



Full wwPDB EM Validation Report ⓘ

Nov 13, 2024 – 10:52 AM JST

PDB ID : 8Y37
EMDB ID : EMD-38874
Title : Cryo-EM structure of Staphylococcus aureus (15B196) 50S ribosome in complex with MCX-190.
Authors : Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on : 2024-01-28
Resolution : 2.53 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

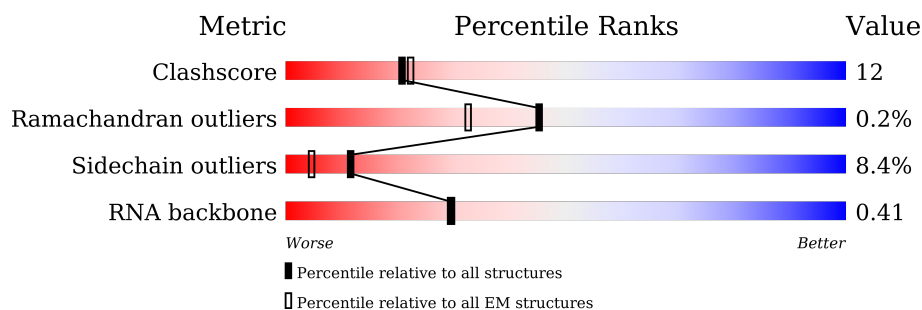
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 Å.

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




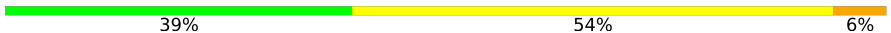

















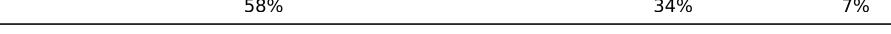


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	47	60% 36% .
2	2	43	79% 21%
3	3	64	73% 25% .
4	4	37	57% 41% .
5	A	2921	52% 39% 8% .
6	B	115	50% 38% 11%
7	C	274	65% 32% ..
8	D	215	65% 33% .

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Mol	Chain	Length	Quality of chain
9	E	206	 75% 21% .
10	F	175	 39% 54% 6%
11	G	175	 58% 39% .
12	H	145	 70% 30% .
13	I	122	 52% 46% .
14	J	146	 77% 21% .
15	K	137	 58% 39% .
16	L	120	 70% 29% .
17	M	119	 64% 31% 5%
18	N	114	 61% 33% 5%
19	O	116	 74% 24% .
20	P	102	 66% 30% . .
21	Q	117	 72% 21% . .
22	R	89	 56% 35% 9%
23	S	103	 58% 38% .
24	T	94	 52% 43% 5%
25	U	82	 65% 32% .
26	V	58	 66% 28% 7%
27	W	67	 58% 34% 7%
28	X	58	 83% 17%
29	Y	59	 73% 24% . .
30	Z	48	 79% 19% .

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 88301 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2884	Total	C	N	O	P	0	0
			61838	27611	11307	20036	2884		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	274	Total	C	N	O	S	0	0
			2090	1301	415	369	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1317	835	223	253	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	175	Total	C	N	O	S	0	0
			1259	788	239	229	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			891	557	174	159	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O		0	0
			889	563	175	151			

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	112	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	94	Total	C	N	O		0	0
			711	456	127	128			

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	82	Total	C	N	O		0	0
			615	380	121	114			

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	58	Total	C	N	O		0	0
			445	277	96	72			

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	67	Total	C	N	O		0	0
			541	333	102	106			

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	58	Total	C	N	O	0	0
			449	280	85	84		

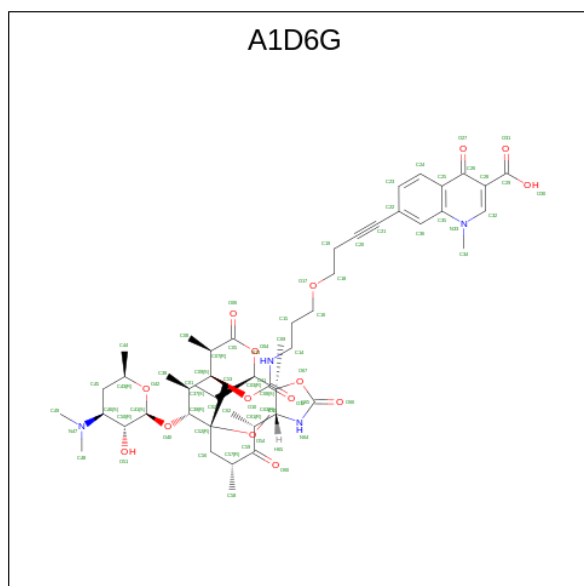
- Molecule 29 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	59	Total	C	N	O	S	0	0
			370	225	68	76	1		

- Molecule 30 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	48	Total	C	N	O	S	0	0
			361	222	77	59	3		

- Molecule 31 is 7-[4-[3-[(1 {S},2 {R},5 {R},6 {S},7 {S},8 {R},9 {R},11 {R},13 {R},14 {R})-8-[(2 {S},3 {R},4 {S},6 {R})-4-(dimethylamino)-6-methyl-3-oxidanyl-oxan-2-yl]oxy-2-ethyl-9-methoxy-1,5,7,9,11,13-hexamethyl-4,12,16-tris(oxidanylidene)-3,17-dioxo-15-azabicyclo [12.3.0]heptadecan-6-yl]oxycarbonylamino]propoxy]but-1-ynyl]-1-methyl-4-oxidanylidene-quinoline-3-carboxylic acid (three-letter code: A1D6G) (formula: C₅₀H₇₂N₄O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	N	O	0
			69	50	4	15	

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	12	Total	Mg	0
			12	12	

- Molecule 33 is water.

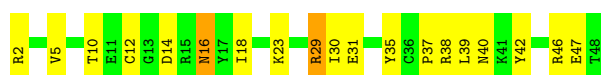
Mol	Chain	Residues	Atoms		AltConf
33	A	6	Total	O	0
			6	6	

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Large ribosomal subunit protein bL33B

Chain 1: 



- Molecule 2: Large ribosomal subunit protein bL34

Chain 2: 



- Molecule 3: Large ribosomal subunit protein bL35

Chain 3: 



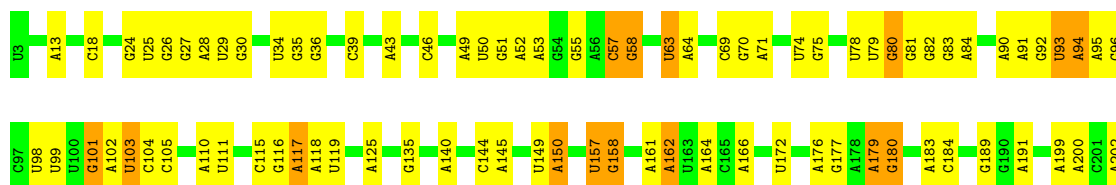
- Molecule 4: Large ribosomal subunit protein bL36

Chain 4: 



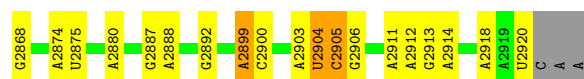
- Molecule 5: 23S ribosomal RNA

Chain A: 

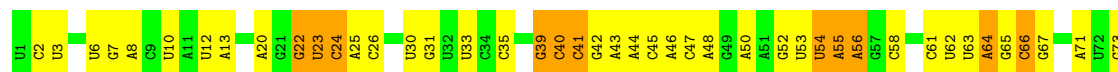


U1493	C1400	A1303	G1207	G1133	A1064	A972	G890	U	C674	A574	U482	G393	G291	U209
G1494	G1401	G1304	A1208	U1134	A1065	A973	A891	G	A677	G575	A489	G396	U292	A210
G1495	A1402	U1305	U1215	C1136	G1066	U974	U896	A757	A678	U576	A489	U397	U293	G214
G1496		A1306	U1216	U1137	A1070	U975	U898	G774	A679	U577	A490	C398	G294	G215
A1497	G1405	G1307	U1217	U1138	A1071	U976	U899	A775	A680	G578	G492	U399	G297	G216
U1498	U1408	G1308	G1218	A1139	A1072	A977	U899	U786	A682	C580	A493	U400	U298	G215
U1499	U1415	A1310	G1219	U1140	A1073	A985	G900	U787	G683	A581	A493	U401	U299	A216
G1500	U1416	A1311	A1220	A1141	U1077	A989	G901	A788	U684	G582	G496	U402	G300	G217
G1501	A1421	G1315	G1225	A1142	U1077	A989	G902	U788	U685	A583	U497	U403	U301	G218
A1502	A1422	G1316	G1226	A1143	U1077	A990	G903	A789	U686	A584	U498	U404	A302	A219
U1503	C1423	G1317	U1227	U1144	G1080	A991	G904	U790	U687	A585	C502	U405	G303	A220
U1504		A1312	A1228	A1145	U1081	A992		U791	A688	A586	A503	G406	G304	G221
G		A1313	C1229	C1146	G1082	C993	C910	A792	A689	U533		A406	A305	
G1506	G1426	C1326	G1229	A1147	U1084	G1000	A911	A793	U690	U606	A506	G409	A224	A225
A1507	U1427	C1327	U1230	C1148	U1085	G1001	U917	G802	A691	G606	C507	G410	U309	A226
C1508		U1328	G1234	U1149	U1086	A1001	U918	G803	A692	C607	U510	A411	C310	G227
U1509	A1432	G1329	C1235	U1150	G1087	U1002	C921	G804	U693	C608	G511	A412	U311	A228
U1510	U1433	U1330	G1236	G1151	C1088	A1003	G922	G805	U694	U614	A512	A417	U312	A229
C1511	U1434	U1331	U1237	U1152	C1089	A1004	G923	A809	U695	A615	G513	C421	A	A230
U1512	C1435	C1332	G1238	C1153	U1090	G1005	G924	A810	U696	G616	G514	G422	C	A231
A1513	C1436	U1333	G1239	G1154	G1091	G1012	G925	G815	U697	A617	G515	G423	U	U232
		U1334	G1240	U1155	A1092	G1013	G926	G816	A698	A618	A516	A427	G	U233
C1516	A1440	U1335	G1241	G1156	C1093	A1017	G927	U702	U699	U619	A517		G317	U234
		U1336	G1242	U1157	A1094	A1018	C928	A703	U700	G620	A518	A430	A318	C234
A1520	A1443	G1336	U1243	G1158	A1095	A1019	C929	A704	A701	A621	G519	A431	G319	G235
A1521	U1444	U1337	C1244	C1159	C1096	A1020	C	G822	A702	A622	G520	G432	U320	U238
G1522	A1445	C1338	U1245	U1160	U1097	A1021	U	G823	A703	C623	U521	U433	C323	
U1523	U1446	U1339	G1246	U1161	A1098	A1022	U	A827	G711	G624	G522	G434	C324	U242
G1524	U1447	U1340	U1247	U1162	G1099	A1023	U	A828	G712	A625	G523	A435	A324	U243
U1525	U1448	U1341	G1248	G1163	G1100	A1024	U	U829	A715	G626	A524	A436	A325	A244
G1526	U1449	U1342	U1249	U1164	A1101	G1025	U	U830	C716	U631	A525	A437	A326	
U1527	U1450	U1343	G1250	G1165	U1102	C1026	G	A834	G717	U632	A526	U438	G327	G248
G1528	U1451	U1344	U1251	G1166	U1103	G1027	G937	U835	A720	A633	G527	C440	A329	G251
U1529	U1452	U1345	G1252	U1167	U1104	A1028	U939	G836	A721	A634	G528	C441	C252	G252
A1530	U1453	U1346	U1253	G1168	U1105	G1029	U940	G837	A722	A635	G529	C442	G333	G253
U1531	U1454	U1347	G1254	G1169	U1106	A1030	A941	A838	U731	G643	G534	A447	A394	A254
U1532	U1455	U1348	U1255	U1170	U1107	C1031	C942	U839	U732	C644	G535	A448	U335	G255
A	U1456	U1349	G1256	G1171	U1108	A1032	C943	G850	U733	A645	A537	U449	U336	
G	U1457	U1350	U1257	U1172	U1109	C1033	C944	G851	G746	A646	G540	U450	G350	G267
G	U1458	U1351	G1258	U1173	U1110	A1034	A945	U852	G747	G647	G541	U451	G351	A268
U1533	U1459	U1352	U1259	G1174	U1111	C1035	U941	U853	G748	G648	G542	U452	G352	C270
	U1460	U1353	G1260	U1175	U1112	A1036	A946	G854	G749	G649	A548	A458	A352	C271
G1534	U1461	U1354	U1261	U1176	U1113	C1037	U942	U855	U750	U650	A549	C459	A353	C272
U1535	U1462	U1355	G1262	U1177	U1114	A1038	C943	U856	U751	U651	A550	C460	A354	A273
A1537	U1463	U1356	U1263	U1178	U1115	C1039	C944	U857	U752	U652	A551	C461	A355	
A1538	U1464	U1357	G1264	U1179	U1116	C1040	A947	U858	U753	U653	A552	C462	A356	A278
U1539	U1465	U1358	U1265	U1180	U1117	A1041	U943	U859	U754	U654	A553	U463	A357	A279
U1540	U1466	U1359	G1266	U1181	U1118	A1042	C944	U860	U755	U655	A554	U464	A358	C280
C1541	U1467	U1360	U1267	U1182	U1119	C1043	A945	U861	U756	U656	A555	U465	A359	G283
G1542	U1468	U1361	U1268	U1183	U1120	A1044	C946	U862	U757	U657	A556	U466	A360	C284
U1543	U1469	U1362	U1269	U1184	U1121	A1045	A946	U863	U758	U658	A557	U467	A361	U285
U1544	U1470	U1363	G1270	U1185	U1122	C1046	C947	U864	U759	U659	A558	U468	A362	U286
U1545	U1471	U1364	U1271	U1186	U1123	A1047	A947	U865	U760	U660	A559	U469	A363	
A1546	U1472	U1365	U1272	U1187	U1124	C1048	C948	U866	U761	U661	A560	U470	A364	A278
	U1473	U1366	G1273	U1188	U1125	A1049	C949	U867	U762	U662	A561	U471	A365	A279
U1547	U1474	U1367	U1274	U1189	U1126	A1050	A948	U868	U763	U663	A562	U472	A366	C280
A1548	U1475	U1368	G1275	U1190	U1127	A1051	C949	U869	U764	U664	A563	U473	A367	G283
U1549	U1476	U1369	U1276	U1191	U1128	A1052	A949	U870	U765	U665	A564	U474	A368	C284
G1550	U1477	U1370	C1277	U1192	U1129	C1053	C950	U871	U766	U666	A565	U475	A369	U285
U1551	U1478	U1371	U1278	U1193	U1130	A1054	C951	U872	U767	U667	A566	U476	A370	U286
U1552	U1479	U1372	G1279	U1194	U1131	A1055	A950	U873	U768	U668	A567	U477	A371	
A1553	U1480	U1373	U1280	U1195	U1132	A1056	C951	U874	U769	U669	A568	U478	A372	A287
U1554	U1481	U1374	U1281	U1196	U1133	A1057	C952	U875	U770	U670	A569	U479	A373	C288
A1555	U1482	U1375	G1282	U1197	U1134	C1058	C953	U876	U771	U671	A570	U480	A374	U289
U1556	U1483	U1376	U1283	U1198	U1135	A1059	C954	U877	U772	U672	A571	U481	A375	U290
	U1484	U1377	U1284	U1199	U1136	A1060	A951	U878	U773	U673	A572	U482	A376	
U1557	U1485	U1378	G1285	U1200	U1137	A1061	C952	U879	U774	U674	A573	U483	A377	
A1558	U1486	U1379	U1286	U1201	U1138	A1062	C953	U880	U775	U675	A574	U484	A378	
U1559	U1487	U1380	U1287	U1202	U1139	A1063	C954	U881	U776	U676	A575	U485	A379	
U1560	U1488	U1381	U1288	U1203	U1140	A1064	C955	U882	U777	U677	A576	U486	A380	
U1561	U1489	U1382	G1289	U1204	U1141	A1065	C956	U883	U778	U678	A577	U487	A381	
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		U1385	U1292	U1207	U1144	A1068	C959	U886	U781	U681	A580	U490	A384	
		U1386	U1293	U1208	U1145	A1069	C960	U887	U782	U682	A581	U491	A385	
		U1387	U1294	U1209	U1146	A1070	C961	U888	U783	U683	A582	U492	A386	
		U1388	U1295	U1210	U1147	A1071	C962	U889	U784	U684	A583	U493	A387	
		U1389	U1296	U1211	U1148	A1072	C963	U890	U785	U685	A584	U494	A388	
		U1390	U1297	U1212	U1149	A1073	C964	U891	U786	U686	A585	U495	A389	
		U1391	U1298	U1213	U1150	A1074	C965	U892	U787	U687	A586	U496	A390	
		U1392	U1299	U1214	U1151	A1075	C966	U893	U788	U688	A587	U497	A391	
		U1393	U1300	U1215	U1152	A1076	C967	U894	U789	U689	A588	U498	A392	
		U1394	U1301	U1216	U1153	A1077	C968	U895	U790	U690	A589	U499	A393	
		U1395	U1302	U1217	U1154	A1078	C969	U896	U791	U691	A590	U500	A394	
		U1396	U1303	U1218	U1155	A1079	C970	U897	U792	U692	A591	U501	A395	
		U1397	U1304	U1219	U1156	A1080	C971	U898	U793	U693	A592	U502	A396	
		U1398	U1305	U1220	U1157	A1081	C972	U899	U794	U694	A593	U503	A397	
		U1399	U1306	U1221	U1158	A1082	C973	U900	U795	U695	A594	U504	A398	
		U1400	U1307	U1222	U1159	A1083	C974	U901	U796	U696	A595	U505	A399	
		U1401	U1308	U1223	U1160	A1084	C975	U902	U797	U697	A596	U506	A400	
		U1402	U1309	U1224	U1161	A1085	C976	U903	U798	U698	A597	U507	A401	
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		U												

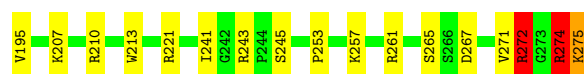
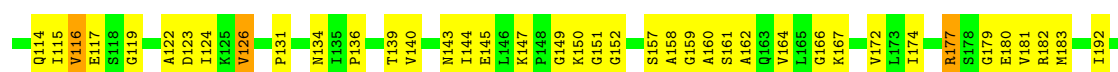
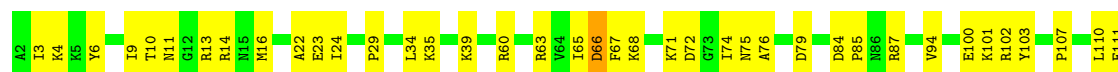
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U1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	A1637	G1638	G1639	U1640	G1641	G1644	G1651	A1652	A1653	A1654	G1655	C1656	G1657	A1658	G1659	A1660	C1661	A1662	G1663	A1666	C1669	A1670	A1671	G1672	A1678	A1679	A1680	U1681	A1684	G1687	A1689	A1690	G1691	G1692	G1693	A1698	A1699	G1700	U1701	U1707	U1708	A1709					
A1712	A1713	C1714	G1717	A1718	C1719	A1723	A1726	C1727	U1736	C1737	C1738	G1739	G1740	C1743	G1751	C1752	C1753	C1754	U1755	U1756	A1757	A1758	A1759	G1760	G1761	U1762	A1763	A1764	A1765	C1766	C1769	C1770	A1771	G1783	A1789	G1790	G1791	A1796	G1797	A1800	C1801	U1802	G1803	U1804	U1805	U1806	U1807	U1808						
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A1998	G1999	U2003	A2008	U2009	U2018	U2019	U2020	C2021	U2022	C2023	A2024	A2025	C2026	G2029	A2032	C2035	G2036	G2037	A2040	G2048	U2049	A2050	A2057	A2058	G2059	A2060	U2061	G2062	C2070	G2075	A2076	C2077	C2082	G2083	G2084	A2085	A2086	G2088	A2089	C2090	C2091	C2092	C2093	U2095										
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• Molecule 6: 5S ribosomal RNA



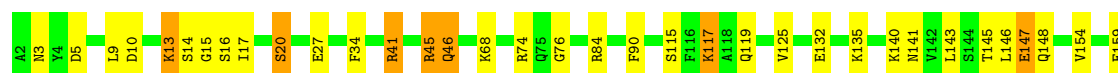
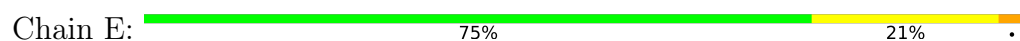
• Molecule 7: Large ribosomal subunit protein uL2



• Molecule 8: Large ribosomal subunit protein uL3



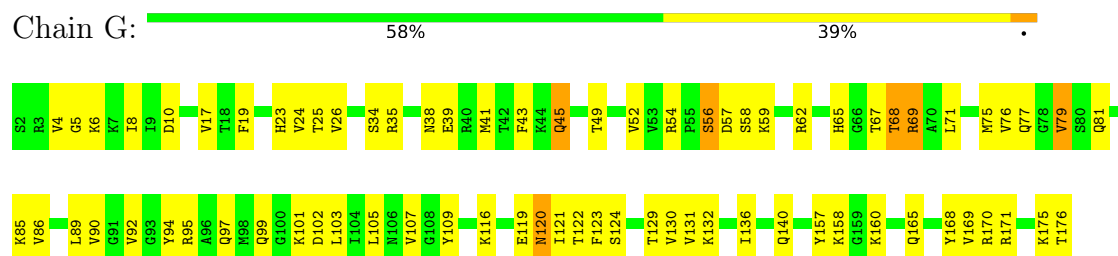
• Molecule 9: Large ribosomal subunit protein uL4



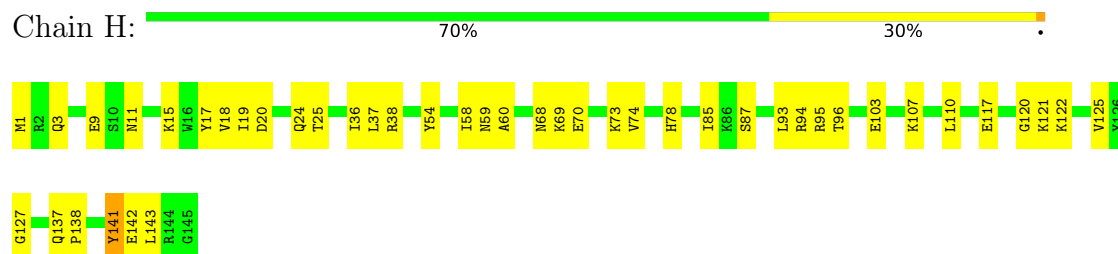
- Molecule 10: Large ribosomal subunit protein uL5



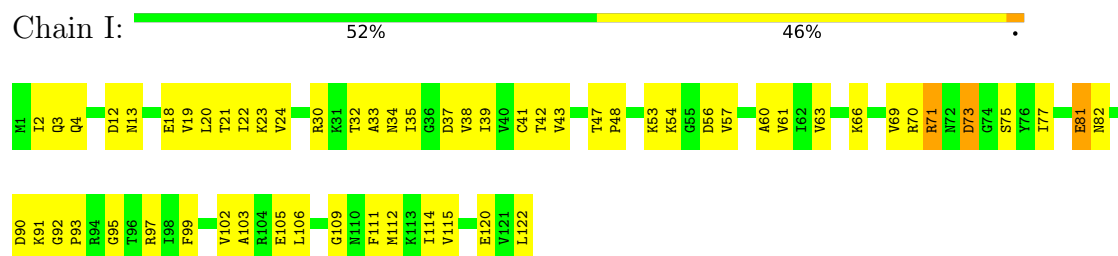
- Molecule 11: Large ribosomal subunit protein uL6



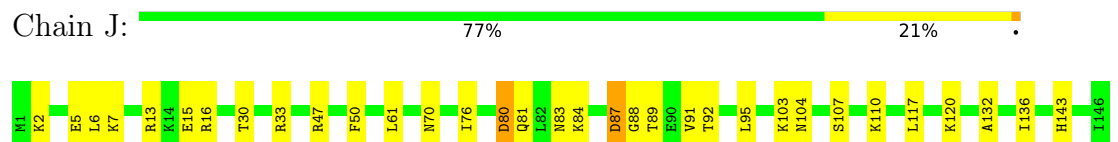
- Molecule 12: Large ribosomal subunit protein uL13



- Molecule 13: Large ribosomal subunit protein uL14

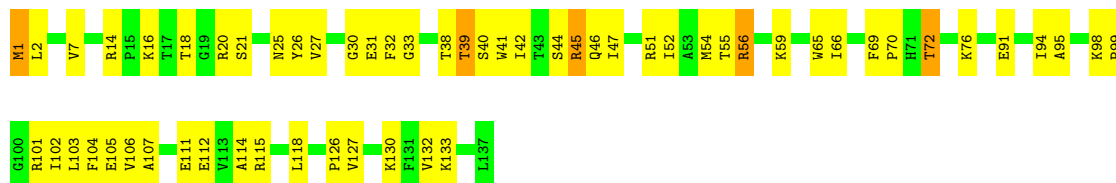


- Molecule 14: Large ribosomal subunit protein uL15



- Molecule 15: Large ribosomal subunit protein uL16

Chain K:  58% 39%



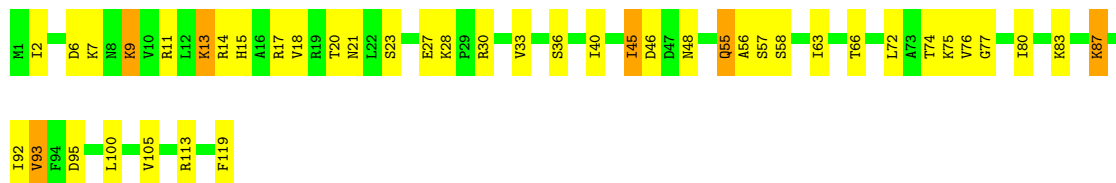
- Molecule 16: Large ribosomal subunit protein bL17

