:41:ARG:HH22	29:X:1041:C:P	2.38	0.46
29:X:1316:U:H2'	29:X:1317:G:C8	2.50	0.46
29:X:2243:U:H2'	29:X:2244:U:H6	1.78	0.46
29:X:2256:G:N2	29:X:2275:C:N4	2.63	0.46
29:X:2276:G:C2	29:X:2277:G:C8	3.04	0.46
29:X:661:U:H2'	29:X:662:C:O4'	2.16	0.46
29:X:669:G:N3	29:X:669:G:C2'	2.79	0.46
29:X:68:G:H2'	29:X:69:C:C6	2.51	0.46
1:O:208:ALA:HB3	1:O:220:LEU:HB2	1.98	0.46
2:A:155:LEU:HD23	29:X:1799:G:N2	2.31	0.46
4:C:119:ALA:HB1	4:C:190:ALA:HB2	1.98	0.46
14:M:65:SER:HA	14:M:81:PHE:O	2.15	0.46
15:N:49:ASP:HA	15:N:52:ASN:HB2	1.98	0.46
29:X:1194:A:C2	29:X:1195:G:H1'	2.50	0.46
29:X:1271:G:H5''	29:X:1272:A:OP1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2266:A:H4'	29:X:2267:A:C2	2.50	0.46
29:X:2325:G:H8	29:X:2325:G:P	2.38	0.46
29:X:389:A:C8	29:X:2413:G:H4'	2.51	0.46
30:Y:6:C:H2'	30:Y:7:C:H6	1.79	0.46
8:G:81:VAL:HG11	8:G:156:HIS:CD2	2.41	0.46
21:T:43:THR:HB	29:X:2331:G:O3'	2.15	0.46
29:X:1234:U:H2'	29:X:1235:G:O4'	2.16	0.46
29:X:1319:G:O2'	29:X:1320:G:H5'	2.16	0.46
29:X:2821:A:H2'	29:X:2822:G:C8	2.51	0.46
4:C:42:THR:HG1	29:X:39:G:H21	1.62	0.46
29:X:691:G:C6	29:X:692:C:C4	3.04	0.46
29:X:818:G:N7	29:X:1187:G:C6	2.84	0.46
26:1:27:ASN:C	26:1:29:ARG:H	2.18	0.46
5:D:135:GLN:HA	5:D:138:PHE:CE1	2.50	0.46
8:G:148:LEU:HD12	8:G:149:LYS:H	1.80	0.46
15:N:85:ARG:HD3	15:N:116:ALA:O	2.16	0.46
17:P:109:ARG:HD2	29:X:748:G:OP2	2.15	0.46
17:P:50:VAL:O	17:P:54:GLU:HG3	2.15	0.46
20:S:23:ALA:N	20:S:32:PHE:HE2	2.14	0.46
22:U:17:SER:HB3	22:U:18:VAL:HB	1.98	0.46
29:X:1019:U:C4	29:X:1020:C:H5	2.34	0.46
29:X:1209:G:N2	29:X:1210:G:H22	2.14	0.46
29:X:2014:A:H2'	29:X:2015:A:C8	2.51	0.46
29:X:2204:A:H2	29:X:2219:U:H3	1.63	0.46
29:X:2247:A:H2'	29:X:2248:C:C6	2.51	0.46
29:X:69:C:H2'	29:X:70:G:C8	2.51	0.46
26:1:41:ASP:OD2	26:1:43:VAL:HG23	2.16	0.45
3:B:2:LYS:HA	3:B:84:PHE:CE1	2.51	0.45
4:C:34:GLN:O	4:C:37:SER:OG	2.22	0.45
9:H:20:MET:HG2	9:H:21:CYS:O	2.16	0.45
9:H:85:ASP:OD1	9:H:87:SER:N	2.43	0.45
10:I:113:GLU:HG2	10:I:114:ILE:N	2.30	0.45
15:N:78:THR:HB	15:N:117:ARG:CZ	2.46	0.45
29:X:1150:U:H2'	29:X:1151:A:H8	1.80	0.45
29:X:1210:G:H4'	29:X:1211:A:H5''	1.96	0.45
29:X:1285:G:N2	29:X:1328:G:H5'	2.30	0.45
29:X:2339:U:H2'	29:X:2340:G:H8	1.80	0.45
29:X:2330:G:N2	29:X:2386:U:O2	2.49	0.45
29:X:562:U:O2'	29:X:572:A:H8	1.97	0.45
29:X:733:G:C8	29:X:761:A:C6	3.04	0.45
29:X:862:G:H2'	29:X:863:A:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:13:GLU:C	26:1:49:PHE:HB3	2.37	0.45
2:A:83:GLU:OE1	2:A:104:TYR:OH	2.28	0.45
3:B:195:LEU:HB2	14:M:3:THR:HG22	1.98	0.45
4:C:156:ASN:HA	4:C:159:ARG:HB2	1.98	0.45
6:E:24:PHE:CD1	6:E:37:TYR:HB2	2.51	0.45
9:H:13:ASN:HD21	9:H:109:ARG:HG2	1.80	0.45
15:N:74:MET:CE	15:N:110:VAL:HG13	2.44	0.45
17:P:71:VAL:HG12	17:P:126:ILE:HD12	1.97	0.45
19:R:18:LYS:HA	19:R:36:VAL:HG11	1.98	0.45
24:W:22:ALA:C	24:W:24:GLY:H	2.20	0.45
2:A:157:ARG:HH11	29:X:1818:U:H6	1.64	0.45
29:X:2327:A:C5	29:X:2388:A:N1	2.85	0.45
29:X:2418:A:H2'	29:X:2419:U:O4'	2.16	0.45
29:X:392:C:H2'	29:X:393:G:C8	2.51	0.45
29:X:399:U:H2'	29:X:400:G:O4'	2.16	0.45
2:A:49:ILE:HG13	29:X:779:U:OP1	2.16	0.45
25:Z:38:GLY:HA3	25:Z:48:ASN:HD22	1.80	0.45
9:H:13:ASN:HD21	9:H:109:ARG:N	2.13	0.45
9:H:43:ARG:HD3	9:H:44:TYR:CE2	2.51	0.45
14:M:70:LYS:HD3	14:M:72:SER:HB2	1.99	0.45
19:R:58:VAL:HA	29:X:483:A:H5'	1.97	0.45
29:X:1499:U:H2'	29:X:1500:A:C8	2.52	0.45
29:X:1840:G:C6	29:X:1841:U:C4	3.04	0.45
29:X:2060:A:C2	29:X:2502:G:C5	3.04	0.45
29:X:2307:G:C6	29:X:2308:G:H1'	2.52	0.45
29:X:2615:U:C2	29:X:2616:C:C5	3.04	0.45
29:X:2616:C:H2'	29:X:2617:C:H6	1.81	0.45
29:X:2680:C:O2'	29:X:2681:C:H5'	2.16	0.45
5:D:92:ARG:HD3	30:Y:47:A:H8	1.80	0.45
8:G:41:TRP:HB3	8:G:163:PRO:HB3	1.98	0.45
10:I:45:LYS:HB2	10:I:45:LYS:HE3	1.54	0.45
15:N:8:ILE:HD11	29:X:1215:G:O3'	2.17	0.45
17:P:109:ARG:CG	17:P:109:ARG:HH11	2.29	0.45
22:U:29:GLY:C	22:U:31:GLY:N	2.69	0.45
8:G:56:THR:HG21	29:X:1005:C:O2'	2.16	0.45
29:X:1330:C:O2'	29:X:1331:C:H5'	2.16	0.45
2:A:250:TRP:CE2	29:X:1805:A:H5''	2.51	0.45
29:X:2371:G:C2	29:X:2372:G:C5	3.04	0.45
29:X:497:A:H2'	29:X:498:G:C8	2.52	0.45
29:X:926:C:O2'	29:X:928:C:N4	2.50	0.45
28:3:6:THR:HG23	28:3:62:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:130:THR:HG22	4:C:160:ALA:O	2.16	0.45
4:C:59:TYR:CD1	4:C:64:THR:HG21	2.52	0.45
9:H:97:VAL:HG11	9:H:126:ILE:HD13	1.98	0.45
17:P:86:LEU:HA	17:P:86:LEU:HD23	1.79	0.45
18:Q:48:VAL:HG11	18:Q:82:LEU:HG	1.99	0.45
29:X:1196:C:O2'	29:X:1227:G:O2'	2.32	0.45
29:X:1365:A:H5'	29:X:1366:A:OP2	2.16	0.45
29:X:2056:G:C2	29:X:2057:A:C8	3.04	0.45
29:X:2195:U:H2'	29:X:2196:C:C6	2.51	0.45
29:X:2347:C:H2'	29:X:2348:U:H6	1.79	0.45
29:X:2615:U:H2'	29:X:2616:C:H6	1.82	0.45
29:X:309:A:N6	29:X:1210:G:O2'	2.49	0.45
29:X:875:G:C6	29:X:876:C:C2	3.05	0.45
25:Z:7:PRO:HA	29:X:2615:U:N1	2.31	0.45
8:G:71:THR:HB	8:G:76:GLN:NE2	2.30	0.45
17:P:75:ALA:HB1	17:P:128:VAL:HG22	1.99	0.45
23:V:27:GLU:O	23:V:31:GLN:HG3	2.16	0.45
24:W:2:LYS:HB3	24:W:54:GLN:HB3	1.98	0.45
29:X:306:U:O2'	29:X:1211:A:N7	2.50	0.45
29:X:1370:C:H2'	29:X:1371:G:O4'	2.17	0.45
29:X:1686:C:H2'	29:X:1687:G:O4'	2.17	0.45
29:X:2599:G:N3	29:X:2600:A:C8	2.85	0.45
4:C:103:GLY:O	4:C:106:MET:N	2.49	0.45
13:L:31:VAL:O	13:L:32:TYR:HB2	2.17	0.45
13:L:47:ARG:C	13:L:49:GLN:H	2.20	0.45
19:R:85:ASP:CG	19:R:108:VAL:HG21	2.37	0.45
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.32	0.45
22:U:22:GLY:O	22:U:39:LYS:HG3	2.16	0.45
22:U:61:TRP:O	22:U:62:LEU:HD12	2.16	0.45
29:X:1163:G:N3	29:X:1164:A:C8	2.84	0.45
29:X:1201:A:C2	29:X:1245:G:C4	3.05	0.45
2:A:202:LYS:HB2	29:X:1820:U:C2	2.51	0.45
29:X:2532:G:C6	29:X:2533:A:C5	3.05	0.45
29:X:2837:A:H2'	29:X:2838:G:C8	2.52	0.45
29:X:733:G:O6	29:X:761:A:C8	2.70	0.45
29:X:83:G:H21	29:X:84:A:N6	2.15	0.45
29:X:902:C:H2'	29:X:903:C:H6	1.81	0.45
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.16	0.45
11:J:36:ILE:HD12	20:S:76:ARG:HD2	1.99	0.45
29:X:2094:G:N2	29:X:2196:C:O2	2.50	0.45
29:X:2339:U:H2'	29:X:2340:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2516:G:C2'	29:X:2517:C:H5'	2.47	0.45
29:X:2727:G:H2'	29:X:2728:U:H6	1.81	0.45
29:X:2901:C:H2'	29:X:2902:A:C8	2.51	0.45
29:X:814:C:H2'	29:X:815:C:H6	1.82	0.45
29:X:91:A:H4'	29:X:92:G:O5'	2.16	0.45
24:W:11:GLY:HA2	29:X:969:G:O3'	2.16	0.45
30:Y:48:A:H2'	30:Y:49:C:C6	2.52	0.45
17:P:56:LEU:HD22	25:Z:28:PRO:HD2	1.99	0.45
27:2:16:HIS:HB2	27:2:44:VAL:HG21	1.99	0.45
5:D:74:ILE:HA	5:D:79:LEU:CB	2.47	0.45
20:S:3:LEU:HD23	20:S:32:PHE:HB2	1.99	0.45
24:W:32:ARG:HG2	24:W:33:GLU:N	2.32	0.45
29:X:1124:C:C2	29:X:1125:G:C8	3.05	0.45
16:O:85:GLY:HA3	29:X:1224:G:O3'	2.16	0.45
29:X:1608:A:H1'	29:X:1610:A:OP2	2.17	0.45
29:X:1849:G:H2'	29:X:1850:G:C8	2.52	0.45
29:X:1922:G:H8	29:X:1922:G:OP2	2.00	0.45
29:X:2004:G:C6	29:X:2005:A:C4	3.05	0.45
29:X:2721:A:H2'	29:X:2722:G:O4'	2.17	0.45
29:X:27:G:HO2'	29:X:28:A:P	2.36	0.45
29:X:440:G:C2	29:X:441:U:C2	3.04	0.45
29:X:878:A:H1'	29:X:899:A:N7	2.31	0.45
7:F:11:GLN:HB3	29:X:1061:U:C5	2.52	0.45
10:I:114:ILE:HD13	10:I:114:ILE:HA	1.81	0.45
11:J:27:TYR:HB2	11:J:137:VAL:HB	1.99	0.45
13:L:101:LYS:O	13:L:104:ALA:HB3	2.17	0.45
20:S:111:GLY:HA3	20:S:172:LEU:O	2.17	0.45
22:U:54:ASN:C	22:U:56:GLN:H	2.14	0.45
16:O:87:ARG:NH2	29:X:1222:C:OP1	2.50	0.45
29:X:2291:U:H2'	29:X:2292:C:C6	2.51	0.45
29:X:2404:C:C2	29:X:2405:G:C8	3.04	0.45
29:X:729:G:H2'	29:X:1775:U:O2	2.17	0.45
30:Y:54:U:H4'	30:Y:54:U:OP1	2.17	0.45
2:A:148:VAL:HB	2:A:151:LYS:HE2	1.99	0.44
3:B:176:ARG:HH21	14:M:16:ILE:HA	1.82	0.44
18:Q:4:TYR:CE2	23:V:23:LYS:HB2	2.52	0.44
19:R:61:SER:HA	19:R:65:PRO:HA	1.99	0.44
20:S:3:LEU:HG	20:S:32:PHE:HD1	1.80	0.44
29:X:1069:A:H4'	29:X:1070:A:H8	1.82	0.44
29:X:2101:G:N2	29:X:2189:U:O2	2.50	0.44
29:X:2307:G:C8	29:X:2308:G:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:33:ILE:HA	3:B:33:ILE:HD13	1.73	0.44
4:C:120:VAL:N	4:C:190:ALA:HB2	2.33	0.44
9:H:85:ASP:OD1	9:H:87:SER:HB3	2.17	0.44
10:I:21:ARG:HG2	10:I:21:ARG:NH1	2.31	0.44
12:K:65:LEU:O	12:K:68:GLN:HG3	2.17	0.44
23:V:31:GLN:O	23:V:35:GLY:N	2.51	0.44
29:X:1950:G:C8	29:X:1951:U:C5	3.05	0.44
29:X:382:G:N2	29:X:393:G:C4	2.86	0.44
17:P:40:LEU:HB3	25:Z:25:LEU:HD13	1.98	0.44
1:O:74:THR:O	1:O:92:SER:HA	2.17	0.44
26:1:46:HIS:CE1	29:X:2372:G:HO2'	2.35	0.44
28:3:35:GLY:N	28:3:36:LYS:HA	2.33	0.44
4:C:168:SER:HB2	4:C:183:HIS:NE2	2.32	0.44
4:C:67:ALA:HA	29:X:1255:U:C6	2.51	0.44
11:J:27:TYR:CB	11:J:137:VAL:HB	2.47	0.44
12:K:28:LEU:HD23	12:K:28:LEU:C	2.37	0.44
29:X:1435:C:H42	29:X:1557:G:H1	1.63	0.44
29:X:219:G:H4'	29:X:386:G:C5	2.52	0.44
29:X:2347:C:H5	29:X:2382:G:H1'	1.83	0.44
29:X:2521:C:H2'	29:X:2522:U:O4'	2.16	0.44
29:X:440:G:H2'	29:X:441:U:C6	2.52	0.44
29:X:981:A:H5''	29:X:982:C:OP2	2.17	0.44
27:2:16:HIS:CB	27:2:44:VAL:HG21	2.48	0.44
28:3:17:THR:HG23	28:3:18:GLY:N	2.31	0.44
2:A:30:GLU:O	2:A:34:THR:HG23	2.18	0.44
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.51	0.44
29:X:1136:G:H2'	29:X:1137:G:C8	2.52	0.44
18:Q:54:SER:HB2	29:X:1341:A:O3'	2.17	0.44
29:X:1763:G:O2'	29:X:1958:C:OP1	2.31	0.44
1:O:1:LYS:HB2	29:X:2131:G:C8	2.53	0.44
29:X:2696:U:H2'	29:X:2697:G:C8	2.53	0.44
29:X:1729:C:H1'	29:X:2860:A:H1'	1.98	0.44
29:X:538:G:C2	29:X:539:G:C8	3.06	0.44
29:X:651(B):C:H5''	29:X:653:U:O5'	2.17	0.44
30:Y:33:C:H42	30:Y:53:G:H1	1.64	0.44
2:A:108:PRO:HA	2:A:196:VAL:O	2.18	0.44
8:G:68:PRO:HA	15:N:67:ALA:HB3	1.99	0.44
11:J:36:ILE:HG22	11:J:37:ALA:O	2.18	0.44
13:L:60:LYS:O	13:L:61:SER:OG	2.23	0.44
16:O:50:ASP:HA	16:O:53:LYS:HE3	1.99	0.44
16:O:78:VAL:O	16:O:79:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:3:HIS:NE2	18:Q:44:GLN:HG3	2.32	0.44
29:X:1118:A:H2'	29:X:1119:U:O4'	2.17	0.44
29:X:1324:G:O2'	29:X:1326:U:OP2	2.28	0.44
29:X:1593:G:H2'	29:X:1594:A:C8	2.52	0.44
29:X:1598:C:H2'	29:X:1599:C:H6	1.82	0.44
29:X:1901:A:H2'	29:X:1902:C:H6	1.82	0.44
29:X:2247:A:H2'	29:X:2248:C:H6	1.82	0.44
29:X:600:C:O2	29:X:604:C:H4'	2.16	0.44
29:X:624:C:O2'	29:X:657:U:H5''	2.17	0.44
29:X:996:A:N3	29:X:997:G:C8	2.86	0.44
30:Y:3:A:C6	30:Y:4:C:N4	2.86	0.44
2:A:43:ARG:HA	2:A:48:ARG:O	2.17	0.44
3:B:144:ARG:NH1	29:X:2572:A:O2'	2.50	0.44
3:B:60:ASN:HB3	3:B:62:PRO:CD	2.45	0.44
5:D:79:LEU:HD21	29:X:2310:A:N3	2.32	0.44
5:D:80:ARG:HD3	5:D:83:MET:HB3	1.99	0.44
7:F:79:ARG:HB3	7:F:84:ILE:O	2.17	0.44
8:G:115:ALA:O	8:G:119:LEU:HB2	2.18	0.44
8:G:65:LYS:O	8:G:66:HIS:HB3	2.18	0.44
14:M:69:ARG:HD2	14:M:78:GLU:OE2	2.17	0.44
29:X:1664:A:H61	29:X:1996:C:H42	1.66	0.44
29:X:189:G:H2'	29:X:190:A:O4'	2.17	0.44
29:X:2018:G:C6	29:X:2019:A:C6	3.05	0.44
29:X:2498:C:O2'	29:X:2499:C:H5'	2.17	0.44
25:Z:7:PRO:HA	29:X:2615:U:C2	2.53	0.44
29:X:620:G:H4'	29:X:621:A:H5''	1.99	0.44
27:2:26:SER:O	27:2:30:ILE:HG13	2.18	0.44
3:B:180:ASN:O	3:B:181:LEU:HD23	2.17	0.44
4:C:112:GLN:C	4:C:114:GLY:H	2.21	0.44
7:F:91:PRO:HA	7:F:135:GLY:HA2	2.00	0.44
8:G:106:TYR:CD2	29:X:2642:G:H5'	2.53	0.44
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.99	0.44
17:P:118:LYS:HD2	17:P:120:ARG:NH2	2.32	0.44
17:P:31:VAL:O	17:P:122:SER:N	2.48	0.44
18:Q:88:ILE:HG13	18:Q:88:ILE:O	2.18	0.44
20:S:152:ILE:HG22	20:S:154:LEU:HD23	1.99	0.44
21:T:21:LEU:HD21	21:T:41:ARG:HH21	1.83	0.44
21:T:6:GLY:HA3	21:T:7:VAL:HA	1.66	0.44
22:U:22:GLY:H	22:U:39:LYS:HB2	1.81	0.44
23:V:25:LEU:HD23	23:V:25:LEU:HA	1.72	0.44
29:X:1533:C:H2'	29:X:1534:C:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1592:U:H2'	29:X:1593:G:C8	2.53	0.44
29:X:1993:U:C2	29:X:1994:C:C6	3.06	0.44
29:X:2720:U:C2	29:X:2721:A:C8	3.06	0.44
29:X:72:A:N1	29:X:111:A:O2'	2.46	0.44
25:Z:3:LYS:HA	29:X:2577:A:O2'	2.18	0.44
1:0:39:VAL:HG11	1:0:185:TYR:CD2	2.52	0.44
3:B:120:TRP:O	3:B:121:ASN:HB2	2.17	0.44
3:B:31:CYS:HA	3:B:32:PRO:HD3	1.89	0.44
5:D:72:LYS:HA	5:D:81:GLN:HA	1.99	0.44
6:E:133:VAL:HG12	6:E:141:VAL:HG13	2.00	0.44
3:B:19:ARG:HA	9:H:84:ALA:O	2.16	0.44
10:I:73:GLU:HG3	10:I:105:PRO:O	2.17	0.44
11:J:71:PRO:HA	11:J:96:SER:HB2	2.00	0.44
15:N:11:ARG:O	15:N:15:LYS:HG3	2.18	0.44
21:T:14:ARG:HE	21:T:14:ARG:HB2	1.48	0.44
22:U:48:LYS:CG	22:U:49:LYS:H	2.19	0.44
29:X:2004:G:C4	29:X:2005:A:C8	3.06	0.44
29:X:2302:C:H42	29:X:2314:G:H1	1.64	0.44
29:X:2511:U:H2'	29:X:2512:C:C6	2.53	0.44
3:B:140:SER:HB2	29:X:2578:G:N7	2.33	0.44
11:J:70:PHE:CE2	29:X:871:C:H4'	2.53	0.44
30:Y:65:A:H2'	30:Y:66:G:H8	1.82	0.44
1:0:60:LEU:HA	1:0:61:PRO:HD3	1.87	0.44
1:0:66:ARG:HH11	1:0:156:ARG:HG3	1.83	0.44
20:S:67:LYS:HE3	20:S:92:VAL:HG21	1.99	0.44
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.82	0.44
29:X:1327:C:H2'	29:X:1328:G:C8	2.53	0.44
29:X:2372:G:C2	29:X:2373:A:N7	2.86	0.44
29:X:2650:U:O2'	29:X:2651:C:H5'	2.18	0.44
29:X:2774:C:H2'	29:X:2775:A:O4'	2.18	0.44
29:X:448:U:O4	29:X:583:G:H1'	2.17	0.44
2:A:218:LYS:HB3	2:A:218:LYS:HE3	1.86	0.43
3:B:175:ILE:HG12	3:B:182:ILE:HG12	1.99	0.43
7:F:112:MET:HG3	7:F:113:PRO:HD3	1.99	0.43
11:J:14:PHE:O	11:J:15:ARG:HG2	2.18	0.43
11:J:52:ARG:HH12	11:J:53:ILE:HG12	1.81	0.43
20:S:104:SER:HA	20:S:139:THR:HA	2.00	0.43
20:S:172:LEU:HD22	20:S:173:PRO:HD2	2.00	0.43
29:X:1054:A:H2'	29:X:1055:G:H8	1.83	0.43
29:X:1091:G:N2	29:X:1101:U:H1'	2.32	0.43
29:X:1242:A:C4	29:X:1243:C:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:165(B):G:H2'	29:X:165(C):G:O4'	2.18	0.43
29:X:1995:U:H3'	29:X:1996:C:H2'	2.00	0.43
29:X:2476:A:H5'	29:X:2476:A:H8	1.83	0.43
29:X:1782:C:H2'	29:X:2608:G:O2'	2.17	0.43
22:U:46:LEU:O	29:X:397:A:H5'	2.18	0.43
29:X:784:A:N7	29:X:792:G:C4	2.86	0.43
1:0:4:ARG:HG2	1:0:5:ALA:H	1.83	0.43
26:1:40:TYR:HA	26:1:46:HIS:HA	2.00	0.43
4:C:152:THR:HG23	4:C:189:ASP:OD2	2.17	0.43
4:C:176:ASN:HD21	4:C:179:ASP:HB2	1.84	0.43
7:F:19:PRO:HB2	7:F:20:ALA:H	1.66	0.43
7:F:90:THR:OG1	7:F:93:LYS:HB2	2.18	0.43
11:J:76:THR:HA	11:J:92:GLU:H	1.84	0.43
20:S:112:LEU:HG	20:S:113:VAL:N	2.32	0.43
22:U:27:ASP:HA	22:U:32:ARG:NH2	2.21	0.43
22:U:70:LEU:HB3	22:U:79:GLU:OE2	2.18	0.43
29:X:1036:G:C2	29:X:1120:G:C4	3.06	0.43
29:X:1422:G:H2'	29:X:1423:A:H8	1.83	0.43
29:X:1510:U:O2'	29:X:1511:G:OP1	2.32	0.43
29:X:13:A:N3	29:X:15:G:O6	2.50	0.43
29:X:2075:U:H3'	29:X:2238:G:H21	1.83	0.43
29:X:2320:A:H5''	29:X:2321:G:C4	2.53	0.43
29:X:2508:G:C4	29:X:2509:G:C8	3.06	0.43
29:X:2536:G:H2'	29:X:2537:U:O4'	2.17	0.43
29:X:2881:U:H2'	29:X:2882:C:C6	2.53	0.43
29:X:733:G:N7	29:X:761:A:C5	2.86	0.43
29:X:787:U:C5	29:X:791:C:N3	2.87	0.43
30:Y:39:C:H5''	30:Y:40:C:C5	2.53	0.43
30:Y:7:C:H2'	30:Y:8:C:H6	1.84	0.43
25:Z:28:PRO:HB2	25:Z:30:LEU:HG	1.99	0.43
1:0:33:PHE:HB3	1:0:34:ASP:H	1.58	0.43
1:0:64:THR:HG22	1:0:65:GLY:H	1.83	0.43
2:A:40:THR:C	2:A:42:GLY:H	2.21	0.43
3:B:72:VAL:O	3:B:73:ALA:HB3	2.18	0.43
6:E:19:ALA:HB1	6:E:24:PHE:HD2	1.83	0.43
12:K:24:GLN:HB3	12:K:44:LEU:CD2	2.45	0.43
13:L:8:ARG:HB2	13:L:8:ARG:NH1	2.31	0.43
16:O:73:LYS:HB2	16:O:82:ARG:HB2	1.99	0.43
19:R:100:ASP:HB2	19:R:103:LYS:CG	2.48	0.43
19:R:38:LEU:HB3	19:R:47:VAL:CG2	2.48	0.43
23:V:11:ALA:HA	23:V:14:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:51:SER:OG	29:X:1814:G:H4'	2.17	0.43
25:Z:43:HIS:N	29:X:2884:U:O4	2.48	0.43
30:Y:39:C:H5'	30:Y:40:C:OP2	2.18	0.43
28:3:29:LYS:HE2	29:X:2418:A:P	2.59	0.43
9:H:116:ARG:HG3	9:H:116:ARG:O	2.18	0.43
9:H:3:MET:O	9:H:6:SER:HB2	2.19	0.43
13:L:33:ARG:CZ	13:L:33:ARG:HB2	2.48	0.43
15:N:11:ARG:HH22	29:X:29:U:C4'	2.31	0.43
16:O:28:GLU:O	16:O:31:ASP:HB2	2.18	0.43
29:X:1164:A:C2	29:X:1165:U:C2	3.06	0.43
29:X:1644:C:O2	29:X:1644:C:H2'	2.18	0.43
9:H:5:GLN:HG2	29:X:1668:A:H5''	1.99	0.43
29:X:1676:A:N6	29:X:1677:A:C6	2.86	0.43
29:X:2212:A:C5'	29:X:2213:U:H5	2.31	0.43
29:X:2392:A:C8	29:X:2429:G:C2	3.06	0.43
29:X:2691:C:H2'	29:X:2692:C:H6	1.83	0.43
29:X:655:A:H4'	29:X:656:G:H5'	2.00	0.43
30:Y:83:C:N4	30:Y:98:C:N3	2.67	0.43
5:D:111:ILE:CG2	5:D:114:PHE:HB2	2.47	0.43
29:X:1094:U:O2'	29:X:1096:A:N7	2.46	0.43
25:Z:10:LYS:HG3	29:X:1263:U:H1'	2.00	0.43
29:X:1641:A:N6	29:X:1642:G:C2	2.86	0.43
29:X:1909:C:H6	29:X:1909:C:O5'	2.02	0.43
29:X:2691:C:H5''	29:X:2872:G:C5'	2.48	0.43
25:Z:30:LEU:HD23	25:Z:30:LEU:HA	1.82	0.43
11:J:46:ASN:HA	11:J:49:GLU:HB2	2.00	0.43
15:N:97:ASP:O	15:N:101:ARG:HB2	2.19	0.43
20:S:50:GLY:O	20:S:51:LEU:HB3	2.18	0.43
29:X:1061:U:H3'	29:X:1062:G:H5''	2.00	0.43
29:X:1078:C:N3	29:X:1088:A:H5'	2.34	0.43
29:X:1511:G:C6	29:X:1512:C:C4	3.06	0.43
29:X:24:G:N2	29:X:25:U:H1'	2.33	0.43
29:X:2856:A:H2'	29:X:2857:G:O4'	2.19	0.43
29:X:516:C:C2'	29:X:517:C:H5'	2.47	0.43
29:X:980:A:H62	29:X:981:A:N6	2.15	0.43
25:Z:18:MET:HE2	25:Z:18:MET:HB3	1.90	0.43
28:3:29:LYS:HZ3	28:3:41:ILE:HG12	1.82	0.43
4:C:145:THR:O	4:C:146:GLU:HG3	2.18	0.43
5:D:92:ARG:NH1	30:Y:46:G:H3'	2.34	0.43
6:E:99:THR:O	6:E:101:LYS:N	2.51	0.43
15:N:28:ARG:HG2	15:N:28:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:53:VAL:HG12	19:R:54:ILE:H	1.84	0.43
29:X:1835:G:H1'	29:X:1931:U:C2	2.53	0.43
29:X:858:U:O2	29:X:2268:A:H2'	2.19	0.43
29:X:2311:A:H5''	29:X:2312:U:OP2	2.19	0.43
29:X:2462:U:H2'	29:X:2463:C:C6	2.54	0.43
29:X:2689:U:P	29:X:2719:G:H22	2.41	0.43
29:X:2721:A:H1'	29:X:2873:A:O2'	2.19	0.43
17:P:9:ARG:NH2	29:X:307:G:OP1	2.48	0.43
29:X:643:A:C2	29:X:644:A:C4	3.07	0.43
29:X:747:U:O2	29:X:2014:A:H1'	2.18	0.43
2:A:229:VAL:HG11	29:X:784:A:C4	2.53	0.43
29:X:920:G:H2'	29:X:921:G:O4'	2.19	0.43
25:Z:3:LYS:HE3	25:Z:3:LYS:HB3	1.71	0.43
2:A:157:ARG:HH12	29:X:1817:G:H3'	1.84	0.43
2:A:85:ASP:HA	2:A:86:PRO:HD3	1.79	0.43
2:A:99:ASP:OD2	29:X:1491:A:H5'	2.19	0.43
8:G:133:GLY:HA3	29:X:1137:G:O2'	2.19	0.43
9:H:100:ASN:C	9:H:100:ASN:OD1	2.57	0.43
10:I:81:GLN:NE2	10:I:113:GLU:OE2	2.51	0.43
10:I:133:VAL:HG11	10:I:140:VAL:CG2	2.48	0.43
11:J:39:GLU:HA	11:J:40:PRO:HD3	1.62	0.43
11:J:6:LYS:O	11:J:71:PRO:HG2	2.19	0.43
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.54	0.43
29:X:1179:G:N1	29:X:1180:U:C4	2.87	0.43
29:X:1619:G:H2'	29:X:1620:G:H8	1.84	0.43
29:X:2290:G:N2	29:X:2373:A:O2'	2.47	0.43
29:X:2330:G:N2	29:X:2386:U:C2	2.87	0.43
29:X:2543:G:C6	29:X:2544:G:C6	3.06	0.43
4:C:78:VAL:HG13	29:X:448:U:H1'	2.00	0.43
29:X:902:C:H2'	29:X:903:C:C6	2.54	0.43
4:C:130:THR:HG21	29:X:320:U:H2'	2.00	0.43
13:L:67:THR:O	13:L:71:VAL:HG12	2.19	0.43
15:N:24:PHE:O	15:N:29:SER:HB3	2.18	0.43
17:P:21:ARG:HH22	29:X:496:G:H4'	1.84	0.43
18:Q:34:THR:HB	18:Q:37:GLU:HG3	2.00	0.43
19:R:35:LYS:HB3	19:R:35:LYS:HE3	1.76	0.43
29:X:1175:G:H2'	29:X:1176:C:C6	2.54	0.43
29:X:1745:G:O2'	29:X:1746:C:H5'	2.19	0.43
29:X:1864:U:H2'	29:X:1874:G:C8	2.54	0.43
29:X:2327:A:H3'	29:X:2328:A:C8	2.53	0.43
29:X:2521:C:C4	29:X:2522:U:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2716:A:C2'	29:X:2717:G:H5'	2.49	0.43
29:X:2717:G:C6	29:X:2718:G:C5	3.07	0.43
1:O:109:VAL:O	1:O:134:PRO:HD3	2.18	0.43
2:A:259:THR:OG1	29:X:1798:U:H5'	2.19	0.43
6:E:139:GLN:HB3	6:E:143:GLN:OE1	2.19	0.43
8:G:90:LEU:HD12	8:G:90:LEU:HA	1.86	0.43
14:M:19:ASP:O	14:M:20:HIS:ND1	2.52	0.43
15:N:32:TYR:O	15:N:35:ALA:HB3	2.18	0.43
15:N:60:LEU:HA	15:N:63:GLN:HG3	2.01	0.43
16:O:78:VAL:CG1	16:O:80:TYR:HB2	2.49	0.43
17:P:8:PHE:HE1	17:P:17:GLN:HB2	1.83	0.43
21:T:55:ARG:HG2	21:T:55:ARG:H	1.68	0.43
29:X:1151:A:H2'	29:X:1152:C:C6	2.54	0.43
29:X:1842:G:H2'	29:X:1843:C:C6	2.53	0.43
29:X:1885:A:H3'	29:X:1886:A:H8	1.84	0.43
29:X:222:G:H2'	29:X:223:A:C8	2.54	0.43
29:X:2376:A:H2'	29:X:2377:A:O4'	2.19	0.43
29:X:2474:C:H5''	29:X:2475:C:OP2	2.19	0.43
29:X:2655:G:O2'	29:X:2664:G:O6	2.26	0.43
29:X:335:C:H2'	29:X:336:C:C6	2.52	0.43
29:X:591:G:C6	29:X:592(A):C:N4	2.86	0.43
1:O:72:VAL:HG13	1:O:110:VAL:HB	2.00	0.42
6:E:25:LYS:HE2	6:E:25:LYS:HB3	1.81	0.42
9:H:83:ARG:HH21	9:H:89:ILE:HD11	1.83	0.42
11:J:69:ILE:HG21	11:J:104:MET:HG2	2.00	0.42
14:M:104:LEU:CD2	14:M:106:TYR:HE2	2.32	0.42
16:O:16:GLU:HG2	16:O:96:LEU:HD23	2.01	0.42
16:O:72:ARG:HA	16:O:82:ARG:O	2.19	0.42
23:V:63:LYS:HG2	23:V:66:GLN:NE2	2.34	0.42
29:X:1014:A:H2'	29:X:1015:U:H6	1.84	0.42
29:X:1312:U:H4'	29:X:1313:U:O5'	2.19	0.42
29:X:1795:C:H2'	29:X:1796:U:O4'	2.18	0.42
29:X:2349:G:O6	29:X:2382:G:N2	2.35	0.42
29:X:2507:C:C4	29:X:2583:G:C6	3.07	0.42
29:X:1637:A:H4'	29:X:2711:A:O2'	2.18	0.42
29:X:2732:G:H3'	29:X:2733:A:O4'	2.19	0.42
29:X:638:G:N1	29:X:649:G:N1	2.67	0.42
29:X:638:G:N2	29:X:650:C:H1'	2.34	0.42
29:X:684:G:C2	29:X:794:A:C2	3.07	0.42
29:X:844:U:H5'	29:X:845:G:OP2	2.19	0.42
2:A:161:THR:O	2:A:196:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:123:ALA:HB3	29:X:2511:U:O3'	2.18	0.42
4:C:74:VAL:O	4:C:77:PHE:HB2	2.19	0.42
5:D:155:THR:HG21	29:X:2314:G:H1'	2.01	0.42
8:G:100:TYR:OH	8:G:126:VAL:HG13	2.19	0.42
10:I:142:LEU:HA	10:I:143:PRO:HD3	1.91	0.42
19:R:77:HIS:HD2	29:X:328:U:C5'	2.29	0.42
20:S:1:MET:HE1	20:S:52:PHE:HB3	2.01	0.42
20:S:66:VAL:HG22	20:S:83:PHE:CE1	2.53	0.42
10:I:31:GLY:HA2	29:X:1190:G:H5''	2.01	0.42
29:X:1365:A:H2'	29:X:1365:A:N3	2.34	0.42