Chain L:  70% 29%



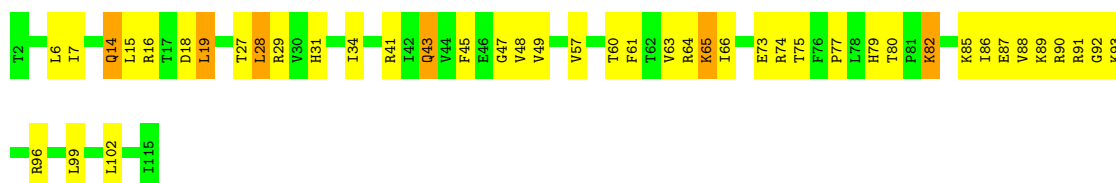
- Molecule 17: Large ribosomal subunit protein uL18

Chain M:  64% 31% 5%



- Molecule 18: Large ribosomal subunit protein bL19

Chain N:  61% 33% 5%



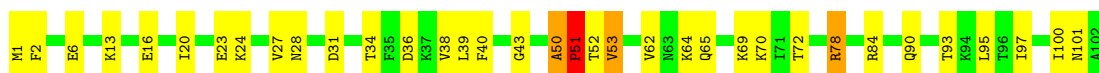
- Molecule 19: Large ribosomal subunit protein bL20

Chain O:  74% 24%



- Molecule 20: Large ribosomal subunit protein bL21

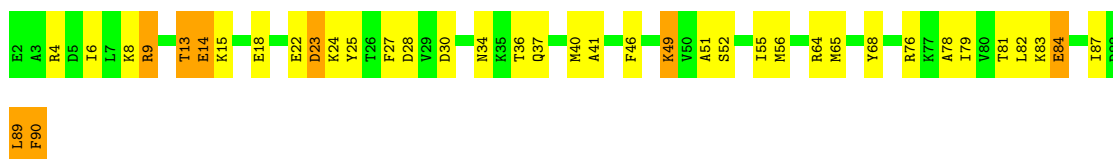
Chain P:  66% 30%



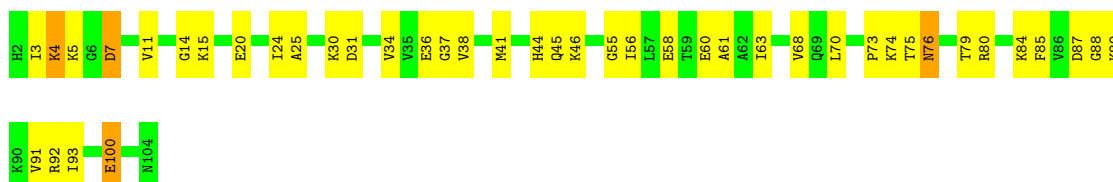
- Molecule 21: Large ribosomal subunit protein uL22



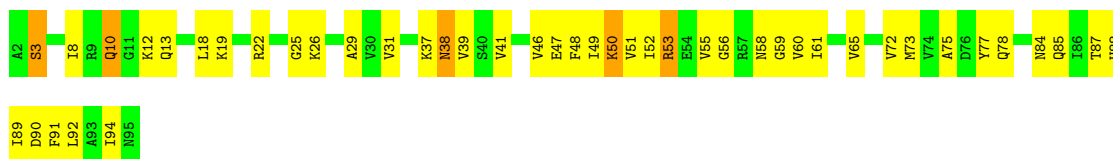
- Molecule 22: Large ribosomal subunit protein uL23



- Molecule 23: Large ribosomal subunit protein uL24



- Molecule 24: Large ribosomal subunit protein bL25

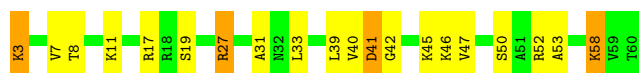


- Molecule 25: Large ribosomal subunit protein bL27



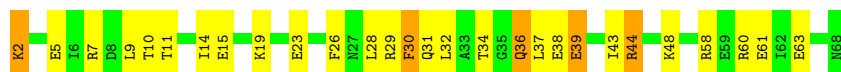
- Molecule 26: Large ribosomal subunit protein bL28





- Molecule 27: Large ribosomal subunit protein uL29

Chain W: 58% 34% 7%



- Molecule 28: Large ribosomal subunit protein uL30

Chain X: 83% 17%



- Molecule 29: Large ribosomal subunit protein bL31B

Chain Y: 73% 24% . .



- Molecule 30: Large ribosomal subunit protein bL32

Chain Z: 79% 19% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68392	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1D6G, OMG, 2MA, 5MU, MA6, 2MG, 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	1	0.60	0/395	0.88	0/530
2	2	0.44	0/371	0.71	0/484
3	3	0.57	0/526	0.80	0/690
4	4	0.74	0/299	0.90	0/393
5	A	0.54	0/69095	0.83	3/107748 (0.0%)
6	B	0.51	0/2733	0.86	1/4257 (0.0%)
7	C	0.59	0/2125	0.86	0/2853
8	D	0.65	0/1651	0.82	0/2215
9	E	0.66	0/1595	0.82	2/2154 (0.1%)
10	F	0.48	0/1332	0.78	0/1798
11	G	0.59	0/1277	0.77	0/1731
12	H	0.43	0/1165	0.67	0/1570
13	I	0.57	0/925	0.76	0/1242
14	J	0.39	0/1100	0.63	0/1467
15	K	0.52	0/1095	0.68	0/1472
16	L	0.43	0/936	0.69	0/1253
17	M	0.58	0/900	0.79	0/1205
18	N	0.41	0/901	0.67	0/1209
19	O	0.39	0/954	0.65	0/1264
20	P	0.50	0/800	0.73	1/1070 (0.1%)
21	Q	0.49	0/861	0.73	0/1161
22	R	0.48	0/723	0.68	0/966
23	S	0.46	0/779	0.70	0/1043
24	T	0.41	0/719	0.65	0/969
25	U	0.50	0/621	0.71	0/825
26	V	0.69	0/451	0.84	0/603
27	W	0.33	0/542	0.67	0/722
28	X	0.32	0/451	0.55	0/606
29	Y	0.36	0/378	0.63	0/521
30	Z	0.58	0/367	0.81	0/490
All	All	0.54	0/96067	0.81	7/144511 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
7	C	0	2
9	E	0	2
20	P	0	2
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	46	GLN	CB-CA-C	-7.80	94.81	110.40
20	P	51	PRO	N-CA-C	-6.95	94.04	112.10
9	E	46	GLN	N-CA-CB	6.32	121.97	110.60
5	A	278	A	OP1-P-O3'	5.97	118.34	105.20
5	A	440	C	OP2-P-O3'	5.15	116.53	105.20
5	A	1528	G	P-O3'-C3'	5.08	125.79	119.70
6	B	20	A	OP2-P-O3'	5.04	116.29	105.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	29	ARG	Sidechain
7	C	272	ARG	Sidechain
7	C	274	ARG	Sidechain
9	E	41	ARG	Sidechain
9	E	45	ARG	Sidechain
20	P	78	ARG	Sidechain
20	P	84	ARG	Sidechain

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	1	390	0	395	32	0
2	2	367	0	415	7	0
3	3	521	0	586	16	0
4	4	296	0	340	16	0
5	A	61838	0	31093	513	0
6	B	2445	0	1240	40	0
7	C	2090	0	2201	106	0
8	D	1627	0	1667	79	0
9	E	1572	0	1619	49	0
10	F	1317	0	1323	195	0
11	G	1259	0	1221	94	0
12	H	1143	0	1134	51	0
13	I	918	0	981	68	0
14	J	1086	0	1125	30	0
15	K	1071	0	1123	73	0
16	L	932	0	983	34	0
17	M	891	0	925	38	0
18	N	889	0	937	52	0
19	O	942	0	1014	44	0
20	P	790	0	830	34	0
21	Q	853	0	905	29	0
22	R	715	0	748	64	0
23	S	770	0	809	47	0
24	T	711	0	740	52	0
25	U	615	0	622	26	0
26	V	445	0	466	23	0
27	W	541	0	563	38	0
28	X	449	0	491	9	0
29	Y	370	0	243	36	0
30	Z	361	0	361	9	0
31	A	69	0	0	1	0
32	A	12	0	0	0	0
33	A	6	0	0	1	0
All	All	88301	0	57100	1695	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 12.

All (1695) 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)
11:G:59:LYS:HD3	11:G:62:ARG:NH2	1.59	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:89:ASP:OD1	19:O:89:ASP:O	1.65	1.14
21:Q:66:THR:HG22	21:Q:66:THR:O	1.39	1.14
28:X:6:ILE:HD11	28:X:47:ILE:HD11	1.28	1.14
11:G:54:ARG:NH1	11:G:62:ARG:HG2	1.64	1.13
24:T:12:LYS:O	24:T:12:LYS:HG2	1.49	1.13
10:F:9:ASN:HA	10:F:13:THR:CG2	1.77	1.13
10:F:50:LEU:O	10:F:54:VAL:HG23	1.50	1.12
20:P:1:MET:HE1	20:P:43:GLY:HA3	1.29	1.12
1:1:12:CYS:SG	1:1:39:LEU:CD1	2.39	1.11
10:F:9:ASN:HA	10:F:13:THR:HG21	1.17	1.10
11:G:54:ARG:HH11	11:G:62:ARG:HG2	1.10	1.10
26:V:58:LYS:HE2	26:V:58:LYS:HA	1.21	1.09
24:T:47:GLU:O	24:T:51:VAL:HG23	1.53	1.08
10:F:59:LEU:HD21	10:F:141:ILE:HG21	1.36	1.08
18:N:27:THR:HG22	18:N:48:VAL:HG22	1.13	1.07
10:F:54:VAL:HG11	10:F:64:LYS:HE3	1.08	1.06
7:C:66:ASP:O	7:C:66:ASP:OD1	1.72	1.06
12:H:141:TYR:CE1	12:H:142:GLU:O	2.08	1.06
1:1:12:CYS:SG	1:1:39:LEU:HD11	1.95	1.05
10:F:54:VAL:CG1	10:F:64:LYS:HE3	1.85	1.05
10:F:130:LEU:HG	10:F:131:GLY:H	1.13	1.04
10:F:7:LYS:HD2	10:F:173:PHE:CZ	1.93	1.03
11:G:86:VAL:HG22	11:G:132:LYS:HG2	1.34	1.03
29:Y:8:GLU:OE1	29:Y:8:GLU:N	1.92	1.03
21:Q:52:MET:HA	21:Q:52:MET:HE3	1.39	1.03
10:F:57:LEU:H	10:F:60:ILE:HD13	1.24	1.02
10:F:66:LEU:HD12	10:F:66:LEU:O	1.59	1.02
22:R:64:ARG:HB2	22:R:64:ARG:HH11	1.20	1.01
6:B:55:A:H4'	10:F:27:GLU:OE1	1.59	1.01
24:T:47:GLU:OE1	24:T:47:GLU:N	1.93	1.01
10:F:54:VAL:HG11	10:F:64:LYS:CE	1.91	1.00
10:F:107:SER:O	10:F:136:LEU:HD21	1.59	1.00
10:F:79:LEU:HD11	10:F:85:ILE:HG12	1.40	0.99
10:F:8:PHE:O	10:F:13:THR:HG23	1.61	0.99
29:Y:9:TYR:CZ	29:Y:26:GLY:HA2	1.97	0.98
16:L:34:GLU:OE2	16:L:105:LYS:HE3	1.60	0.98
5:A:1644:C:P	22:R:76:ARG:HH12	1.85	0.98
10:F:62:GLY:HA3	10:F:95:ARG:HH21	1.27	0.97
7:C:167:LYS:HD2	7:C:172:VAL:HG22	1.47	0.96
8:D:38:LYS:HG3	8:D:96:VAL:CG1	1.96	0.96
11:G:41:MET:CE	11:G:65:HIS:HA	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:144:C:C5'	22:R:37:GLN:NE2	2.29	0.95
1:1:18:ILE:HG21	5:A:2446:U:C5'	1.95	0.94
9:E:141:ASN:O	9:E:145:THR:HG23	1.64	0.94
8:D:128:GLN:OE1	8:D:132:LYS:HD2	1.68	0.94
10:F:152:MET:HE2	10:F:154:ILE:HD11	1.47	0.94
24:T:8:ILE:HD11	24:T:65:VAL:HG13	1.49	0.94
11:G:35:ARG:HG3	11:G:75:MET:HE3	1.48	0.94
26:V:58:LYS:HE2	26:V:58:LYS:CA	1.97	0.94
21:Q:66:THR:O	21:Q:66:THR:CG2	2.14	0.93
11:G:26:VAL:CG1	11:G:79:VAL:HG11	1.99	0.92
5:A:2711:U:OP1	18:N:60:THR:HG21	1.69	0.92
24:T:75:ALA:HB2	24:T:92:LEU:HD22	1.50	0.92
9:E:167:ALA:HA	9:E:170:ILE:HD12	1.52	0.92
27:W:10:THR:O	27:W:11:THR:HG22	1.68	0.92
10:F:65:PRO:HB2	10:F:87:ALA:HB1	1.51	0.92
18:N:31:HIS:CD2	18:N:85:LYS:HD3	2.05	0.92
14:J:91:VAL:HG23	14:J:95:LEU:HD12	1.52	0.92
7:C:143:ASN:ND2	7:C:152:GLY:HA3	1.84	0.91
10:F:95:ARG:CD	29:Y:1:MET:HB3	1.99	0.91
5:A:144:C:C5'	22:R:37:GLN:HE21	1.82	0.91
8:D:38:LYS:CG	8:D:96:VAL:CG1	2.49	0.91
15:K:51:ARG:O	15:K:55:THR:HG23	1.70	0.91
10:F:59:LEU:HD23	10:F:141:ILE:HD13	1.52	0.91
1:1:14:ASP:HB3	1:1:38:ARG:HH21	1.33	0.91
10:F:4:LEU:HD12	10:F:7:LYS:HD3	1.50	0.91
14:J:132:ALA:O	14:J:136:ILE:HD12	1.70	0.91
8:D:14:GLN:CD	8:D:22:LEU:HD21	1.92	0.91
26:V:58:LYS:HA	26:V:58:LYS:CE	1.93	0.90
22:R:64:ARG:NH1	22:R:64:ARG:CB	2.35	0.90
15:K:1:MET:C	15:K:2:LEU:HD12	1.92	0.90
10:F:59:LEU:CD2	10:F:141:ILE:HG21	2.00	0.90
11:G:59:LYS:CD	11:G:62:ARG:NH2	2.34	0.90
18:N:34:ILE:HD11	18:N:43:GLN:HE21	1.34	0.89
22:R:14:GLU:O	22:R:18:GLU:HG3	1.70	0.89
11:G:26:VAL:HG12	11:G:79:VAL:HG11	1.52	0.89
10:F:60:ILE:HG21	10:F:137:ILE:CG2	2.01	0.89
10:F:60:ILE:H	10:F:60:ILE:HD12	1.37	0.89
10:F:132:VAL:O	10:F:133:LYS:HD3	1.70	0.89
13:I:102:VAL:CG1	13:I:106:LEU:HD12	2.03	0.89
1:1:18:ILE:HG21	5:A:2446:U:H5''	1.52	0.89
25:U:35:ASP:OD1	25:U:77:PHE:CD1	2.26	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:7:VAL:HG12	4:4:25:VAL:HG23	1.55	0.88
13:I:38:VAL:HG13	13:I:60:ALA:O	1.74	0.88
15:K:31:GLU:CD	15:K:32:PHE:CE2	2.47	0.87
11:G:81:GLN:O	11:G:81:GLN:CD	2.13	0.87
15:K:42:ILE:CG2	15:K:47:ILE:HD11	2.04	0.87
18:N:45:PHE:HE2	18:N:63:VAL:HG11	1.39	0.87
9:E:132:GLU:OE1	9:E:132:GLU:N	2.08	0.87
18:N:27:THR:HG22	18:N:48:VAL:CG2	2.03	0.87
19:O:8:THR:O	19:O:8:THR:HG22	1.75	0.87
10:F:130:LEU:HG	10:F:131:GLY:N	1.90	0.87
3:3:7:HIS:CE1	5:A:254:A:OP1	2.28	0.86
11:G:59:LYS:HD3	11:G:62:ARG:HH21	1.36	0.86
22:R:64:ARG:HH11	22:R:64:ARG:CB	1.88	0.86
18:N:45:PHE:CE2	18:N:63:VAL:HG11	2.09	0.86
10:F:137:ILE:HG22	10:F:138:PHE:H	1.39	0.86
10:F:51:ASP:HA	10:F:54:VAL:HG23	1.58	0.86
8:D:107:VAL:HG12	8:D:188:VAL:HG13	1.57	0.85
10:F:17:MET:O	10:F:17:MET:SD	2.34	0.85
27:W:63:GLU:OE1	27:W:63:GLU:HA	1.76	0.85
1:1:10:THR:HG22	1:1:46:ARG:HH12	1.41	0.85
10:F:130:LEU:CG	10:F:131:GLY:H	1.87	0.85
8:D:99:TYR:O	8:D:100:GLU:OE2	1.93	0.85
10:F:62:GLY:HA3	10:F:95:ARG:NH2	1.92	0.85
21:Q:2:GLU:HG2	21:Q:106:VAL:CG1	2.07	0.85
22:R:64:ARG:HB2	22:R:64:ARG:NH1	1.91	0.85
25:U:83:ASP:O	25:U:84:LYS:HD2	1.75	0.85
28:X:17:GLU:OE1	28:X:20:ARG:HD2	1.77	0.84
11:G:99:GLN:HG3	11:G:99:GLN:O	1.74	0.84
11:G:121:ILE:HG22	11:G:123:PHE:CE1	2.12	0.84
28:X:6:ILE:CD1	28:X:47:ILE:HD11	2.06	0.84
3:3:53:SER:O	3:3:56:LYS:HG2	1.78	0.84
26:V:41:ASP:OD1	26:V:41:ASP:O	1.95	0.84
11:G:121:ILE:HD11	11:G:140:GLN:HB3	1.59	0.84
12:H:78:HIS:HD2	12:H:85:ILE:CD1	1.90	0.84
10:F:63:GLN:HE22	29:Y:1:MET:HB2	1.43	0.84
22:R:84:GLU:OE1	22:R:84:GLU:O	1.95	0.84
5:A:1855:G:O6	7:C:221:ARG:HD3	1.77	0.83
7:C:84:ASP:OD1	7:C:87:ARG:HG3	1.78	0.83
20:P:1:MET:CE	20:P:43:GLY:HA3	2.07	0.83
10:F:106:VAL:O	10:F:136:LEU:HD22	1.76	0.83
23:S:30:LYS:O	23:S:31:ASP:OD1	1.95	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:115:SER:O	9:E:119:GLN:HG3	1.76	0.83
10:F:152:MET:CE	10:F:154:ILE:HD11	2.08	0.83
10:F:95:ARG:HD3	29:Y:1:MET:HB3	1.58	0.83
10:F:25:VAL:HG23	10:F:26:MET:HE2	1.58	0.83
21:Q:52:MET:HA	21:Q:52:MET:CE	2.08	0.83
27:W:10:THR:O	27:W:11:THR:CG2	2.27	0.83
18:N:77:PRO:O	18:N:80:THR:HG22	1.79	0.82
23:S:36:GLU:HA	23:S:60:GLU:OE2	1.79	0.82
26:V:7:VAL:HG23	26:V:8:THR:N	1.93	0.82
10:F:149:VAL:HG23	10:F:149:VAL:O	1.77	0.82
7:C:111:GLU:HG2	7:C:114:GLN:NE2	1.95	0.82
4:4:7:VAL:CG2	4:4:36:GLN:O	2.27	0.82
10:F:50:LEU:O	10:F:54:VAL:CG2	2.27	0.82
10:F:59:LEU:HD23	10:F:141:ILE:CD1	2.09	0.82
18:N:45:PHE:HE2	18:N:63:VAL:CG1	1.91	0.82
5:A:427:A:H61	5:A:439:U:H5	1.25	0.82
6:B:40:C:O2	10:F:66:LEU:CD2	2.27	0.82
13:I:63:VAL:HG12	13:I:106:LEU:HD11	1.61	0.81
21:Q:66:THR:HA	21:Q:69:LEU:HD12	1.61	0.81
15:K:42:ILE:HG21	15:K:47:ILE:HD11	1.63	0.81
5:A:1884:G:H21	5:A:1912:A:H2	1.29	0.81
10:F:107:SER:O	10:F:136:LEU:CD2	2.29	0.81
27:W:31:GLN:HB2	27:W:36:GLN:HG3	1.63	0.81
1:1:5:VAL:HG13	1:1:47:GLU:HG3	1.63	0.81
8:D:15:VAL:HG22	8:D:25:VAL:CG1	2.10	0.81
14:J:104:ASN:O	14:J:104:ASN:OD1	1.99	0.81
9:E:27:GLU:OE1	9:E:27:GLU:HA	1.79	0.80
26:V:40:VAL:CG1	26:V:45:LYS:HB3	2.11	0.80
1:1:12:CYS:SG	1:1:39:LEU:HD12	2.18	0.80
10:F:107:SER:HA	10:F:136:LEU:HD13	1.63	0.80
9:E:140:LYS:HD3	9:E:170:ILE:HG23	1.64	0.80
7:C:124:ILE:O	7:C:124:ILE:HG22	1.81	0.80
11:G:86:VAL:CG2	11:G:132:LYS:HG2	2.12	0.80
10:F:63:GLN:HE22	29:Y:1:MET:CB	1.94	0.79
10:F:25:VAL:HG23	10:F:26:MET:CE	2.13	0.79
10:F:31:ILE:HG23	10:F:96:MET:SD	2.21	0.79
12:H:20:ASP:OD1	12:H:58:ILE:HG12	1.82	0.79
7:C:140:VAL:HG13	7:C:161:SER:HB2	1.65	0.79
10:F:59:LEU:HD21	10:F:141:ILE:CG2	2.10	0.79
5:A:63:U:O2	22:R:65:MET:HE1	1.82	0.79
5:A:2403:A:N3	17:M:113:ARG:NH2	2.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:25:GLY:O	24:T:26:LYS:HD3	1.81	0.79
20:P:50:ALA:HB3	20:P:51:PRO:HD3	1.64	0.79
7:C:23:GLU:OE1	7:C:23:GLU:N	2.14	0.78
17:M:15:HIS:CE1	17:M:95:ASP:OD2	2.37	0.78
5:A:2419:A:H2	5:A:2451:C:H42	1.32	0.78
5:A:2918:A:H5'	12:H:137:GLN:HE21	1.48	0.78
10:F:138:PHE:HB2	10:F:141:ILE:HG13	1.64	0.78
23:S:74:LYS:HD3	23:S:74:LYS:N	1.97	0.78
10:F:132:VAL:C	10:F:133:LYS:HD3	2.03	0.78
13:I:12:ASP:OD1	13:I:95:GLY:HA3	1.83	0.78
15:K:51:ARG:HH11	15:K:55:THR:HG21	1.46	0.78
18:N:45:PHE:CE2	18:N:63:VAL:CG1	2.66	0.78
1:I:14:ASP:HB3	1:I:38:ARG:NH2	1.98	0.78
7:C:111:GLU:HG2	7:C:114:GLN:HE21	1.48	0.78
4:4:7:VAL:HG23	4:4:36:GLN:O	1.84	0.78
18:N:64:ARG:HD2	18:N:73:GLU:OE2	1.83	0.77
12:H:78:HIS:HD2	12:H:85:ILE:HD13	1.48	0.77
15:K:101:ARG:O	15:K:103:LEU:HD12	1.83	0.77
5:A:144:C:H5''	22:R:37:GLN:NE2	1.97	0.77
21:Q:17:VAL:HG12	21:Q:43:SER:HB3	1.66	0.77
22:R:84:GLU:O	22:R:84:GLU:CD	2.23	0.77
10:F:117:VAL:HG22	10:F:175:MET:HB2	1.66	0.77
5:A:1854:U:C5	7:C:221:ARG:HD2	2.19	0.77
8:D:133:ARG:HG3	8:D:173:MET:HG3	1.66	0.77
10:F:51:ASP:HA	10:F:54:VAL:CG2	2.15	0.77
12:H:141:TYR:CD1	12:H:142:GLU:O	2.37	0.77
15:K:31:GLU:HG2	15:K:32:PHE:CD2	2.20	0.76
5:A:63:U:O2	22:R:65:MET:CE	2.33	0.76
5:A:292:U:H1'	5:A:293:U:H5'	1.67	0.76
10:F:35:VAL:HG12	10:F:155:VAL:CG2	2.16	0.76
10:F:95:ARG:HD2	29:Y:1:MET:HB3	1.66	0.76
26:V:7:VAL:CG2	26:V:8:THR:N	2.48	0.76
5:A:506:A:H2	5:A:515:G:H21	1.33	0.76
8:D:128:GLN:HG3	8:D:173:MET:HE3	1.67	0.76
10:F:54:VAL:HG12	10:F:64:LYS:HG3	1.68	0.76
10:F:60:ILE:HD12	10:F:60:ILE:N	2.00	0.76
11:G:176:THR:HG22	11:G:176:THR:O	1.85	0.75
27:W:19:LYS:O	27:W:23:GLU:HG2	1.85	0.75
10:F:63:GLN:OE1	29:Y:1:MET:HA	1.86	0.75
17:M:15:HIS:O	17:M:18:VAL:HG22	1.85	0.75
21:Q:1:MET:SD	21:Q:1:MET:O	2.44	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:15:LEU:HD22	18:N:79:HIS:CE1	2.20	0.75
6:B:71:A:C2	24:T:38:ASN:ND2	2.54	0.75
5:A:656:G:H21	5:A:660:A:H2	1.33	0.74
9:E:17:ILE:HD13	9:E:196:GLU:HG2	1.68	0.74
7:C:144:ILE:HD13	7:C:174:ILE:HD11	1.67	0.74
5:A:1578:A:H8	5:A:1588:U:H3	1.34	0.74
7:C:182:ARG:HG2	7:C:182:ARG:HH11	1.51	0.74
11:G:26:VAL:HG12	11:G:79:VAL:HG21	1.70	0.74
7:C:117:GLU:HG3	7:C:122:ALA:HB1	1.69	0.74
5:A:1478:A:H61	5:A:1605:A:H61	1.35	0.74
5:A:2338:A:C2	10:F:76:THR:OG1	2.41	0.74
17:M:14:ARG:O	17:M:18:VAL:HG13	1.88	0.74
7:C:145:GLU:HG2	7:C:151:GLY:C	2.08	0.73
8:D:27:VAL:HG23	8:D:194:VAL:CG1	2.18	0.73
26:V:7:VAL:CG2	26:V:8:THR:H	2.01	0.73
5:A:2684:A:H1'	5:A:2692:A:N6	2.02	0.73
10:F:115:GLN:HG3	10:F:119:LYS:NZ	2.01	0.73
20:P:1:MET:C	20:P:1:MET:SD	2.66	0.73
21:Q:1:MET:HG3	21:Q:111:LYS:O	1.88	0.73
22:R:14:GLU:O	22:R:18:GLU:CG	2.36	0.73
5:A:2403:A:C2	17:M:113:ARG:NH2	2.56	0.73
8:D:38:LYS:CG	8:D:96:VAL:HG11	2.18	0.73
10:F:54:VAL:CG1	10:F:64:LYS:HG3	2.18	0.73
21:Q:9:THR:O	21:Q:9:THR:HG22	1.88	0.73
26:V:17:ARG:HH11	26:V:17:ARG:HG3	1.54	0.73
5:A:144:C:H4'	22:R:37:GLN:HE21	1.54	0.73
5:A:2575:G:H1'	13:I:23:LYS:NZ	2.03	0.72
5:A:2341:A:H4'	10:F:155:VAL:HG21	1.71	0.72
6:B:71:A:H2	24:T:38:ASN:ND2	1.86	0.72
8:D:38:LYS:HG2	8:D:96:VAL:HG11	1.71	0.72
10:F:4:LEU:CD1	10:F:7:LYS:HD3	2.19	0.72
5:A:1847:U:H5	7:C:177:ARG:HH12	1.36	0.72
10:F:69:LYS:HG3	10:F:84:PRO:HA	1.71	0.72
18:N:85:LYS:HE3	18:N:87:GLU:OE2	1.89	0.72
9:E:154:VAL:HG22	9:E:193:VAL:CG2	2.19	0.72
8:D:128:GLN:OE1	8:D:132:LYS:CD	2.36	0.72
10:F:8:PHE:HA	10:F:12:VAL:HG23	1.71	0.72
5:A:1644:C:P	22:R:76:ARG:NH1	2.61	0.72
14:J:84:LYS:HG3	14:J:84:LYS:O	1.87	0.72
5:A:144:C:H5'	22:R:37:GLN:HE21	1.53	0.72
5:A:1644:C:OP1	22:R:76:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:15:VAL:HG22	8:D:25:VAL:HG11	1.69	0.72
15:K:65:TRP:HH2	15:K:107:ALA:HB3	1.54	0.72
15:K:101:ARG:O	15:K:103:LEU:CD1	2.37	0.72
23:S:4:LYS:HE2	23:S:92:ARG:NH1	2.05	0.72
4:4:7:VAL:CG1	4:4:25:VAL:HG23	2.19	0.72
18:N:47:GLY:HA3	18:N:63:VAL:CG1	2.19	0.72
10:F:7:LYS:HD2	10:F:173:PHE:CE2	2.24	0.71
22:R:64:ARG:NH1	22:R:64:ARG:HB3	2.03	0.71
7:C:79:ASP:C	7:C:79:ASP:OD1	2.28	0.71
10:F:65:PRO:CB	10:F:87:ALA:HB1	2.20	0.71
10:F:152:MET:N	10:F:152:MET:SD	2.62	0.71
6:B:91:C:OP2	24:T:19:LYS:NZ	2.23	0.71
15:K:112:GLU:OE1	15:K:112:GLU:N	2.23	0.71
5:A:144:C:C4'	22:R:37:GLN:HE21	2.04	0.71
5:A:721:A:H8	5:A:2096:G:H21	1.38	0.71
11:G:119:GLU:OE1	11:G:119:GLU:N	2.23	0.71
21:Q:40:ASN:CG	21:Q:40:ASN:O	2.28	0.71
6:B:40:C:C2	10:F:66:LEU:HD22	2.26	0.71
16:L:26:ILE:CD1	16:L:71:ILE:HD11	2.21	0.71
24:T:8:ILE:CD1	24:T:65:VAL:HG13	2.19	0.71
5:A:2306:G:N7	25:U:22:ARG:NH2	2.37	0.70
5:A:2918:A:H5'	12:H:137:GLN:NE2	2.06	0.70
11:G:41:MET:HE2	11:G:65:HIS:HA	1.71	0.70
23:S:3:ILE:HD12	23:S:4:LYS:N	2.06	0.70
5:A:1846:A:H2	7:C:275:LYS:HB3	1.54	0.70
8:D:27:VAL:HG23	8:D:194:VAL:HG11	1.72	0.70
17:M:63:ILE:O	17:M:72:LEU:HD21	1.91	0.70
21:Q:2:GLU:OE2	21:Q:72:LYS:HD2	1.90	0.70
7:C:181:VAL:HG22	7:C:272:ARG:HG3	1.74	0.70
11:G:69:ARG:C	11:G:69:ARG:HD3	2.11	0.70
13:I:13:ASN:ND2	13:I:97:ARG:HB3	2.07	0.70
10:F:57:LEU:N	10:F:60:ILE:HD13	2.02	0.70
5:A:2859:G:H4'	16:L:45:GLU:OE1	1.92	0.70
10:F:63:GLN:NE2	29:Y:1:MET:HB2	2.05	0.70
17:M:46:ASP:OD1	17:M:48:ASN:N	2.25	0.70
18:N:34:ILE:HD11	18:N:43:GLN:NE2	2.06	0.70
16:L:26:ILE:HD12	16:L:71:ILE:HD11	1.72	0.70
5:A:1483:A:H62	5:A:1599:G:H8	1.40	0.69
15:K:25:ASN:C	15:K:26:TYR:HD1	1.94	0.69
15:K:70:PRO:HA	15:K:95:ALA:HB2	1.74	0.69
7:C:74:ILE:HD12	7:C:74:ILE:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:99:TYR:CD2	8:D:103:GLN:NE2	2.60	0.69
14:J:83:ASN:ND2	14:J:117:LEU:HA	2.07	0.69
8:D:99:TYR:HD2	8:D:103:GLN:NE2	1.91	0.69
24:T:22:ARG:HD2	24:T:87:THR:HG22	1.75	0.69
13:I:32:THR:CG2	13:I:33:ALA:N	2.55	0.69
11:G:38:ASN:HB3	11:G:41:MET:HG3	1.73	0.69
13:I:90:ASP:C	13:I:90:ASP:OD1	2.31	0.69
17:M:100:LEU:H	17:M:100:LEU:HD12	1.55	0.69
9:E:193:VAL:O	9:E:193:VAL:HG23	1.93	0.69
10:F:5:LYS:HZ2	10:F:94:GLU:HG3	1.57	0.69
18:N:14:GLN:HG3	18:N:14:GLN:O	1.92	0.69
15:K:42:ILE:HG22	15:K:47:ILE:HD11	1.74	0.69
26:V:40:VAL:HG12	26:V:45:LYS:HB3	1.73	0.69
10:F:60:ILE:HG21	10:F:137:ILE:HG21	1.75	0.68
10:F:63:GLN:NE2	29:Y:1:MET:HA	2.08	0.68
27:W:15:GLU:OE1	27:W:15:GLU:N	2.26	0.68
7:C:34:LEU:HD21	7:C:63:ARG:HG3	1.73	0.68
12:H:9:GLU:HG3	12:H:9:GLU:O	1.93	0.68
19:O:89:ASP:OD1	19:O:89:ASP:C	2.31	0.68
24:T:75:ALA:CB	24:T:92:LEU:HD22	2.23	0.68
15:K:114:ALA:O	15:K:118:LEU:HG	1.93	0.68
13:I:102:VAL:CG1	13:I:106:LEU:CD1	2.72	0.68
5:A:1290:G:N2	19:O:33:LYS:HG2	2.08	0.68
10:F:63:GLN:HE22	29:Y:1:MET:CA	2.06	0.68
20:P:2:PHE:HE1	20:P:13:LYS:HG3	1.58	0.68
28:X:6:ILE:HD11	28:X:47:ILE:CD1	2.18	0.68
7:C:164:VAL:HG13	7:C:172:VAL:HG11	1.74	0.68
12:H:141:TYR:HE1	12:H:142:GLU:O	1.77	0.68
6:B:40:C:C2	10:F:66:LEU:CD2	2.77	0.68
11:G:99:GLN:O	11:G:99:GLN:CG	2.41	0.68
5:A:578:G:N2	19:O:48:ARG:HH22	1.92	0.68
10:F:149:VAL:O	10:F:149:VAL:CG2	2.41	0.68
13:I:93:PRO:HB3	13:I:114:ILE:HD11	1.75	0.68
19:O:105:ALA:HB1	20:P:40:PHE:HZ	1.59	0.68
15:K:103:LEU:HD12	15:K:103:LEU:N	2.09	0.67
23:S:74:LYS:N	23:S:74:LYS:CD	2.56	0.67
5:A:144:C:H5'	22:R:37:GLN:NE2	2.07	0.67
10:F:60:ILE:H	10:F:60:ILE:CD1	2.07	0.67
12:H:68:ASN:O	12:H:68:ASN:OD1	2.12	0.67
23:S:24:ILE:CG1	23:S:34:VAL:HG13	2.24	0.67
8:D:128:GLN:HG3	8:D:173:MET:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:63:GLN:NE2	29:Y:1:MET:CA	2.58	0.67
16:L:92:ARG:HG2	16:L:93:TYR:CE1	2.29	0.67
13:I:12:ASP:OD1	13:I:13:ASN:N	2.27	0.67
25:U:83:ASP:O	25:U:84:LYS:CD	2.42	0.67
5:A:2314:A:H62	5:A:2371:U:H3	1.41	0.67
14:J:80:ASP:C	14:J:80:ASP:OD1	2.33	0.67
30:Z:29:GLU:HG2	30:Z:36:TYR:CE1	2.28	0.67
6:B:41:C:H4'	29:Y:3:GLN:H	1.60	0.67
9:E:3:ASN:OD1	9:E:16:SER:HB3	1.95	0.67
17:M:92:ILE:C	17:M:92:ILE:HD12	2.14	0.67
8:D:37:GLN:OE1	8:D:76:HIS:HE1	1.77	0.67
13:I:32:THR:HG22	13:I:33:ALA:N	2.09	0.67
14:J:83:ASN:HD21	14:J:117:LEU:HA	1.58	0.67
10:F:161:ASN:HB2	10:F:165:GLU:OE1	1.95	0.67
15:K:42:ILE:HG21	15:K:47:ILE:CD1	2.25	0.67
27:W:31:GLN:O	27:W:36:GLN:HG3	1.94	0.67
5:A:2037:G:H5''	21:Q:42:ALA:HB2	1.77	0.66
20:P:1:MET:SD	20:P:1:MET:O	2.53	0.66
5:A:1084:U:H3	5:A:1159:A:H61	1.43	0.66
23:S:79:THR:HG23	23:S:80:ARG:O	1.95	0.66
9:E:125:VAL:HG13	9:E:194:ILE:HG23	1.77	0.66
17:M:33:VAL:HG11	17:M:105:VAL:HG22	1.77	0.66
19:O:104:LYS:H	19:O:104:LYS:CE	2.08	0.66
3:3:7:HIS:HD2	3:3:10:ALA:N	1.94	0.66
3:3:7:HIS:HD2	3:3:10:ALA:H	1.42	0.66
11:G:5:GLY:HA2	11:G:69:ARG:HG3	1.78	0.66
5:A:2496:A:O2'	15:K:56:ARG:NH1	2.29	0.66
7:C:74:ILE:HD12	7:C:74:ILE:N	2.10	0.66
29:Y:9:TYR:OH	29:Y:26:GLY:HA2	1.95	0.66
5:A:2575:G:H1'	13:I:23:LYS:HZ2	1.60	0.66
11:G:35:ARG:HG3	11:G:75:MET:CE	2.25	0.66
5:A:2341:A:H5'	10:F:35:VAL:HG11	1.77	0.66
16:L:34:GLU:OE2	16:L:105:LYS:CE	2.42	0.66
9:E:20:SER:N	9:E:203:GLU:OE2	2.29	0.66
10:F:109:PRO:CG	10:F:110:ARG:HH11	2.09	0.66
13:I:102:VAL:HG12	13:I:106:LEU:HD12	1.77	0.65
12:H:78:HIS:CD2	12:H:85:ILE:HD12	2.31	0.65
14:J:104:ASN:OD1	14:J:104:ASN:C	2.34	0.65
5:A:1290:G:N2	19:O:33:LYS:CG	2.60	0.65
15:K:51:ARG:NH1	15:K:55:THR:HG21	2.10	0.65
21:Q:1:MET:SD	21:Q:1:MET:C	2.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2085:MA6:H91	33:A:3101:HOH:O	1.96	0.65
28:X:17:GLU:CD	28:X:20:ARG:HD2	2.15	0.65
5:A:1478:A:H61	5:A:1605:A:N6	1.94	0.65
6:B:40:C:H1'	10:F:66:LEU:HD23	1.79	0.65
8:D:21:GLU:N	8:D:21:GLU:OE1	2.29	0.65
25:U:49:ARG:HG2	25:U:49:ARG:HH11	1.62	0.65
10:F:9:ASN:HA	10:F:13:THR:HG23	1.73	0.65
10:F:55:GLU:OE1	10:F:55:GLU:O	2.14	0.65
11:G:86:VAL:HG22	11:G:132:LYS:CG	2.18	0.65
13:I:47:THR:HG23	13:I:48:PRO:HD2	1.78	0.65
6:B:2:C:H41	6:B:113:G:H1	1.45	0.64
12:H:78:HIS:CD2	12:H:85:ILE:CD1	2.77	0.64
15:K:42:ILE:CG2	15:K:47:ILE:CD1	2.74	0.64
17:M:55:GLN:OE1	17:M:56:ALA:CA	2.45	0.64
15:K:42:ILE:HG21	15:K:47:ILE:CG1	2.27	0.64
23:S:24:ILE:HG12	23:S:34:VAL:HG13	1.80	0.64
1:I:18:ILE:HG21	5:A:2446:U:H5'	1.78	0.64
9:E:159:GLU:OE2	9:E:177:THR:HG21	1.98	0.64
10:F:35:VAL:CG1	10:F:155:VAL:HG22	2.27	0.64
15:K:118:LEU:HD23	15:K:118:LEU:N	2.11	0.64
24:T:92:LEU:H	24:T:92:LEU:HD23	1.62	0.64
5:A:1216:U:H2'	5:A:1218:G:H8	1.62	0.64
15:K:42:ILE:CG2	15:K:47:ILE:CG1	2.76	0.64
22:R:8:LYS:HE3	22:R:30:ASP:HA	1.80	0.64
5:A:2432:G:H2'	5:A:2438:A:H61	1.62	0.64
10:F:63:GLN:CD	29:Y:1:MET:HA	2.18	0.64
19:O:104:LYS:H	19:O:104:LYS:CD	2.10	0.64
5:A:144:C:H4'	22:R:37:GLN:NE2	2.13	0.64
7:C:115:ILE:HD12	7:C:115:ILE:N	2.12	0.64
10:F:59:LEU:HD23	10:F:141:ILE:CG1	2.28	0.64
10:F:91:LEU:HD12	10:F:95:ARG:HB2	1.80	0.64
12:H:70:GLU:OE1	12:H:70:GLU:HA	1.97	0.64
5:A:2231:C:H5''	7:C:150:LYS:HD2	1.78	0.63
7:C:71:LYS:HG3	7:C:102:ARG:NH2	2.14	0.63
10:F:9:ASN:CA	10:F:13:THR:CG2	2.67	0.63
7:C:34:LEU:CD2	7:C:63:ARG:HG3	2.27	0.63
7:C:117:GLU:HG3	7:C:122:ALA:CB	2.28	0.63
10:F:8:PHE:C	10:F:13:THR:HG23	2.17	0.63
11:G:23:HIS:NE2	11:G:34:SER:HB3	2.13	0.63
20:P:62:VAL:HG22	20:P:95:LEU:CD2	2.28	0.63
7:C:144:ILE:HD13	7:C:174:ILE:CD1	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:167:ALA:HA	9:E:170:ILE:CD1	2.28	0.63
23:S:73:PRO:HG2	23:S:74:LYS:HD3	1.81	0.63
1:1:10:THR:CG2	1:1:46:ARG:HH12	2.10	0.63
11:G:69:ARG:HD3	11:G:69:ARG:O	1.98	0.63
8:D:38:LYS:HG3	8:D:96:VAL:HG13	1.77	0.63
8:D:38:LYS:HD3	8:D:96:VAL:HG12	1.80	0.63
10:F:107:SER:HA	10:F:136:LEU:CD1	2.28	0.63
1:1:35:TYR:O	1:1:37:PRO:HD3	1.99	0.63
5:A:2575:G:N3	13:I:23:LYS:NZ	2.47	0.63
7:C:124:ILE:O	7:C:124:ILE:CG2	2.47	0.63
5:A:2859:G:C4'	16:L:45:GLU:OE1	2.46	0.63
7:C:143:ASN:HD21	7:C:152:GLY:HA3	1.63	0.63
3:3:7:HIS:HE1	5:A:254:A:OP1	1.81	0.62
11:G:57:ASP:O	11:G:62:ARG:NE	2.32	0.62
15:K:2:LEU:HD12	15:K:2:LEU:N	2.10	0.62
8:D:15:VAL:HG23	8:D:23:ILE:HB	1.80	0.62
11:G:59:LYS:CD	11:G:62:ARG:HH21	2.06	0.62
25:U:35:ASP:OD1	25:U:77:PHE:HD1	1.82	0.62
1:1:2:ARG:NH2	5:A:2312:C:OP2	2.33	0.62
9:E:164:GLU:HG3	9:E:175:VAL:HG11	1.80	0.62
13:I:112:MET:HA	13:I:112:MET:HE3	1.82	0.62
9:E:193:VAL:CG2	9:E:193:VAL:O	2.47	0.62
18:N:27:THR:CG2	18:N:48:VAL:HG22	2.08	0.62
16:L:92:ARG:HG2	16:L:93:TYR:CD1	2.35	0.62
19:O:104:LYS:H	19:O:104:LYS:HE2	1.64	0.62
7:C:9:ILE:HD12	7:C:10:THR:OG1	2.00	0.62
7:C:253:PRO:HB2	7:C:257:LYS:HG3	1.80	0.62
8:D:107:VAL:HG13	8:D:195:ILE:HG13	1.82	0.62
5:A:351:G:O2'	23:S:15:LYS:NZ	2.33	0.62
5:A:502:C:C5	22:R:68:TYR:CZ	2.88	0.62
8:D:95:ASP:C	8:D:95:ASP:OD1	2.38	0.62
10:F:31:ILE:HD12	10:F:158:THR:CG2	2.29	0.61
4:4:17:ILE:HD13	4:4:26:ILE:HD13	1.81	0.61
11:G:81:GLN:O	11:G:81:GLN:OE1	2.18	0.61
30:Z:24:VAL:HG13	30:Z:25:PRO:HD2	1.81	0.61
8:D:38:LYS:CD	8:D:96:VAL:HG12	2.30	0.61
10:F:59:LEU:CD2	10:F:141:ILE:HD13	2.29	0.61
15:K:27:VAL:HG13	15:K:105:GLU:HG2	1.83	0.61
8:D:38:LYS:CG	8:D:96:VAL:HG12	2.29	0.61
9:E:117:LYS:HE3	9:E:186:ILE:O	2.00	0.61
4:4:17:ILE:HD11	4:4:26:ILE:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:103:LEU:HD21	11:G:105:LEU:HG	1.82	0.61
20:P:62:VAL:HG22	20:P:95:LEU:HD21	1.83	0.61
22:R:22:GLU:OE1	22:R:24:LYS:HG3	2.00	0.61
5:A:1512:U:H2'	5:A:1513:A:C8	2.36	0.61
11:G:169:VAL:O	11:G:171:ARG:HG2	2.00	0.61
13:I:91:LYS:HE3	13:I:111:PHE:CZ	2.35	0.61
3:3:17:THR:OG1	3:3:21:GLN:HB2	2.01	0.61
10:F:35:VAL:CG1	10:F:155:VAL:CG2	2.78	0.61
10:F:150:ARG:NE	10:F:150:ARG:HA	2.16	0.61
5:A:2499:G:H21	5:A:2505:A:H62	1.48	0.60
9:E:154:VAL:HG22	9:E:193:VAL:HG21	1.82	0.60
18:N:34:ILE:CD1	18:N:43:GLN:HG2	2.31	0.60
10:F:54:VAL:CG1	10:F:64:LYS:CE	2.63	0.60
11:G:23:HIS:CE1	11:G:34:SER:HB3	2.36	0.60
22:R:4:ARG:CZ	27:W:23:GLU:OE1	2.49	0.60
14:J:84:LYS:O	14:J:84:LYS:CG	2.50	0.60
9:E:154:VAL:HG22	9:E:193:VAL:HG22	1.84	0.60
5:A:1378:U:C6	22:R:79:ILE:HD13	2.37	0.60
13:I:13:ASN:HD22	13:I:97:ARG:HB3	1.65	0.60
5:A:2328:A:H61	5:A:2342:U:H3	1.48	0.60
10:F:60:ILE:CG2	10:F:137:ILE:CG2	2.79	0.60
10:F:115:GLN:HG3	10:F:119:LYS:HZ3	1.65	0.60
13:I:90:ASP:OD1	13:I:90:ASP:O	2.19	0.59
26:V:40:VAL:HG11	26:V:45:LYS:HB3	1.81	0.59
27:W:10:THR:O	27:W:10:THR:CG2	2.50	0.59
9:E:17:ILE:CD1	9:E:196:GLU:HG2	2.31	0.59
13:I:105:GLU:OE1	13:I:105:GLU:N	2.35	0.59
23:S:3:ILE:HD12	23:S:3:ILE:C	2.23	0.59
7:C:16:MET:HE1	7:C:207:LYS:HG3	1.85	0.59
7:C:66:ASP:O	7:C:66:ASP:CG	2.41	0.59
9:E:17:ILE:HD11	9:E:200:LYS:HE3	1.85	0.59
10:F:51:ASP:CA	10:F:54:VAL:HG23	2.30	0.59
13:I:12:ASP:OD2	13:I:95:GLY:N	2.33	0.59
7:C:65:ILE:HD11	7:C:67:PHE:CZ	2.38	0.59
5:A:1218:G:H2'	5:A:1219:G:C8	2.37	0.59
7:C:65:ILE:HG22	7:C:103:TYR:HB2	1.84	0.59
15:K:25:ASN:C	15:K:26:TYR:CD1	2.75	0.59
8:D:15:VAL:HG22	8:D:25:VAL:HG13	1.85	0.59
11:G:8:ILE:C	11:G:69:ARG:HH21	2.05	0.59
23:S:55:GLY:C	23:S:56:ILE:HD12	2.23	0.59
15:K:2:LEU:N	15:K:2:LEU:CD1	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:22:ARG:HD2	2:2:31:VAL:HG21	1.84	0.59
7:C:160:ALA:H	7:C:195:VAL:HG22	1.68	0.59
7:C:164:VAL:HG13	7:C:172:VAL:CG1	2.32	0.59
22:R:6:ILE:HD11	22:R:41:ALA:HB2	1.83	0.59
22:R:64:ARG:HB3	22:R:64:ARG:CZ	2.33	0.59
19:O:36:LYS:O	19:O:40:MET:HG3	2.02	0.59
1:1:14:ASP:OD1	1:1:16:ASN:ND2	2.35	0.59
5:A:2231:C:H5''	7:C:147:LYS:HD3	1.83	0.59
10:F:137:ILE:HG22	10:F:138:PHE:N	2.12	0.58
23:S:30:LYS:C	23:S:31:ASP:OD1	2.41	0.58
27:W:31:GLN:HA	27:W:34:THR:OG1	2.03	0.58
19:O:8:THR:O	19:O:8:THR:CG2	2.46	0.58
5:A:1529:U:H3'	5:A:1530:A:C8	2.38	0.58
8:D:56:LYS:HE3	8:D:66:ASN:O	2.04	0.58
8:D:191:GLU:OE1	8:D:191:GLU:N	2.30	0.58
17:M:72:LEU:O	17:M:76:VAL:HG23	2.03	0.58
1:1:10:THR:HG22	1:1:46:ARG:NH1	2.16	0.58
7:C:140:VAL:CG1	7:C:161:SER:HB2	2.33	0.58
8:D:15:VAL:CG2	8:D:25:VAL:HG11	2.33	0.58
11:G:103:LEU:HD23	11:G:103:LEU:C	2.24	0.58
13:I:73:ASP:OD1	13:I:75:SER:HB3	2.03	0.58
20:P:23:GLU:OE1	20:P:23:GLU:HA	2.03	0.58
23:S:87:ASP:HB3	23:S:89:LYS:NZ	2.18	0.58
5:A:925:G:H3'	5:A:926:G:C8	2.39	0.58
5:A:1254:C:OP1	19:O:11:ARG:HD2	2.03	0.58
5:A:630:G:N7	14:J:33:ARG:NH1	2.51	0.58
22:R:34:ASN:OD1	22:R:37:GLN:HG3	2.02	0.58
28:X:4:LEU:C	28:X:4:LEU:HD12	2.24	0.58
5:A:1115:G:N1	5:A:1136:C:OP2	2.36	0.58
10:F:8:PHE:HA	10:F:12:VAL:CG2	2.33	0.58
23:S:56:ILE:HD12	23:S:56:ILE:N	2.18	0.58
24:T:31:VAL:HG12	24:T:91:PHE:HB2	1.86	0.58
5:A:2084:G:O6	5:A:2085:MA6:H92	2.04	0.58
27:W:63:GLU:OE1	27:W:63:GLU:CA	2.50	0.58
21:Q:2:GLU:HG2	21:Q:106:VAL:HG12	1.85	0.58
2:2:22:ARG:HD2	2:2:31:VAL:CG2	2.34	0.57
11:G:41:MET:HE1	11:G:65:HIS:HA	1.84	0.57
5:A:534:G:H4'	21:Q:49:LYS:HE3	1.85	0.57
5:A:1401:G:OP1	26:V:3:LYS:HE3	2.04	0.57
5:A:2085:MA6:H93	31:A:3000:A1D6G:O51	2.05	0.57
9:E:154:VAL:HA	9:E:193:VAL:HG22	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:89:VAL:HA	29:Y:2:LYS:HE2	1.86	0.57
11:G:56:SER:OG	11:G:57:ASP:N	2.36	0.57
15:K:38:THR:OG1	15:K:127:VAL:HG23	2.04	0.57
6:B:40:C:O2	10:F:66:LEU:HD23	2.04	0.57
12:H:117:GLU:O	12:H:121:LYS:HG3	2.04	0.57
29:Y:38:GLU:OE1	29:Y:38:GLU:N	2.37	0.57
30:Z:8:THR:HG23	30:Z:12:ARG:HB3	1.86	0.57
5:A:1039:C:C5	12:H:1:MET:HA	2.39	0.57
20:P:72:THR:HG23	20:P:72:THR:O	2.04	0.57
22:R:36:THR:O	22:R:40:MET:HG3	2.03	0.57
23:S:100:GLU:O	23:S:100:GLU:CD	2.42	0.57
24:T:10:GLN:CD	24:T:10:GLN:N	2.58	0.57
26:V:17:ARG:HB2	26:V:27:ARG:HG3	1.87	0.57
5:A:150:A:H61	5:A:179:A:H2	1.52	0.57
21:Q:1:MET:CG	21:Q:111:LYS:O	2.52	0.57
3:3:21:GLN:HB3	3:3:49:LEU:HD22	1.87	0.57
17:M:55:GLN:OE1	17:M:56:ALA:N	2.38	0.57
23:S:100:GLU:CD	23:S:100:GLU:C	2.63	0.57
7:C:29:PRO:HB2	7:C:34:LEU:HD11	1.87	0.57
10:F:31:ILE:HD12	10:F:158:THR:HG23	1.85	0.57
12:H:141:TYR:CD1	12:H:141:TYR:C	2.78	0.57
22:R:84:GLU:CD	22:R:84:GLU:C	2.63	0.57
5:A:437:A:H2'	5:A:438:U:H5'	1.86	0.57
7:C:65:ILE:HG22	7:C:103:TYR:CB	2.35	0.57
10:F:58:GLU:HG3	29:Y:7:PRO:HG3	1.86	0.57
12:H:20:ASP:OD1	12:H:58:ILE:CG1	2.51	0.57
15:K:31:GLU:OE2	15:K:32:PHE:CZ	2.58	0.57
5:A:2338:A:H2	10:F:76:THR:OG1	1.85	0.57
24:T:8:ILE:HD11	24:T:65:VAL:CG1	2.30	0.57
5:A:2049:U:OP2	30:Z:12:ARG:NH2	2.37	0.56
6:B:54:U:H1'	6:B:55:A:H8	1.68	0.56
7:C:13:ARG:O	7:C:13:ARG:HG3	2.04	0.56
10:F:63:GLN:HE22	29:Y:1:MET:HA	1.65	0.56
18:N:47:GLY:HA3	18:N:63:VAL:HG13	1.86	0.56