29:X:1885:A:H3'	29:X:1886:A:C8	2.54	0.42
29:X:2306:U:H5'	29:X:2307:G:C8	2.54	0.42
29:X:2747:G:O6	29:X:2755:C:H5''	2.19	0.42
17:P:134:LYS:HB2	29:X:2797:A:N6	2.35	0.42
29:X:347:C:H2'	29:X:348:G:H5'	2.01	0.42
29:X:704:G:H1'	29:X:726:G:N2	2.34	0.42
29:X:875:G:H2'	29:X:876:C:O4'	2.19	0.42
3:B:134:TRP:HE1	3:B:139:GLY:H	1.67	0.42
3:B:174:GLU:HB3	3:B:183:LEU:HB2	2.02	0.42
3:B:5:LEU:HD22	3:B:195:LEU:HD11	2.01	0.42
10:I:97:ARG:HB2	10:I:97:ARG:HE	1.53	0.42
11:J:17:ARG:HB3	11:J:42:TRP:HZ2	1.84	0.42
11:J:61:ARG:HA	11:J:62:GLY:HA2	1.66	0.42
17:P:25:PHE:HD1	17:P:127:ILE:HD11	1.84	0.42
20:S:143:ILE:HA	20:S:171:VAL:HG12	2.01	0.42
21:T:37:LEU:HD11	21:T:61:ALA:N	2.34	0.42
29:X:1821:A:O5'	29:X:1821:A:H8	2.03	0.42
29:X:2472:G:H2'	29:X:2475:C:H42	1.84	0.42
29:X:2711:A:N6	29:X:2714:G:C5	2.88	0.42
29:X:2825:C:H5''	29:X:2826:A:OP2	2.19	0.42
29:X:816:C:N3	29:X:1192:G:C2	2.87	0.42
29:X:925:A:H2'	29:X:926:C:O4'	2.19	0.42
1:O:95:LEU:HD13	1:O:98:ARG:HB2	2.00	0.42
28:3:29:LYS:HZ1	28:3:41:ILE:HG23	1.83	0.42
4:C:116:LYS:HB3	4:C:185:ARG:HD3	2.02	0.42
4:C:48:ARG:HB3	4:C:48:ARG:HE	1.43	0.42
8:G:52:GLY:O	8:G:55:ALA:HB3	2.19	0.42
11:J:76:THR:HG22	11:J:91:VAL:HA	2.00	0.42
13:L:15:ARG:HE	13:L:91:ARG:HH11	1.66	0.42
14:M:15:GLY:O	14:M:18:GLN:HG2	2.20	0.42
24:W:22:ALA:C	24:W:24:GLY:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1097:U:H2'	29:X:1098:A:O4'	2.18	0.42
29:X:1504:G:H2'	29:X:1505:U:O4'	2.19	0.42
29:X:170:C:O2'	29:X:171:A:H5'	2.20	0.42
29:X:231:C:O2	29:X:621:A:O2'	2.34	0.42
10:I:65:PHE:CE1	29:X:2404:C:H1'	2.54	0.42
29:X:2513:G:C2	29:X:2514:U:C2	3.07	0.42
29:X:820:A:H1'	29:X:943:U:O2'	2.19	0.42
26:1:34:LYS:HE3	26:1:51:ALA:O	2.19	0.42
5:D:126:GLY:O	5:D:160:ALA:HB3	2.20	0.42
5:D:64:LYS:HA	5:D:65:PRO:HD3	1.78	0.42
10:I:116:ARG:HG2	10:I:117:ALA:N	2.35	0.42
10:I:12:SER:O	29:X:660:G:N2	2.52	0.42
11:J:13:GLN:HB3	11:J:14:PHE:CD2	2.54	0.42
9:H:134:LEU:HA	14:M:48:GLN:HE22	1.84	0.42
16:O:64:GLY:HA3	16:O:90:PHE:CZ	2.55	0.42
18:Q:68:PHE:CD1	29:X:65:C:H1'	2.55	0.42
21:T:36:ILE:HD11	29:X:2364:C:O2	2.19	0.42
29:X:1745:G:C6	29:X:1746:C:N4	2.88	0.42
29:X:2280:G:C2'	29:X:2281:C:H5'	2.50	0.42
29:X:2332:U:H4'	29:X:2336:A:H62	1.85	0.42
29:X:2501:C:H5'	29:X:2502:G:OP1	2.18	0.42
29:X:2697:G:C2	29:X:2711:A:C2	3.06	0.42
29:X:740:U:C2	29:X:741:G:C8	3.08	0.42
29:X:980:A:N6	29:X:981:A:N6	2.67	0.42
30:Y:78:A:H2'	30:Y:79:U:O4'	2.19	0.42
1:O:43:LEU:H	1:O:167:VAL:HG12	1.84	0.42
28:3:17:THR:CG2	28:3:21:LYS:H	2.29	0.42
28:3:39:ASP:HB3	28:3:42:ARG:NH2	2.33	0.42
6:E:45:GLN:HG3	6:E:49:GLN:O	2.19	0.42
9:H:13:ASN:ND2	9:H:108:THR:HB	2.35	0.42
12:K:100:VAL:HG12	12:K:101:GLY:N	2.33	0.42
17:P:36:ARG:NH1	29:X:1266:G:C8	2.87	0.42
19:R:15:HIS:CD2	19:R:16:PHE:HD2	2.37	0.42
29:X:1235:G:C6	29:X:1236:G:N1	2.87	0.42
29:X:1309:G:N2	29:X:1611:C:H5'	2.34	0.42
29:X:14:A:C5	29:X:526:A:N1	2.87	0.42
2:A:86:PRO:HG3	29:X:1567:A:H2'	2.02	0.42
29:X:1675:C:H2'	29:X:1676:A:O4'	2.20	0.42
29:X:2836:G:C6	29:X:2837:A:N6	2.87	0.42
8:G:33:ILE:CD1	29:X:537:U:H4'	2.49	0.42
18:Q:73:ASN:HA	29:X:58:G:OP1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:19:THR:HB	30:Y:93:G:O5'	2.20	0.42
1:O:132:LEU:HD11	29:X:2169:A:O2'	2.20	0.42
27:2:6:GLN:HA	27:2:7:PRO:HD2	1.85	0.42
8:G:42:VAL:HG22	8:G:164:GLN:HB2	2.02	0.42
11:J:15:ARG:HB3	11:J:16:GLY:H	1.51	0.42
22:U:22:GLY:HA3	22:U:39:LYS:CE	2.50	0.42
29:X:1111:A:O2'	29:X:1112:G:H4'	2.19	0.42
29:X:1223:G:C6	29:X:1227:G:C6	3.07	0.42
15:N:33:ARG:HD3	29:X:1252:G:O4'	2.20	0.42
29:X:1587:A:H5'	29:X:1587:A:H8	1.85	0.42
29:X:1652:A:H3'	29:X:1653:G:C8	2.55	0.42
29:X:1665:A:C2'	29:X:1666:G:H5'	2.50	0.42
29:X:2263:C:H2'	29:X:2264:C:H6	1.85	0.42
3:B:144:ARG:NH1	29:X:2572:A:N3	2.68	0.42
29:X:2599:G:C4	29:X:2600:A:C8	3.08	0.42
29:X:2884:U:C5	29:X:2885:C:C2	3.08	0.42
29:X:537:U:H2'	29:X:538:G:C8	2.55	0.42
29:X:848:G:N2	29:X:932:U:H1'	2.34	0.42
25:Z:51:TYR:CD2	25:Z:54:GLY:O	2.73	0.42
1:O:12:ARG:HG3	1:O:217:SER:O	2.20	0.42
28:3:16:ILE:HG12	28:3:65:GLY:O	2.20	0.42
2:A:159:ALA:HB1	2:A:198:ASN:HB3	2.00	0.42
2:A:42:GLY:O	2:A:50:THR:N	2.49	0.42
2:A:67:PHE:HB3	2:A:153:ALA:H	1.84	0.42
6:E:22:GLY:HA3	6:E:39:THR:HG22	2.00	0.42
9:H:90:ARG:NH2	14:M:78:GLU:OE1	2.53	0.42
10:I:81:GLN:HB3	10:I:82:ASP:H	1.50	0.42
15:N:39:LEU:HA	15:N:39:LEU:HD23	1.72	0.42
29:X:1107:G:N1	29:X:1108:U:O2	2.53	0.42
29:X:1126:A:H4'	29:X:1127:A:C5'	2.50	0.42
29:X:1142:A:O2'	29:X:1143:A:H5''	2.20	0.42
29:X:1452:U:C2	29:X:1458:U:O2	2.73	0.42
29:X:1770:G:C5	29:X:1771:C:C5	3.08	0.42
29:X:2037:G:C6	29:X:2038:G:C6	3.08	0.42
29:X:472:A:C3'	29:X:473:G:H5'	2.50	0.42
29:X:501:A:H8	29:X:501:A:O5'	2.02	0.42
29:X:637:A:H4'	29:X:638:G:O5'	2.19	0.42
29:X:907:U:HO2'	29:X:908:G:C5'	2.32	0.42
8:G:65:LYS:NZ	8:G:65:LYS:HB2	2.33	0.42
12:K:33:ARG:HB2	12:K:114:GLU:CB	2.46	0.42
16:O:57:GLN:H	16:O:97:GLY:CA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1297:C:C2	29:X:1298:C:C5	3.08	0.42
29:X:1344:U:H4'	29:X:1384:A:C6	2.54	0.42
29:X:1739:C:H2'	29:X:1740:G:C8	2.54	0.42
29:X:1858:G:O2'	29:X:1883:G:N2	2.45	0.42
29:X:2140:G:H2'	29:X:2141:C:C6	2.54	0.42
29:X:2556:C:H2'	29:X:2557:G:O4'	2.20	0.42
29:X:622:G:C6	29:X:623:G:N7	2.88	0.42
29:X:646:A:N3	29:X:2350:C:O2'	2.52	0.42
29:X:841:G:H1	29:X:937:C:H42	1.66	0.42
11:J:66:TYR:HE2	29:X:873:A:HO2'	1.62	0.42
4:C:118:VAL:O	4:C:188:ILE:HG12	2.20	0.42
5:D:148:LYS:H	5:D:148:LYS:HG3	1.55	0.42
6:E:61:HIS:O	6:E:65:HIS:HB2	2.19	0.42
7:F:1:MET:HB3	7:F:2:ARG:HH11	1.84	0.42
15:N:36:PHE:O	15:N:39:LEU:HB2	2.19	0.42
18:Q:53:ILE:HG13	18:Q:80:VAL:HG13	2.02	0.42
21:T:23:VAL:HG22	21:T:26:PHE:CZ	2.55	0.42
29:X:2030:A:H4'	29:X:2031:A:C8	2.55	0.42
29:X:2342:C:O2'	29:X:2374:G:H5''	2.19	0.42
29:X:2667:C:H2'	29:X:2668:G:O4'	2.20	0.42
29:X:2773:C:H2'	29:X:2774:C:H6	1.84	0.42
29:X:403:U:H5''	29:X:404:C:OP1	2.19	0.42
29:X:537:U:H2'	29:X:538:G:H8	1.85	0.42
29:X:603:G:C5	29:X:625:G:C2	3.07	0.42
29:X:700:G:N2	29:X:732:C:H5	2.18	0.42
29:X:761:A:O5'	29:X:761:A:H8	2.03	0.42
30:Y:67:C:O2'	30:Y:68:A:H5'	2.20	0.42
2:A:161:THR:H	2:A:196:VAL:HB	1.85	0.41
3:B:105:THR:HB	3:B:197:VAL:HG12	2.02	0.41
3:B:2:LYS:HA	3:B:84:PHE:HE1	1.85	0.41
4:C:193:LEU:HD12	4:C:193:LEU:HA	1.85	0.41
6:E:126:PRO:HD2	6:E:130:ARG:O	2.20	0.41
9:H:111:PHE:HD1	9:H:111:PHE:N	2.18	0.41
9:H:23:ARG:HA	9:H:23:ARG:HD2	1.88	0.41
12:K:39:THR:O	12:K:42:LYS:N	2.53	0.41
19:R:76:LEU:HD23	19:R:76:LEU:HA	1.90	0.41
20:S:5:ALA:HB1	20:S:7:PRO:HD3	2.01	0.41
21:T:4:LYS:HA	21:T:4:LYS:HD3	1.82	0.41
29:X:1019:U:C4	29:X:1020:C:C5	3.08	0.41
29:X:1212:G:HO2'	29:X:1213:A:P	2.43	0.41
29:X:121:G:O5'	29:X:121:G:H8	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1263:U:C4	29:X:1264:G:C6	3.08	0.41
29:X:1794:A:H2'	29:X:1795:C:H6	1.85	0.41
29:X:1786:A:H1'	29:X:1938:A:N6	2.35	0.41
29:X:2114:A:N6	29:X:2119:A:H62	2.17	0.41
29:X:2219:U:N3	29:X:2220:C:H1'	2.34	0.41
29:X:2307:G:H1'	29:X:2311:A:N6	2.35	0.41
29:X:2455:G:C6	29:X:2456:C:N4	2.88	0.41
29:X:2532:G:C5	29:X:2533:A:C5	3.08	0.41
29:X:310:A:O3'	29:X:311:A:H8	2.03	0.41
29:X:466:A:N3	29:X:683:U:H1'	2.35	0.41
1:0:41:PHE:CE2	1:0:189:ILE:HG12	2.55	0.41
2:A:14:ARG:HB3	2:A:14:ARG:HE	1.62	0.41
4:C:26:VAL:HB	4:C:106:MET:HE1	2.02	0.41
9:H:115:ALA:O	9:H:117:GLU:N	2.54	0.41
22:U:20:ARG:O	22:U:43:ARG:NH2	2.53	0.41
29:X:1511:G:C6	29:X:1512:C:N4	2.88	0.41
29:X:2218:U:N3	29:X:2219:U:O4	2.53	0.41
29:X:2260:C:H2'	29:X:2261:C:H6	1.83	0.41
29:X:582:G:H2'	29:X:583:G:C8	2.56	0.41
29:X:935:U:H2'	29:X:936:C:C6	2.55	0.41
30:Y:75:A:C8	30:Y:107:C:C2	3.07	0.41
30:Y:7:C:H2'	30:Y:8:C:C6	2.56	0.41
10:I:57:ILE:HB	28:3:9:MET:HE2	2.02	0.41
2:A:78:LYS:HA	2:A:116:THR:HA	2.01	0.41
2:A:169:GLU:HB3	2:A:170:SER:H	1.57	0.41
5:D:5:LYS:HE2	5:D:100:LEU:HG	2.02	0.41
8:G:140:GLN:O	8:G:144:MET:HG3	2.21	0.41
10:I:98:LEU:O	10:I:99:VAL:HG13	2.21	0.41
11:J:135:ARG:HB3	11:J:136:GLU:H	1.68	0.41
11:J:23:LYS:HB3	11:J:24:GLY:H	1.72	0.41
15:N:25:TRP:O	15:N:28:ARG:HB2	2.20	0.41
21:T:41:ARG:HH11	29:X:2387:U:H1'	1.86	0.41
29:X:1760:C:C2'	29:X:1761:C:H5'	2.50	0.41
29:X:1985:G:H2'	29:X:1986:G:H8	1.84	0.41
29:X:2043:C:C4	29:X:2777:G:C2	3.08	0.41
29:X:2187:C:C2	29:X:2188:U:H1'	2.55	0.41
12:K:96:ARG:NE	29:X:2882:C:OP1	2.47	0.41
29:X:2809:A:C2	29:X:2891:A:C4	3.08	0.41
29:X:612:G:C2	29:X:616:A:C6	3.09	0.41
29:X:648:G:C6	29:X:649:G:C6	3.08	0.41
17:P:40:LEU:HB3	25:Z:25:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:130:ARG:HD3	1:O:130:ARG:HA	1.98	0.41
4:C:192:ALA:O	4:C:195:ILE:HG13	2.19	0.41
5:D:150:ARG:HB3	5:D:151:GLY:H	1.60	0.41
7:F:53:ILE:HA	7:F:54:PRO:HD2	1.93	0.41
4:C:28:HIS:CB	10:I:6:LEU:HD13	2.50	0.41
12:K:22:ARG:HG2	12:K:69:ASP:O	2.20	0.41
15:N:62:ILE:HG23	15:N:76:TYR:CE1	2.54	0.41
16:O:40:VAL:HB	16:O:46:VAL:H	1.85	0.41
17:P:107:ILE:HG13	17:P:107:ILE:O	2.21	0.41
20:S:26:LYS:N	20:S:26:LYS:HD3	2.35	0.41
3:B:146:THR:HG23	29:X:1130:U:C5	2.56	0.41
29:X:1282:U:H2'	29:X:1283:G:O4'	2.21	0.41
29:X:2335:A:O2'	29:X:2336:A:OP2	2.31	0.41
29:X:2389:G:H5''	29:X:2390:U:O5'	2.20	0.41
29:X:2513:G:H2'	29:X:2514:U:C6	2.55	0.41
29:X:2554:U:H2'	29:X:2555:U:C6	2.55	0.41
29:X:2547:U:C5	29:X:2566:A:C5	3.09	0.41
29:X:2684:U:N3	29:X:2685:G:C8	2.88	0.41
29:X:2720:U:H2'	29:X:2721:A:H8	1.84	0.41
29:X:2728:U:C2	29:X:2729:C:C5	3.08	0.41
29:X:2833:U:O2'	29:X:2834:A:H5'	2.18	0.41
29:X:2896:U:H2'	29:X:2897:U:C6	2.55	0.41
29:X:713:G:N2	29:X:718:A:OP2	2.53	0.41
29:X:701:G:C2	29:X:732:C:C5	3.08	0.41
2:A:18:THR:HG23	2:A:211:ARG:NH1	2.35	0.41
4:C:19:LEU:HB3	4:C:20:PRO:CA	2.51	0.41
4:C:22:VAL:HG13	4:C:106:MET:CG	2.47	0.41
9:H:130:ALA:HA	9:H:131:PRO:HD3	1.83	0.41
18:Q:50:VAL:HG22	18:Q:82:LEU:HD12	2.02	0.41
19:R:85:ASP:HB2	19:R:92:THR:HG21	2.02	0.41
29:X:1022:G:H22	29:X:1142:A:H2	1.68	0.41
29:X:1591:A:H2'	29:X:1592:U:C6	2.55	0.41
29:X:1999:C:O2	29:X:2687:U:O2'	2.36	0.41
29:X:2075:U:H3'	29:X:2238:G:N2	2.34	0.41
29:X:223:A:H2'	29:X:224:G:O4'	2.21	0.41
29:X:2427:C:H5''	29:X:2428:G:OP1	2.21	0.41
29:X:602:A:H4'	29:X:603:G:O5'	2.19	0.41
29:X:693:A:H2'	29:X:694:U:O4'	2.21	0.41
25:Z:10:LYS:HD2	29:X:1262:A:N3	2.35	0.41
4:C:27:LEU:HA	4:C:27:LEU:HD23	1.83	0.41
5:D:125:ARG:H	5:D:125:ARG:HG2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:24:PHE:CE2	6:E:43:VAL:HG13	2.55	0.41
11:J:126:LEU:HA	11:J:127:PRO:HD3	1.85	0.41
11:J:11:ARG:HB3	11:J:12:LYS:H	1.48	0.41
11:J:24:GLY:HA2	11:J:25:GLY:HA2	1.59	0.41
12:K:3:HIS:CG	12:K:3:HIS:O	2.72	0.41
14:M:55:ILE:CG1	14:M:67:THR:HG22	2.50	0.41
14:M:90:GLN:OE1	14:M:91:VAL:N	2.35	0.41
17:P:18:VAL:HG23	17:P:19:LYS:H	1.85	0.41
29:X:1229:A:C2'	29:X:1230:G:H5'	2.50	0.41
29:X:1360:G:N7	29:X:1361:G:C8	2.89	0.41
29:X:1535:U:O2'	29:X:1537:G:N2	2.53	0.41
29:X:2075:U:C4	29:X:2238:G:C6	3.09	0.41
13:L:18:ARG:HH22	29:X:2292:C:P	2.43	0.41
29:X:23:G:C2	29:X:24:G:C8	3.08	0.41
29:X:2541:A:HO2'	29:X:2765:A:H2	1.64	0.41
29:X:320:U:H5''	29:X:321:C:OP1	2.21	0.41
29:X:600:C:N4	29:X:601:G:C5	2.89	0.41
29:X:663:G:C6	29:X:664:G:C5	3.08	0.41
29:X:681:G:H2'	29:X:682:G:O4'	2.20	0.41
29:X:78:C:H42	29:X:108:G:H1	1.69	0.41
29:X:833:A:H2'	29:X:834:C:C6	2.56	0.41
2:A:134:ARG:NH2	2:A:135:PHE:HE2	2.19	0.41
3:B:134:TRP:CZ2	3:B:139:GLY:HA2	2.56	0.41
3:B:1:MET:O	3:B:84:PHE:HD1	2.03	0.41
5:D:10:ASP:HA	5:D:13:ARG:HD2	2.02	0.41
10:I:45:LYS:HB3	10:I:46:GLY:O	2.20	0.41
12:K:17:ARG:HE	12:K:17:ARG:HB2	1.15	0.41
19:R:10:HIS:ND1	19:R:44:GLN:OE1	2.54	0.41
23:V:24:GLU:OE1	23:V:46:LEU:HD21	2.21	0.41
29:X:1464:G:H2'	29:X:1465:G:C8	2.55	0.41
29:X:1936:A:C2	29:X:1945:G:C8	3.08	0.41
29:X:2457:U:O2	29:X:2495:G:C2	2.74	0.41
29:X:2498:C:OP2	29:X:2499:C:OP2	2.38	0.41
29:X:2507:C:C2	29:X:2583:G:C2	3.09	0.41
29:X:2547:U:C5	29:X:2566:A:C8	3.08	0.41
29:X:489:G:C2	29:X:491:G:H1'	2.56	0.41
29:X:651(B):C:OP2	29:X:653:U:H5'	2.21	0.41
29:X:650:C:C2	29:X:651:G:N7	2.89	0.41
29:X:781:A:H2	29:X:1776:G:N3	2.19	0.41
1:O:205:LEU:HD13	1:O:222:LEU:HD22	2.03	0.41
28:3:33:ASN:O	28:3:36:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:34:VAL:HG12	3:B:35:GLN:N	2.36	0.41
3:B:61:LYS:N	3:B:62:PRO:HD2	2.36	0.41
5:D:156:ILE:HG13	5:D:156:ILE:H	1.52	0.41
6:E:8:PRO:HD2	6:E:69:ARG:NH1	2.35	0.41
7:F:70:LYS:HB3	7:F:71:THR:H	1.59	0.41
12:K:28:LEU:HD23	12:K:29:LEU:HD23	2.02	0.41
15:N:66:ASN:OD1	15:N:70:ARG:HD2	2.21	0.41
15:N:77:SER:HB2	29:X:1152:C:O4'	2.21	0.41
16:O:7:THR:CB	16:O:22:VAL:HG11	2.44	0.41
16:O:22:VAL:HG12	16:O:23:GLU:H	1.84	0.41
18:Q:20:MET:HB2	18:Q:25:TYR:CE1	2.55	0.41
29:X:1154:G:OP2	29:X:1154:G:H8	2.03	0.41
10:I:62:LYS:HD2	29:X:2394:C:H5''	2.03	0.41
29:X:7:G:H2'	29:X:8:A:C8	2.56	0.41
29:X:872:A:C6	29:X:906:A:C2	3.09	0.41
27:2:19:ARG:NH1	29:X:124:G:H2'	2.36	0.41
5:D:71:LYS:HB2	5:D:71:LYS:HE3	1.90	0.41
7:F:41:PHE:O	7:F:45:THR:HG23	2.20	0.41
9:H:13:ASN:ND2	9:H:109:ARG:H	2.18	0.41
16:O:11:GLN:N	16:O:11:GLN:HE21	2.19	0.41
21:T:57:HIS:N	21:T:57:HIS:CD2	2.88	0.41
22:U:47:HIS:HB3	29:X:397:A:OP1	2.20	0.41
29:X:1197:G:H2'	29:X:1198:U:H6	1.85	0.41
29:X:150:C:H6	29:X:150:C:OP1	2.04	0.41
29:X:208:C:H2'	29:X:209:C:C6	2.55	0.41
5:D:125:ARG:HG3	29:X:2315:U:O2'	2.21	0.41
29:X:2508:G:H2'	29:X:2509:G:H8	1.85	0.41
29:X:2862:G:C6	29:X:2863:U:C4	3.09	0.41
29:X:518:G:H2'	29:X:519:U:C6	2.56	0.41
29:X:657:U:H2'	29:X:658:A:H8	1.82	0.41
29:X:677:A:C4	29:X:678:C:C5	3.09	0.41
29:X:852:A:H61	29:X:926:C:H42	1.69	0.41
9:H:124:MET:N	9:H:124:MET:SD	2.94	0.41
11:J:41:ALA:HB2	11:J:128:ILE:CG2	2.51	0.41
13:L:65:THR:HG1	30:Y:52:G:P	2.42	0.41
16:O:57:GLN:H	16:O:97:GLY:HA2	1.85	0.41
21:T:43:THR:O	21:T:43:THR:HG22	2.21	0.41
29:X:1127:A:H2'	29:X:1127:A:N3	2.36	0.41
29:X:1146:G:H2'	29:X:1147:A:O4'	2.21	0.41
29:X:1168:A:C2	29:X:1182:G:C2	3.09	0.41
15:N:13:ARG:HH12	29:X:1251:C:H3'	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1360:G:C8	29:X:1361:G:C8	3.09	0.41
29:X:2250:G:N3	29:X:2250:G:O4'	2.52	0.41
29:X:2673:G:N3	29:X:2674:A:C8	2.89	0.41
29:X:2690:C:N4	29:X:2713:U:O3'	2.54	0.41
19:R:10:HIS:NE2	29:X:327:G:H1'	2.36	0.41
29:X:864:G:H2'	29:X:865:C:C6	2.56	0.41
13:L:32:TYR:CZ	30:Y:9:G:H5'	2.56	0.41
25:Z:49:CYS:HB2	25:Z:51:TYR:HD1	1.86	0.41
28:3:17:THR:CG2	28:3:20:GLY:H	2.28	0.41
5:D:22:TYR:CD1	5:D:28:VAL:HG22	2.56	0.41
7:F:10:LEU:HD13	7:F:27:LEU:HD13	2.02	0.41
9:H:55:VAL:HB	9:H:68:ASP:H	1.85	0.41
10:I:97:ARG:O	10:I:98:LEU:HB2	2.21	0.41
17:P:51:GLN:O	17:P:54:GLU:HB2	2.21	0.41
21:T:69:PHE:HB2	29:X:856:C:H4'	2.03	0.41
29:X:1301:A:H2	29:X:1625(A):G:N3	2.19	0.41
29:X:1659:U:H2'	29:X:1660:C:O5'	2.21	0.41
29:X:177:G:O2'	29:X:178:U:OP2	2.39	0.41
29:X:2727:G:H2'	29:X:2728:U:C6	2.55	0.41
29:X:2749:A:OP2	29:X:2750:A:O2'	2.31	0.41
29:X:2752:C:H2'	29:X:2753:A:O4'	2.20	0.41
29:X:2818:G:O2'	29:X:2819:G:H5'	2.20	0.41
29:X:600:C:N4	29:X:601:G:C6	2.89	0.41
29:X:704:G:N3	29:X:726:G:C2	2.89	0.41
29:X:934:G:C4	29:X:935:U:C5	3.09	0.41
29:X:946:G:H2'	29:X:947:G:C8	2.55	0.41
30:Y:39:C:C5	30:Y:40:C:C4	3.09	0.41
4:C:161:ALA:HB1	4:C:167:VAL:HG21	2.03	0.40
7:F:73:PRO:C	7:F:75:SER:H	2.24	0.40
8:G:140:GLN:O	8:G:143:ALA:HB3	2.21	0.40
8:G:51:LEU:CD1	8:G:88:VAL:HG11	2.51	0.40
11:J:14:PHE:HD1	11:J:88:LYS:HE3	1.86	0.40
12:K:3:HIS:NE2	12:K:5:LYS:HD3	2.37	0.40
13:L:33:ARG:NH2	13:L:103:LEU:HD12	2.29	0.40
14:M:22:ARG:NE	14:M:24:LEU:HD21	2.35	0.40
19:R:16:PHE:CE2	19:R:81:VAL:HG11	2.55	0.40
20:S:9:THR:HA	20:S:10:PRO:HD3	1.88	0.40
21:T:23:VAL:HG22	21:T:26:PHE:CE2	2.56	0.40
22:U:32:ARG:HG2	22:U:34:THR:N	2.36	0.40
22:U:66:ALA:O	22:U:70:LEU:HB2	2.20	0.40
29:X:100:U:H4'	29:X:101:U:H5''	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1422:G:H2'	29:X:1423:A:C8	2.55	0.40
29:X:1499:U:H2'	29:X:1500:A:H8	1.86	0.40
29:X:1445:G:N3	29:X:1547:U:C2	2.89	0.40
29:X:1788:C:H2'	29:X:1789:A:C8	2.56	0.40
29:X:1904:G:O2'	29:X:1928:A:N1	2.43	0.40
29:X:2186:A:H2'	29:X:2187:C:C6	2.56	0.40
29:X:718:A:H3'	29:X:719:G:O4'	2.21	0.40
27:2:34:ARG:CZ	27:2:39:ARG:HD2	2.51	0.40
6:E:24:PHE:HB2	6:E:37:TYR:CE1	2.55	0.40
9:H:87:SER:HA	14:M:80:VAL:O	2.21	0.40
14:M:18:GLN:C	14:M:20:HIS:H	2.25	0.40
29:X:1324:G:N2	29:X:1331:C:C2	2.89	0.40
29:X:1414:G:HO2'	29:X:1415:A:H8	1.68	0.40
29:X:1634:U:H4'	29:X:1635:G:OP2	2.22	0.40
29:X:2280:G:C2	29:X:2281:C:C6	3.10	0.40
29:X:2489:G:C6	29:X:2490:G:C6	3.09	0.40
29:X:1955:U:H5	29:X:2557:G:N2	2.20	0.40
3:B:140:SER:HB2	29:X:2575:C:O2'	2.21	0.40
29:X:2715:C:C2	29:X:2716:A:C8	3.08	0.40
29:X:1729:C:O2'	29:X:2859:A:N3	2.35	0.40
29:X:2895:C:H2'	29:X:2896:U:C6	2.55	0.40
29:X:312:G:OP1	29:X:332:A:H5''	2.22	0.40
15:N:31:GLN:CD	29:X:580:C:H4'	2.41	0.40
29:X:670:A:H4'	29:X:671:C:O5'	2.21	0.40
29:X:866:A:H2'	29:X:866:A:N3	2.34	0.40
29:X:864:G:N2	29:X:913:U:O2	2.54	0.40
29:X:981:A:N1	29:X:2027:G:O2'	2.41	0.40
1:0:95:LEU:HD22	1:0:98:ARG:HD2	2.02	0.40
2:A:152:GLY:O	2:A:154:GLN:HG3	2.21	0.40
3:B:134:TRP:O	3:B:134:TRP:CG	2.74	0.40
3:B:4:ILE:HG12	3:B:5:LEU:N	2.36	0.40
4:C:171:PRO:HB2	4:C:172:VAL:HG23	2.04	0.40
5:D:38:GLU:HG2	5:D:53:ALA:HB1	2.02	0.40
19:R:62:MET:HA	19:R:63:THR:HA	1.80	0.40
29:X:1121:C:H2'	29:X:1122:G:O4'	2.22	0.40
29:X:1150:U:H2'	29:X:1151:A:C8	2.57	0.40
29:X:1163:G:C2	29:X:1164:A:C8	3.09	0.40
29:X:1487:G:H2'	29:X:1488:G:H8	1.87	0.40
29:X:1755:U:H5''	29:X:1756:A:OP2	2.20	0.40
2:A:44:ASN:HB2	29:X:1812:U:O2'	2.21	0.40
29:X:1783:A:C6	29:X:2587:A:C2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2662:A:O5'	29:X:2662:A:H8	2.04	0.40
29:X:2691:C:C2	29:X:2692:C:C5	3.10	0.40
29:X:2697:G:N1	29:X:2711:A:C2	2.90	0.40
30:Y:46:G:C2	30:Y:50:U:O2	2.75	0.40
3:B:102:ILE:HD11	3:B:184:VAL:HG21	2.02	0.40
3:B:6:GLY:HA3	3:B:27:LEU:O	2.21	0.40
3:B:55:ALA:O	3:B:59:VAL:HG23	2.22	0.40
3:B:33:ILE:HG12	3:B:89:ASP:HA	2.02	0.40
11:J:76:THR:HG22	11:J:91:VAL:H	1.87	0.40
12:K:28:LEU:CD2	12:K:115:LEU:HD11	2.49	0.40
13:L:32:TYR:O	13:L:32:TYR:CG	2.75	0.40
13:L:8:ARG:C	13:L:10:LYS:H	2.25	0.40
29:X:1180:U:H2'	29:X:1181:U:H6	1.87	0.40
15:N:10:ARG:HG3	29:X:1251:C:OP1	2.21	0.40
29:X:1485:C:H2'	29:X:1486:G:O4'	2.22	0.40
29:X:166:G:H2'	29:X:167:A:O4'	2.22	0.40
1:O:32:LYS:HE3	29:X:2128:C:H5'	2.02	0.40
29:X:954:G:O2'	29:X:2274:A:N1	2.33	0.40
10:I:62:LYS:HG3	29:X:2394:C:OP1	2.21	0.40
29:X:2519:U:C6	29:X:2541:A:N6	2.89	0.40
14:M:100:ARG:O	29:X:2848:G:H3'	2.20	0.40
29:X:817:C:O2'	29:X:839:U:H5''	2.21	0.40
25:Z:7:PRO:HA	29:X:2615:U:C6	2.57	0.40
2:A:227:ASN:OD1	29:X:784:A:H5''	2.22	0.40
6:E:55:PRO:HB2	6:E:56:SER:H	1.57	0.40
7:F:115:LEU:C	7:F:117:ALA:H	2.25	0.40
18:Q:89:GLU:HG3	18:Q:89:GLU:H	1.65	0.40
21:T:11:LYS:HB2	21:T:11:LYS:HE2	1.81	0.40
29:X:1196:C:N3	29:X:1197:G:N7	2.69	0.40
29:X:1197:G:C4	29:X:1198:U:C5	3.09	0.40
29:X:127:A:H5''	29:X:128:C:O4'	2.21	0.40
29:X:1319:G:C6	29:X:1320:G:O6	2.75	0.40
29:X:1354:A:H2'	29:X:1355:G:O4'	2.22	0.40
29:X:1478:G:C6	29:X:1479:G:C5	3.10	0.40
29:X:1413:G:N2	29:X:1587:A:C8	2.90	0.40
29:X:1731:A:H61	29:X:1741:U:H3	1.68	0.40
29:X:179:A:H2'	29:X:180:C:O4'	2.22	0.40
29:X:676:A:H8	29:X:2069:G:H21	1.65	0.40
29:X:2194:U:H2'	29:X:2195:U:O4'	2.22	0.40
29:X:2468:G:N2	29:X:2481:G:H2'	2.34	0.40
29:X:2469:A:N6	29:X:2481:G:O2'	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:296:C:H2'	29:X:297:C:C6	2.55	0.40
29:X:617:A:H2'	29:X:618:C:C6	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	222/224 (99%)	135 (61%)	65 (29%)	22 (10%)	0	1
2	A	272/274 (99%)	238 (88%)	25 (9%)	9 (3%)	4	15
3	B	203/205 (99%)	168 (83%)	24 (12%)	11 (5%)	2	6
4	C	195/197 (99%)	151 (77%)	30 (15%)	14 (7%)	1	3
5	D	175/177 (99%)	124 (71%)	39 (22%)	12 (7%)	1	3
6	E	169/171 (99%)	130 (77%)	22 (13%)	17 (10%)	0	1
7	F	142/144 (99%)	99 (70%)	34 (24%)	9 (6%)	1	4
8	G	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	10
9	H	132/134 (98%)	103 (78%)	19 (14%)	10 (8%)	1	2
10	I	139/141 (99%)	104 (75%)	23 (16%)	12 (9%)	1	2
11	J	134/136 (98%)	102 (76%)	20 (15%)	12 (9%)	1	1
12	K	111/113 (98%)	95 (86%)	11 (10%)	5 (4%)	2	9
13	L	102/104 (98%)	65 (64%)	21 (21%)	16 (16%)	0	0
14	M	107/109 (98%)	93 (87%)	7 (6%)	7 (6%)	1	3
15	N	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	5	20
16	O	92/94 (98%)	75 (82%)	11 (12%)	6 (6%)	1	3
17	P	125/127 (98%)	99 (79%)	16 (13%)	10 (8%)	1	2
18	Q	91/93 (98%)	87 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	R	108/110 (98%)	84 (78%)	14 (13%)	10 (9%)	0	1
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	0	1
21	T	82/84 (98%)	68 (83%)	11 (13%)	3 (4%)	3	13
22	U	70/72 (97%)	38 (54%)	16 (23%)	16 (23%)	0	0
23	V	64/66 (97%)	55 (86%)	5 (8%)	4 (6%)	1	4
24	W	53/55 (96%)	48 (91%)	3 (6%)	2 (4%)	3	13
25	Z	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	2	5
26	1	52/54 (96%)	33 (64%)	13 (25%)	6 (12%)	0	1
27	2	45/47 (96%)	40 (89%)	3 (7%)	2 (4%)	2	10
28	3	63/65 (97%)	47 (75%)	12 (19%)	4 (6%)	1	4
All	All	3431/3487 (98%)	2670 (78%)	512 (15%)	249 (7%)	1	3