25:U:49:ARG:HG2	25:U:49:ARG:NH1	2.18	0.56
5:A:1183:G:OP2	12:H:73:LYS:NZ	2.36	0.56
10:F:115:GLN:HG3	10:F:119:LYS:HZ2	1.69	0.56
15:K:51:ARG:HH11	15:K:51:ARG:HG2	1.70	0.56
5:A:1259:U:OP1	20:P:69:LYS:NZ	2.38	0.56
6:B:47:C:H2'	6:B:48:A:C8	2.41	0.56
10:F:7:LYS:CD	10:F:173:PHE:CZ	2.81	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:25:ALA:HB3	23:S:34:VAL:HG12	1.86	0.56
5:A:144:C:H5''	22:R:37:GLN:HE22	1.69	0.56
5:A:320:U:H5	5:A:326:A:N7	2.04	0.56
5:A:435:A:H1'	5:A:458:A:H4'	1.87	0.56
8:D:186:VAL:HG22	8:D:196:LEU:HB3	1.87	0.56
13:I:71:ARG:HH11	18:N:74:ARG:CZ	2.19	0.56
15:K:46:GLN:HE22	15:K:126:PRO:HG3	1.69	0.56
22:R:25:TYR:CE2	22:R:82:LEU:HD21	2.40	0.56
10:F:94:GLU:O	10:F:98:GLU:OE1	2.23	0.56
17:M:46:ASP:OD1	17:M:46:ASP:C	2.42	0.56
25:U:27:LYS:O	25:U:29:LEU:HG	2.04	0.56
5:A:1065:A:H62	5:A:1185:U:H3	1.52	0.56
5:A:1044:A:H2'	5:A:1045:A:C8	2.40	0.56
5:A:1051:C:OP1	12:H:38:ARG:NH1	2.37	0.56
10:F:2:ASN:CB	10:F:5:LYS:HE2	2.35	0.56
24:T:84:ASN:O	24:T:85:GLN:HG3	2.06	0.56
7:C:115:ILE:HD12	7:C:115:ILE:H	1.70	0.56
11:G:103:LEU:HD23	11:G:103:LEU:O	2.06	0.56
24:T:8:ILE:HG22	24:T:8:ILE:O	2.04	0.56
8:D:44:ASP:OD1	8:D:44:ASP:O	2.23	0.56
10:F:109:PRO:HB2	10:F:110:ARG:HD2	1.87	0.56
11:G:6:LYS:N	11:G:65:HIS:HE1	2.04	0.56
25:U:19:LYS:NZ	25:U:19:LYS:HB3	2.20	0.56
1:1:35:TYR:HD1	1:1:42:TYR:CE1	2.24	0.56
5:A:2405:A:O2'	17:M:28:LYS:NZ	2.39	0.56
5:A:2618:C:N4	5:A:2619:G:O6	2.39	0.56
17:M:28:LYS:HG2	17:M:93:VAL:HG22	1.88	0.56
4:4:17:ILE:HD11	4:4:26:ILE:HG21	1.88	0.55
5:A:1479:G:H2'	5:A:1480:G:C8	2.41	0.55
7:C:65:ILE:HD11	7:C:67:PHE:CE1	2.42	0.55
5:A:926:G:H21	5:A:941:A:H62	1.54	0.55
11:G:59:LYS:CE	11:G:62:ARG:HH22	2.19	0.55
17:M:113:ARG:HG3	17:M:119:PHE:CE1	2.40	0.55
5:A:1003:A:H2'	5:A:1004:A:C8	2.42	0.55
10:F:35:VAL:HG12	10:F:155:VAL:HG23	1.86	0.55
22:R:27:PHE:HZ	22:R:87:ILE:HG21	1.70	0.55
5:A:2222:U:H2'	5:A:2223:C:C6	2.41	0.55
10:F:17:MET:O	10:F:17:MET:CE	2.54	0.55
17:M:113:ARG:HG3	17:M:119:PHE:CZ	2.42	0.55
5:A:2098:A:H2'	5:A:2099:G:C8	2.42	0.55
6:B:73:G:N3	24:T:88:HIS:CE1	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:12:LYS:NZ	5:A:252:C:O2	2.40	0.55
18:N:16:ARG:HD3	18:N:79:HIS:HA	1.86	0.55
3:3:35:ASN:HB3	5:A:2417:U:H5'	1.89	0.55
4:4:19:ARG:HB2	4:4:24:MET:SD	2.47	0.55
16:L:106:GLN:NE2	16:L:118:ILE:HD12	2.22	0.55
18:N:28:LEU:HD12	18:N:28:LEU:O	2.07	0.55
22:R:84:GLU:OE1	22:R:84:GLU:N	2.36	0.55
1:1:31:GLU:HG3	1:1:46:ARG:HG3	1.87	0.55
4:4:5:PRO:HG2	5:A:2492:C:H4'	1.89	0.55
5:A:1954:A:H2'	5:A:1955:A:C8	2.40	0.55
8:D:10:ILE:HB	8:D:27:VAL:HG13	1.89	0.55
17:M:15:HIS:HE1	17:M:95:ASP:OD2	1.89	0.55
23:S:41:MET:O	23:S:58:GLU:HA	2.07	0.55
5:A:1886:A:H62	5:A:1910:G:H21	1.55	0.55
5:A:2048:G:OP1	30:Z:9:SER:OG	2.24	0.55
11:G:26:VAL:HG12	11:G:79:VAL:CG1	2.32	0.55
24:T:46:VAL:HG12	24:T:50:LYS:NZ	2.20	0.55
4:4:7:VAL:HG12	4:4:25:VAL:CG2	2.34	0.54
5:A:1290:G:H21	19:O:33:LYS:CG	2.20	0.54
6:B:54:U:H1'	6:B:55:A:C8	2.42	0.54
17:M:17:ARG:O	17:M:20:THR:HG22	2.07	0.54
5:A:1290:G:H21	19:O:33:LYS:HG2	1.71	0.54
5:A:1545:U:O4	5:A:1546:A:N6	2.41	0.54
15:K:21:SER:OG	15:K:101:ARG:HB2	2.06	0.54
15:K:40:SER:OG	15:K:41:TRP:N	2.40	0.54
5:A:1868:U:C2	5:A:1869:G:C8	2.96	0.54
9:E:140:LYS:HD3	9:E:170:ILE:CG2	2.35	0.54
10:F:110:ARG:HB2	10:F:136:LEU:HD23	1.90	0.54
5:A:2432:G:H2'	5:A:2438:A:N6	2.21	0.54
10:F:36:VAL:HG12	10:F:57:LEU:HD21	1.89	0.54
10:F:104:ILE:HD12	10:F:104:ILE:O	2.08	0.54
12:H:70:GLU:OE1	12:H:70:GLU:CA	2.53	0.54
13:I:71:ARG:HH11	18:N:74:ARG:NH2	2.06	0.54
21:Q:4:LYS:HD2	21:Q:106:VAL:HG22	1.90	0.54
23:S:89:LYS:N	23:S:89:LYS:HD2	2.22	0.54
5:A:1529:U:H5'	5:A:1530:A:N7	2.23	0.54
6:B:43:A:O4'	10:F:92:ARG:NE	2.40	0.54
16:L:95:GLU:O	16:L:97:GLN:NE2	2.40	0.54
7:C:22:ALA:HB3	7:C:23:GLU:OE1	2.07	0.54
11:G:54:ARG:NH1	11:G:62:ARG:CG	2.55	0.54
19:O:107:ALA:O	19:O:111:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:6:GLU:HB2	20:P:39:LEU:HD11	1.90	0.54
22:R:55:ILE:HD12	22:R:78:ALA:HB2	1.89	0.54
27:W:44:ARG:HD2	27:W:48:LYS:NZ	2.22	0.54
29:Y:9:TYR:CE1	29:Y:26:GLY:HA2	2.40	0.54
5:A:901:G:H2'	5:A:902:A:C8	2.42	0.54
5:A:1847:U:OP1	7:C:177:ARG:NH1	2.41	0.54
15:K:102:ILE:C	15:K:103:LEU:HD12	2.28	0.54
18:N:29:ARG:HD3	18:N:89:LYS:HD3	1.90	0.54
5:A:2122:A:H2'	5:A:2123:A:O4'	2.08	0.54
6:B:41:C:H4'	29:Y:1:MET:O	2.08	0.54
11:G:43:PHE:CE1	11:G:52:VAL:HG13	2.42	0.54
24:T:52:ILE:O	24:T:56:GLY:N	2.38	0.54
24:T:94:ILE:HD12	24:T:94:ILE:N	2.23	0.54
27:W:31:GLN:HB2	27:W:36:GLN:CG	2.36	0.54
5:A:1378:U:C6	22:R:79:ILE:CD1	2.91	0.54
8:D:21:GLU:O	8:D:21:GLU:HG2	2.07	0.54
19:O:88:ILE:HA	20:P:50:ALA:O	2.08	0.54
21:Q:2:GLU:HG2	21:Q:106:VAL:HG11	1.87	0.54
7:C:183:MET:CE	7:C:271:VAL:HG22	2.37	0.54
12:H:54:TYR:CE1	12:H:122:LYS:HD2	2.43	0.54
16:L:34:GLU:CD	16:L:105:LYS:HE3	2.28	0.54
19:O:104:LYS:H	19:O:104:LYS:HD3	1.72	0.54
22:R:9:ARG:HG2	22:R:28:ASP:HB3	1.90	0.54
23:S:87:ASP:HB3	23:S:89:LYS:HZ2	1.73	0.54
27:W:5:GLU:O	27:W:9:LEU:HG	2.08	0.54
27:W:10:THR:O	27:W:10:THR:HG22	2.06	0.54
6:B:64:A:H1'	6:B:66:C:N4	2.22	0.53
10:F:83:MET:O	10:F:85:ILE:HG13	2.08	0.53
12:H:58:ILE:HG13	12:H:59:ASN:N	2.23	0.53
13:I:35:ILE:HD13	13:I:69:VAL:HG13	1.89	0.53
3:3:27:ALA:HB1	5:A:2419:A:O2'	2.08	0.53
6:B:64:A:N6	6:B:104:A:H2'	2.23	0.53
6:B:73:G:N3	24:T:88:HIS:HE1	2.06	0.53
7:C:182:ARG:HG2	7:C:182:ARG:NH1	2.22	0.53
5:A:896:U:H2'	5:A:897:A:C8	2.44	0.53
5:A:1484:G:H3'	5:A:1485:G:H8	1.73	0.53
7:C:274:ARG:HA	7:C:274:ARG:HH11	1.72	0.53
8:D:128:GLN:CG	8:D:173:MET:HE3	2.38	0.53
7:C:144:ILE:HD11	7:C:162:ALA:HB3	1.90	0.53
9:E:34:PHE:CE1	14:J:6:LEU:HD13	2.43	0.53
18:N:41:ARG:HG3	18:N:41:ARG:O	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:60:THR:CG2	18:N:60:THR:O	2.55	0.53
19:O:102:ASP:OD1	19:O:104:LYS:HE2	2.08	0.53
24:T:49:ILE:HG22	24:T:53:ARG:NH1	2.23	0.53
5:A:1526:G:H8	5:A:1528:G:H5''	1.74	0.53
10:F:137:ILE:CG2	10:F:138:PHE:H	2.18	0.53
15:K:51:ARG:NH1	15:K:51:ARG:HG2	2.24	0.53
13:I:22:ILE:HD11	13:I:42:THR:HG23	1.90	0.53
10:F:9:ASN:CA	10:F:13:THR:HG23	2.36	0.53
25:U:35:ASP:CG	25:U:77:PHE:HD1	2.12	0.53
5:A:1463:A:H2	5:A:1625:U:H3	1.57	0.53
8:D:14:GLN:NE2	8:D:22:LEU:HD21	2.23	0.53
17:M:30:ARG:HH21	17:M:45:ILE:HG12	1.74	0.53
27:W:58:ARG:NH1	27:W:61:GLU:OE2	2.39	0.53
5:A:792:5MU:H4'	21:Q:92:ARG:HH12	1.74	0.53
5:A:2136:U:H3'	5:A:2147:G:OP1	2.09	0.53
5:A:2511:G:OP1	15:K:45:ARG:HD2	2.08	0.53
10:F:54:VAL:CG1	10:F:64:LYS:CG	2.86	0.53
5:A:1080:G:H1	5:A:1163:U:H3	1.57	0.53
5:A:1885:G:H1'	5:A:1911:A:H62	1.72	0.53
5:A:2372:G:H4'	5:A:2373:A:H5''	1.91	0.53
8:D:191:GLU:HG2	8:D:192:ASN:N	2.24	0.53
13:I:32:THR:CG2	13:I:33:ALA:H	2.20	0.53
15:K:51:ARG:NH2	15:K:52:ILE:HG12	2.24	0.53
24:T:37:LYS:HG3	24:T:38:ASN:N	2.23	0.53
3:3:4:MET:HE1	5:A:636:A:H1'	1.91	0.52
5:A:1089:C:H4'	5:A:1090:A:H5''	1.90	0.52
5:A:2540:A:H2'	5:A:2541:U:C6	2.45	0.52
6:B:55:A:C4'	10:F:27:GLU:OE1	2.47	0.52
11:G:41:MET:SD	11:G:65:HIS:HA	2.49	0.52
11:G:81:GLN:CD	11:G:81:GLN:C	2.67	0.52
1:1:2:ARG:NE	5:A:2312:C:OP2	2.40	0.52
5:A:2163:A:H62	5:A:2183:G:H21	1.57	0.52
13:I:71:ARG:HD2	18:N:74:ARG:HH21	1.73	0.52
13:I:91:LYS:HD2	13:I:111:PHE:CE1	2.43	0.52
18:N:65:LYS:HG3	18:N:66:ILE:N	2.24	0.52
5:A:458:A:C5	5:A:459:C:H1'	2.44	0.52
8:D:14:GLN:OE1	8:D:22:LEU:HD21	2.09	0.52
13:I:63:VAL:HG12	13:I:106:LEU:CD1	2.37	0.52
5:A:2146:A:H62	5:A:2195:G:H22	1.58	0.52
10:F:7:LYS:O	10:F:12:VAL:HG23	2.10	0.52
10:F:31:ILE:CD1	10:F:156:ILE:HG22	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1478:A:N6	5:A:1605:A:H61	2.06	0.52
7:C:29:PRO:CB	7:C:34:LEU:HD11	2.39	0.52
10:F:66:LEU:CD1	10:F:68:THR:CG2	2.88	0.52
12:H:37:LEU:HD11	12:H:110:LEU:HD11	1.91	0.52
23:S:11:VAL:HG12	23:S:68:VAL:HG12	1.91	0.52
5:A:2838:C:OP2	16:L:38:LYS:NZ	2.40	0.52
5:A:2854:A:H2'	5:A:2899:A:H61	1.75	0.52
7:C:68:LYS:HG2	7:C:151:GLY:CA	2.40	0.52
25:U:34:ALA:N	25:U:37:GLN:OE1	2.38	0.52
5:A:352:A:H4'	23:S:14:GLY:HA2	1.92	0.52
5:A:1669:C:H2'	5:A:1670:A:O4'	2.10	0.52
10:F:55:GLU:OE1	10:F:55:GLU:CA	2.57	0.52
10:F:59:LEU:CD2	10:F:141:ILE:CG2	2.80	0.52
5:A:1758:A:H61	5:A:1771:A:H62	1.57	0.52
12:H:19:ILE:HD11	12:H:36:ILE:HD13	1.92	0.52
15:K:42:ILE:HG22	15:K:47:ILE:CD1	2.40	0.52
20:P:38:VAL:HG12	20:P:53:VAL:HG13	1.90	0.52
2:2:31:VAL:HG12	2:2:34:ARG:NH2	2.25	0.52
5:A:221:G:H22	5:A:238:U:H4'	1.75	0.52
20:P:50:ALA:CB	20:P:51:PRO:HD3	2.37	0.52
5:A:388:A:H2'	5:A:389:A:H2	1.74	0.52
5:A:1150:A:H3'	5:A:1151:G:H8	1.74	0.52
5:A:2774:G:O2'	11:G:67:THR:HG23	2.09	0.52
7:C:210:ARG:HA	7:C:213:TRP:CE3	2.44	0.52
14:J:95:LEU:O	14:J:95:LEU:HD22	2.09	0.52
16:L:102:ARG:HH22	16:L:122:VAL:HG23	1.74	0.52
20:P:27:VAL:CG2	20:P:31:ASP:HB2	2.40	0.52
23:S:75:THR:O	23:S:76:ASN:OD1	2.27	0.52
24:T:46:VAL:O	24:T:50:LYS:HG3	2.09	0.52
5:A:548:A:H4'	5:A:549:U:H5'	1.92	0.51
5:A:1055:A:OP1	19:O:75:SER:OG	2.28	0.51
5:A:2760:A:C6	8:D:216:LYS:HG2	2.45	0.51
5:A:2760:A:C5	8:D:216:LYS:HE2	2.45	0.51
7:C:182:ARG:HH11	7:C:182:ARG:CG	2.22	0.51
10:F:32:ASP:C	10:F:32:ASP:OD1	2.46	0.51
10:F:32:ASP:OD2	17:M:2:ILE:HD11	2.10	0.51
11:G:57:ASP:O	11:G:62:ARG:CD	2.58	0.51
15:K:21:SER:OG	15:K:98:LYS:HB2	2.10	0.51
29:Y:55:HIS:ND1	29:Y:58:TYR:O	2.43	0.51
5:A:921:C:H2'	5:A:922:G:C8	2.45	0.51
5:A:2581:U:H2'	5:A:2582:U:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:107:VAL:HG13	8:D:195:ILE:CG1	2.40	0.51
11:G:121:ILE:HG22	11:G:123:PHE:HE1	1.71	0.51
13:I:97:ARG:O	13:I:99:PHE:CE1	2.63	0.51
24:T:46:VAL:HG12	24:T:50:LYS:HE3	1.92	0.51
5:A:943:C:H2'	5:A:944:G:C8	2.46	0.51
5:A:2231:C:C5'	7:C:147:LYS:HD3	2.40	0.51
7:C:274:ARG:O	7:C:275:LYS:HB2	2.10	0.51
17:M:55:GLN:OE1	17:M:56:ALA:HA	2.10	0.51
24:T:46:VAL:HG12	24:T:50:LYS:CE	2.40	0.51
5:A:324:A:H2'	5:A:325:A:O4'	2.11	0.51
8:D:10:ILE:HG21	18:N:6:LEU:HD11	1.91	0.51
10:F:69:LYS:HG3	10:F:84:PRO:CA	2.39	0.51
24:T:39:VAL:HG12	24:T:41:VAL:HG13	1.93	0.51
5:A:1315:C:H2'	5:A:1316:G:H8	1.75	0.51
5:A:1871:U:H3'	5:A:1872:G:H8	1.74	0.51
5:A:2144:A:C8	5:A:2176:C:H5'	2.46	0.51
7:C:94:VAL:HG22	7:C:102:ARG:O	2.10	0.51
10:F:60:ILE:HG21	10:F:137:ILE:HG23	1.90	0.51
13:I:42:THR:HG22	13:I:57:VAL:HG22	1.92	0.51
13:I:111:PHE:O	13:I:115:VAL:HG23	2.10	0.51
23:S:7:ASP:OD1	23:S:7:ASP:N	2.36	0.51
23:S:24:ILE:HG13	23:S:34:VAL:HG13	1.92	0.51
24:T:46:VAL:CG1	24:T:50:LYS:HE3	2.41	0.51
5:A:291:G:H2'	5:A:292:U:C2	2.46	0.51
5:A:1590:C:H2'	5:A:1591:G:C8	2.45	0.51
5:A:2316:G:O6	5:A:2370:U:H5	1.93	0.51
10:F:2:ASN:HA	10:F:5:LYS:HE2	1.93	0.51
10:F:5:LYS:NZ	10:F:94:GLU:HG3	2.24	0.51
10:F:59:LEU:HD23	10:F:141:ILE:HG12	1.93	0.51
11:G:89:LEU:HD22	11:G:95:ARG:O	2.11	0.51
12:H:78:HIS:HD2	12:H:85:ILE:HD12	1.65	0.51
23:S:87:ASP:O	23:S:89:LYS:HD2	2.11	0.51
24:T:8:ILE:HD12	24:T:41:VAL:HG12	1.92	0.51
5:A:631:U:H1'	9:E:90:PHE:HB3	1.93	0.51
5:A:674:C:O2	5:A:684:U:O2'	2.28	0.51
5:A:1265:G:N7	19:O:16:LYS:NZ	2.59	0.51
5:A:1576:A:N3	5:A:1576:A:H2'	2.26	0.51
8:D:27:VAL:HG23	8:D:194:VAL:HG13	1.91	0.51
10:F:25:VAL:CG2	10:F:26:MET:CE	2.88	0.51
15:K:65:TRP:HZ3	15:K:106:VAL:C	2.12	0.51
25:U:35:ASP:OD1	25:U:77:PHE:CE1	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:47:ASN:OD1	8:D:47:ASN:O	2.28	0.51
5:A:396:G:H2'	5:A:397:U:O4'	2.11	0.51
5:A:1261:G:N7	20:P:70:LYS:NZ	2.56	0.51
5:A:2599:A:OP1	5:A:2601:G:H4'	2.10	0.51
7:C:111:GLU:CG	7:C:114:GLN:HE21	2.19	0.51
11:G:176:THR:O	11:G:176:THR:CG2	2.54	0.51
21:Q:52:MET:CE	21:Q:52:MET:CA	2.81	0.51
6:B:2:C:N4	6:B:113:G:H1	2.08	0.50
7:C:79:ASP:OD1	7:C:79:ASP:O	2.29	0.50
10:F:31:ILE:HA	10:F:158:THR:HG22	1.93	0.50
11:G:26:VAL:CG1	11:G:79:VAL:CG1	2.80	0.50
13:I:2:ILE:HD11	13:I:82:ASN:OD1	2.10	0.50
15:K:103:LEU:CD1	15:K:103:LEU:N	2.74	0.50
7:C:157:SER:O	7:C:195:VAL:HG21	2.11	0.50
5:A:1992:C:H2'	5:A:1993:A:C8	2.46	0.50
8:D:118:VAL:HG12	8:D:183:LEU:HD12	1.93	0.50
10:F:143:TYR:O	10:F:146:VAL:HG22	2.11	0.50
23:S:76:ASN:CG	23:S:76:ASN:O	2.48	0.50
25:U:23:ASP:OD1	25:U:24:SER:N	2.43	0.50
1:1:40:ASN:O	1:1:40:ASN:OD1	2.30	0.50
5:A:327:G:H1	5:A:399:U:H3	1.59	0.50
5:A:1819:G:O2'	5:A:1857:C:OP1	2.27	0.50
11:G:90:VAL:O	11:G:94:TYR:HD2	1.93	0.50
17:M:83:LYS:O	17:M:87:LYS:HG2	2.11	0.50
20:P:27:VAL:HG22	20:P:28:ASN:N	2.27	0.50
24:T:61:ILE:HD13	24:T:61:ILE:N	2.25	0.50
5:A:648:G:O6	14:J:103:LYS:NZ	2.45	0.50
5:A:2338:A:O2'	10:F:79:LEU:HD22	2.12	0.50
8:D:33:ASN:HB2	8:D:105:VAL:HB	1.92	0.50
9:E:159:GLU:OE2	9:E:177:THR:CG2	2.59	0.50
19:O:104:LYS:HD3	19:O:104:LYS:N	2.26	0.50
1:1:5:VAL:CG1	1:1:47:GLU:HG3	2.40	0.50
3:3:4:MET:CE	5:A:636:A:H1'	2.42	0.50
10:F:55:GLU:OE1	10:F:55:GLU:HA	2.12	0.50
10:F:60:ILE:HG12	10:F:137:ILE:HG22	1.94	0.50
11:G:59:LYS:CE	11:G:62:ARG:NH2	2.74	0.50
19:O:78:ARG:N	19:O:78:ARG:CD	2.75	0.50
5:A:660:A:H8	9:E:182:ASN:HB3	1.77	0.50
5:A:681:G:N7	14:J:110:LYS:HE3	2.27	0.50
5:A:738:U:O2'	5:A:1390:A:N3	2.44	0.50
5:A:2036:G:C2	5:A:2037:G:C8	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:72:ASP:O	7:C:74:ILE:HD12	2.10	0.50
8:D:67:LYS:HA	8:D:86:ARG:HH22	1.76	0.50
18:N:31:HIS:NE2	18:N:85:LYS:HD3	2.25	0.50
5:A:52:A:H2'	5:A:53:A:H8	1.77	0.50
5:A:1753:U:H1'	5:A:2880:A:H1'	1.94	0.50
9:E:164:GLU:HA	9:E:175:VAL:HG21	1.92	0.50
16:L:91:GLU:OE1	16:L:91:GLU:N	2.44	0.50
5:A:1401:G:OP1	26:V:3:LYS:CE	2.59	0.50
9:E:195:THR:HG22	9:E:197:ALA:H	1.76	0.50
19:O:116:ALA:O	19:O:117:LEU:C	2.50	0.50
1:1:12:CYS:SG	1:1:39:LEU:CG	3.00	0.49
5:A:665:G:H4'	5:A:666:A:H5''	1.94	0.49
5:A:1806:U:H5	5:A:1811:A:N7	2.10	0.49
5:A:2622:G:N2	5:A:2625:A:OP2	2.39	0.49
13:I:93:PRO:HD3	13:I:114:ILE:CD1	2.42	0.49
15:K:42:ILE:CG2	15:K:47:ILE:HG13	2.42	0.49
18:N:61:PHE:O	18:N:75:THR:HG23	2.12	0.49
19:O:104:LYS:CD	19:O:104:LYS:N	2.74	0.49
22:R:14:GLU:HG2	22:R:15:LYS:N	2.27	0.49
24:T:46:VAL:CG1	24:T:50:LYS:NZ	2.75	0.49
5:A:787:U:H2'	5:A:788:A:C8	2.47	0.49
5:A:1072:A:N6	5:A:1169:G:H2'	2.27	0.49
8:D:99:TYR:O	8:D:100:GLU:CD	2.50	0.49
10:F:56:GLU:HA	10:F:60:ILE:CD1	2.41	0.49
16:L:100:TYR:O	16:L:101:THR:HG23	2.13	0.49
26:V:17:ARG:HG3	26:V:17:ARG:NH1	2.23	0.49
5:A:502:C:C6	22:R:68:TYR:CE1	3.00	0.49
5:A:2867:U:H2'	5:A:2868:G:O4'	2.13	0.49
8:D:5:ILE:HG21	8:D:195:ILE:CD1	2.41	0.49
12:H:58:ILE:HG13	12:H:59:ASN:H	1.77	0.49
18:N:60:THR:O	18:N:60:THR:HG23	2.12	0.49
26:V:7:VAL:HG22	26:V:8:THR:H	1.76	0.49
27:W:26:PHE:CE1	27:W:30:PHE:CD1	3.01	0.49
5:A:2154:G:H2'	5:A:2155:C:C6	2.47	0.49
10:F:108:LEU:HB2	29:Y:51:SER:HA	1.94	0.49
12:H:78:HIS:CD2	12:H:85:ILE:HD13	2.39	0.49
15:K:72:THR:HB	15:K:94:ILE:HG12	1.95	0.49
16:L:24:LEU:HD23	16:L:44:VAL:HG21	1.94	0.49
22:R:36:THR:CG2	22:R:40:MET:HE3	2.42	0.49
25:U:71:ILE:HD12	25:U:72:ASP:O	2.13	0.49
5:A:689:A:H5''	5:A:689:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2142:G:N2	5:A:2188:C:OP1	2.45	0.49
5:A:2775:A:H5''	11:G:4:VAL:HG21	1.93	0.49
10:F:58:GLU:HB2	10:F:64:LYS:HA	1.94	0.49
10:F:66:LEU:HD12	10:F:66:LEU:C	2.30	0.49
11:G:119:GLU:HB3	11:G:120:ASN:OD1	2.12	0.49
17:M:6:ASP:OD1	17:M:7:LYS:N	2.45	0.49
20:P:2:PHE:HE1	20:P:13:LYS:CG	2.26	0.49
27:W:2:LYS:O	27:W:2:LYS:HD2	2.13	0.49
9:E:164:GLU:HG3	9:E:175:VAL:CG1	2.42	0.49
12:H:103:GLU:HB2	12:H:125:VAL:HG11	1.95	0.49
5:A:52:A:H2'	5:A:53:A:C8	2.48	0.49
5:A:144:C:C4'	22:R:37:GLN:NE2	2.70	0.49
5:A:1846:A:H3'	7:C:177:ARG:HG2	1.94	0.49
5:A:2431:C:H2'	5:A:2432:G:O4'	2.12	0.49
6:B:44:A:H5''	17:M:7:LYS:HE3	1.95	0.49
9:E:5:ASP:HA	9:E:13:LYS:NZ	2.28	0.49
5:A:162:A:H8	5:A:2244:G:H21	1.61	0.49
5:A:1699:A:N6	5:A:2032:A:O2'	2.46	0.49
5:A:2540:A:OP1	8:D:168:LYS:HE2	2.13	0.49
11:G:45:GLN:O	11:G:45:GLN:HG2	2.13	0.49
11:G:168:TYR:CE2	11:G:170:ARG:HG2	2.48	0.49
12:H:74:VAL:CG2	12:H:87:SER:HB2	2.42	0.49
13:I:19:VAL:HG22	13:I:20:LEU:N	2.28	0.49
13:I:32:THR:HG23	13:I:33:ALA:H	1.77	0.49
15:K:30:GLY:CA	15:K:65:TRP:CZ3	2.96	0.49
15:K:31:GLU:CG	15:K:32:PHE:CE2	2.96	0.49
5:A:293:U:H2'	5:A:294:G:O4'	2.13	0.49
5:A:579:U:H5'	19:O:42:SER:OG	2.13	0.49
5:A:677:A:H2'	5:A:678:A:C8	2.48	0.49
5:A:897:A:H5'	28:X:45:GLY:HA3	1.94	0.49
5:A:1198:G:OP2	19:O:58:ARG:NH2	2.40	0.49
5:A:1754:C:H2'	5:A:1755:U:C6	2.48	0.49
5:A:2328:A:N6	5:A:2342:U:H3	2.09	0.49
22:R:15:LYS:HA	22:R:18:GLU:HG3	1.95	0.49
5:A:852:U:C2	5:A:853:G:C8	3.01	0.49
5:A:1932:C:H4'	5:A:1956:G:H8	1.77	0.49
5:A:2123:A:C2	5:A:2124:U:C5	3.00	0.49
6:B:55:A:H2'	6:B:56:A:C8	2.48	0.49
7:C:166:GLY:O	7:C:172:VAL:HG13	2.13	0.49
5:A:1290:G:N2	19:O:33:LYS:HG3	2.28	0.48
8:D:27:VAL:CG2	8:D:194:VAL:HG11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:27:THR:OG1	18:N:90:ARG:HG2	2.13	0.48
19:O:111:THR:O	19:O:115:ASP:OD2	2.31	0.48
4:4:26:ILE:CG1	4:4:26:ILE:O	2.62	0.48
5:A:1315:C:H5'	16:L:20:LEU:CD2	2.43	0.48
16:L:94:THR:HG23	16:L:95:GLU:HG3	1.95	0.48
22:R:49:LYS:N	22:R:84:GLU:OE2	2.46	0.48
22:R:51:ALA:HB2	22:R:83:LYS:HG3	1.95	0.48
24:T:3:SER:O	24:T:3:SER:OG	2.31	0.48
29:Y:1:MET:O	29:Y:1:MET:HG3	2.12	0.48
1:1:18:ILE:CG2	5:A:2446:U:H5'	2.42	0.48
1:1:35:TYR:CD1	1:1:42:TYR:CE1	3.00	0.48
5:A:43:A:H62	5:A:482:U:H3	1.59	0.48
5:A:707:G:H5''	14:J:16:ARG:HB3	1.94	0.48
5:A:1097:U:H4'	5:A:1098:A:OP2	2.12	0.48
5:A:1315:C:H5'	16:L:20:LEU:HD21	1.96	0.48
5:A:2858:G:C4	5:A:2859:G:C8	3.01	0.48
7:C:119:GLY:O	7:C:131:PRO:HD3	2.13	0.48
5:A:157:U:H3'	5:A:158:G:H5''	1.95	0.48
5:A:2632:U:H2'	5:A:2633:C:C6	2.49	0.48
10:F:35:VAL:HG12	10:F:155:VAL:HG22	1.87	0.48
5:A:1821:U:H2'	5:A:1822:C:C6	2.48	0.48
15:K:47:ILE:HG23	15:K:104:PHE:CZ	2.48	0.48
5:A:297:G:H4'	5:A:304:G:O3'	2.12	0.48
5:A:1485:G:O2'	5:A:1672:G:OP1	2.24	0.48
6:B:73:G:H2'	6:B:74:G:O4'	2.13	0.48
10:F:43:ALA:HB2	10:F:49:VAL:CG2	2.44	0.48
10:F:66:LEU:CD1	10:F:88:LYS:HB3	2.42	0.48
29:Y:9:TYR:CZ	29:Y:26:GLY:CA	2.84	0.48
5:A:93:U:H1'	5:A:94:A:H5'	1.95	0.48
5:A:881:G:C6	5:A:882:C:C5	3.02	0.48
5:A:1495:C:H4'	5:A:1496:G:C4	2.49	0.48
5:A:1855:G:O6	7:C:221:ARG:CD	2.57	0.48
10:F:90:THR:H	29:Y:2:LYS:HE2	1.78	0.48
11:G:101:LYS:O	11:G:102:ASP:OD1	2.30	0.48
16:L:70:GLU:OE1	16:L:80:THR:HG22	2.14	0.48
19:O:76:TYR:O	19:O:80:MET:HG2	2.13	0.48
5:A:144:C:H2'	5:A:145:A:C8	2.49	0.48
5:A:529:A:C8	23:S:44:HIS:HD2	2.31	0.48
5:A:1701:U:OP1	8:D:149:ARG:N	2.47	0.48
5:A:2338:A:O2'	10:F:79:LEU:CD2	2.62	0.48
23:S:87:ASP:O	23:S:89:LYS:CE	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:231:A:H61	5:A:465:C:C5'	2.26	0.48
16:L:73:ASN:HB2	16:L:77:THR:OG1	2.13	0.48
22:R:22:GLU:OE1	22:R:23:ASP:N	2.47	0.48
5:A:702:U:H2'	5:A:703:A:C8	2.49	0.48
5:A:1279:C:C2	5:A:1280:U:C5	3.02	0.48
5:A:1400:C:O2'	5:A:1836:A:N3	2.37	0.48
10:F:109:PRO:HG2	10:F:110:ARG:HH11	1.79	0.48
13:I:30:ARG:NH2	13:I:37:ASP:OD2	2.46	0.48
19:O:76:TYR:CZ	19:O:80:MET:HG3	2.48	0.48
27:W:32:LEU:C	27:W:32:LEU:HD23	2.35	0.48
10:F:66:LEU:CD1	10:F:68:THR:HG22	2.45	0.47
12:H:85:ILE:HG23	12:H:85:ILE:O	2.13	0.47
15:K:111:GLU:OE2	15:K:115:ARG:NH2	2.45	0.47
20:P:16:GLU:HA	20:P:97:ILE:HB	1.96	0.47
5:A:2272:U:H5''	5:A:2273:G:H5'	1.96	0.47
11:G:8:ILE:CB	11:G:69:ARG:NH2	2.77	0.47
14:J:2:LYS:HB2	14:J:5:GLU:HG3	1.94	0.47
28:X:5:GLN:HG3	28:X:36:VAL:HG22	1.96	0.47
6:B:64:A:H1'	6:B:66:C:H41	1.78	0.47
11:G:59:LYS:HE2	11:G:62:ARG:HH22	1.77	0.47
5:A:1300:G:C6	5:A:1301:U:C4	3.02	0.47
5:A:1737:U:O2'	7:C:14:ARG:NH1	2.47	0.47
5:A:2318:U:H2'	5:A:2319:U:C6	2.50	0.47
5:A:2662:U:O2'	8:D:90:GLU:OE1	2.32	0.47
5:A:2817:A:H1'	5:A:2818:A:H5'	1.96	0.47
5:A:2903:A:H5'	5:A:2904:U:H5''	1.96	0.47
8:D:93:ASN:OD1	8:D:94:VAL:N	2.47	0.47
10:F:95:ARG:HH22	29:Y:9:TYR:HB2	1.78	0.47
12:H:85:ILE:O	12:H:85:ILE:CG2	2.63	0.47
23:S:3:ILE:HD12	23:S:4:LYS:O	2.14	0.47
24:T:60:VAL:C	24:T:61:ILE:HD13	2.35	0.47
5:A:1693:G:C6	5:A:2036:G:O6	2.68	0.47
10:F:106:VAL:HG21	10:F:139:PRO:HG3	1.96	0.47
13:I:81:GLU:OE1	13:I:82:ASN:O	2.32	0.47
24:T:22:ARG:CD	24:T:87:THR:HG22	2.42	0.47
5:A:1072:A:H2'	5:A:1073:A:C8	2.50	0.47
5:A:1633:A:H1'	5:A:1634:A:H5'	1.96	0.47
5:A:2224:U:H2'	5:A:2251:G:H1	1.80	0.47
5:A:2400:U:H2'	5:A:2401:C:C6	2.50	0.47
9:E:5:ASP:HB2	9:E:13:LYS:HE2	1.97	0.47
11:G:26:VAL:HG21	11:G:76:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:15:LYS:HD2	12:H:17:TYR:OH	2.14	0.47
24:T:75:ALA:CA	24:T:92:LEU:HD22	2.45	0.47
25:U:83:ASP:OD1	25:U:83:ASP:N	2.47	0.47
29:Y:18:THR:HG21	29:Y:49:ASP:O	2.14	0.47
1:1:35:TYR:HD1	1:1:42:TYR:CD1	2.32	0.47
5:A:388:A:H8	5:A:389:A:C2	2.33	0.47
5:A:512:A:H5''	5:A:512:A:H8	1.80	0.47
5:A:1084:U:H2'	5:A:1085:U:O4'	2.15	0.47
5:A:1206:G:N2	20:P:90:GLN:OE1	2.47	0.47
5:A:1522:G:H2'	5:A:1559:G:N2	2.30	0.47
5:A:2786:G:H1'	5:A:2787:C:H5'	1.95	0.47
7:C:100:GLU:OE2	7:C:102:ARG:HD3	2.15	0.47
7:C:181:VAL:HG23	7:C:271:VAL:HB	1.96	0.47
11:G:81:GLN:OE1	11:G:81:GLN:CA	2.61	0.47
12:H:20:ASP:OD1	12:H:58:ILE:CD1	2.62	0.47
14:J:95:LEU:HD13	14:J:95:LEU:C	2.34	0.47
24:T:12:LYS:O	24:T:12:LYS:CG	2.34	0.47
8:D:54:GLU:O	8:D:85:LYS:HD3	2.15	0.47
17:M:77:GLY:O	17:M:80:ILE:HG22	2.13	0.47
20:P:62:VAL:HG22	20:P:95:LEU:HD23	1.96	0.47
5:A:593:U:P	20:P:64:LYS:HZ1	2.37	0.47
5:A:2575:G:H1'	13:I:23:LYS:HZ1	1.77	0.47
5:A:2727:G:H2'	5:A:2728:U:C6	2.49	0.47
7:C:181:VAL:O	7:C:271:VAL:HG23	2.14	0.47
10:F:4:LEU:HB2	10:F:101:ASP:OD1	2.14	0.47
11:G:103:LEU:CD2	11:G:105:LEU:HG	2.45	0.47
25:U:48:GLN:OE1	25:U:52:LYS:N	2.46	0.47
1:1:5:VAL:HG11	1:1:30:ILE:HD11	1.97	0.47
5:A:944:G:H2'	5:A:945:A:O4'	2.15	0.47
4:4:17:ILE:CD1	4:4:26:ILE:CG2	2.93	0.46
5:A:26:G:H2'	5:A:27:G:O4'	2.15	0.46
6:B:64:A:H61	6:B:104:A:H2'	1.80	0.46
7:C:157:SER:O	7:C:195:VAL:CG2	2.63	0.46
8:D:169:MET:HE3	8:D:169:MET:HB3	1.72	0.46
14:J:70:ASN:OD1	14:J:70:ASN:O	2.33	0.46
24:T:25:GLY:C	24:T:26:LYS:HD3	2.36	0.46
27:W:19:LYS:HB3	27:W:19:LYS:NZ	2.29	0.46
27:W:31:GLN:CB	27:W:36:GLN:HG3	2.40	0.46
5:A:684:U:C2	5:A:685:C:C5	3.03	0.46
13:I:42:THR:HA	13:I:56:ASP:O	2.15	0.46
13:I:73:ASP:OD1	13:I:75:SER:CB	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:36:ASP:OD1	20:P:36:ASP:N	2.45	0.46
24:T:78:GLN:HB2	24:T:88:HIS:H	1.80	0.46
5:A:350:G:H8	5:A:373:A:N6	2.14	0.46
5:A:687:G:C2	5:A:689:A:H5'	2.50	0.46
5:A:1929:C:H5''	7:C:241:ILE:HB	1.96	0.46
5:A:2279:G:C8	25:U:12:LYS:HD2	2.51	0.46
7:C:76:ALA:HB3	7:C:116:VAL:HG12	1.97	0.46
11:G:160:LYS:HB3	11:G:160:LYS:HE2	1.70	0.46
18:N:34:ILE:HD11	18:N:43:GLN:HG2	1.96	0.46
5:A:1804:U:H5	5:A:1814:A:N1	2.14	0.46
5:A:2645:G:H21	8:D:163:VAL:HG21	1.81	0.46
7:C:139:THR:HG21	7:C:192:ILE:HD12	1.97	0.46
21:Q:2:GLU:OE2	21:Q:72:LYS:CD	2.62	0.46
22:R:27:PHE:HE2	27:W:30:PHE:HZ	1.63	0.46
5:A:720:A:OP1	9:E:76:GLY:HA3	2.16	0.46
10:F:92:ARG:O	10:F:96:MET:CE	2.64	0.46
20:P:27:VAL:CG2	20:P:28:ASN:N	2.79	0.46
5:A:924:G:H2'	5:A:925:G:C8	2.51	0.46
5:A:2146:A:N6	5:A:2195:G:H22	2.13	0.46
5:A:2294:A:H5''	5:A:2295:A:H5'	1.97	0.46
5:A:2428:U:H2'	5:A:2429:U:O4'	2.15	0.46
7:C:68:LYS:HG2	7:C:151:GLY:HA2	1.98	0.46
8:D:205:LYS:HE2	8:D:205:LYS:HB2	1.65	0.46
10:F:25:VAL:CG2	10:F:26:MET:HE3	2.45	0.46
14:J:87:ASP:C	14:J:89:THR:H	2.18	0.46
15:K:31:GLU:HG2	15:K:32:PHE:CE2	2.50	0.46
15:K:42:ILE:O	15:K:94:ILE:HA	2.16	0.46
24:T:55:VAL:HG21	24:T:59:GLY:HA3	1.98	0.46
27:W:38:GLU:OE1	27:W:38:GLU:HA	2.14	0.46
29:Y:1:MET:O	29:Y:3:GLN:N	2.48	0.46
5:A:82:G:H22	5:A:102:A:P	2.38	0.46
5:A:1422:A:H1'	5:A:1423:C:C6	2.51	0.46
5:A:1823:U:H2'	5:A:1824:C:C6	2.50	0.46
7:C:180:GLU:OE2	7:C:182:ARG:HD2	2.15	0.46
15:K:31:GLU:CD	15:K:32:PHE:CZ	2.88	0.46
18:N:88:VAL:O	18:N:88:VAL:HG12	2.15	0.46
4:4:7:VAL:HG21	4:4:23:VAL:O	2.16	0.46
5:A:1336:G:N1	5:A:1684:A:OP2	2.42	0.46
5:A:2144:A:H1'	5:A:2175:G:H4'	1.97	0.46
5:A:2854:A:H2'	5:A:2899:A:N6	2.31	0.46
11:G:92:VAL:HG23	11:G:92:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:55:GLN:CD	17:M:55:GLN:C	2.75	0.46
5:A:578:G:H21	19:O:48:ARG:HH22	1.58	0.46
5:A:1829:A:H2'	5:A:1830:A:C8	2.50	0.46
7:C:68:LYS:CD	7:C:149:GLY:O	2.64	0.46
11:G:5:GLY:HA2	11:G:69:ARG:CG	2.46	0.46
13:I:112:MET:HA	13:I:112:MET:CE	2.46	0.46
16:L:106:GLN:NE2	16:L:118:ILE:CD1	2.79	0.46
19:O:45:TYR:CD1	19:O:48:ARG:NH2	2.84	0.46
5:A:901:G:H2'	5:A:902:A:H8	1.80	0.46
5:A:1128:A:C8	5:A:1129:A:C8	3.04	0.46
5:A:1577:G:N2	5:A:1589:U:H3	2.14	0.46
5:A:1726:A:OP2	5:A:1743:G:N2	2.47	0.46
5:A:2124:U:C4	5:A:2125:U:C4	3.04	0.46
5:A:2403:A:H2	17:M:113:ARG:NH2	2.12	0.46
10:F:106:VAL:HG21	10:F:139:PRO:CG	2.46	0.46
11:G:123:PHE:N	11:G:123:PHE:CD1	2.84	0.46
13:I:102:VAL:HG13	13:I:106:LEU:CD1	2.45	0.46
15:K:30:GLY:HA2	15:K:65:TRP:CH2	2.50	0.46
30:Z:29:GLU:OE1	30:Z:34:GLY:O	2.34	0.46
5:A:270:C:H4'	5:A:323:C:H1'	1.99	0.45
5:A:1000:G:N2	5:A:1003:A:H3'	2.32	0.45
5:A:1290:G:C2	19:O:33:LYS:HG3	2.51	0.45
6:B:43:A:O4'	10:F:92:ARG:CD	2.64	0.45
12:H:93:LEU:HA	12:H:93:LEU:HD23	1.77	0.45
13:I:91:LYS:HE3	13:I:111:PHE:CE1	2.51	0.45
14:J:15:GLU:OE2	14:J:16:ARG:O	2.34	0.45
19:O:78:ARG:N	19:O:78:ARG:HD3	2.31	0.45
3:3:24:ARG:HD2	14:J:61:LEU:HD21	1.98	0.45
5:A:660:A:C8	9:E:182:ASN:HB3	2.51	0.45
5:A:1225:G:H3'	5:A:1226:G:H8	1.81	0.45
5:A:1308:C:H5''	5:A:1309:G:C5'	2.46	0.45
5:A:1758:A:H5''	5:A:1759:G:H21	1.80	0.45
5:A:1818:A:C2'	5:A:1819:G:H5'	2.47	0.45
6:B:22:G:N7	6:B:54:U:H2'	2.30	0.45
13:I:18:GLU:OE2	13:I:19:VAL:N	2.49	0.45
23:S:100:GLU:C	23:S:100:GLU:OE1	2.54	0.45
5:A:29:U:H2'	5:A:30:G:C8	2.52	0.45
5:A:280:C:O2	5:A:280:C:H2'	2.16	0.45
5:A:363:A:OP1	9:E:135:LYS:NZ	2.48	0.45
5:A:962:A:H5''	5:A:2295:A:H61	1.80	0.45
8:D:33:ASN:O	8:D:105:VAL:N	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:17:ILE:CD1	9:E:200:LYS:HE3	2.47	0.45