All (249) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	28	LEU
1	0	30	THR
1	0	45	ILE
1	0	157	ILE
1	0	216	PRO
2	A	170	SER
2	A	242	ALA
3	B	85	ALA
3	B	86	PRO
3	B	117	MET
3	B	121	ASN
4	C	10	ASN
4	C	64	THR
4	C	162	ARG
5	D	33	LYS
5	D	42	SER
5	D	134	GLU
6	E	55	PRO
6	E	65	HIS
6	E	92	VAL
6	E	126	PRO
6	E	165	VAL
7	F	22	PRO

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Mol	Chain	Res	Type
7	F	23	VAL
8	G	66	HIS
8	G	70	PHE
9	H	29	ILE
9	H	47	VAL
10	I	28	LYS
10	I	53	ARG
10	I	81	GLN
10	I	98	LEU
10	I	99	VAL
11	J	13	GLN
11	J	91	VAL
11	J	98	VAL
12	K	4	GLY
12	K	32	GLY
12	K	88	ALA
13	L	21	THR
13	L	23	ALA
13	L	32	TYR
13	L	40	ALA
13	L	45	ASP
13	L	104	ALA
15	N	5	LYS
15	N	7	GLY
16	O	8	GLY
16	O	31	ASP
17	P	50	VAL
17	P	65	SER
17	P	81	HIS
17	P	82	ASN
17	P	88	ASP
19	R	49	GLU
19	R	58	VAL
19	R	60	PRO
20	S	57	GLU
20	S	91	PRO
20	S	125	PRO
20	S	169	VAL
22	U	15	VAL
22	U	56	GLN
22	U	60	VAL
23	V	3	PRO