9:E:146:LEU:O	9:E:148:GLN:OE1	2.34	0.45
10:F:5:LYS:HZ2	10:F:94:GLU:HA	1.81	0.45
11:G:24:VAL:HG12	11:G:25:THR:N	2.31	0.45
12:H:18:VAL:CG2	12:H:138:PRO:HB2	2.47	0.45
20:P:100:ILE:HG22	20:P:101:ASN:N	2.32	0.45
23:S:38:VAL:HG11	23:S:63:ILE:HD13	1.98	0.45
5:A:144:C:H2'	5:A:145:A:H8	1.82	0.45
5:A:896:U:H2'	5:A:897:A:H8	1.80	0.45
5:A:1680:U:H2'	5:A:1681:U:C6	2.51	0.45
5:A:2122:A:C4	5:A:2123:A:C8	3.04	0.45
15:K:65:TRP:CH2	15:K:107:ALA:HB3	2.42	0.45
20:P:20:ILE:HG13	20:P:95:LEU:HB2	1.98	0.45
5:A:1854:U:H5	7:C:221:ARG:HD2	1.79	0.45
7:C:74:ILE:H	7:C:74:ILE:CD1	2.28	0.45
8:D:29:GLU:OE2	8:D:31:LYS:HD3	2.16	0.45
10:F:126:GLY:HA2	10:F:163:ASP:HA	1.97	0.45
12:H:36:ILE:HG22	12:H:37:LEU:N	2.32	0.45
22:R:36:THR:CG2	22:R:40:MET:CE	2.95	0.45
24:T:29:ALA:HA	24:T:88:HIS:CD2	2.52	0.45
27:W:7:ARG:O	27:W:60:ARG:NH2	2.49	0.45
1:1:14:ASP:CB	1:1:38:ARG:HH21	2.19	0.45
5:A:1278:G:C8	5:A:1279:C:C6	3.05	0.45
5:A:2153:A:C4'	5:A:2190:C:H42	2.29	0.45
10:F:111:VAL:H	10:F:136:LEU:HD21	1.81	0.45
12:H:18:VAL:CG1	12:H:58:ILE:HG23	2.47	0.45
26:V:31:ALA:HB3	26:V:33:LEU:HG	1.99	0.45
28:X:4:LEU:HD12	28:X:4:LEU:O	2.17	0.45
5:A:2369:C:H3'	5:A:2370:U:O2	2.17	0.45
7:C:35:LYS:HB3	7:C:35:LYS:HE2	1.82	0.45
23:S:91:VAL:HG22	23:S:92:ARG:N	2.31	0.45
5:A:57:C:H2'	5:A:58:G:O4'	2.17	0.45
5:A:632:U:H2'	5:A:633:A:H8	1.82	0.45
5:A:1712:A:O2'	5:A:1718:G:N7	2.37	0.45
9:E:117:LYS:HB2	9:E:117:LYS:HE2	1.82	0.45
10:F:57:LEU:H	10:F:60:ILE:CD1	2.12	0.45
13:I:13:ASN:ND2	13:I:97:ARG:CB	2.79	0.45
13:I:38:VAL:HG22	13:I:61:VAL:HB	1.98	0.45
18:N:82:LYS:HE2	18:N:82:LYS:HB3	1.52	0.45
20:P:27:VAL:CG2	20:P:31:ASP:CB	2.95	0.45
5:A:523:A:H2'	5:A:524:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:631:U:H2'	5:A:632:U:C6	2.52	0.45
5:A:1712:A:N3	5:A:1714:C:N4	2.65	0.45
5:A:2253:C:C2	5:A:2254:A:C8	3.05	0.45
6:B:86:A:H8	6:B:87:C:H5''	1.82	0.45
10:F:22:TYR:HB3	10:F:27:GLU:HB3	1.99	0.45
16:L:55:ASP:OD1	16:L:55:ASP:O	2.35	0.45
7:C:11:ASN:C	7:C:13:ARG:H	2.19	0.45
8:D:2:THR:O	8:D:94:VAL:HG12	2.17	0.45
9:E:68:LYS:HE3	9:E:68:LYS:HB3	1.75	0.45
22:R:46:PHE:CE2	22:R:87:ILE:HG23	2.52	0.45
27:W:37:LEU:HG	27:W:39:GLU:H	1.81	0.45
5:A:117:A:N3	5:A:180:G:H1'	2.32	0.44
5:A:719:G:H5''	9:E:76:GLY:N	2.32	0.44
5:A:1115:G:N2	5:A:1136:C:OP2	2.50	0.44
5:A:2022:U:H3'	5:A:2023:C:H2'	1.98	0.44
5:A:2330:G:H4'	10:F:123:ASP:HA	1.99	0.44
7:C:60:ARG:HD3	7:C:85:PRO:HB2	1.99	0.44
11:G:90:VAL:O	11:G:94:TYR:CD2	2.71	0.44
12:H:73:LYS:O	12:H:73:LYS:HG3	2.17	0.44
15:K:20:ARG:HD2	15:K:99:PRO:HG2	1.98	0.44
16:L:92:ARG:HD2	16:L:93:TYR:CZ	2.52	0.44
20:P:2:PHE:CE1	20:P:13:LYS:HG3	2.46	0.44
22:R:89:LEU:O	22:R:90:PHE:C	2.54	0.44
4:4:15:LYS:HB3	4:4:15:LYS:HE3	1.66	0.44
5:A:79:U:O2'	5:A:389:A:H1'	2.17	0.44
5:A:672:A:H2'	14:J:76:ILE:HD11	1.98	0.44
5:A:1328:C:C2	5:A:1329:G:C8	3.05	0.44
5:A:1881:A:H4'	5:A:2260:A:H4'	1.98	0.44
5:A:2212:G:H2'	5:A:2213:U:C6	2.52	0.44
6:B:23:U:H4'	6:B:24:C:C2	2.52	0.44
11:G:102:ASP:OD1	11:G:116:LYS:HA	2.17	0.44
13:I:75:SER:HA	18:N:75:THR:O	2.18	0.44
15:K:30:GLY:HA3	15:K:65:TRP:CZ3	2.52	0.44
16:L:55:ASP:OD1	16:L:55:ASP:C	2.55	0.44
26:V:39:LEU:CD1	26:V:42:GLY:O	2.65	0.44
27:W:28:LEU:HD12	27:W:29:ARG:N	2.32	0.44
5:A:24:G:C6	5:A:25:U:C4	3.05	0.44
5:A:1801:C:O2	5:A:1801:C:H2'	2.16	0.44
5:A:2359:C:OP1	25:U:54:TYR:OH	2.29	0.44
17:M:100:LEU:H	17:M:100:LEU:CD1	2.29	0.44
22:R:9:ARG:HG2	22:R:28:ASP:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1489:A:N6	5:A:1509:G:C8	2.85	0.44
5:A:2278:OMG:HM23	5:A:2278:OMG:H1'	1.49	0.44
5:A:2372:G:N3	5:A:2408:C:H2'	2.33	0.44
5:A:2564:U:H2'	5:A:2565:C:C6	2.53	0.44
5:A:1379:A:HO2'	5:A:1381:U:P	2.40	0.44
5:A:1871:U:H3'	5:A:1872:G:C8	2.52	0.44
5:A:2793:G:C2	5:A:2794:C:C6	3.06	0.44
9:E:13:LYS:NZ	9:E:15:GLY:O	2.50	0.44
12:H:59:ASN:O	12:H:127:GLY:HA2	2.16	0.44
18:N:91:ARG:HG3	18:N:92:GLY:H	1.81	0.44
22:R:89:LEU:HD12	27:W:30:PHE:HE2	1.83	0.44
5:A:1312:A:N7	16:L:12:GLN:HG2	2.33	0.44
5:A:2035:C:H2'	5:A:2036:G:H8	1.82	0.44
5:A:2874:A:H2'	5:A:2875:U:C6	2.53	0.44
5:A:1103:G:O6	5:A:1124:A:N6	2.51	0.44
5:A:1806:U:H5'	5:A:1807:A:O5'	2.18	0.44
20:P:39:LEU:HD23	20:P:52:THR:HG22	2.00	0.44
21:Q:14:PRO:HG3	21:Q:78:GLU:HG3	2.00	0.44
22:R:36:THR:HG22	22:R:40:MET:HE3	2.00	0.44
5:A:702:U:H2'	5:A:703:A:H8	1.82	0.44
10:F:34:ILE:HG13	10:F:91:LEU:HB2	1.99	0.44
13:I:71:ARG:HH11	18:N:74:ARG:NE	2.14	0.44
13:I:91:LYS:CE	13:I:109:GLY:O	2.66	0.44
17:M:113:ARG:CG	17:M:119:PHE:CE1	3.00	0.44
5:A:1054:A:OP1	19:O:66:ASN:ND2	2.43	0.44
5:A:1315:C:H2'	5:A:1316:G:C8	2.52	0.44
5:A:1493:U:H5''	5:A:1576:A:C4	2.53	0.44
5:A:2322:C:OP1	17:M:14:ARG:NH2	2.51	0.44
5:A:2512:G:H5''	15:K:46:GLN:OE1	2.17	0.44
10:F:58:GLU:CG	29:Y:7:PRO:HG3	2.47	0.44
10:F:132:VAL:HG22	10:F:152:MET:HE2	2.00	0.44
11:G:23:HIS:C	11:G:23:HIS:ND1	2.71	0.44
11:G:26:VAL:HG12	11:G:79:VAL:CG2	2.45	0.44
19:O:76:TYR:CE1	19:O:80:MET:HG3	2.53	0.44
22:R:23:ASP:OD2	22:R:82:LEU:HD12	2.18	0.44
23:S:3:ILE:CD1	23:S:4:LYS:O	2.66	0.44
29:Y:8:GLU:HG2	29:Y:8:GLU:O	2.18	0.44
5:A:300:G:N1	5:A:467:U:O2'	2.50	0.43
5:A:318:A:H62	5:A:401:U:H3	1.66	0.43
5:A:2670:G:H2'	5:A:2671:A:C8	2.52	0.43
5:A:2701:G:H4'	13:I:30:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:59:LEU:HD12	10:F:59:LEU:HA	1.84	0.43
11:G:122:THR:CG2	11:G:123:PHE:N	2.81	0.43
12:H:15:LYS:HD2	12:H:17:TYR:CZ	2.53	0.43
13:I:21:THR:HB	13:I:39:ILE:HD12	2.00	0.43
22:R:27:PHE:CE2	27:W:30:PHE:HZ	2.35	0.43
5:A:1141:U:H2'	5:A:1142:A:C4	2.53	0.43
5:A:1185:U:H4'	5:A:1186:A:O5'	2.18	0.43
5:A:2123:A:C4	5:A:2124:U:C5	3.06	0.43
5:A:2355:A:H2'	5:A:2356:A:C8	2.53	0.43
10:F:7:LYS:NZ	10:F:172:ASN:HA	2.33	0.43
11:G:17:VAL:HG22	11:G:26:VAL:HG22	1.99	0.43
24:T:72:VAL:HG21	24:T:91:PHE:HB3	1.99	0.43
2:2:2:VAL:N	5:A:1663:G:HO2'	2.16	0.43
5:A:1435:C:H2'	5:A:1436:C:C6	2.54	0.43
8:D:107:VAL:HG21	8:D:193:LYS:HA	2.01	0.43
8:D:173:MET:HE3	8:D:173:MET:HB2	1.80	0.43
10:F:95:ARG:CD	29:Y:1:MET:CB	2.84	0.43
21:Q:40:ASN:O	21:Q:40:ASN:ND2	2.50	0.43
23:S:5:LYS:O	23:S:5:LYS:HG3	2.15	0.43
5:A:300:G:H1	5:A:467:U:HO2'	1.65	0.43
5:A:409:G:H3'	5:A:410:G:C8	2.54	0.43
5:A:491:C:O2	5:A:496:G:H1'	2.18	0.43
7:C:39:LYS:HE2	7:C:39:LYS:HB2	1.67	0.43
7:C:111:GLU:O	7:C:114:GLN:HG3	2.17	0.43
8:D:118:VAL:HG23	8:D:209:VAL:HB	1.99	0.43
10:F:95:ARG:HD2	29:Y:1:MET:CB	2.41	0.43
23:S:37:GLY:N	23:S:60:GLU:OE2	2.48	0.43
24:T:31:VAL:HG12	24:T:91:PHE:CB	2.47	0.43
5:A:78:U:H2'	5:A:79:U:C6	2.53	0.43
5:A:529:A:H5'	23:S:44:HIS:HB3	2.00	0.43
5:A:556:U:H4'	5:A:1273:G:H4'	2.01	0.43
5:A:579:U:O2'	19:O:49:ASP:OD2	2.30	0.43
5:A:1698:A:O2'	8:D:127:PHE:O	2.27	0.43
5:A:1707:U:O2'	5:A:2713:G:H4'	2.17	0.43
5:A:2725:U:H2'	5:A:2726:C:C6	2.53	0.43
13:I:4:GLN:HA	13:I:21:THR:HG23	2.00	0.43
13:I:24:VAL:HG23	13:I:24:VAL:O	2.18	0.43
13:I:77:ILE:HG23	13:I:77:ILE:O	2.18	0.43
13:I:93:PRO:HB3	13:I:114:ILE:CD1	2.46	0.43
15:K:45:ARG:O	15:K:45:ARG:HG3	2.19	0.43
18:N:6:LEU:HD12	18:N:7:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:34:THR:HG23	20:P:34:THR:O	2.18	0.43
20:P:65:GLN:HG2	20:P:93:THR:HG22	2.00	0.43
22:R:52:SER:OG	22:R:81:THR:CG2	2.66	0.43
23:S:45:GLN:OE1	23:S:46:LYS:N	2.51	0.43
27:W:38:GLU:OE1	27:W:38:GLU:CA	2.66	0.43
5:A:81:G:N2	5:A:105:C:C2	2.86	0.43
5:A:786:U:H2'	5:A:787:U:O4'	2.18	0.43
5:A:923:A:H2'	5:A:924:G:C8	2.53	0.43
5:A:1247:G:O2'	5:A:1275:A:N1	2.41	0.43
5:A:1296:C:O2'	5:A:1297:G:H5'	2.19	0.43
5:A:1844:G:H2'	5:A:1845:U:H5'	2.01	0.43
9:E:117:LYS:CE	9:E:186:ILE:O	2.65	0.43
15:K:46:GLN:HE21	15:K:46:GLN:HB2	1.59	0.43
16:L:37:ALA:HA	16:L:40:VAL:HG12	2.00	0.43
21:Q:11:ARG:HH21	21:Q:98:LYS:HB3	1.83	0.43
21:Q:22:ASP:OD1	21:Q:25:ARG:NH1	2.47	0.43
27:W:34:THR:OG1	27:W:36:GLN:HG2	2.18	0.43
1:1:10:THR:CG2	1:1:46:ARG:NH1	2.78	0.43
5:A:2106:U:H2'	5:A:2107:G:O4'	2.19	0.43
5:A:2829:A:H3'	5:A:2830:A:H8	1.84	0.43
7:C:107:PRO:HD2	7:C:110:LEU:HD22	2.01	0.43
10:F:132:VAL:HG22	10:F:152:MET:CE	2.47	0.43
11:G:120:ASN:HD22	11:G:136:ILE:HD11	1.83	0.43
23:S:7:ASP:HB2	23:S:70:LEU:HD21	2.00	0.43
23:S:84:LYS:CE	23:S:93:ILE:HD12	2.48	0.43
24:T:94:ILE:HD12	24:T:94:ILE:H	1.82	0.43
5:A:26:G:O2'	5:A:27:G:O4'	2.34	0.43
5:A:1197:C:H2'	5:A:1198:G:O4'	2.19	0.43
8:D:17:GLY:O	8:D:21:GLU:OE1	2.37	0.43
8:D:128:GLN:CB	8:D:173:MET:HE3	2.49	0.43
11:G:57:ASP:O	11:G:62:ARG:HD3	2.19	0.43
13:I:71:ARG:NH1	18:N:74:ARG:CZ	2.80	0.43
16:L:69:VAL:HG12	16:L:70:GLU:N	2.32	0.43
18:N:45:PHE:HE2	18:N:63:VAL:CB	2.31	0.43
23:S:20:GLU:OE1	23:S:20:GLU:N	2.52	0.43
5:A:103:U:C5	5:A:104:C:C5	3.07	0.43
5:A:430:A:C5	5:A:431:C:C5	3.07	0.43
5:A:525:A:H1'	5:A:526:A:H5''	2.01	0.43
5:A:1893:A:H61	5:A:1903:A:H2'	1.83	0.43
5:A:2135:U:H4'	5:A:2177:U:H1'	2.00	0.43
27:W:10:THR:C	27:W:11:THR:HG22	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:32:LEU:HD12	27:W:37:LEU:HD23	2.01	0.43
5:A:102:A:N7	5:A:103:U:C6	2.87	0.43
5:A:209:U:H2'	5:A:210:A:H8	1.84	0.43
5:A:666:A:H3'	5:A:667:G:H8	1.83	0.43
5:A:2273:G:H2'	5:A:2274:A:H8	1.83	0.43
12:H:15:LYS:CD	12:H:17:TYR:CZ	3.02	0.43
19:O:89:ASP:O	19:O:89:ASP:CG	2.43	0.43
4:4:17:ILE:CD1	4:4:26:ILE:HG21	2.48	0.42
5:A:162:A:H2	5:A:166:A:H61	1.65	0.42
5:A:1094:A:C6	5:A:2778:G:C2	3.07	0.42
5:A:1617:A:H2'	5:A:1618:A:C8	2.53	0.42
5:A:2304:G:OP2	25:U:20:ASN:OD1	2.37	0.42
7:C:63:ARG:O	7:C:65:ILE:HG23	2.19	0.42
14:J:143:HIS:ND1	14:J:143:HIS:O	2.51	0.42
15:K:76:LYS:HB3	15:K:91:GLU:OE1	2.19	0.42
24:T:46:VAL:HG12	24:T:50:LYS:HZ2	1.83	0.42
26:V:40:VAL:CG1	26:V:45:LYS:CB	2.91	0.42
5:A:1490:G:H8	5:A:1592:A:O2'	2.02	0.42
5:A:2799:C:H5'	8:D:181:GLN:NE2	2.34	0.42
6:B:39:G:H3'	6:B:40:C:H6	1.84	0.42
10:F:109:PRO:HA	29:Y:50:ILE:HG12	2.01	0.42
10:F:133:LYS:HD3	10:F:133:LYS:N	2.24	0.42
11:G:92:VAL:O	11:G:92:VAL:CG2	2.67	0.42
13:I:66:LYS:HB3	13:I:66:LYS:HE3	1.85	0.42
15:K:1:MET:HG2	15:K:66:ILE:HG21	2.01	0.42
15:K:1:MET:N	15:K:2:LEU:CD1	2.82	0.42
19:O:33:LYS:HE3	19:O:33:LYS:HB2	1.75	0.42
22:R:13:THR:OG1	22:R:14:GLU:OE1	2.37	0.42
5:A:80:G:H2'	5:A:81:G:O4'	2.19	0.42
5:A:233:U:C5	5:A:235:G:C6	3.08	0.42
5:A:437:A:C2'	5:A:438:U:H5'	2.49	0.42
5:A:1496:G:N7	5:A:1502:A:N1	2.67	0.42
5:A:2161:A:H61	5:A:2184:G:C2'	2.32	0.42
10:F:7:LYS:HE2	10:F:12:VAL:HG22	2.01	0.42
11:G:26:VAL:HG21	11:G:76:VAL:HG12	2.01	0.42
13:I:35:ILE:H	13:I:35:ILE:HD12	1.84	0.42
14:J:91:VAL:HG22	14:J:92:THR:N	2.35	0.42
15:K:31:GLU:OE1	15:K:32:PHE:CE2	2.72	0.42
15:K:111:GLU:HG2	15:K:112:GLU:OE1	2.19	0.42
22:R:84:GLU:OE1	22:R:84:GLU:C	2.57	0.42
5:A:925:G:H3'	5:A:926:G:H8	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1000:G:H2'	5:A:1001:A:H2'	2.01	0.42
8:D:79:LYS:HE2	8:D:79:LYS:HB3	1.78	0.42
8:D:123:LYS:HE3	8:D:204:PRO:HA	2.00	0.42
8:D:128:GLN:CB	8:D:173:MET:CE	2.97	0.42
10:F:69:LYS:HE2	10:F:69:LYS:HB2	1.70	0.42
10:F:75:ALA:HA	10:F:78:ARG:HH12	1.85	0.42
13:I:53:LYS:HB2	13:I:53:LYS:HE2	1.66	0.42
24:T:73:MET:O	24:T:92:LEU:HD23	2.19	0.42
25:U:44:ILE:HG21	25:U:47:ARG:HG2	2.01	0.42
25:U:54:TYR:HD2	25:U:80:LYS:HD3	1.85	0.42
2:2:10:LYS:NZ	5:A:1346:G:OP2	2.48	0.42
5:A:1800:A:N7	5:A:1856:A:H1'	2.34	0.42
5:A:1805:U:H3'	5:A:1811:A:N6	2.34	0.42
5:A:2611:U:H2'	5:A:2612:U:H2'	2.00	0.42
10:F:67:VAL:O	10:F:69:LYS:HD3	2.20	0.42
14:J:47:ARG:NH2	14:J:50:PHE:HD1	2.18	0.42
14:J:80:ASP:OD1	14:J:81:GLN:N	2.52	0.42
15:K:26:TYR:CD1	15:K:26:TYR:N	2.87	0.42
16:L:92:ARG:CG	16:L:93:TYR:CE1	3.01	0.42
18:N:28:LEU:HD21	18:N:49:VAL:CG2	2.49	0.42
19:O:102:ASP:OD1	19:O:104:LYS:CE	2.67	0.42
21:Q:34:ALA:HB3	30:Z:27:MET:CE	2.50	0.42
23:S:85:PHE:HD1	23:S:88:GLY:C	2.23	0.42
24:T:48:PHE:CE2	24:T:89:ILE:HD13	2.54	0.42
27:W:11:THR:HB	27:W:60:ARG:HH11	1.85	0.42
5:A:115:C:HO2'	5:A:125:A:H8	1.61	0.42
5:A:390:A:H2'	5:A:391:A:C8	2.55	0.42
5:A:503:A:N1	5:A:516:A:H5''	2.35	0.42
5:A:1378:U:H3'	5:A:1434:U:O2	2.20	0.42
5:A:1726:A:H2'	5:A:1727:C:C6	2.55	0.42
5:A:2253:C:H2'	5:A:2254:A:O4'	2.19	0.42
5:A:2392:G:H4'	25:U:68:PHE:CZ	2.54	0.42
5:A:2859:G:C4	5:A:2860:U:C5	3.07	0.42
7:C:24:ILE:N	7:C:24:ILE:CD1	2.83	0.42
11:G:24:VAL:HG12	11:G:25:THR:H	1.84	0.42
18:N:85:LYS:HG2	18:N:86:ILE:N	2.35	0.42
5:A:351:G:H2'	5:A:352:A:C8	2.55	0.42
5:A:1235:C:C2	5:A:1236:G:C8	3.08	0.42
5:A:1751:G:H1'	5:A:1783:G:N3	2.35	0.42
5:A:1928:A:H2'	5:A:1929:C:C6	2.55	0.42
5:A:2608:G:OP2	5:A:2608:G:N2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:107:PRO:HD2	7:C:110:LEU:HB2	2.01	0.42
13:I:90:ASP:OD1	13:I:92:GLY:N	2.53	0.42
14:J:6:LEU:C	14:J:6:LEU:HD12	2.40	0.42
20:P:24:LYS:NZ	20:P:24:LYS:HB3	2.35	0.42
23:S:45:GLN:OE1	23:S:45:GLN:CA	2.67	0.42
24:T:13:GLN:HB3	24:T:18:LEU:CD2	2.50	0.42
5:A:328:G:H1'	5:A:329:A:H5'	2.00	0.42
5:A:502:C:H6	22:R:68:TYR:CE1	2.37	0.42
5:A:1152:U:C5	5:A:1153:C:C2	3.07	0.42
5:A:1203:U:C2	5:A:1204:G:C8	3.08	0.42
5:A:1804:U:O2	5:A:1804:U:O4'	2.37	0.42
5:A:2332:U:O4	10:F:40:VAL:HG12	2.19	0.42
5:A:2415:A:H5'	5:A:2416:G:OP2	2.19	0.42
5:A:2652:G:H2'	5:A:2653:C:O4'	2.20	0.42
5:A:2859:G:O4'	16:L:45:GLU:OE1	2.38	0.42
8:D:18:GLU:O	8:D:21:GLU:OE1	2.37	0.42
10:F:7:LYS:O	10:F:7:LYS:HG2	2.20	0.42
10:F:44:VAL:HB	10:F:78:ARG:HB2	2.01	0.42
11:G:121:ILE:CG2	11:G:123:PHE:CE1	2.96	0.42
15:K:31:GLU:HG2	15:K:32:PHE:N	2.34	0.42
27:W:9:LEU:HB2	27:W:14:ILE:HD11	2.01	0.42
3:3:56:LYS:NZ	3:3:56:LYS:HB3	2.34	0.42
5:A:227:G:H21	5:A:234:C:H41	1.66	0.42
5:A:1053:A:C8	5:A:1197:C:O2'	2.72	0.42
5:A:1426:G:H2'	5:A:1427:U:O4'	2.20	0.42
10:F:13:THR:O	10:F:17:MET:HB2	2.20	0.42
11:G:131:VAL:HG12	11:G:132:LYS:N	2.34	0.42
13:I:20:LEU:O	13:I:41:CYS:HB2	2.19	0.42
13:I:43:VAL:HG23	13:I:54:LYS:HA	2.00	0.42
15:K:54:MET:HE2	15:K:54:MET:HB2	1.80	0.42
18:N:93:LYS:O	18:N:93:LYS:HG2	2.20	0.42
22:R:56:MET:CE	22:R:79:ILE:HD11	2.49	0.42
22:R:89:LEU:HD12	27:W:30:PHE:CE2	2.54	0.42
5:A:388:A:H8	5:A:389:A:H2	1.68	0.42
5:A:1306:A:H1'	5:A:2040:A:N6	2.35	0.42
5:A:1630:A:H1'	5:A:1631:G:C8	2.54	0.42
5:A:2435:U:H2'	5:A:2436:G:C8	2.55	0.42
5:A:2707:C:H5'	8:D:202:PRO:HA	2.01	0.42
6:B:53:U:H2'	6:B:54:U:C6	2.54	0.42
7:C:16:MET:CE	7:C:207:LYS:HG3	2.50	0.42
11:G:81:GLN:OE1	11:G:81:GLN:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:35:ILE:HG21	13:I:103:ALA:HB3	2.00	0.42
18:N:15:LEU:HD22	18:N:79:HIS:NE2	2.35	0.42
26:V:46:LYS:C	26:V:47:VAL:HG13	2.40	0.42
5:A:242:U:H2'	5:A:243:U:O4'	2.20	0.41
5:A:272:C:H3'	5:A:298:U:O4	2.20	0.41
5:A:864:A:N7	5:A:1227:U:C5	2.88	0.41
5:A:1335:C:H2'	5:A:1336:G:O4'	2.20	0.41
5:A:1476:G:H8	5:A:1476:G:H5''	1.85	0.41
5:A:1868:U:N3	5:A:1869:G:N7	2.68	0.41
5:A:2142:G:O2'	5:A:2192:G:N1	2.45	0.41
5:A:2346:U:OP2	5:A:2346:U:C6	2.73	0.41
5:A:2793:G:H2'	5:A:2793:G:N3	2.34	0.41
6:B:61:C:H2'	6:B:62:U:C6	2.55	0.41
7:C:100:GLU:HG3	7:C:101:LYS:N	2.35	0.41
7:C:117:GLU:CG	7:C:122:ALA:HB1	2.46	0.41
7:C:126:VAL:O	7:C:126:VAL:HG12	2.19	0.41
8:D:128:GLN:CG	8:D:173:MET:CE	2.96	0.41
23:S:41:MET:CE	23:S:61:ALA:HB2	2.50	0.41
4:4:7:VAL:HG13	4:4:34:GLN:HB3	2.02	0.41
5:A:305:A:H62	5:A:410:G:H21	1.67	0.41
5:A:398:C:H2'	5:A:399:U:O4'	2.20	0.41
5:A:1692:C:H5	5:A:2036:G:H1	1.68	0.41
5:A:2680:U:H2'	5:A:2681:A:C2	2.55	0.41
6:B:73:G:H21	24:T:88:HIS:CE1	2.37	0.41
10:F:5:LYS:NZ	10:F:94:GLU:HA	2.36	0.41
11:G:10:ASP:OD1	11:G:69:ARG:CZ	2.68	0.41
11:G:120:ASN:OD1	11:G:120:ASN:N	2.52	0.41
15:K:69:PHE:HA	15:K:70:PRO:HD3	1.85	0.41
16:L:105:LYS:HA	16:L:117:VAL:HG12	2.02	0.41
19:O:104:LYS:HE2	19:O:104:LYS:N	2.33	0.41
22:R:64:ARG:CB	22:R:64:ARG:CZ	2.85	0.41
25:U:19:LYS:HB3	25:U:19:LYS:HZ3	1.84	0.41
27:W:28:LEU:HD13	27:W:43:ILE:HG12	2.02	0.41
3:3:48:ARG:HH11	3:3:48:ARG:HG2	1.85	0.41
5:A:269:G:H21	5:A:322:A:H8	1.63	0.41
5:A:441:C:H2'	5:A:442:G:H8	1.84	0.41
5:A:1512:U:H2'	5:A:1513:A:H8	1.85	0.41
5:A:2228:C:H2'	5:A:2229:C:C6	2.55	0.41
5:A:2345:A:H5'	5:A:2346:U:OP2	2.20	0.41
6:B:45:C:H2'	6:B:46:A:O4'	2.21	0.41
7:C:68:LYS:HD2	7:C:149:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:69:ARG:C	11:G:69:ARG:CD	2.81	0.41
29:Y:18:THR:HG22	29:Y:53:ASP:OD2	2.20	0.41
5:A:26:G:C2'	5:A:27:G:O4'	2.69	0.41
5:A:35:G:C6	5:A:492:G:N2	2.89	0.41
5:A:512:A:H3'	5:A:513:G:O4'	2.20	0.41
5:A:648:G:N1	5:A:669:C:N3	2.68	0.41
5:A:687:G:N2	5:A:689:A:H5'	2.36	0.41
5:A:1867:G:C5	5:A:1868:U:C5	3.09	0.41
5:A:2101:U:O2'	5:A:2624:G:H1'	2.20	0.41
5:A:2115:A:H2'	5:A:2116:U:O4'	2.21	0.41
5:A:2319:U:O2'	5:A:2320:C:H5'	2.21	0.41
5:A:2803:A:C2	5:A:2805:A:C2	3.08	0.41
7:C:100:GLU:OE2	7:C:102:ARG:CD	2.68	0.41
9:E:5:ASP:HA	9:E:13:LYS:HZ1	1.86	0.41
10:F:36:VAL:CG1	10:F:57:LEU:CD2	2.98	0.41
17:M:9:LYS:H	17:M:9:LYS:HG2	1.37	0.41
26:V:7:VAL:HG21	26:V:53:ALA:HB1	2.02	0.41
2:2:19:PHE:HB2	5:A:125:A:C2	2.55	0.41
3:3:7:HIS:CD2	3:3:10:ALA:H	2.31	0.41
5:A:1088:C:H5'	5:A:1092:A:H1'	2.02	0.41
5:A:1751:G:H1'	5:A:1783:G:C4	2.55	0.41
5:A:1816:A:H2'	5:A:1817:C:O4'	2.20	0.41
5:A:1818:A:N6	5:A:1855:G:O2'	2.52	0.41
5:A:1862:G:H1	5:A:1932:C:H5	1.67	0.41
5:A:2273:G:H2'	5:A:2274:A:C8	2.55	0.41
5:A:2536:G:C6	5:A:2537:C:C5	3.09	0.41
5:A:2541:U:H2'	5:A:2542:C:C6	2.55	0.41
7:C:261:ARG:H	7:C:261:ARG:HG2	1.67	0.41
11:G:157:TYR:O	11:G:171:ARG:NH2	2.53	0.41
21:Q:39:THR:OG1	30:Z:25:PRO:HG3	2.21	0.41
5:A:110:A:C6	5:A:111:U:C4	3.08	0.41
5:A:644:C:O2'	5:A:645:A:H8	2.02	0.41
5:A:1303:A:O4'	5:A:1305:U:C6	2.73	0.41
5:A:2863:G:C2	5:A:2864:A:C8	3.08	0.41
6:B:45:C:O3'	17:M:100:LEU:HD13	2.20	0.41
9:E:3:ASN:OD1	9:E:16:SER:CB	2.67	0.41
9:E:167:ALA:CA	9:E:170:ILE:HD12	2.36	0.41
10:F:55:GLU:OE1	10:F:55:GLU:C	2.59	0.41
10:F:95:ARG:HH22	29:Y:9:TYR:CB	2.33	0.41
11:G:68:THR:HA	11:G:71:LEU:HB2	2.01	0.41
12:H:60:ALA:HB3	12:H:127:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:20:LEU:HD12	13:I:21:THR:N	2.35	0.41
16:L:102:ARG:NH2	16:L:122:VAL:HG23	2.35	0.41
18:N:34:ILE:HD12	18:N:43:GLN:HG2	2.02	0.41
1:1:14:ASP:OD1	1:1:14:ASP:C	2.59	0.41
5:A:219:A:C8	5:A:478:A:N6	2.88	0.41
5:A:1329:G:H2'	5:A:1330:U:C6	2.55	0.41
5:A:1856:A:C8	5:A:1857:C:C5	3.09	0.41
5:A:2591:A:O2'	5:A:2592:A:O5'	2.26	0.41
8:D:18:GLU:O	8:D:21:GLU:OE2	2.39	0.41
9:E:140:LYS:CD	9:E:170:ILE:CG2	2.97	0.41
10:F:138:PHE:CB	10:F:141:ILE:HG13	2.42	0.41
10:F:159:THR:O	10:F:159:THR:HG22	2.21	0.41
11:G:130:VAL:O	11:G:130:VAL:HG12	2.20	0.41
12:H:38:ARG:HH11	12:H:38:ARG:HG3	1.85	0.41
12:H:68:ASN:O	12:H:68:ASN:CG	2.58	0.41
14:J:88:GLY:N	14:J:120:LYS:O	2.50	0.41
15:K:38:THR:OG1	15:K:127:VAL:CG2	2.69	0.41
17:M:40:ILE:HG23	17:M:76:VAL:HG21	2.01	0.41
18:N:14:GLN:O	18:N:14:GLN:CG	2.65	0.41
18:N:60:THR:OG1	18:N:75:THR:HG22	2.20	0.41
18:N:99:LEU:HB3	18:N:102:LEU:HD13	2.02	0.41
25:U:35:ASP:OD1	25:U:35:ASP:N	2.54	0.41
25:U:57:GLU:CD	25:U:57:GLU:N	2.73	0.41
2:2:4:ARG:O	2:2:7:GLN:OE1	2.39	0.41
5:A:1238:U:O4'	19:O:4:VAL:HG23	2.20	0.41
5:A:1326:C:H2'	5:A:1327:C:H6	1.86	0.41
5:A:1542:C:H6	5:A:1542:C:H2'	1.77	0.41
5:A:1712:A:N3	5:A:1714:C:C4	2.89	0.41
5:A:1989:C:H4'	5:A:1990:C:C5	2.56	0.41
5:A:2107:G:H5'	26:V:19:SER:CB	2.51	0.41
5:A:2109:A:H3'	5:A:2110:G:H8	1.86	0.41
11:G:26:VAL:HG13	11:G:79:VAL:HG11	1.95	0.41
26:V:39:LEU:HA	26:V:39:LEU:HD12	1.84	0.41
5:A:285:U:H6	5:A:285:U:H2'	1.75	0.41
5:A:409:G:H3'	5:A:410:G:H8	1.85	0.41
5:A:774:G:O4'	7:C:207:LYS:NZ	2.53	0.41
5:A:902:A:O2'	5:A:903:G:H5'	2.20	0.41
5:A:1415:A:H1'	5:A:1416:U:C5	2.55	0.41
5:A:1501:G:H2'	5:A:1502:A:C8	2.56	0.41
5:A:2026:C:H5''	5:A:2750:C:O2'	2.20	0.41
5:A:2725:U:C2	5:A:2726:C:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:183:MET:HE3	7:C:271:VAL:HG22	2.02	0.41
8:D:14:GLN:OE1	8:D:22:LEU:HD11	2.20	0.41
10:F:36:VAL:HG12	10:F:36:VAL:O	2.21	0.41
15:K:31:GLU:HG2	15:K:32:PHE:CG	2.54	0.41
25:U:77:PHE:CD1	25:U:77:PHE:N	2.88	0.41
1:1:35:TYR:CD1	1:1:42:TYR:HE1	2.39	0.41
1:1:46:ARG:NH1	1:1:46:ARG:HB2	2.36	0.41
5:A:101:G:H4'	5:A:102:A:O4'	2.21	0.41
5:A:441:C:H2'	5:A:442:G:C8	2.55	0.41
5:A:1358:A:H3'	5:A:1359:A:H8	1.86	0.41
5:A:1432:A:O2'	5:A:1434:U:C6	2.74	0.41
5:A:1595:C:C2'	5:A:1596:G:H5'	2.51	0.41
5:A:2434:A:OP1	5:A:2434:A:C8	2.75	0.41
5:A:2553:G:C2	5:A:2554:C:H1'	2.56	0.41
6:B:67:G:O6	6:B:104:A:H2	2.04	0.41
9:E:146:LEU:O	9:E:147:GLU:HG3	2.21	0.41
10:F:66:LEU:O	10:F:66:LEU:CD1	2.49	0.41
10:F:142:ASP:HB3	10:F:144:ASP:H	1.86	0.41
11:G:23:HIS:CE1	11:G:24:VAL:O	2.74	0.41
11:G:158:LYS:HA	11:G:171:ARG:NH2	2.35	0.41
12:H:24:GLN:HE21	12:H:143:LEU:HD12	1.85	0.41
12:H:69:LYS:HE2	12:H:69:LYS:HB3	1.83	0.41
13:I:71:ARG:NH1	18:N:74:ARG:NE	2.69	0.41
18:N:19:LEU:O	18:N:19:LEU:HD23	2.20	0.41
21:Q:11:ARG:HH11	21:Q:11:ARG:C	2.24	0.41
27:W:44:ARG:CD	27:W:48:LYS:NZ	2.84	0.41
5:A:303:G:H2'	5:A:304:G:O4'	2.21	0.40
5:A:710:C:H2'	5:A:711:G:H8	1.86	0.40
5:A:1708:A:N3	5:A:1709:A:C8	2.88	0.40
5:A:2617:A:H2'	5:A:2618:C:C6	2.56	0.40
5:A:2905:C:N4	30:Z:39:SER:OG	2.47	0.40
6:B:55:A:H2'	6:B:56:A:H8	1.85	0.40
7:C:6:TYR:CD2	7:C:16:MET:HG2	2.56	0.40
7:C:111:GLU:H	7:C:114:GLN:NE2	2.18	0.40
7:C:181:VAL:CG2	7:C:271:VAL:HB	2.51	0.40
8:D:49:ILE:HD12	8:D:51:VAL:HG23	2.03	0.40
10:F:5:LYS:NZ	10:F:94:GLU:CG	2.84	0.40
12:H:141:TYR:C	12:H:141:TYR:HD1	2.24	0.40
15:K:26:TYR:HD1	15:K:26:TYR:N	2.19	0.40
15:K:42:ILE:HG21	15:K:47:ILE:HG12	2.00	0.40
16:L:22:THR:O	16:L:26:ILE:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:112:LYS:HE3	19:O:112:LYS:HB2	1.82	0.40
23:S:56:ILE:N	23:S:56:ILE:CD1	2.85	0.40
1:1:12:CYS:SG	1:1:39:LEU:HG	2.61	0.40
5:A:82:G:H22	5:A:102:A:H5''	1.87	0.40
5:A:437:A:O5'	5:A:438:U:OP2	2.39	0.40
5:A:1113:A:H4'	5:A:1140:A:O2'	2.21	0.40
5:A:1229:G:OP1	14:J:30:THR:OG1	2.39	0.40
5:A:1723:A:H2	5:A:1791:G:O4'	2.04	0.40
5:A:2564:U:H2'	5:A:2565:C:H6	1.87	0.40
9:E:34:PHE:CD1	14:J:6:LEU:HD13	2.57	0.40
12:H:18:VAL:CG1	12:H:58:ILE:CG2	2.99	0.40
12:H:95:ARG:CG	12:H:96:THR:HG23	2.51	0.40
24:T:84:ASN:O	24:T:85:GLN:CG	2.68	0.40
5:A:421:C:H2'	5:A:422:G:H8	1.86	0.40
5:A:491:C:H2'	5:A:492:G:O4'	2.20	0.40
5:A:2091:C:H2'	5:A:2092:C:C6	2.56	0.40
5:A:2300:A:H2'	5:A:2301:A:C8	2.56	0.40
9:E:146:LEU:C	9:E:147:GLU:HG3	2.41	0.40
11:G:19:PHE:CD1	11:G:45:GLN:NE2	2.89	0.40
24:T:49:ILE:O	24:T:53:ARG:HG2	2.21	0.40
1:1:14:ASP:CB	1:1:38:ARG:NH2	2.79	0.40
5:A:310:C:O2'	5:A:311:U:H2'	2.21	0.40
5:A:851:C:C2	5:A:852:U:C5	3.09	0.40
5:A:858:U:H2'	5:A:859:C:C6	2.57	0.40
5:A:1308:C:H5''	5:A:1309:G:H5'	2.04	0.40
5:A:1565:U:C4	5:A:1566:G:N7	2.90	0.40
5:A:2590:U:C2	5:A:2592:A:OP2	2.74	0.40
6:B:46:A:H2'	6:B:47:C:O4'	2.22	0.40
7:C:16:MET:HB2	7:C:16:MET:HE2	1.79	0.40
7:C:158:ALA:HA	7:C:195:VAL:HG23	2.03	0.40
7:C:159:GLY:H	7:C:195:VAL:HG23	1.86	0.40
7:C:182:ARG:NH1	7:C:182:ARG:CG	2.78	0.40
8:D:27:VAL:CG2	8:D:194:VAL:CG1	2.97	0.40
10:F:132:VAL:CG2	10:F:152:MET:CE	2.99	0.40
10:F:140:GLU:H	10:F:140:GLU:HG3	1.58	0.40
11:G:89:LEU:H	11:G:129:THR:HG23	1.86	0.40
12:H:18:VAL:HG23	12:H:138:PRO:HB2	2.04	0.40
12:H:107:LYS:NZ	12:H:120:GLY:O	2.55	0.40
15:K:33:GLY:O	15:K:132:VAL:CG2	2.70	0.40
15:K:39:THR:HB	15:K:98:LYS:HA	2.03	0.40
17:M:13:LYS:O	17:M:17:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:72:LEU:HD23	17:M:75:LYS:HG3	2.03	0.40
17:M:92:ILE:HD12	17:M:93:VAL:N	2.36	0.40
22:R:52:SER:OG	22:R:81:THR:HG21	2.22	0.40
27:W:19:LYS:HB3	27:W:19:LYS:HZ2	1.86	0.40
5:A:234:C:OP2	5:A:235:G:O4'	2.40	0.40
5:A:2677:C:H2'	5:A:2678:C:C6	2.56	0.40
5:A:2727:G:H2'	5:A:2728:U:H6	1.86	0.40
7:C:274:ARG:HA	7:C:274:ARG:HD3	1.55	0.40
10:F:60:ILE:HG12	10:F:137:ILE:CG2	2.52	0.40
10:F:137:ILE:HD11	10:F:152:MET:HE1	2.04	0.40
11:G:86:VAL:HG12	11:G:165:GLN:CB	2.52	0.40
15:K:101:ARG:O	15:K:103:LEU:HD11	2.17	0.40
16:L:99:GLY:O	16:L:100:TYR:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	45/47 (96%)	41 (91%)	4 (9%)	0	100	100
2	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
3	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
4	4	35/37 (95%)	30 (86%)	5 (14%)	0	100	100
7	C	272/274 (99%)	241 (89%)	29 (11%)	2 (1%)	19	33
8	D	213/215 (99%)	196 (92%)	17 (8%)	0	100	100
9	E	204/206 (99%)	187 (92%)	17 (8%)	0	100	100
10	F	173/175 (99%)	140 (81%)	31 (18%)	2 (1%)	11	19
11	G	173/175 (99%)	155 (90%)	18 (10%)	0	100	100
12	H	143/145 (99%)	129 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
14	J	144/146 (99%)	136 (94%)	8 (6%)	0	100	100
15	K	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
16	L	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
17	M	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
18	N	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
19	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
20	P	100/102 (98%)	94 (94%)	4 (4%)	2 (2%)	6	10
21	Q	110/117 (94%)	104 (94%)	6 (6%)	0	100	100
22	R	87/89 (98%)	82 (94%)	5 (6%)	0	100	100
23	S	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
24	T	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
25	U	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
26	V	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
27	W	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
28	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
29	Y	57/59 (97%)	52 (91%)	4 (7%)	1 (2%)	7	12
30	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
All	All	3071/3132 (98%)	2819 (92%)	245 (8%)	7 (0%)	45	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	Y	2	LYS
7	C	126	VAL
20	P	51	PRO
10	F	76	THR
20	P	50	ALA
7	C	179	GLY
10	F	139	PRO