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Mol	Chain	Res	Type
24	W	23	LEU
24	W	36	ASP
25	Z	36	CYS
26	1	32	GLN
26	1	46	HIS
27	2	44	VAL
28	3	34	THR
1	0	17	SER
1	0	29	ALA
1	0	62	HIS
1	0	87	ALA
1	0	138	SER
2	A	45	ASN
2	A	198	ASN
3	B	34	VAL
3	B	118	LYS
4	C	9	GLN
4	C	11	GLY
4	C	22	VAL
4	C	124	ASP
4	C	155	GLU
4	C	172	VAL
4	C	190	ALA
5	D	35	VAL
5	D	40	LEU
5	D	132	ILE
6	E	18	ASN
6	E	58	ALA
6	E	100	GLY
6	E	110	SER
7	F	47	ASP
7	F	82	ALA
8	G	36	ASN
8	G	165	VAL
9	H	37	GLY
9	H	71	LYS
10	I	78	SER
10	I	103	ASN
11	J	11	ARG
11	J	21	ASP
11	J	46	ASN
11	J	97	VAL

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Mol	Chain	Res	Type
12	K	20	LEU
12	K	109	THR
13	L	55	SER
13	L	56	SER
16	O	16	GLU
17	P	64	ALA
19	R	110	SER
20	S	16	GLU
20	S	50	GLY
20	S	88	TYR
20	S	128	ARG
20	S	156	GLU
21	T	14	ARG
22	U	18	VAL
22	U	29	GLY
22	U	30	VAL
22	U	32	ARG
22	U	55	GLY
22	U	76	LYS
23	V	4	SER
26	1	4	ALA
26	1	48	VAL
28	3	46	LYS
28	3	52	LYS
1	0	61	PRO
1	0	86	GLY
1	0	108	ALA
1	0	146	ALA
2	A	52	ARG
2	A	169	GLU
3	B	94	ASP
3	B	133	LYS
5	D	133	LYS
6	E	7	GLN
6	E	19	ALA
6	E	42	THR
6	E	173	ALA
7	F	19	PRO
7	F	98	LYS
9	H	14	SER
9	H	69	VAL
10	I	27	ASP

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Mol	Chain	Res	Type
10	I	45	LYS
10	I	86	THR
10	I	91	ASP
11	J	23	LYS
13	L	52	ALA
13	L	53	ALA
13	L	96	TYR
17	P	89	ARG
19	R	75	ALA
19	R	78	ALA
20	S	6	LYS
20	S	14	LEU
22	U	12	ASN
22	U	14	VAL
22	U	41	VAL
22	U	48	LYS
26	1	7	ARG
26	1	44	ALA
27	2	7	PRO
28	3	45	GLY
1	0	33	PHE
2	A	26	LYS
2	A	226	MET
3	B	60	ASN
4	C	159	ARG
5	D	81	GLN
5	D	145	MET
6	E	24	PHE
6	E	112	PRO
6	E	136	ILE
8	G	95	LEU
9	H	22	ILE
9	H	32	LYS
9	H	42	LYS
9	H	70	VAL
11	J	45	SER
13	L	59	LEU
13	L	93	SER
14	M	10	GLY
14	M	16	ILE
16	O	29	ALA
16	O	44	GLN