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	44/45 (98%)	41 (93%)	3 (7%)	13	25
2	2	39/39 (100%)	38 (97%)	1 (3%)	41	66
3	3	55/55 (100%)	50 (91%)	5 (9%)	7	14
4	4	35/35 (100%)	29 (83%)	6 (17%)	1	3
7	C	220/221 (100%)	204 (93%)	16 (7%)	11	22
8	D	173/173 (100%)	160 (92%)	13 (8%)	11	21
9	E	168/168 (100%)	153 (91%)	15 (9%)	8	15
10	F	139/154 (90%)	121 (87%)	18 (13%)	3	6
11	G	123/153 (80%)	107 (87%)	16 (13%)	3	6
12	H	122/123 (99%)	117 (96%)	5 (4%)	26	47
13	I	100/100 (100%)	92 (92%)	8 (8%)	10	19
14	J	109/112 (97%)	104 (95%)	5 (5%)	23	42
15	K	108/114 (95%)	95 (88%)	13 (12%)	4	7
16	L	96/101 (95%)	92 (96%)	4 (4%)	25	46
17	M	86/95 (90%)	71 (83%)	15 (17%)	1	2
18	N	93/100 (93%)	84 (90%)	9 (10%)	6	12
19	O	96/96 (100%)	92 (96%)	4 (4%)	25	46
20	P	84/86 (98%)	82 (98%)	2 (2%)	44	68
21	Q	89/94 (95%)	82 (92%)	7 (8%)	10	19
22	R	78/80 (98%)	70 (90%)	8 (10%)	6	11
23	S	81/88 (92%)	77 (95%)	4 (5%)	21	40
24	T	75/82 (92%)	67 (89%)	8 (11%)	5	10
25	U	60/64 (94%)	53 (88%)	7 (12%)	4	8
26	V	44/49 (90%)	37 (84%)	7 (16%)	2	3
27	W	58/60 (97%)	53 (91%)	5 (9%)	8	16
28	X	52/52 (100%)	50 (96%)	2 (4%)	28	51
29	Y	23/56 (41%)	20 (87%)	3 (13%)	3	6
30	Z	36/44 (82%)	35 (97%)	1 (3%)	38	63
All	All	2486/2639 (94%)	2276 (92%)	210 (8%)	11	17

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	16	ASN
1	1	23	LYS
1	1	29	ARG
2	2	15	LYS
3	3	31	HIS
3	3	52	LYS
3	3	56	LYS
3	3	62	LEU
3	3	65	LYS
4	4	4	ARG
4	4	8	LYS
4	4	11	CYS
4	4	12	GLU
4	4	15	LYS
4	4	22	LYS
7	C	3	ILE
7	C	4	LYS
7	C	66	ASP
7	C	75	ASN
7	C	116	VAL
7	C	123	ASP
7	C	134	ASN
7	C	136	PRO
7	C	177	ARG
7	C	243	ARG
7	C	245	SER
7	C	265	SER
7	C	267	ASP
7	C	272	ARG
7	C	274	ARG
7	C	275	LYS
8	D	13	THR
8	D	54	GLU
8	D	55	ASP
8	D	61	LYS
8	D	78	LYS
8	D	108	ASP
8	D	137	SER
8	D	138	ARG
8	D	158	SER
8	D	170	PRO
8	D	193	LYS

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Mol	Chain	Res	Type
8	D	200	ASN
8	D	205	LYS
9	E	9	LEU
9	E	10	ASP
9	E	13	LYS
9	E	14	SER
9	E	20	SER
9	E	41	ARG
9	E	45	ARG
9	E	46	GLN
9	E	74	ARG
9	E	84	ARG
9	E	117	LYS
9	E	143	LEU
9	E	147	GLU
9	E	161	VAL
9	E	176	THR
10	F	17	MET
10	F	20	PHE
10	F	24	SER
10	F	38	MET
10	F	45	GLN
10	F	72	LYS
10	F	78	ARG
10	F	85	ILE
10	F	95	ARG
10	F	120	LYS
10	F	128	TYR
10	F	133	LYS
10	F	143	TYR
10	F	148	LYS
10	F	150	ARG
10	F	152	MET
10	F	156	ILE
10	F	168	GLU
11	G	39	GLU
11	G	45	GLN
11	G	49	THR
11	G	56	SER
11	G	58	SER
11	G	68	THR
11	G	69	ARG