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Mol	Chain	Res	Type
16	O	45	THR
17	P	19	LYS
17	P	87	GLU
20	S	38	ALA
22	U	10	LYS
1	0	158	GLU
1	0	191	ALA
1	0	197	PRO
1	0	203	VAL
3	B	128	SER
4	C	15	ILE
6	E	107	ILE
10	I	90	ARG
11	J	15	ARG
11	J	30	PHE
13	L	46	SER
13	L	91	ARG
14	M	7	ILE
14	M	15	GLY
14	M	25	PRO
14	M	26	ASP
14	M	83	PHE
19	R	51	VAL
19	R	64	ASN
20	S	51	LEU
21	T	74	LYS
22	U	47	HIS
25	Z	53	ASP
1	0	100	ALA
2	A	210	GLY
3	B	73	ALA
5	D	123	ASP
7	F	25	PRO
7	F	94	ALA
11	J	37	ALA
13	L	51	LEU
19	R	52	ASN
19	R	108	VAL
20	S	32	PHE
20	S	37	LYS
22	U	40	ARG
25	Z	15	LYS

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Mol	Chain	Res	Type
4	C	18	PRO
7	F	83	GLY
20	S	110	GLY
1	0	89	VAL
4	C	20	PRO
5	D	41	GLY
8	G	34	PRO
17	P	61	PRO
20	S	58	GLY
21	T	30	VAL
1	0	198	GLY
15	N	8	ILE
20	S	124	ALA
23	V	43	VAL
5	D	137	ILE
23	V	18	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	0	167/167 (100%)	150 (90%)	17 (10%)	7	22
2	A	214/214 (100%)	190 (89%)	24 (11%)	6	18
3	B	155/155 (100%)	139 (90%)	16 (10%)	7	22
4	C	157/157 (100%)	137 (87%)	20 (13%)	4	13
5	D	153/153 (100%)	131 (86%)	22 (14%)	3	9
6	E	136/136 (100%)	114 (84%)	22 (16%)	2	7
7	F	107/107 (100%)	97 (91%)	10 (9%)	9	27
8	G	118/118 (100%)	108 (92%)	10 (8%)	10	31
9	H	103/103 (100%)	76 (74%)	27 (26%)	0	1
10	I	108/108 (100%)	85 (79%)	23 (21%)	1	3
11	J	110/110 (100%)	89 (81%)	21 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	90/90 (100%)	78 (87%)	12 (13%)	4	11
13	L	74/74 (100%)	52 (70%)	22 (30%)	0	1
14	M	92/92 (100%)	79 (86%)	13 (14%)	3	10
15	N	96/96 (100%)	86 (90%)	10 (10%)	7	21
16	O	75/75 (100%)	57 (76%)	18 (24%)	0	2
17	P	109/109 (100%)	92 (84%)	17 (16%)	2	8
18	Q	75/75 (100%)	69 (92%)	6 (8%)	12	33
19	R	91/91 (100%)	76 (84%)	15 (16%)	2	7
20	S	149/149 (100%)	117 (78%)	32 (22%)	1	3
21	T	62/62 (100%)	48 (77%)	14 (23%)	1	2
22	U	57/57 (100%)	42 (74%)	15 (26%)	0	1
23	V	54/54 (100%)	48 (89%)	6 (11%)	6	19
24	W	48/48 (100%)	43 (90%)	5 (10%)	7	21
25	Z	51/51 (100%)	43 (84%)	8 (16%)	2	8
26	1	38/38 (100%)	30 (79%)	8 (21%)	1	3
27	2	40/40 (100%)	33 (82%)	7 (18%)	2	6
28	3	51/51 (100%)	40 (78%)	11 (22%)	1	3
All	All	2780/2780 (100%)	2349 (84%)	431 (16%)	2	8

All (431) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	11	ASP
1	0	12	ARG
1	0	16	TYR
1	0	24	LEU
1	0	25	VAL
1	0	26	LYS
1	0	38	GLU
1	0	52	GLN
1	0	64	THR
1	0	70	VAL
1	0	110	VAL
1	0	141	VAL
1	0	152	LEU
1	0	157	ILE

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Mol	Chain	Res	Type
1	0	166	VAL
1	0	186	GLN
1	0	212	THR
2	A	10	THR
2	A	13	ARG
2	A	14	ARG
2	A	18	THR
2	A	35	GLU
2	A	63	ARG
2	A	68	LYS
2	A	71	ASP
2	A	96	HIS
2	A	99	ASP
2	A	117	VAL
2	A	134	ARG
2	A	164	GLN
2	A	165	VAL
2	A	168	LYS
2	A	183	ARG
2	A	200	GLU
2	A	204	ILE
2	A	233	HIS
2	A	247	VAL
2	A	252	LYS
2	A	261	ARG
2	A	271	VAL
2	A	273	ARG
3	B	19	ARG
3	B	86	PRO
3	B	87	ASP
3	B	91	VAL
3	B	116	VAL
3	B	132	LYS
3	B	136	ARG
3	B	138	PRO
3	B	140	SER
3	B	143	GLN
3	B	144	ARG
3	B	145	LYS
3	B	152	LYS
3	B	162	MET
3	B	184	VAL

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Mol	Chain	Res	Type
3	B	205	SER
4	C	38	ARG
4	C	48	ARG
4	C	51	VAL
4	C	62	LYS
4	C	84	PHE
4	C	87	LYS
4	C	94	THR
4	C	102	LEU
4	C	110	SER
4	C	117	LEU
4	C	121	ASP
4	C	131	LYS
4	C	143	ASP
4	C	145	THR
4	C	152	THR
4	C	172	VAL
4	C	181	LEU
4	C	185	ARG
4	C	188	ILE
4	C	198	GLU
5	D	34	ILE
5	D	40	LEU
5	D	46	ASP
5	D	66	ILE
5	D	80	ARG
5	D	89	VAL
5	D	90	THR
5	D	92	ARG
5	D	115	ARG
5	D	117	ILE
5	D	125	ARG
5	D	142	THR
5	D	145	MET
5	D	148	LYS
5	D	150	ARG
5	D	152	MET
5	D	153	ASP
5	D	154	ILE
5	D	155	THR
5	D	156	ILE
5	D	158	THR

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Mol	Chain	Res	Type
5	D	159	THR
6	E	6	LYS
6	E	35	VAL
6	E	38	ASN
6	E	40	GLU
6	E	43	VAL
6	E	44	ARG
6	E	50	LEU
6	E	64	LEU
6	E	67	LEU
6	E	69	ARG
6	E	72	VAL
6	E	81	ASP
6	E	84	THR
6	E	90	ARG
6	E	105	MET
6	E	106	ASN
6	E	113	VAL
6	E	114	ILE
6	E	130	ARG
6	E	140	LEU
6	E	149	ARG
6	E	165	VAL
7	F	2	ARG
7	F	36	GLU
7	F	50	ASP
7	F	63	ARG
7	F	84	ILE
7	F	99	LEU
7	F	102	ASP
7	F	119	SER
7	F	136	VAL
7	F	137	THR
8	G	31	THR
8	G	33	ILE
8	G	65	LYS
8	G	69	ASP
8	G	94	LYS
8	G	96	ASP
8	G	111	LYS
8	G	122	HIS
8	G	156	HIS

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Mol	Chain	Res	Type
8	G	167	LYS
9	H	3	MET
9	H	8	LEU
9	H	9	ASP
9	H	13	ASN
9	H	22	ILE
9	H	25	LEU
9	H	29	ILE
9	H	35	THR
9	H	36	THR
9	H	41	ASN
9	H	43	ARG
9	H	46	HIS
9	H	54	SER
9	H	65	LYS
9	H	68	ASP
9	H	78	SER
9	H	83	ARG
9	H	89	ILE
9	H	90	ARG
9	H	109	ARG
9	H	111	PHE
9	H	116	ARG
9	H	117	GLU
9	H	120	ASP
9	H	122	ARG
9	H	126	ILE
9	H	127	VAL
10	I	4	HIS
10	I	5	ASP
10	I	27	ASP
10	I	29	THR
10	I	35	LYS
10	I	50	GLU
10	I	57	ILE
10	I	65	PHE
10	I	70	THR
10	I	73	GLU
10	I	77	LEU
10	I	80	LEU
10	I	81	GLN
10	I	91	ASP

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Mol	Chain	Res	Type
10	I	93	LEU
10	I	94	GLU
10	I	96	TYR
10	I	97	ARG
10	I	99	VAL
10	I	103	ASN
10	I	114	ILE
10	I	121	HIS
10	I	140	VAL
11	J	10	PHE
11	J	11	ARG
11	J	17	ARG
11	J	26	ASP
11	J	48	ILE
11	J	60	ARG
11	J	82	THR
11	J	84	MET
11	J	91	VAL
11	J	92	GLU
11	J	93	TYR
11	J	95	VAL
11	J	99	LYS
11	J	102	ARG
11	J	111	THR
11	J	112	GLU
11	J	113	GLU
11	J	132	MET
11	J	133	VAL
11	J	137	VAL
11	J	140	GLU
12	K	17	ARG
12	K	31	GLU
12	K	33	ARG
12	K	36	THR
12	K	56	LYS
12	K	59	ASP
12	K	60	LEU
12	K	64	ARG
12	K	68	GLN
12	K	73	LYS
12	K	83	VAL
12	K	112	LEU

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Mol	Chain	Res	Type
13	L	8	ARG
13	L	13	THR
13	L	14	ARG
13	L	16	LYS
13	L	17	VAL
13	L	30	SER
13	L	36	LYS
13	L	37	HIS
13	L	38	ILE
13	L	39	TYR
13	L	42	ILE
13	L	43	ILE
13	L	47	ARG
13	L	55	SER
13	L	60	LYS
13	L	66	ASP
13	L	67	THR
13	L	71	VAL
13	L	91	ARG
13	L	93	SER
13	L	105	ASP
13	L	108	ARG
14	M	2	GLN
14	M	3	THR
14	M	5	ILE
14	M	6	LYS
14	M	7	ILE
14	M	14	ARG
14	M	37	THR
14	M	38	LYS
14	M	58	ASN
14	M	65	SER
14	M	71	ILE
14	M	99	VAL
14	M	101	ARG
15	N	8	ILE
15	N	9	VAL
15	N	19	LYS
15	N	51	ARG
15	N	59	ARG
15	N	74	MET
15	N	76	TYR

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Mol	Chain	Res	Type
15	N	77	SER
15	N	80	ILE
15	N	87	ASN
16	O	6	GLN
16	O	7	THR
16	O	10	LYS
16	O	11	GLN
16	O	14	VAL
16	O	16	GLU
16	O	18	ASP
16	O	26	GLN
16	O	31	ASP
16	O	34	GLU
16	O	50	ASP
16	O	53	LYS
16	O	56	VAL
16	O	59	GLU
16	O	62	GLU
16	O	65	ARG
16	O	69	ILE
16	O	84	THR
17	P	9	ARG
17	P	17	GLN
17	P	25	PHE
17	P	32	ARG
17	P	36	ARG
17	P	45	ILE
17	P	48	LYS
17	P	49	SER
17	P	63	SER
17	P	65	SER
17	P	66	GLU
17	P	93	LYS
17	P	98	ASP
17	P	103	LEU
17	P	105	ARG
17	P	109	ARG
17	P	122	SER
18	Q	40	ASP
18	Q	62	ARG
18	Q	64	ARG
18	Q	80	VAL

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Mol	Chain	Res	Type
18	Q	82	LEU
18	Q	91	LEU
19	R	5	SER
19	R	18	LYS
19	R	46	VAL
19	R	51	VAL
19	R	53	VAL
19	R	66	GLN
19	R	81	VAL
19	R	98	ILE
19	R	99	VAL
19	R	102	LYS
19	R	103	LYS
19	R	104	VAL
19	R	106	VAL
19	R	112	LYS
19	R	113	THR
20	S	3	LEU
20	S	4	THR
20	S	13	LYS
20	S	15	ASP
20	S	22	VAL
20	S	24	TYR
20	S	25	ASN
20	S	27	GLU
20	S	48	THR
20	S	49	THR
20	S	55	THR
20	S	57	GLU
20	S	61	THR
20	S	65	LEU
20	S	67	LYS
20	S	83	PHE
20	S	87	THR
20	S	95	SER
20	S	96	VAL
20	S	100	THR
20	S	103	ARG
20	S	109	GLN
20	S	112	LEU
20	S	117	VAL
20	S	119	ASN

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Mol	Chain	Res	Type
20	S	120	LEU
20	S	140	LYS
20	S	151	ASP
20	S	166	LEU
20	S	167	THR
20	S	171	VAL
20	S	175	ARG
21	T	7	VAL
21	T	10	SER
21	T	11	LYS
21	T	19	LYS
21	T	23	VAL
21	T	31	VAL
21	T	32	LYS
21	T	37	LEU
21	T	38	VAL
21	T	46	LYS
21	T	51	VAL
21	T	64	ASP
21	T	80	SER
21	T	85	GLN
22	U	8	THR
22	U	12	ASN
22	U	14	VAL
22	U	19	ILE
22	U	23	LYS
22	U	25	ARG
22	U	32	ARG
22	U	33	LYS
22	U	35	THR
22	U	42	GLN
22	U	49	LYS
22	U	63	SER
22	U	67	ILE
22	U	70	LEU
22	U	78	ILE
23	V	10	GLN
23	V	16	LYS
23	V	21	ARG
23	V	46	LEU
23	V	47	ARG
23	V	55	THR

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Mol	Chain	Res	Type
24	W	3	ILE
24	W	10	ILE
24	W	34	VAL
24	W	51	LEU
24	W	53	VAL
25	Z	3	LYS
25	Z	9	LYS
25	Z	20	ARG
25	Z	23	HIS
25	Z	32	GLU
25	Z	49	CYS
25	Z	57	VAL
25	Z	58	LEU
26	1	7	ARG
26	1	18	THR
26	1	24	THR
26	1	28	ARG
26	1	32	GLN
26	1	43	VAL
26	1	47	VAL
26	1	49	PHE
27	2	1	MET
27	2	12	ARG
27	2	24	THR
27	2	25	LYS
27	2	26	SER
27	2	42	LEU
27	2	45	SER
28	3	7	HIS
28	3	17	THR
28	3	22	VAL
28	3	26	LYS
28	3	29	LYS
28	3	31	HIS
28	3	32	GLN
28	3	39	ASP
28	3	46	LYS
28	3	50	LEU
28	3	62	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	129	ASN
2	A	231	HIS
4	C	10	ASN
5	D	118	ASN
5	D	120	ASN
5	D	127	ASN
8	G	161	GLN
9	H	41	ASN
14	M	58	ASN
15	N	91	ASN
18	Q	86	GLN
19	R	69	GLN
19	R	77	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	655 (23%)	41 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	690 (23%)	42 (1%)

All (690) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	13	A
29	X	14	A
29	X	22	C
29	X	28	A
29	X	46	C
29	X	51	G
29	X	55	G
29	X	59	C
29	X	64	A
29	X	65	C
29	X	68	G
29	X	71	A
29	X	74	A
29	X	75	G
29	X	92	G
29	X	93	A
29	X	95	A
29	X	97	G

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Mol	Chain	Res	Type
29	X	102	G
29	X	104	C
29	X	110	G
29	X	118	A
29	X	120	U
29	X	121	G
29	X	125	A
29	X	126	A
29	X	137	U
29	X	149	G
29	X	161	A
29	X	167	A
29	X	168	A
29	X	170	C
29	X	171	A
29	X	173	C
29	X	175	C
29	X	176	A
29	X	184	A
29	X	187	G
29	X	188	A
29	X	193	A
29	X	194	A
29	X	195	A
29	X	196	G
29	X	200	A
29	X	201	U
29	X	202	U
29	X	205	A
29	X	220	G
29	X	221	C
29	X	222	G
29	X	223	A
29	X	224	G
29	X	233	G
29	X	238	G
29	X	310	A
29	X	311	A
29	X	312	G
29	X	314	U
29	X	316	C
29	X	324	A

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Mol	Chain	Res	Type
29	X	328	U
29	X	329	G
29	X	332	A
29	X	333	G
29	X	334	U
29	X	338	G
29	X	339	U
29	X	345	A
29	X	346	A
29	X	347	C
29	X	349	A
29	X	350	G
29	X	386	G
29	X	387	U
29	X	390	A
29	X	391	A
29	X	395	U
29	X	396	G
29	X	401	A
29	X	404	C
29	X	405	C
29	X	406	G
29	X	409	C
29	X	411	G
29	X	412	A
29	X	441	U
29	X	449	A
29	X	451	C
29	X	454	A
29	X	456	U
29	X	458	G
29	X	470	A
29	X	472	A
29	X	475	U
29	X	479	A
29	X	480	A
29	X	481	G
29	X	483	A
29	X	494	G
29	X	499	U
29	X	501	A
29	X	502	A

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Mol	Chain	Res	Type
29	X	503	A
29	X	504	G
29	X	505	A
29	X	506	G
29	X	508	A
29	X	509	C
29	X	510	C
29	X	511	U
29	X	517	C
29	X	522	A
29	X	530	G
29	X	531	C
29	X	532	A
29	X	533	G
29	X	545	U
29	X	546	U
29	X	547	A
29	X	548	U
29	X	549	G
29	X	550	C
29	X	555	U
29	X	563	G
29	X	569	U
29	X	573	G
29	X	574	C
29	X	575	A
29	X	583	G
29	X	586	A
29	X	592	A
29	X	592(A)	C
29	X	600	C
29	X	602	A
29	X	614	A
29	X	615	A
29	X	621	A
29	X	623	G
29	X	627	A
29	X	634	G
29	X	637	A
29	X	643	A
29	X	644	A
29	X	645	U

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Mol	Chain	Res	Type
29	X	651(B)	C
29	X	653	U
29	X	654	U
29	X	655	A
29	X	669	G
29	X	670	A
29	X	682	G
29	X	686	G
29	X	690	A
29	X	714	U
29	X	716	A
29	X	718	A
29	X	719	G
29	X	720	G
29	X	730	A
29	X	734	A
29	X	739	G
29	X	740	U
29	X	747	U
29	X	752	C
29	X	761	A
29	X	762	U
29	X	765	G
29	X	776	G
29	X	782	A
29	X	784	A
29	X	785	G
29	X	792	G
29	X	793	A
29	X	801	G
29	X	805	G
29	X	808	A
29	X	812	C
29	X	819	A
29	X	826	U
29	X	827	U
29	X	828	G
29	X	832	U
29	X	835	A
29	X	844	U
29	X	845	G
29	X	859	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	X	866	A
29	X	874	G
29	X	910	A
29	X	915	C
29	X	920	G
29	X	921	G
29	X	926	C
29	X	928	C
29	X	929	G
29	X	945	A
29	X	946	G
29	X	958	U
29	X	961	C
29	X	962	U
29	X	974	G
29	X	983	A
29	X	984	A
29	X	989	G
29	X	990	A
29	X	996	A
29	X	997	G
29	X	1003	G
29	X	1008	U
29	X	1009	A
29	X	1011	A
29	X	1012	U
29	X	1013	G
29	X	1022	G
29	X	1023	U
29	X	1026	U
29	X	1033	U
29	X	1038	C
29	X	1044	A
29	X	1045	U
29	X	1046	A
29	X	1047	G
29	X	1049	C
29	X	1057	A
29	X	1060	U
29	X	1061	U
29	X	1067	A
29	X	1068	G

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Mol	Chain	Res	Type
29	X	1070	A
29	X	1071	G
29	X	1075	C
29	X	1078	C
29	X	1080	C
29	X	1083	C
29	X	1087	G
29	X	1088	A
29	X	1089	G
29	X	1096	A
29	X	1097	U
29	X	1102	C
29	X	1109	C
29	X	1111	A
29	X	1112	G
29	X	1117	G
29	X	1122	G
29	X	1127	A
29	X	1128	A
29	X	1130	U
29	X	1131	G
29	X	1134	C
29	X	1135	G
29	X	1138	G
29	X	1140	U
29	X	1141	C
29	X	1142	A
29	X	1143	A
29	X	1147	A
29	X	1154	G
29	X	1156	A
29	X	1169	A
29	X	1172(B)	C
29	X	1173	A
29	X	1175	G
29	X	1181	U
29	X	1193	G
29	X	1195	G
29	X	1210	G
29	X	1213	A
29	X	1217	C
29	X	1225	A

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Mol	Chain	Res	Type
29	X	1226	A
29	X	1227	G
29	X	1253	G
29	X	1256	G
29	X	1257	C
29	X	1271	G
29	X	1272	A
29	X	1273	U
29	X	1275	A
29	X	1276	A
29	X	1284	A
29	X	1287	A
29	X	1288	U
29	X	1294	U
29	X	1298	C
29	X	1300	U
29	X	1301	A
29	X	1318	G
29	X	1319	G
29	X	1321	A
29	X	1329	U
29	X	1332	G
29	X	1338	G
29	X	1341	A
29	X	1346	G
29	X	1357	U
29	X	1360	G
29	X	1365	A
29	X	1368	G
29	X	1378	A
29	X	1379	U
29	X	1390	U
29	X	1391	C
29	X	1395	A
29	X	1413	G
29	X	1414	G
29	X	1415	A
29	X	1418	G
29	X	1428	C
29	X	1437	C
29	X	1444	U
29	X	1445	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	X	1459	A
29	X	1460	U
29	X	1468	G
29	X	1474	U
29	X	1482	G
29	X	1489	U
29	X	1490	C
29	X	1491	A
29	X	1498	C
29	X	1507	A
29	X	1508	C
29	X	1509	A
29	X	1511	G
29	X	1525	G
29	X	1529	G
29	X	1532	U
29	X	1536	C
29	X	1537	G
29	X	1546	G
29	X	1558	A
29	X	1559	C
29	X	1566	A
29	X	1569	A
29	X	1578	U
29	X	1583	G
29	X	1585	U
29	X	1586	G
29	X	1587	A
29	X	1602	U
29	X	1608	A
29	X	1609	A
29	X	1610	A
29	X	1613	G
29	X	1615	C
29	X	1616	A
29	X	1634	U
29	X	1639	U
29	X	1644	C
29	X	1648	C
29	X	1651	G
29	X	1652	A
29	X	1653	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	X	1660	C
29	X	1674	G
29	X	1675	C
29	X	1694	C
29	X	1697	A
29	X	1700	A
29	X	1734	C
29	X	1735	U
29	X	1736	U
29	X	1737	C
29	X	1738	G
29	X	1747	G
29	X	1750	G
29	X	1754	A
29	X	1758	G
29	X	1761	C
29	X	1763	G
29	X	1773	A
29	X	1781	C
29	X	1784	A
29	X	1791	A
29	X	1797	C
29	X	1800	C
29	X	1801	C
29	X	1808	A
29	X	1816	C
29	X	1819	A
29	X	1829	A
29	X	1833	C
29	X	1843	C
29	X	1858	G
29	X	1862	G
29	X	1876	A
29	X	1880	U
29	X	1886	A
29	X	1892	C
29	X	1900	A
29	X	1901	A
29	X	1903	G
29	X	1906	G
29	X	1907	G
29	X	1910	G

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Mol	Chain	Res	Type
29	X	1912	A
29	X	1913	A
29	X	1914	C
29	X	1915	U
29	X	1916	A
29	X	1920	C
29	X	1922	G
29	X	1926	U
29	X	1936	A
29	X	1938	A
29	X	1940	U
29	X	1941	C
29	X	1951	U
29	X	1955	U
29	X	1963	U
29	X	1966	A
29	X	1967	C
29	X	1968	G
29	X	1970	A
29	X	1971	A
29	X	1972	G
29	X	1991	U
29	X	1992	G
29	X	1993	U
29	X	1996	C
29	X	1997	A
29	X	2016	U
29	X	2023	G
29	X	2031	A
29	X	2035	G
29	X	2036	C
29	X	2043	C
29	X	2046	G
29	X	2049	G
29	X	2055	C
29	X	2056	G
29	X	2060	A
29	X	2061	G
29	X	2062	A
29	X	2066	C
29	X	2069	G
29	X	2075	U

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Mol	Chain	Res	Type
29	X	2076	U
29	X	2077	A
29	X	2092	U
29	X	2093	G
29	X	2110	G
29	X	2111	C
29	X	2112	G
29	X	2114	A
29	X	2116	G
29	X	2117	A
29	X	2118	U
29	X	2119	A
29	X	2121	G
29	X	2123	G
29	X	2124	G
29	X	2125	G
29	X	2126	A
29	X	2127	G
29	X	2128	C
29	X	2132	C
29	X	2133	G
29	X	2134	A
29	X	2136	A
29	X	2137	C
29	X	2138	U
29	X	2139	G
29	X	2140	G
29	X	2142	C
29	X	2143	U
29	X	2144	U
29	X	2145	U
29	X	2146	U
29	X	2151	U
29	X	2152	C
29	X	2157	G
29	X	2158	A
29	X	2164	C
29	X	2167	U
29	X	2168	G
29	X	2170	A
29	X	2171	A
29	X	2173	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	X	2175	C
29	X	2179	C
29	X	2182	A
29	X	2188	U
29	X	2190	G
29	X	2197	U
29	X	2198	A
29	X	2205	A
29	X	2210	A
29	X	2211	A
29	X	2212	A
29	X	2213	U
29	X	2217	U
29	X	2220	C
29	X	2221	G
29	X	2225	A
29	X	2238	G
29	X	2239	G
29	X	2250	G
29	X	2251	G
29	X	2270	U
29	X	2273	A
29	X	2280	G
29	X	2283	C
29	X	2287	A
29	X	2288	A
29	X	2289	G
29	X	2305	U
29	X	2306	U
29	X	2307	G
29	X	2308	G
29	X	2309	A
29	X	2311	A
29	X	2320	A
29	X	2321	G
29	X	2322	A
29	X	2327	A
29	X	2333	A
29	X	2334	G
29	X	2335	A
29	X	2336	A
29	X	2346	A

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Mol	Chain	Res	Type
29	X	2350	C
29	X	2352	A
29	X	2357	G
29	X	2361	C
29	X	2372	G
29	X	2379	C
29	X	2382	G
29	X	2383	G
29	X	2385	C
29	X	2390	U
29	X	2392	A
29	X	2396	G
29	X	2400	G
29	X	2402	A
29	X	2406	U
29	X	2407	G
29	X	2410	G
29	X	2414	G
29	X	2423	U
29	X	2425	A
29	X	2428	G
29	X	2429	G
29	X	2430	A
29	X	2431	U
29	X	2434	A
29	X	2439	A
29	X	2440	C
29	X	2441	C
29	X	2447	G
29	X	2448	A
29	X	2462	U
29	X	2463	C
29	X	2469	A
29	X	2474	C
29	X	2476	A
29	X	2478	A
29	X	2481	G
29	X	2484	G
29	X	2491	U
29	X	2498	C
29	X	2499	C
29	X	2500	U

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Mol	Chain	Res	Type
29	X	2501	C
29	X	2502	G
29	X	2505	G
29	X	2515	C
29	X	2518	A
29	X	2519	U
29	X	2529	G
29	X	2538	C
29	X	2542	A
29	X	2543	G
29	X	2553	G
29	X	2554	U
29	X	2555	U
29	X	2566	A
29	X	2567	G
29	X	2572	A
29	X	2573	C
29	X	2578	G
29	X	2582	G
29	X	2586	C
29	X	2600	A
29	X	2602	A
29	X	2603	G
29	X	2609	U
29	X	2610	C
29	X	2612	C
29	X	2614	A
29	X	2615	U
29	X	2632	A
29	X	2634	A
29	X	2640	G
29	X	2660	A
29	X	2663	G
29	X	2666	C
29	X	2673	G
29	X	2681	C
29	X	2682	G
29	X	2689	U
29	X	2691	C
29	X	2697	G
29	X	2700	G
29	X	2707	C

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Mol	Chain	Res	Type
29	X	2712	C
29	X	2712(A)	A
29	X	2713	U
29	X	2714	G
29	X	2715	C
29	X	2722	G
29	X	2723	C
29	X	2726	U
29	X	2727	G
29	X	2733	A
29	X	2738	A
29	X	2748	A
29	X	2756	U
29	X	2757	A
29	X	2758	A
29	X	2763	G
29	X	2765	A
29	X	2778	A
29	X	2780	G
29	X	2789	C
29	X	2794	U
29	X	2795	U
29	X	2797	A
29	X	2798	U
29	X	2799	C
29	X	2800	A
29	X	2808	U
29	X	2812	A
29	X	2818	G
29	X	2820	A
29	X	2821	A
29	X	2823	A
29	X	2825	C
29	X	2834	A
29	X	2840	C
29	X	2848	G
29	X	2852	G
29	X	2858	C
29	X	2867	C
29	X	2872	G
29	X	2873	A
29	X	2874	C

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Mol	Chain	Res	Type
29	X	2876	G
29	X	2883	A
29	X	2890	G
29	X	2891	A
29	X	2893	G
29	X	2894	U
29	X	2902	A
30	Y	11	G
30	Y	14	C
30	Y	16	U
30	Y	17	A
30	Y	20	A
30	Y	26	G
30	Y	27	A
30	Y	28	A
30	Y	29	C
30	Y	34	C
30	Y	37	C
30	Y	40	C
30	Y	42	U
30	Y	43	G
30	Y	44	C
30	Y	46	G
30	Y	47	A
30	Y	48	A
30	Y	49	C
30	Y	53	G
30	Y	58	G
30	Y	59	A
30	Y	63	A
30	Y	69	G
30	Y	75	A
30	Y	76	U
30	Y	86	A
30	Y	99	G
30	Y	108	G
30	Y	111	C
30	Y	112	A
30	Y	115	G
30	Y	120	G
30	Y	121	G
30	Y	123	U

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	219	G
29	X	310	A
29	X	330	A
29	X	453	C
29	X	501	A
29	X	506	G
29	X	508	A
29	X	614	A
29	X	643	A
29	X	644	A
29	X	669	G
29	X	734	A
29	X	800	A
29	X	929	G
29	X	960	A
29	X	1127	A
29	X	1212	G
29	X	1275	A
29	X	1413	G
29	X	1414	G
29	X	1490	C
29	X	1510	U
29	X	1585	U
29	X	1586	G
29	X	1608	A
29	X	1610	A
29	X	1662	U
29	X	1997	A
29	X	2022	U
29	X	2035	G
29	X	2051	A
29	X	2060	A
29	X	2347	C
29	X	2351	G
29	X	2430	A
29	X	2468	G
29	X	2553	G
29	X	2714	G
29	X	2756	U
29	X	2778	A
29	X	2873	A
30	Y	16	U

## 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 198 ligands modelled in this entry, 198 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	0	224/224 (100%)	5.93	199 (88%) 0 0	238, 259, 280, 290	0
2	A	274/274 (100%)	0.53	31 (11%) 5 4	93, 135, 154, 161	0
3	B	205/205 (100%)	0.24	7 (3%) 45 40	60, 89, 107, 124	0
4	C	197/197 (100%)	0.37	15 (7%) 13 10	77, 125, 145, 159	0
5	D	177/177 (100%)	1.65	67 (37%) 0 0	155, 174, 190, 197	0
6	E	171/171 (100%)	0.85	35 (20%) 1 0	110, 148, 175, 177	0
7	F	144/144 (100%)	3.56	102 (70%) 0 0	213, 230, 235, 237	0
8	G	142/142 (100%)	0.27	11 (7%) 13 10	79, 112, 127, 144	0
9	H	134/134 (100%)	0.03	5 (3%) 41 37	62, 79, 94, 111	0
10	I	141/141 (100%)	0.98	32 (22%) 0 0	86, 138, 155, 161	0
11	J	136/136 (100%)	1.04	33 (24%) 0 0	94, 113, 135, 141	0
12	K	113/113 (100%)	0.14	3 (2%) 54 50	61, 72, 83, 88	0
13	L	104/104 (100%)	1.48	33 (31%) 0 0	121, 136, 153, 162	0
14	M	109/109 (100%)	-0.19	3 (2%) 53 49	65, 80, 98, 127	0
15	N	117/117 (100%)	0.40	10 (8%) 10 8	80, 107, 127, 133	0
16	O	94/94 (100%)	0.07	8 (8%) 10 8	89, 122, 141, 152	0
17	P	127/127 (100%)	0.40	10 (7%) 12 10	71, 85, 109, 156	0
18	Q	93/93 (100%)	0.94	14 (15%) 2 1	98, 124, 140, 144	0
19	R	110/110 (100%)	0.58	14 (12%) 3 2	110, 121, 146, 157	0
20	S	175/175 (100%)	0.72	35 (20%) 1 0	124, 151, 164, 168	0
21	T	84/84 (100%)	2.25	38 (45%) 0 0	102, 117, 133, 146	0
22	U	72/72 (100%)	2.89	46 (63%) 0 0	117, 148, 161, 164	0
23	V	66/66 (100%)	0.35	8 (12%) 4 3	129, 141, 159, 163	0
24	W	55/55 (100%)	0.70	10 (18%) 1 1	95, 110, 126, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Z	57/57 (100%)	-0.12	1 (1%) 68 67	74, 82, 104, 112	0
26	1	54/54 (100%)	1.45	20 (37%) 0 0	125, 136, 152, 168	0
27	2	47/47 (100%)	0.21	1 (2%) 63 61	91, 108, 116, 117	0
28	3	65/65 (100%)	2.07	32 (49%) 0 0	107, 118, 127, 129	0
29	X	2780/2881 (96%)	-0.13	108 (3%) 39 35	51, 111, 221, 347	0
30	Y	122/122 (100%)	-0.53	4 (3%) 46 41	96, 136, 161, 172	0
All	All	6389/6490 (98%)	0.57	935 (14%) 2 1	51, 119, 242, 347	0

All (935) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	X	2137	C	31.2
29	X	1916	A	26.7
1	0	54	VAL	23.5
29	X	2112	G	20.1
1	0	86	GLY	19.7
29	X	1918	A	19.5
1	0	85	ALA	19.4
29	X	2144	U	18.6
29	X	1917	U	18.5
1	0	223	GLY	18.4
1	0	200	ALA	17.9
1	0	143	ALA	16.7
7	F	1	MET	16.7
1	0	55	ARG	16.6
29	X	2138	U	15.5
1	0	14	LYS	15.4
1	0	209	TYR	15.3
21	T	3	HIS	15.1
29	X	2113	U	14.1
29	X	1919	A	13.7
1	0	222	LEU	13.1
29	X	1914	C	13.1
7	F	25	PRO	12.9
1	0	208	ALA	12.6
1	0	164	THR	12.5
1	0	162	ASP	11.9
29	X	2145	U	11.9
1	0	69	ARG	11.8
1	0	42	ARG	11.7

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Mol	Chain	Res	Type	RSRZ
21	T	2	ALA	11.7
1	0	56	GLY	11.4
29	X	718	A	11.4
29	X	1507	A	11.4
7	F	7	ILE	11.3
1	0	102	GLY	11.3
1	0	193	GLU	11.2
29	X	2146	U	11.2
1	0	49	LYS	11.2
21	T	6	GLY	11.0
29	X	1508	C	11.0
7	F	4	VAL	11.0
1	0	84	ALA	11.0
29	X	2142	C	10.9
1	0	205	LEU	10.8
1	0	207	SER	10.8
1	0	203	VAL	10.6
1	0	204	PHE	10.6
29	X	2111	C	10.4
7	F	136	VAL	10.3
1	0	159	PHE	10.3
1	0	48	ARG	10.2
1	0	165	GLY	10.2
29	X	2143	U	10.1
29	X	2133	G	10.0
1	0	78	ASN	10.0
1	0	107	ASP	9.9
1	0	124	ALA	9.9
7	F	26	ALA	9.8
1	0	210	LEU	9.8
1	0	174	ALA	9.7
29	X	2125	G	9.5
1	0	39	VAL	9.5
1	0	206	ARG	9.4
29	X	1911	U	9.4
29	X	1915	U	9.4
29	X	2126	A	9.3
1	0	218	ILE	9.3
1	0	170	PRO	9.2
1	0	142	GLY	9.2
1	0	90	VAL	9.1
1	0	157	ILE	9.1

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Mol	Chain	Res	Type	RSRZ
21	T	4	LYS	9.1
1	0	163	LYS	9.0
29	X	1509	A	8.9
1	0	194	GLY	8.9
29	X	1173	A	8.9
1	0	219	PRO	8.9
13	L	40	ALA	8.8
7	F	12	LEU	8.8
1	0	198	GLY	8.7
1	0	87	ALA	8.6
29	X	2134	A	8.6
1	0	103	PHE	8.6
1	0	199	THR	8.5
7	F	5	ALA	8.5
1	0	113	PRO	8.5
1	0	82	ALA	8.4
1	0	189	ILE	8.4
1	0	28	LEU	8.3
1	0	13	ASN	8.3
1	0	88	ASP	8.3
1	0	67	SER	8.3
29	X	717	C	8.3
1	0	19	ASP	8.3
1	0	144	ASP	8.3
1	0	99	ILE	8.3
22	U	28	GLY	8.2
29	X	716	A	8.2
3	B	205	SER	8.2
1	0	217	SER	8.1
1	0	202	GLY	8.1
1	0	136	PRO	8.0
1	0	161	ASN	8.0
1	0	15	GLN	8.0
5	D	73	SER	7.9
29	X	2132	C	7.9
1	0	74	THR	7.9
21	T	5	LYS	7.9
1	0	145	VAL	7.9
29	X	2141	C	7.8
7	F	137	THR	7.8
7	F	96	VAL	7.7
13	L	58	ALA	7.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	L	53	ALA	7.7
29	X	2796	U	7.5
1	0	196	LYS	7.5
20	S	92	VAL	7.5
1	0	50	SER	7.4
1	0	33	PHE	7.4
4	C	196	VAL	7.4
7	F	58	THR	7.4
1	0	201	LYS	7.4
1	0	216	PRO	7.3
1	0	53	ASN	7.3
7	F	18	THR	7.3
29	X	1912	A	7.2
13	L	33	ARG	7.2
1	0	89	VAL	7.2
22	U	16	ASN	7.2
1	0	44	GLY	7.1
7	F	6	GLY	7.1
29	X	715	G	7.1
7	F	2	ARG	7.0
1	0	121	GLN	7.0
1	0	100	ALA	7.0
1	0	93	ASP	6.9
1	0	6	LEU	6.9
1	0	81	ALA	6.9
1	0	140	THR	6.9
29	X	1172(C)	G	6.9
5	D	146	VAL	6.9
29	X	2139	G	6.9
7	F	67	PHE	6.9
22	U	25	ARG	6.8
1	0	146	ALA	6.8
1	0	129	PRO	6.8
7	F	29	GLN	6.7
7	F	20	ALA	6.7
29	X	2150	G	6.7
22	U	15	VAL	6.7
5	D	31	ILE	6.7
29	X	2110	G	6.7
22	U	75	TYR	6.6
7	F	23	VAL	6.6
1	0	92	SER	6.6

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Mol	Chain	Res	Type	RSRZ
29	X	2147	G	6.6
5	D	139	PRO	6.5
27	2	1	MET	6.5
28	3	23	MET	6.5
29	X	1536	C	6.5
13	L	59	LEU	6.5
1	0	83	GLU	6.5
7	F	66	THR	6.4
1	0	40	HIS	6.4
5	D	42	SER	6.4
1	0	101	GLY	6.4
29	X	1174	A	6.4
20	S	15	ASP	6.4
1	0	80	GLN	6.4
1	0	79	VAL	6.4
29	X	1910	G	6.3
1	0	41	PHE	6.3
29	X	1078	C	6.3
7	F	27	LEU	6.2
1	0	98	ARG	6.2
1	0	171	ILE	6.2
7	F	68	ILE	6.2
22	U	45	ASN	6.2
7	F	92	ASN	6.2
21	T	7	VAL	6.2
29	X	2602	A	6.2
22	U	27	ASP	6.1
22	U	52	ARG	6.1
7	F	95	LYS	6.1
7	F	24	GLY	6.1
22	U	26	ALA	6.1
29	X	1920	C	6.1
1	0	47	PRO	6.0
1	0	122	LYS	6.0
7	F	119	SER	6.0
1	0	120	GLY	6.0
1	0	134	PRO	6.0
1	0	135	ASN	6.0
13	L	12	ARG	6.0
5	D	62	LEU	6.0
7	F	138	VAL	6.0
1	0	20	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
29	X	1175	G	5.9
29	X	2114	A	5.9
1	0	95	LEU	5.9
1	0	91	GLY	5.9
5	D	71	LYS	5.9
17	P	134	LYS	5.9
18	Q	27	PHE	5.8
1	0	180	ASN	5.8
22	U	12	ASN	5.8
5	D	74	ILE	5.8
29	X	2797	A	5.8
1	0	76	GLY	5.8
1	0	197	PRO	5.7
7	F	94	ALA	5.7
1	0	141	VAL	5.7
1	0	104	MET	5.7
7	F	32	ALA	5.7
21	T	71	ASN	5.7
13	L	54	ALA	5.7
30	Y	123	U	5.7
1	0	185	TYR	5.7
1	0	215	GLY	5.6
22	U	13	LEU	5.6
1	0	45	ILE	5.5
5	D	72	LYS	5.5
1	0	147	GLY	5.5
29	X	1913	A	5.5
29	X	2182	A	5.5
7	F	101	TRP	5.5
13	L	14	ARG	5.5
1	0	34	ASP	5.5
5	D	43	SER	5.4
28	3	55	TRP	5.4
1	0	57	THR	5.4
1	0	188	LEU	5.4
30	Y	2	C	5.4
1	0	18	ILE	5.4
29	X	2109	U	5.4
1	0	125	ARG	5.4
5	D	145	MET	5.4
7	F	113	PRO	5.4
22	U	8	THR	5.4

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Mol	Chain	Res	Type	RSRZ
6	E	123	PHE	5.3
20	S	74	ARG	5.3
1	0	96	ILE	5.3
7	F	120	VAL	5.3
10	I	74	VAL	5.3
7	F	143	ASN	5.3
21	T	69	PHE	5.3
1	0	75	LYS	5.2
28	3	22	VAL	5.2
28	3	51	ALA	5.2
1	0	106	PHE	5.2
1	0	123	LEU	5.2
1	0	114	ASP	5.2
22	U	57	VAL	5.2
1	0	119	ILE	5.1
1	0	7	GLU	5.1
1	0	4	ARG	5.1
5	D	61	THR	5.1
4	C	20	PRO	5.0
29	X	1075	C	5.0
10	I	67	ASN	5.0
7	F	37	PHE	5.0
7	F	55	VAL	5.0
5	D	66	ILE	5.0
1	0	73	ILE	5.0
7	F	62	ASP	5.0
7	F	30	TYR	5.0
1	0	68	VAL	4.9
7	F	56	GLU	4.9
13	L	51	LEU	4.9
1	0	117	ALA	4.9
5	D	141	ILE	4.9
29	X	2794	U	4.9
5	D	81	GLN	4.9
21	T	84	ALA	4.9
1	0	32	LYS	4.9
20	S	14	LEU	4.9
7	F	3	ARG	4.8
7	F	43	ALA	4.8
5	D	175	LEU	4.8
28	3	16	ILE	4.8
7	F	112	MET	4.8

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Mol	Chain	Res	Type	RSRZ
10	I	51	GLY	4.8
1	0	151	GLY	4.8
7	F	142	PRO	4.8
22	U	60	VAL	4.8
21	T	82	GLU	4.8
7	F	14	ALA	4.8
7	F	121	GLU	4.8
13	L	39	TYR	4.8
1	0	11	ASP	4.7
7	F	57	ILE	4.7
1	0	97	GLU	4.7
20	S	11	LYS	4.7
21	T	49	GLN	4.7
29	X	1506	C	4.7
22	U	35	THR	4.7
4	C	150	LEU	4.6
1	0	182	SER	4.6
5	D	136	LEU	4.6
29	X	2136	A	4.6
29	X	2127	G	4.6
1	0	17	SER	4.6
26	1	21	TYR	4.6
1	0	126	LEU	4.6
21	T	74	LYS	4.6
16	O	72	ARG	4.6
26	1	22	TYR	4.6
28	3	9	MET	4.6
1	0	111	ALA	4.6
21	T	72	LYS	4.6
1	0	133	LEU	4.5
28	3	14	ILE	4.5
1	0	178	SER	4.5
10	I	48	PHE	4.5
5	D	99	PHE	4.5
1	0	52	GLN	4.5
22	U	14	VAL	4.5
5	D	65	PRO	4.5
22	U	44	ALA	4.5
29	X	2154	G	4.5
7	F	97	GLY	4.5
7	F	102	ASP	4.5
21	T	83	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
29	X	2181	G	4.5
21	T	73	GLY	4.4
28	3	52	LYS	4.4
24	W	6	VAL	4.4
13	L	60	LYS	4.4
21	T	65	GLY	4.4
12	K	69	ASP	4.4
29	X	2108	C	4.4
22	U	70	LEU	4.4
22	U	61	TRP	4.4
1	0	155	GLY	4.4
26	1	20	PHE	4.4
21	T	45	PHE	4.4
5	D	20	PHE	4.4
13	L	52	ALA	4.4
20	S	171	VAL	4.4
1	0	61	PRO	4.4
20	S	34	LEU	4.4
1	0	5	ALA	4.3
20	S	73	LYS	4.3
10	I	108	LEU	4.3
11	J	105	PHE	4.3
1	0	118	GLN	4.3
13	L	89	PHE	4.3
29	X	2135	A	4.3
28	3	50	LEU	4.3
7	F	127	VAL	4.3
26	1	11	LYS	4.3
28	3	10	ALA	4.3
1	0	110	VAL	4.3
29	X	2131	G	4.3
7	F	13	PRO	4.2
16	O	74	TYR	4.2
7	F	8	VAL	4.2
1	0	1	LYS	4.2
5	D	172	SER	4.2
22	U	62	LEU	4.2
6	E	163	ARG	4.2
6	E	133	VAL	4.2
1	0	148	MET	4.2
6	E	162	VAL	4.2
29	X	1737	C	4.2

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Mol	Chain	Res	Type	RSRZ
8	G	99	VAL	4.2
8	G	112	THR	4.1
2	A	235	GLY	4.1
22	U	43	ARG	4.1
23	V	66	GLN	4.1
28	3	25	PHE	4.1
29	X	1074	G	4.1
10	I	75	VAL	4.1
1	0	115	MET	4.1
1	0	183	ALA	4.1
10	I	60	LEU	4.1
28	3	12	ARG	4.1
7	F	34	ILE	4.1
24	W	50	LEU	4.1
1	0	3	TYR	4.1
13	L	62	GLY	4.1
26	1	23	THR	4.1
1	0	116	MET	4.1
1	0	220	LEU	4.1
2	A	147	LEU	4.1
1	0	156	ARG	4.0
1	0	172	GLY	4.0
5	D	125	ARG	4.0
29	X	1537	G	4.0
10	I	62	LYS	4.0
1	0	36	THR	4.0
22	U	24	ALA	4.0
5	D	36	VAL	3.9
19	R	55	THR	3.9
5	D	60	ILE	3.9
21	T	8	GLY	3.9
29	X	2169	A	3.9
1	0	149	VAL	3.9
10	I	68	VAL	3.9
22	U	69	THR	3.9
29	X	2178	C	3.9
7	F	51	ALA	3.9
29	X	2795	U	3.9
15	N	48	ARG	3.9
22	U	10	LYS	3.9
18	Q	94	GLN	3.8
20	S	12	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
29	X	2180	U	3.8
7	F	83	GLY	3.8
29	X	2170	A	3.8
5	D	169	LEU	3.8
7	F	125	ASN	3.8
7	F	118	GLY	3.8
13	L	93	SER	3.8
29	X	2149	G	3.8
22	U	33	LYS	3.8
28	3	54	GLU	3.8
26	1	1	ALA	3.8
11	J	119	PHE	3.8
22	U	47	HIS	3.8
3	B	1	MET	3.8
1	0	37	VAL	3.8
1	0	51	ASP	3.8
18	Q	42	ILE	3.8
1	0	10	VAL	3.8
1	0	224	GLY	3.7
6	E	168	GLN	3.7
29	X	1921	G	3.7
1	0	109	VAL	3.7
1	0	179	GLY	3.7
26	1	19	GLY	3.7
7	F	22	PRO	3.7
6	E	114	ILE	3.7
1	0	8	GLY	3.7
13	L	30	SER	3.7
22	U	58	LYS	3.7
1	0	195	ALA	3.7
5	D	49	ALA	3.7
7	F	60	TYR	3.7
1	0	152	LEU	3.7
1	0	158	GLU	3.7
17	P	133	ASN	3.7
11	J	59	PHE	3.7
29	X	2140	G	3.7
7	F	54	PRO	3.7
20	S	65	LEU	3.7
29	X	1079	C	3.6
18	Q	12	ILE	3.6
26	1	13	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	A	111	LEU	3.6
13	L	31	VAL	3.6
10	I	69	GLY	3.6
18	Q	84	GLU	3.6
7	F	63	ARG	3.6
7	F	140	GLY	3.6
7	F	44	GLN	3.6
6	E	105	MET	3.6
21	T	79	ILE	3.6
1	0	128	GLY	3.6
2	A	2	ALA	3.6
11	J	106	GLU	3.6
7	F	19	PRO	3.6
2	A	91	ARG	3.5
6	E	17	VAL	3.5
11	J	114	GLN	3.5
16	O	73	LYS	3.5
2	A	237	GLU	3.5
5	D	144	ASP	3.5
5	D	85	VAL	3.5
5	D	138	PHE	3.5
1	0	60	LEU	3.5
18	Q	91	LEU	3.5
1	0	72	VAL	3.5
1	0	62	HIS	3.5
29	X	2152	C	3.5
13	L	94	TYR	3.5
19	R	59	LYS	3.5
26	1	39	LYS	3.5
2	A	12	SER	3.4
29	X	1510	U	3.4
10	I	45	LYS	3.4
11	J	139	ASP	3.4
8	G	100	TYR	3.4
10	I	102	LYS	3.4
7	F	114	ASP	3.4
5	D	108	LEU	3.4
28	3	60	LEU	3.4
7	F	70	LYS	3.4
1	0	94	GLU	3.4
22	U	11	LYS	3.4
22	U	73	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
23	V	36	GLN	3.4
30	Y	43	G	3.4
7	F	15	GLY	3.4
10	I	122	VAL	3.4
20	S	114	ASP	3.4
22	U	23	LYS	3.3
4	C	125	ILE	3.3
5	D	142	THR	3.3
28	3	62	LEU	3.3
5	D	67	ILE	3.3
12	K	22	ARG	3.3
1	0	184	ASN	3.3
28	3	30	ARG	3.3
29	X	2116	G	3.3
2	A	242	ALA	3.3
13	L	57	ALA	3.3
20	S	91	PRO	3.3
6	E	111	HIS	3.3
21	T	20	TYR	3.3
5	D	76	ASN	3.3
5	D	140	GLU	3.3
20	S	1	MET	3.3
7	F	144	ALA	3.3
28	3	64	ARG	3.3
28	3	32	GLN	3.3
5	D	41	GLY	3.3
5	D	173	MET	3.2
7	F	91	PRO	3.2
23	V	37	LEU	3.2
13	L	61	SER	3.2
28	3	21	LYS	3.2
29	X	1538	G	3.2
1	0	70	VAL	3.2
7	F	141	GLY	3.2
21	T	59	LEU	3.2
6	E	169	ILE	3.2
11	J	69	ILE	3.2
26	1	2	ALA	3.2
26	1	26	LYS	3.2
10	I	123	ASP	3.2
13	L	34	SER	3.2
29	X	2107	U	3.2

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Mol	Chain	Res	Type	RSRZ
7	F	123	ALA	3.2
7	F	11	GLN	3.2
7	F	21	PRO	3.2
21	T	61	ALA	3.2
22	U	51	ILE	3.2
4	C	123	PHE	3.2
20	S	83	PHE	3.2
22	U	39	LYS	3.2
1	0	112	THR	3.2
29	X	2168	G	3.2
1	0	31	ALA	3.2
5	D	100	LEU	3.2
1	0	64	THR	3.1
15	N	47	TYR	3.1
29	X	2153	G	3.1
7	F	61	ALA	3.1
11	J	36	ILE	3.1
1	0	190	SER	3.1
21	T	66	LYS	3.1
29	X	1535	U	3.1
11	J	65	ILE	3.1
10	I	50	GLU	3.1
29	X	1176	C	3.1
1	0	22	ALA	3.1
7	F	48	LYS	3.1
1	0	77	GLU	3.1
29	X	1076	C	3.1
1	0	127	LEU	3.1
6	E	89	LEU	3.1
28	3	46	LYS	3.1
5	D	29	PRO	3.1
19	R	101	GLY	3.1
26	1	6	PRO	3.1
1	0	169	ALA	3.1
7	F	84	ILE	3.1
21	T	53	MET	3.0
24	W	7	ARG	3.0
15	N	25	TRP	3.0
20	S	72	ASP	3.0
11	J	26	ASP	3.0
5	D	168	ALA	3.0
7	F	64	SER	3.0

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Mol	Chain	Res	Type	RSRZ
15	N	12	ARG	3.0
6	E	173	ALA	3.0
22	U	34	THR	3.0
29	X	2104	U	3.0
7	F	35	MET	3.0
20	S	66	VAL	3.0
29	X	1172(B)	C	3.0
4	C	180	ILE	3.0
5	D	147	ASP	3.0
11	J	121	LEU	3.0
28	3	15	LYS	3.0
13	L	9	ARG	3.0
20	S	3	LEU	2.9
29	X	1540	A	2.9
18	Q	48	VAL	2.9
7	F	99	LEU	2.9
5	D	143	TYR	2.9
29	X	714	U	2.9
1	0	186	GLN	2.9
5	D	34	ILE	2.9
2	A	108	PRO	2.9
5	D	103	LEU	2.9
11	J	118	ALA	2.9
13	L	29	LEU	2.9
18	Q	7	LEU	2.9
10	I	73	GLU	2.9
10	I	103	ASN	2.9
20	S	123	VAL	2.9
11	J	37	ALA	2.9
20	S	51	LEU	2.9
24	W	1	MET	2.9
29	X	2187	C	2.9
7	F	131	ALA	2.9
13	L	18	ARG	2.9
3	B	3	GLY	2.9
7	F	17	ALA	2.9
9	H	134	LEU	2.9
1	0	173	LYS	2.9
2	A	275	LYS	2.9
28	3	66	LYS	2.9
5	D	59	LEU	2.9
19	R	46	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
21	T	52	GLY	2.9
20	S	33	ALA	2.9
28	3	58	MET	2.9
29	X	1026	U	2.9
8	G	131	VAL	2.9
21	T	11	LYS	2.8
5	D	69	LYS	2.8
23	V	34	ALA	2.8
28	3	61	MET	2.8
1	0	35	GLU	2.8
21	T	70	ILE	2.8
21	T	63	SER	2.8
13	L	84	ILE	2.8
1	0	160	ARG	2.8
1	0	191	ALA	2.8
5	D	176	PRO	2.8
6	E	159	GLY	2.8
11	J	100	PRO	2.8
5	D	89	VAL	2.8
28	3	24	ALA	2.8
7	F	10	LEU	2.8
5	D	58	ALA	2.8
15	N	20	ARG	2.8
11	J	126	LEU	2.8
2	A	236	GLY	2.7
22	U	36	GLY	2.7
6	E	37	TYR	2.7
7	F	110	THR	2.7
11	J	11	ARG	2.7
5	D	109	PRO	2.7
19	R	75	ALA	2.7
28	3	53	ALA	2.7
4	C	188	ILE	2.7
6	E	46	ASP	2.7
20	S	169	VAL	2.7
17	P	46	ARG	2.7
28	3	65	GLY	2.7
5	D	154	ILE	2.7
1	0	25	VAL	2.7
13	L	97	HIS	2.7
16	O	83	ARG	2.7
20	S	54	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
12	K	29	LEU	2.7
22	U	74	PRO	2.7
1	0	176	PHE	2.7
6	E	150	LYS	2.7
16	O	71	ILE	2.7
1	0	105	ASP	2.7
24	W	25	LEU	2.7
9	H	11	ALA	2.7
26	1	49	PHE	2.7
10	I	87	THR	2.7
7	F	50	ASP	2.7
11	J	107	VAL	2.7
7	F	28	GLY	2.7
11	J	33	TYR	2.7
2	A	106	LEU	2.7
1	0	108	ALA	2.7
29	X	2183	G	2.7
22	U	78	ILE	2.6
6	E	175	LYS	2.6
13	L	95	LYS	2.6
16	O	81	ARG	2.6
4	C	21	GLU	2.6
6	E	15	VAL	2.6
1	0	150	ARG	2.6
29	X	2129	C	2.6
4	C	147	LYS	2.6
20	S	93	GLU	2.6
5	D	132	ILE	2.6
1	0	65	GLY	2.6
10	I	104	ARG	2.6
11	J	103	VAL	2.6
5	D	135	GLN	2.6
10	I	72	TYR	2.6
11	J	32	ASP	2.6
22	U	65	ASN	2.6
26	1	53	ALA	2.6
19	R	68	GLY	2.6
9	H	1	MET	2.6
24	W	3	ILE	2.6
13	L	85	LYS	2.6
1	0	175	SER	2.6
21	T	67	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
5	D	165	GLU	2.6
22	U	54	ASN	2.6
29	X	1077	A	2.6
7	F	59	ILE	2.6
2	A	234	GLY	2.6
7	F	31	GLY	2.6
5	D	158	THR	2.6
4	C	149	LEU	2.6
20	S	23	ALA	2.6
29	X	1756	A	2.5
6	E	25	LYS	2.5
7	F	33	ASN	2.5
1	0	63	GLY	2.5
1	0	211	THR	2.5
4	C	17	LEU	2.5
5	D	56	GLU	2.5
20	S	134	LEU	2.5
23	V	2	LYS	2.5
26	1	0	ALA	2.5
11	J	117	GLU	2.5
28	3	20	GLY	2.5
2	A	68	LYS	2.5
10	I	112	GLY	2.5
14	M	104	LEU	2.5
20	S	69	VAL	2.5
1	0	46	ASP	2.5
2	A	190	TYR	2.5
10	I	76	LYS	2.5
11	J	7	ARG	2.5
14	M	54	VAL	2.5
10	I	101	ARG	2.5
6	E	115	ILE	2.5
19	R	57	ASN	2.5
29	X	614	A	2.5
29	X	652	A	2.5
2	A	255	LYS	2.5
18	Q	76	LYS	2.5
28	3	29	LYS	2.5
28	3	2	PRO	2.5
10	I	113	GLU	2.5
24	W	53	VAL	2.5
2	A	145	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	231	HIS	2.5
7	F	41	PHE	2.4
11	J	104	MET	2.4
11	J	132	MET	2.4
29	X	2122	U	2.4
29	X	2173	A	2.4
1	0	192	LEU	2.4
8	G	102	ARG	2.4
13	L	11	LEU	2.4
15	N	90	LEU	2.4
11	J	101	GLY	2.4
8	G	51	LEU	2.4
17	P	116	ILE	2.4
6	E	43	VAL	2.4
17	P	92	VAL	2.4
26	1	12	MET	2.4
19	R	60	PRO	2.4
23	V	35	GLY	2.4
6	E	156	ALA	2.4
6	E	27	LYS	2.4
3	B	54	LYS	2.4
7	F	82	ALA	2.4
11	J	60	ARG	2.4
9	H	8	LEU	2.4
6	E	122	THR	2.4
7	F	47	ASP	2.4
1	0	132	LEU	2.4
24	W	51	LEU	2.4
21	T	26	PHE	2.4
1	0	166	VAL	2.4
8	G	41	TRP	2.4
7	F	109	LYS	2.4
11	J	99	LYS	2.4
1	0	138	SER	2.3
7	F	105	LEU	2.3
1	0	153	LYS	2.3
1	0	2	ARG	2.3
29	X	2123	G	2.3
2	A	55	GLY	2.3
2	A	64	ILE	2.3
2	A	105	ILE	2.3
5	D	156	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
22	U	37	ILE	2.3
21	T	9	SER	2.3
3	B	84	PHE	2.3
22	U	56	GLN	2.3
6	E	167	GLU	2.3
10	I	30	ALA	2.3
22	U	66	ALA	2.3
7	F	52	ILE	2.3
18	Q	62	ARG	2.3
24	W	17	VAL	2.3
29	X	2334	G	2.3
1	O	177	GLU	2.3
2	A	208	LYS	2.3
17	P	107	ILE	2.3
17	P	108	PRO	2.3
22	U	76	LYS	2.3
10	I	114	ILE	2.3
18	Q	51	ILE	2.3
20	S	130	ILE	2.3
10	I	96	TYR	2.3
16	O	70	TYR	2.3
16	O	80	TYR	2.3
19	R	83	LEU	2.3
23	V	33	ALA	2.3
29	X	293	A	2.3
29	X	2148	G	2.3
7	F	130	THR	2.3
21	T	41	ARG	2.3
2	A	241	GLY	2.3
5	D	57	LEU	2.3
5	D	137	ILE	2.3
6	E	160	LYS	2.3
23	V	30	PHE	2.3
2	A	40	THR	2.2
3	B	94	ASP	2.2
2	A	104	TYR	2.2
10	I	49	PHE	2.2
18	Q	37	GLU	2.2
29	X	1092	C	2.2
25	Z	56	GLN	2.2
22	U	20	ARG	2.2
19	R	76	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
21	T	48	GLY	2.2
28	3	7	HIS	2.2
6	E	107	ILE	2.2
11	J	10	PHE	2.2
7	F	98	LYS	2.2
11	J	19	THR	2.2
26	1	52	ALA	2.2
6	E	62	ARG	2.2
14	M	106	TYR	2.2
7	F	139	GLU	2.2
6	E	172	LYS	2.2
7	F	76	TYR	2.2
29	X	2179	C	2.2
11	J	63	GLY	2.2
17	P	98	ASP	2.2
19	R	52	ASN	2.2
4	C	186	LEU	2.2
4	C	38	ARG	2.2
7	F	90	THR	2.2
26	1	37	LEU	2.2
11	J	102	ARG	2.2
28	3	36	LYS	2.2
5	D	25	VAL	2.2
6	E	23	VAL	2.2
1	0	43	LEU	2.2
10	I	56	LEU	2.2
26	1	29	ARG	2.2
18	Q	38	ILE	2.2
20	S	10	PRO	2.2
2	A	62	TYR	2.2
19	R	40	LEU	2.2
21	T	37	LEU	2.2
21	T	10	SER	2.2
5	D	101	GLU	2.2
9	H	75	VAL	2.2
1	0	12	ARG	2.2
4	C	143	ASP	2.2
20	S	172	LEU	2.2
1	0	221	ALA	2.2
2	A	239	ARG	2.2
8	G	98	LYS	2.2
20	S	120	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
17	P	45	ILE	2.1
22	U	72	LYS	2.1
2	A	103	ARG	2.1
22	U	40	ARG	2.1
15	N	39	LEU	2.1
15	N	40	LEU	2.1
2	A	221	GLN	2.1
22	U	53	GLU	2.1
15	N	57	PHE	2.1
29	X	2798	U	2.1
17	P	105	ARG	2.1
7	F	124	ALA	2.1
13	L	79	ALA	2.1
2	A	16	MET	2.1
30	Y	14	C	2.1
13	L	13	THR	2.1
5	D	134	GLU	2.1
19	R	100	ASP	2.1
21	T	85	GLN	2.1
7	F	93	LYS	2.1
21	T	25	LYS	2.1
29	X	2189	U	2.1
5	D	16	LEU	2.1
13	L	75	LEU	2.1
15	N	53	LYS	2.1
10	I	58	ALA	2.1
11	J	67	ILE	2.1
4	C	148	VAL	2.1
5	D	105	ASN	2.1
6	E	128	PRO	2.1
18	Q	29	VAL	2.1
20	S	30	VAL	2.1
29	X	2117	A	2.1
8	G	106	TYR	2.1
20	S	84	TYR	2.1
6	E	95	ARG	2.1
19	R	67	GLY	2.1
20	S	13	LYS	2.1
6	E	41	LEU	2.0
6	E	109	TYR	2.0
7	F	122	ALA	2.0
8	G	109	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
10	I	44	GLY	2.0
1	0	38	GLU	2.0
6	E	101	LYS	2.0
11	J	39	GLU	2.0
7	F	103	GLN	2.0
13	L	49	GLN	2.0
10	I	59	ARG	2.0
7	F	40	ALA	2.0
20	S	79	ILE	2.0
5	D	32	GLU	2.0
8	G	101	THR	2.0
3	B	95	ILE	2.0
26	1	4	ALA	2.0
29	X	2151	U	2.0
29	X	1539	A	2.0
7	F	65	PHE	2.0
5	D	170	LEU	2.0
20	S	44	ARG	2.0
2	A	233	HIS	2.0
5	D	50	ILE	2.0
29	X	1909	C	2.0
5	D	88	LYS	2.0
21	T	62	LEU	2.0
24	W	13	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6108	1/1	0.36	0.64	120,120,120,120	0
31	MG	X	6119	1/1	0.46	0.53	128,128,128,128	0
31	MG	X	6177	1/1	0.48	0.59	113,113,113,113	0
31	MG	X	6159	1/1	0.49	0.44	111,111,111,111	0
31	MG	X	6093	1/1	0.52	0.69	106,106,106,106	0
31	MG	X	6046	1/1	0.56	0.40	91,91,91,91	0
31	MG	X	6167	1/1	0.56	0.57	103,103,103,103	0
31	MG	X	6183	1/1	0.58	0.71	105,105,105,105	0
31	MG	X	6179	1/1	0.61	0.54	117,117,117,117	0
31	MG	X	6175	1/1	0.64	0.41	121,121,121,121	0
31	MG	X	6098	1/1	0.65	1.04	97,97,97,97	0
31	MG	X	6144	1/1	0.65	0.37	87,87,87,87	0
31	MG	X	6162	1/1	0.67	0.81	111,111,111,111	0
31	MG	X	6041	1/1	0.69	0.35	83,83,83,83	0
31	MG	X	6038	1/1	0.71	0.67	85,85,85,85	0
31	MG	X	6099	1/1	0.72	0.68	89,89,89,89	0
31	MG	X	6186	1/1	0.72	1.02	134,134,134,134	0
31	MG	X	6133	1/1	0.73	1.20	111,111,111,111	0
31	MG	X	6170	1/1	0.73	1.97	127,127,127,127	0
31	MG	X	6191	1/1	0.74	1.56	101,101,101,101	0
31	MG	X	6141	1/1	0.74	0.60	122,122,122,122	0
31	MG	X	6138	1/1	0.75	0.78	94,94,94,94	0
31	MG	X	6058	1/1	0.76	0.52	97,97,97,97	0
31	MG	X	6085	1/1	0.76	0.36	101,101,101,101	0
31	MG	X	6187	1/1	0.77	0.57	92,92,92,92	0
31	MG	X	6111	1/1	0.77	0.70	98,98,98,98	0
31	MG	X	6113	1/1	0.77	0.53	115,115,115,115	0
31	MG	X	6192	1/1	0.77	0.69	138,138,138,138	0
31	MG	X	6014	1/1	0.78	0.42	91,91,91,91	0
31	MG	X	6048	1/1	0.78	0.80	102,102,102,102	0
31	MG	X	6117	1/1	0.78	0.36	90,90,90,90	0
31	MG	X	6020	1/1	0.78	0.34	79,79,79,79	0
31	MG	X	6180	1/1	0.78	1.59	101,101,101,101	0
31	MG	X	6156	1/1	0.79	0.63	105,105,105,105	0
31	MG	X	6107	1/1	0.79	0.75	113,113,113,113	0
31	MG	X	6121	1/1	0.79	0.80	99,99,99,99	0
31	MG	X	6146	1/1	0.80	1.51	129,129,129,129	0
31	MG	X	6022	1/1	0.80	0.40	77,77,77,77	0
31	MG	X	6006	1/1	0.81	0.48	69,69,69,69	0
31	MG	X	6164	1/1	0.81	0.99	124,124,124,124	0
31	MG	X	6122	1/1	0.81	0.46	100,100,100,100	0
31	MG	X	6171	1/1	0.82	0.80	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6110	1/1	0.82	0.38	130,130,130,130	0
31	MG	X	6157	1/1	0.82	0.31	111,111,111,111	0
31	MG	X	6100	1/1	0.83	0.59	97,97,97,97	0
31	MG	X	6090	1/1	0.83	0.45	117,117,117,117	0
31	MG	X	6155	1/1	0.83	0.33	115,115,115,115	0
31	MG	X	6013	1/1	0.83	0.57	76,76,76,76	0
31	MG	X	6136	1/1	0.83	0.81	122,122,122,122	0
31	MG	X	6018	1/1	0.83	0.46	74,74,74,74	0
31	MG	X	6080	1/1	0.83	0.71	108,108,108,108	0
31	MG	X	6154	1/1	0.83	1.09	113,113,113,113	0
31	MG	Y	205	1/1	0.83	0.90	129,129,129,129	0
31	MG	X	6016	1/1	0.84	0.35	77,77,77,77	0
31	MG	X	6109	1/1	0.84	0.31	101,101,101,101	0
31	MG	X	6190	1/1	0.84	1.33	129,129,129,129	0
31	MG	X	6028	1/1	0.84	0.33	88,88,88,88	0
31	MG	X	6172	1/1	0.84	0.66	124,124,124,124	0
31	MG	X	6011	1/1	0.85	0.45	89,89,89,89	0
31	MG	X	6174	1/1	0.85	0.72	87,87,87,87	0
31	MG	X	6030	1/1	0.85	1.19	83,83,83,83	0
31	MG	X	6052	1/1	0.85	0.52	97,97,97,97	0
31	MG	X	6003	1/1	0.85	0.49	70,70,70,70	0
31	MG	X	6137	1/1	0.85	0.57	135,135,135,135	0
31	MG	X	6173	1/1	0.85	1.91	102,102,102,102	0
31	MG	X	6142	1/1	0.86	0.77	89,89,89,89	0
31	MG	X	6012	1/1	0.86	0.50	82,82,82,82	0
31	MG	X	6127	1/1	0.86	0.59	122,122,122,122	0
31	MG	X	6143	1/1	0.86	1.04	100,100,100,100	0
31	MG	X	6074	1/1	0.86	0.74	80,80,80,80	0
31	MG	X	6158	1/1	0.86	2.46	114,114,114,114	0
31	MG	X	6105	1/1	0.86	1.40	118,118,118,118	0
31	MG	X	6066	1/1	0.86	1.08	84,84,84,84	0
31	MG	X	6151	1/1	0.86	0.34	98,98,98,98	0
31	MG	X	6072	1/1	0.86	0.56	102,102,102,102	0
31	MG	X	6135	1/1	0.86	0.76	91,91,91,91	0
31	MG	X	6124	1/1	0.87	1.14	107,107,107,107	0
31	MG	X	6160	1/1	0.87	0.68	104,104,104,104	0
31	MG	Y	204	1/1	0.87	0.96	109,109,109,109	0
31	MG	X	6189	1/1	0.87	0.75	120,120,120,120	0
31	MG	X	6147	1/1	0.87	1.00	82,82,82,82	0
31	MG	X	6023	1/1	0.87	0.52	97,97,97,97	0
31	MG	Y	201	1/1	0.87	0.85	112,112,112,112	0
31	MG	X	6034	1/1	0.88	0.81	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6176	1/1	0.88	0.50	107,107,107,107	0
31	MG	X	6008	1/1	0.88	0.42	81,81,81,81	0
31	MG	X	6114	1/1	0.88	0.55	91,91,91,91	0
31	MG	X	6083	1/1	0.88	0.80	91,91,91,91	0
31	MG	X	6182	1/1	0.88	0.97	120,120,120,120	0
31	MG	X	6149	1/1	0.88	0.59	94,94,94,94	0
31	MG	X	6123	1/1	0.88	0.48	130,130,130,130	0
31	MG	X	6057	1/1	0.88	0.99	93,93,93,93	0
31	MG	X	6165	1/1	0.88	0.99	99,99,99,99	0
31	MG	X	6027	1/1	0.89	1.04	86,86,86,86	0
31	MG	X	6039	1/1	0.89	1.17	104,104,104,104	0
31	MG	X	6037	1/1	0.89	0.41	86,86,86,86	0
31	MG	X	6132	1/1	0.89	0.54	94,94,94,94	0
31	MG	X	6035	1/1	0.89	0.43	86,86,86,86	0
31	MG	X	6115	1/1	0.89	0.74	103,103,103,103	0
31	MG	X	6047	1/1	0.89	0.54	74,74,74,74	0
31	MG	X	6021	1/1	0.90	0.70	75,75,75,75	0
31	MG	X	6168	1/1	0.90	0.84	107,107,107,107	0
31	MG	X	6055	1/1	0.90	0.64	90,90,90,90	0
31	MG	X	6067	1/1	0.90	0.49	79,79,79,79	0
31	MG	X	6059	1/1	0.90	0.46	87,87,87,87	0
31	MG	X	6017	1/1	0.91	0.48	83,83,83,83	0
31	MG	X	6104	1/1	0.91	0.59	86,86,86,86	0
31	MG	X	6064	1/1	0.91	0.63	96,96,96,96	0
31	MG	X	6075	1/1	0.91	0.85	103,103,103,103	0
31	MG	X	6140	1/1	0.91	1.02	97,97,97,97	0
31	MG	X	6019	1/1	0.91	0.81	77,77,77,77	0
31	MG	X	6082	1/1	0.91	0.76	83,83,83,83	0
31	MG	X	6015	1/1	0.91	0.55	77,77,77,77	0
31	MG	X	6071	1/1	0.91	0.40	81,81,81,81	0
31	MG	X	6188	1/1	0.91	0.44	98,98,98,98	0
31	MG	X	6051	1/1	0.91	0.39	69,69,69,69	0
31	MG	X	6001	1/1	0.92	0.56	69,69,69,69	0
31	MG	X	6084	1/1	0.92	0.30	93,93,93,93	0
31	MG	X	6010	1/1	0.92	0.83	69,69,69,69	0
31	MG	X	6045	1/1	0.92	1.03	89,89,89,89	0
31	MG	X	6076	1/1	0.92	0.73	102,102,102,102	0
31	MG	X	6004	1/1	0.92	0.36	76,76,76,76	0
31	MG	Y	202	1/1	0.92	0.43	125,125,125,125	0
31	MG	X	6095	1/1	0.92	0.85	79,79,79,79	0
31	MG	X	6056	1/1	0.92	0.88	85,85,85,85	0
31	MG	X	6101	1/1	0.93	0.87	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6097	1/1	0.93	1.26	93,93,93,93	0
31	MG	X	6161	1/1	0.93	0.68	95,95,95,95	0
31	MG	X	6120	1/1	0.93	1.04	102,102,102,102	0
31	MG	X	6092	1/1	0.93	0.26	93,93,93,93	0
31	MG	X	6163	1/1	0.93	0.37	156,156,156,156	0
31	MG	X	6033	1/1	0.93	0.53	98,98,98,98	0
31	MG	X	6002	1/1	0.93	0.33	78,78,78,78	0
31	MG	X	6178	1/1	0.93	0.58	103,103,103,103	0
31	MG	X	6118	1/1	0.93	0.72	90,90,90,90	0
31	MG	X	6024	1/1	0.93	0.61	87,87,87,87	0
31	MG	X	6081	1/1	0.93	0.42	78,78,78,78	0
31	MG	X	6129	1/1	0.93	0.89	104,104,104,104	0
31	MG	X	6094	1/1	0.93	0.45	92,92,92,92	0
31	MG	X	6128	1/1	0.93	0.81	97,97,97,97	0
31	MG	X	6007	1/1	0.93	0.46	70,70,70,70	0
31	MG	X	6150	1/1	0.94	0.69	111,111,111,111	0
31	MG	X	6044	1/1	0.94	0.29	73,73,73,73	0
31	MG	X	6130	1/1	0.94	0.67	108,108,108,108	0
31	MG	X	6078	1/1	0.94	0.57	93,93,93,93	0
31	MG	X	6145	1/1	0.94	0.20	104,104,104,104	0
31	MG	X	6112	1/1	0.94	0.68	84,84,84,84	0
31	MG	X	6029	1/1	0.94	0.43	69,69,69,69	0
31	MG	X	6036	1/1	0.94	0.84	82,82,82,82	0
31	MG	X	6062	1/1	0.94	0.41	85,85,85,85	0
31	MG	X	6169	1/1	0.94	0.57	101,101,101,101	0
31	MG	X	6088	1/1	0.94	0.87	99,99,99,99	0
31	MG	X	6077	1/1	0.94	0.65	98,98,98,98	0
31	MG	X	6026	1/1	0.94	0.41	91,91,91,91	0
31	MG	X	6126	1/1	0.94	1.19	94,94,94,94	0
31	MG	X	6040	1/1	0.94	0.78	80,80,80,80	0
31	MG	X	6106	1/1	0.94	0.54	80,80,80,80	0
31	MG	X	6032	1/1	0.94	0.34	78,78,78,78	0
31	MG	X	6103	1/1	0.94	0.32	117,117,117,117	0
31	MG	X	6091	1/1	0.94	1.11	88,88,88,88	0
31	MG	X	6102	1/1	0.94	0.25	89,89,89,89	0
31	MG	X	6131	1/1	0.94	0.86	101,101,101,101	0
31	MG	X	6068	1/1	0.94	0.66	90,90,90,90	0
31	MG	X	6139	1/1	0.95	0.54	126,126,126,126	0
31	MG	X	6089	1/1	0.95	0.51	90,90,90,90	0
31	MG	X	6031	1/1	0.95	0.53	69,69,69,69	0
31	MG	X	6079	1/1	0.95	0.35	102,102,102,102	0
31	MG	X	6073	1/1	0.95	0.79	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6152	1/1	0.95	0.93	112,112,112,112	0
31	MG	X	6185	1/1	0.95	0.59	109,109,109,109	0
31	MG	M	201	1/1	0.95	0.94	69,69,69,69	0
31	MG	X	6061	1/1	0.95	0.71	83,83,83,83	0
31	MG	X	6054	1/1	0.95	0.54	92,92,92,92	0
31	MG	X	6065	1/1	0.96	0.61	81,81,81,81	0
31	MG	X	6184	1/1	0.96	0.76	102,102,102,102	0
31	MG	X	6153	1/1	0.96	0.62	113,113,113,113	0
31	MG	X	6049	1/1	0.96	0.67	88,88,88,88	0
31	MG	X	6005	1/1	0.96	0.89	69,69,69,69	0
31	MG	X	6063	1/1	0.96	1.29	87,87,87,87	0
31	MG	X	6070	1/1	0.96	0.58	107,107,107,107	0
31	MG	X	6166	1/1	0.96	0.73	106,106,106,106	0
31	MG	X	6069	1/1	0.96	0.51	91,91,91,91	0
31	MG	X	6181	1/1	0.97	0.31	121,121,121,121	0
31	MG	X	6043	1/1	0.97	0.85	69,69,69,69	0
31	MG	X	6060	1/1	0.97	0.68	80,80,80,80	0
31	MG	X	6116	1/1	0.97	0.59	106,106,106,106	0
31	MG	X	6096	1/1	0.97	1.19	89,89,89,89	0
31	MG	X	6025	1/1	0.97	0.45	83,83,83,83	0
31	MG	X	6050	1/1	0.97	0.50	84,84,84,84	0
31	MG	X	6125	1/1	0.97	0.46	123,123,123,123	0
31	MG	Y	203	1/1	0.97	0.97	102,102,102,102	0
31	MG	X	6009	1/1	0.97	0.67	69,69,69,69	0
31	MG	X	6086	1/1	0.98	0.93	87,87,87,87	0
31	MG	X	6087	1/1	0.98	0.54	98,98,98,98	0
31	MG	X	6042	1/1	0.98	0.59	83,83,83,83	0
31	MG	X	6053	1/1	0.99	0.85	91,91,91,91	0
31	MG	X	6148	1/1	0.99	0.57	130,130,130,130	0
31	MG	X	6134	1/1	0.99	0.67	112,112,112,112	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.