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Mol	Chain	Res	Type
11	G	77	GLN
11	G	79	VAL
11	G	85	LYS
11	G	97	GLN
11	G	107	VAL
11	G	109	TYR
11	G	120	ASN
11	G	124	SER
11	G	175	LYS
12	H	3	GLN
12	H	11	ASN
12	H	25	THR
12	H	94	ARG
12	H	141	TYR
13	I	3	GLN
13	I	34	ASN
13	I	70	ARG
13	I	71	ARG
13	I	73	ASP
13	I	81	GLU
13	I	120	GLU
13	I	122	LEU
14	J	7	LYS
14	J	13	ARG
14	J	80	ASP
14	J	87	ASP
14	J	107	SER
15	K	1	MET
15	K	7	VAL
15	K	14	ARG
15	K	16	LYS
15	K	18	THR
15	K	39	THR
15	K	44	SER
15	K	45	ARG
15	K	56	ARG
15	K	59	LYS
15	K	72	THR
15	K	130	LYS
15	K	133	LYS
16	L	29	ARG
16	L	59	ARG

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Mol	Chain	Res	Type
16	L	79	GLN
16	L	102	ARG
17	M	9	LYS
17	M	11	ARG
17	M	13	LYS
17	M	21	ASN
17	M	23	SER
17	M	27	GLU
17	M	36	SER
17	M	45	ILE
17	M	55	GLN
17	M	57	SER
17	M	58	SER
17	M	66	THR
17	M	74	THR
17	M	87	LYS
17	M	93	VAL
18	N	14	GLN
18	N	18	ASP
18	N	19	LEU
18	N	28	LEU
18	N	43	GLN
18	N	57	VAL
18	N	65	LYS
18	N	82	LYS
18	N	96	ARG
19	O	51	ARG
19	O	59	LYS
19	O	78	ARG
19	O	117	LEU
20	P	53	VAL
20	P	78	ARG
21	Q	2	GLU
21	Q	38	LEU
21	Q	43	SER
21	Q	64	MET
21	Q	72	LYS
21	Q	81	THR
21	Q	86	ARG
22	R	9	ARG
22	R	13	THR
22	R	14	GLU

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Mol	Chain	Res	Type
22	R	23	ASP
22	R	49	LYS
22	R	84	GLU
22	R	89	LEU
22	R	90	PHE
23	S	4	LYS
23	S	7	ASP
23	S	76	ASN
23	S	100	GLU
24	T	3	SER
24	T	10	GLN
24	T	38	ASN
24	T	50	LYS
24	T	53	ARG
24	T	58	ASN
24	T	77	TYR
24	T	90	ASP
25	U	12	LYS
25	U	35	ASP
25	U	45	LEU
25	U	53	ILE
25	U	75	VAL
25	U	82	ARG
25	U	84	LYS
26	V	3	LYS
26	V	11	LYS
26	V	27	ARG
26	V	41	ASP
26	V	50	SER
26	V	52	ARG
26	V	58	LYS
27	W	2	LYS
27	W	30	PHE
27	W	36	GLN
27	W	39	GLU
27	W	44	ARG
28	X	10	ARG
28	X	18	THR
29	Y	2	LYS
29	Y	5	ILE
29	Y	9	TYR
30	Z	39	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	7	GLN
3	3	7	HIS
7	C	114	GLN
7	C	143	ASN
8	D	47	ASN
10	F	63	GLN
11	G	65	HIS
12	H	78	HIS
12	H	137	GLN
14	J	83	ASN
15	K	46	GLN
16	L	106	GLN
17	M	15	HIS
18	N	31	HIS
18	N	43	GLN
21	Q	40	ASN
22	R	37	GLN
23	S	76	ASN
24	T	88	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	2875/2921 (98%)	939 (32%)	87 (3%)
6	B	114/115 (99%)	38 (33%)	4 (3%)
All	All	2989/3036 (98%)	977 (32%)	91 (3%)

All (977) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	13	A
5	A	18	C
5	A	28	A
5	A	34	U
5	A	36	G
5	A	39	C
5	A	46	C
5	A	49	A
5	A	50	U
5	A	51	G

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Mol	Chain	Res	Type
5	A	55	G
5	A	57	C
5	A	58	G
5	A	63	U
5	A	64	A
5	A	70	G
5	A	71	A
5	A	74	U
5	A	75	G
5	A	80	G
5	A	83	G
5	A	84	A
5	A	90	A
5	A	91	A
5	A	92	G
5	A	93	U
5	A	94	A
5	A	95	A
5	A	96	G
5	A	98	U
5	A	99	U
5	A	101	G
5	A	103	U
5	A	116	G
5	A	117	A
5	A	118	A
5	A	119	U
5	A	135	G
5	A	140	A
5	A	149	U
5	A	150	A
5	A	157	U
5	A	158	G
5	A	162	A
5	A	164	A
5	A	172	U
5	A	176	A
5	A	177	G
5	A	179	A
5	A	180	G
5	A	183	A
5	A	184	C

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Mol	Chain	Res	Type
5	A	189	G
5	A	191	A
5	A	199	A
5	A	200	A
5	A	202	A
5	A	213	C
5	A	215	G
5	A	216	A
5	A	218	G
5	A	219	A
5	A	224	A
5	A	225	A
5	A	228	A
5	A	229	A
5	A	230	A
5	A	231	A
5	A	232	U
5	A	233	U
5	A	234	C
5	A	235	G
5	A	242	U
5	A	244	A
5	A	248	G
5	A	251	G
5	A	255	G
5	A	267	G
5	A	268	A
5	A	269	G
5	A	270	C
5	A	273	A
5	A	280	C
5	A	283	G
5	A	285	U
5	A	286	U
5	A	289	U
5	A	292	U
5	A	293	U
5	A	294	G
5	A	299	U
5	A	300	G
5	A	301	U
5	A	302	A

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Mol	Chain	Res	Type
5	A	303	G
5	A	305	A
5	A	309	U
5	A	310	C
5	A	311	U
5	A	312	A
5	A	318	A
5	A	321	U
5	A	324	A
5	A	326	A
5	A	327	G
5	A	328	G
5	A	329	A
5	A	333	C
5	A	335	U
5	A	336	U
5	A	353	A
5	A	354	A
5	A	360	A
5	A	372	A
5	A	388	A
5	A	390	A
5	A	392	U
5	A	393	G
5	A	397	U
5	A	399	U
5	A	401	U
5	A	403	U
5	A	404	U
5	A	405	G
5	A	406	A
5	A	411	A
5	A	417	A
5	A	432	G
5	A	433	U
5	A	434	G
5	A	435	A
5	A	436	A
5	A	437	A
5	A	438	U
5	A	447	A
5	A	448	A

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Mol	Chain	Res	Type
5	A	449	U
5	A	451	U
5	A	452	G
5	A	459	C
5	A	460	C
5	A	461	A
5	A	463	C
5	A	468	A
5	A	482	U
5	A	489	A
5	A	490	C
5	A	492	G
5	A	493	A
5	A	497	U
5	A	502	C
5	A	503	A
5	A	506	A
5	A	507	C
5	A	510	U
5	A	512	A
5	A	513	G
5	A	514	G
5	A	516	A
5	A	517	A
5	A	518	A
5	A	520	G
5	A	521	U
5	A	523	A
5	A	525	A
5	A	527	G
5	A	529	A
5	A	530	C
5	A	537	A
5	A	540	G
5	A	549	U
5	A	550	A
5	A	553	A
5	A	554	C
5	A	565	G
5	A	566	U
5	A	567	G
5	A	572	C

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Mol	Chain	Res	Type
5	A	574	A
5	A	575	G
5	A	576	U
5	A	577	A
5	A	578	G
5	A	581	A
5	A	583	A
5	A	591	A
5	A	592	A
5	A	606	G
5	A	608	C
5	A	616	G
5	A	617	A
5	A	618	A
5	A	619	U
5	A	621	A
5	A	623	C
5	A	629	A
5	A	630	G
5	A	643	G
5	A	644	C
5	A	645	A
5	A	646	A
5	A	647	G
5	A	657	U
5	A	658	A
5	A	659	A
5	A	661	U
5	A	666	A
5	A	668	C
5	A	672	A
5	A	682	A
5	A	688	A
5	A	689	A
5	A	690	U
5	A	691	A
5	A	696	G
5	A	698	U
5	A	699	U
5	A	700	A
5	A	715	A
5	A	716	C

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Mol	Chain	Res	Type
5	A	720	A
5	A	722	A
5	A	731	U
5	A	746	G
5	A	749	G
5	A	775	A
5	A	792	5MU
5	A	797	A
5	A	802	G
5	A	805	G
5	A	809	A
5	A	810	A
5	A	815	G
5	A	816	G
5	A	820	G
5	A	821	C
5	A	822	G
5	A	827	A
5	A	828	A
5	A	829	U
5	A	830	U
5	A	834	A
5	A	835	U
5	A	837	G
5	A	838	A
5	A	850	G
5	A	856	U
5	A	857	C
5	A	868	A
5	A	872	U
5	A	873	U
5	A	891	A
5	A	899	U
5	A	904	G
5	A	911	A
5	A	917	U
5	A	922	G
5	A	925	G
5	A	926	G
5	A	927	G
5	A	928	C
5	A	938	G

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Mol	Chain	Res	Type
5	A	939	U
5	A	940	U
5	A	942	C
5	A	943	C
5	A	944	G
5	A	945	A
5	A	951	G
5	A	952	A
5	A	955	A
5	A	957	C
5	A	960	C
5	A	964	U
5	A	965	G
5	A	970	U
5	A	971	U
5	A	973	A
5	A	975	U
5	A	977	A
5	A	985	A
5	A	989	A
5	A	990	G
5	A	992	A
5	A	993	C
5	A	1003	A
5	A	1005	G
5	A	1012	G
5	A	1018	A
5	A	1019	A
5	A	1024	A
5	A	1027	A
5	A	1028	G
5	A	1029	C
5	A	1033	G
5	A	1034	A
5	A	1035	C
5	A	1037	A
5	A	1040	A
5	A	1043	U
5	A	1046	G
5	A	1047	G
5	A	1056	U
5	A	1057	A

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Mol	Chain	Res	Type
5	A	1061	G
5	A	1063	U
5	A	1064	A
5	A	1066	G
5	A	1070	A
5	A	1071	A
5	A	1077	U
5	A	1083	G
5	A	1086	G
5	A	1089	C
5	A	1090	A
5	A	1091	G
5	A	1092	A
5	A	1093	C
5	A	1094	A
5	A	1095	A
5	A	1096	C
5	A	1097	U
5	A	1098	A
5	A	1100	G
5	A	1101	A
5	A	1105	U
5	A	1106	G
5	A	1109	U
5	A	1111	A
5	A	1113	A
5	A	1114	A
5	A	1115	G
5	A	1116	C
5	A	1117	A
5	A	1118	G
5	A	1119	C
5	A	1120	C
5	A	1125	U
5	A	1126	U
5	A	1127	U
5	A	1130	A
5	A	1131	G
5	A	1132	A
5	A	1133	G
5	A	1135	G
5	A	1138	U

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Mol	Chain	Res	Type
5	A	1143	G
5	A	1145	U
5	A	1147	A
5	A	1148	C
5	A	1149	U
5	A	1151	G
5	A	1153	C
5	A	1154	G
5	A	1155	A
5	A	1156	G
5	A	1157	U
5	A	1159	A
5	A	1160	C
5	A	1163	U
5	A	1166	G
5	A	1174	U
5	A	1175	G
5	A	1176	U
5	A	1177	A
5	A	1179	C
5	A	1180	G
5	A	1183	G
5	A	1185	U
5	A	1186	A
5	A	1192	A
5	A	1200	A
5	A	1201	G
5	A	1208	A
5	A	1215	U
5	A	1217	U
5	A	1220	A
5	A	1225	G
5	A	1234	G
5	A	1245	G
5	A	1258	A
5	A	1265	G
5	A	1273	G
5	A	1274	G
5	A	1275	A
5	A	1276	G
5	A	1284	A
5	A	1286	G

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Mol	Chain	Res	Type
5	A	1287	U
5	A	1290	G
5	A	1291	A
5	A	1294	G
5	A	1304	G
5	A	1309	G
5	A	1310	A
5	A	1312	A
5	A	1337	A
5	A	1338	U
5	A	1339	U
5	A	1340	G
5	A	1341	A
5	A	1342	C
5	A	1344	A
5	A	1348	U
5	A	1349	U
5	A	1357	G
5	A	1360	G
5	A	1361	G
5	A	1362	C
5	A	1366	U
5	A	1370	C
5	A	1378	U
5	A	1384	G
5	A	1387	C
5	A	1396	A
5	A	1397	G
5	A	1402	A
5	A	1405	G
5	A	1415	A
5	A	1416	U
5	A	1421	A
5	A	1422	A
5	A	1432	A
5	A	1433	U
5	A	1434	U
5	A	1440	A
5	A	1443	A
5	A	1450	A
5	A	1451	U
5	A	1454	U

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Mol	Chain	Res	Type
5	A	1455	U
5	A	1457	U
5	A	1458	A
5	A	1459	A
5	A	1460	U
5	A	1462	G
5	A	1463	A
5	A	1464	U
5	A	1465	G
5	A	1471	A
5	A	1472	C
5	A	1476	G
5	A	1477	U
5	A	1478	A
5	A	1479	G
5	A	1481	A
5	A	1482	U
5	A	1484	G
5	A	1488	A
5	A	1489	A
5	A	1493	U
5	A	1494	G
5	A	1496	G
5	A	1497	A
5	A	1498	U
5	A	1499	U
5	A	1503	U
5	A	1504	U
5	A	1507	A
5	A	1508	C
5	A	1510	U
5	A	1511	C
5	A	1516	C
5	A	1520	A
5	A	1521	A
5	A	1522	G
5	A	1523	G
5	A	1525	U
5	A	1526	G
5	A	1527	A
5	A	1528	G
5	A	1529	U

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Mol	Chain	Res	Type
5	A	1530	A
5	A	1531	U
5	A	1532	U
5	A	1538	A
5	A	1539	A
5	A	1540	U
5	A	1541	C
5	A	1542	C
5	A	1543	G
5	A	1544	G
5	A	1546	A
5	A	1550	G
5	A	1552	U
5	A	1553	A
5	A	1555	G
5	A	1556	G
5	A	1561	G
5	A	1562	C
5	A	1563	U
5	A	1564	G
5	A	1565	U
5	A	1568	U
5	A	1569	G
5	A	1570	G
5	A	1572	G
5	A	1573	A
5	A	1574	G
5	A	1575	A
5	A	1576	A
5	A	1577	G
5	A	1578	A
5	A	1579	C
5	A	1580	A
5	A	1581	U
5	A	1582	U
5	A	1583	G
5	A	1584	U
5	A	1585	G
5	A	1586	U
5	A	1587	C
5	A	1588	U
5	A	1589	U

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Mol	Chain	Res	Type
5	A	1590	C
5	A	1592	A
5	A	1593	G
5	A	1594	U
5	A	1596	G
5	A	1598	U
5	A	1599	G
5	A	1602	U
5	A	1605	A
5	A	1606	C
5	A	1613	G
5	A	1616	A
5	A	1623	U
5	A	1624	C
5	A	1625	U
5	A	1627	G
5	A	1628	A
5	A	1629	U
5	A	1630	A
5	A	1631	G
5	A	1632	A
5	A	1633	A
5	A	1634	A
5	A	1635	A
5	A	1636	U
5	A	1637	A
5	A	1639	G
5	A	1641	G
5	A	1651	C
5	A	1652	A
5	A	1653	A
5	A	1654	A
5	A	1656	C
5	A	1657	G
5	A	1658	A
5	A	1660	A
5	A	1661	C
5	A	1662	A
5	A	1666	A
5	A	1678	A
5	A	1679	A
5	A	1687	G

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Mol	Chain	Res	Type
5	A	1690	A
5	A	1691	G
5	A	1692	C
5	A	1707	U
5	A	1717	G
5	A	1718	G
5	A	1719	C
5	A	1736	U
5	A	1737	U
5	A	1738	C
5	A	1740	G
5	A	1757	U
5	A	1758	A
5	A	1759	G
5	A	1760	G
5	A	1761	G
5	A	1762	U
5	A	1763	U
5	A	1764	A
5	A	1766	C
5	A	1769	C
5	A	1770	C
5	A	1771	A
5	A	1790	G
5	A	1791	G
5	A	1796	A
5	A	1797	G
5	A	1800	A
5	A	1803	G
5	A	1805	U
5	A	1806	U
5	A	1808	U
5	A	1809	C
5	A	1811	A
5	A	1827	C
5	A	1828	U
5	A	1829	A
5	A	1835	U
5	A	1843	U
5	A	1844	G
5	A	1856	A
5	A	1863	C

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Mol	Chain	Res	Type
5	A	1870	C
5	A	1871	U
5	A	1875	A
5	A	1880	A
5	A	1886	A
5	A	1891	U
5	A	1892	U
5	A	1893	A
5	A	1894	G
5	A	1898	C
5	A	1899	U
5	A	1903	A
5	A	1904	A
5	A	1905	G
5	A	1909	C
5	A	1910	G
5	A	1911	A
5	A	1912	A
5	A	1913	U
5	A	1919	C
5	A	1923	A
5	A	1933	G
5	A	1934	G
5	A	1938	U
5	A	1939	A
5	A	1945	A
5	A	1946	A
5	A	1948	G
5	A	1950	U
5	A	1956	G
5	A	1957	G
5	A	1958	U
5	A	1964	A
5	A	1965	A
5	A	1966	5MU
5	A	1967	U
5	A	1982	U
5	A	1992	C
5	A	1994	C
5	A	1996	A
5	A	1997	A
5	A	1998	A

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Mol	Chain	Res	Type
5	A	1999	G
5	A	2003	U
5	A	2008	A
5	A	2009	U
5	A	2018	U
5	A	2019	G
5	A	2020	U
5	A	2023	C
5	A	2024	A
5	A	2029	G
5	A	2048	G
5	A	2050	A
5	A	2057	A
5	A	2058	A
5	A	2059	G
5	A	2060	A
5	A	2061	U
5	A	2062	G
5	A	2070	C
5	A	2075	G
5	A	2076	A
5	A	2078	A
5	A	2082	C
5	A	2083	G
5	A	2087	A
5	A	2088	G
5	A	2089	A
5	A	2090	C
5	A	2095	U
5	A	2096	G
5	A	2107	G
5	A	2109	A
5	A	2114	G
5	A	2117	A
5	A	2119	U
5	A	2120	G
5	A	2127	G
5	A	2128	G
5	A	2129	C
5	A	2130	A
5	A	2132	A
5	A	2133	G

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Mol	Chain	Res	Type
5	A	2134	C
5	A	2135	U
5	A	2136	U
5	A	2138	U
5	A	2139	A
5	A	2140	C
5	A	2143	G
5	A	2144	A
5	A	2145	U
5	A	2146	A
5	A	2147	G
5	A	2148	G
5	A	2149	U
5	A	2153	A
5	A	2155	C
5	A	2156	C
5	A	2158	U
5	A	2159	U
5	A	2161	A
5	A	2163	A
5	A	2164	C
5	A	2169	G
5	A	2170	C
5	A	2172	C
5	A	2173	U
5	A	2175	G
5	A	2177	U
5	A	2185	A
5	A	2186	G
5	A	2188	C
5	A	2190	C
5	A	2193	G
5	A	2194	U
5	A	2195	G
5	A	2196	G
5	A	2198	A
5	A	2200	A
5	A	2204	C
5	A	2205	C
5	A	2206	C
5	A	2208	A
5	A	2209	G

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Mol	Chain	Res	Type
5	A	2210	C
5	A	2211	U
5	A	2212	G
5	A	2214	G
5	A	2215	U
5	A	2217	G
5	A	2221	U
5	A	2224	U
5	A	2225	A
5	A	2226	A
5	A	2230	G
5	A	2231	C
5	A	2232	A
5	A	2235	A
5	A	2238	U
5	A	2239	A
5	A	2240	U
5	A	2241	C
5	A	2245	G
5	A	2252	A
5	A	2261	G
5	A	2265	G
5	A	2266	G
5	A	2287	C
5	A	2296	A
5	A	2306	G
5	A	2310	C
5	A	2311	U
5	A	2312	C
5	A	2313	A
5	A	2314	A
5	A	2315	A
5	A	2326	G
5	A	2328	A
5	A	2329	U
5	A	2330	G
5	A	2331	G
5	A	2332	U
5	A	2333	U
5	A	2334	G
5	A	2335	G
5	A	2336	A

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Mol	Chain	Res	Type
5	A	2337	A
5	A	2338	A
5	A	2339	U
5	A	2342	U
5	A	2345	A
5	A	2346	U
5	A	2347	A
5	A	2348	G
5	A	2349	A
5	A	2350	G
5	A	2352	G
5	A	2353	U
5	A	2354	A
5	A	2358	G
5	A	2360	A
5	A	2362	A
5	A	2364	G
5	A	2370	U
5	A	2371	U
5	A	2372	G
5	A	2374	C
5	A	2377	C
5	A	2381	A
5	A	2388	A
5	A	2396	A
5	A	2399	G
5	A	2400	U
5	A	2410	G
5	A	2411	A
5	A	2412	C
5	A	2419	A
5	A	2427	G
5	A	2429	U
5	A	2430	C
5	A	2434	A
5	A	2438	A
5	A	2441	G
5	A	2445	A
5	A	2449	C
5	A	2451	C
5	A	2456	G
5	A	2457	A

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Mol	Chain	Res	Type
5	A	2458	U
5	A	2459	A
5	A	2460	A
5	A	2461	A
5	A	2463	G
5	A	2468	C
5	A	2474	G
5	A	2475	A
5	A	2493	C
5	A	2497	G
5	A	2505	A
5	A	2506	U
5	A	2508	G
5	A	2521	G
5	A	2525	C
5	A	2528	C
5	A	2529	G
5	A	2531	U
5	A	2532	G
5	A	2533	U
5	A	2534	C
5	A	2543	G
5	A	2545	A
5	A	2547	C
5	A	2552	G
5	A	2554	C
5	A	2556	G
5	A	2558	A
5	A	2559	G
5	A	2562	G
5	A	2568	A
5	A	2569	A
5	A	2570	G
5	A	2574	U
5	A	2579	U
5	A	2580	G
5	A	2589	U
5	A	2592	A
5	A	2593	A
5	A	2594	G
5	A	2599	A
5	A	2600	C

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Mol	Chain	Res	Type
5	A	2601	G
5	A	2605	G
5	A	2609	G
5	A	2612	U
5	A	2613	C
5	A	2626	G
5	A	2629	A
5	A	2636	U
5	A	2640	U
5	A	2642	U
5	A	2648	G
5	A	2649	U
5	A	2650	G
5	A	2656	A
5	A	2661	A
5	A	2668	A
5	A	2672	G
5	A	2681	A
5	A	2682	G
5	A	2683	U
5	A	2684	A
5	A	2685	C
5	A	2687	A
5	A	2692	A
5	A	2693	C
5	A	2694	C
5	A	2695	G
5	A	2696	G
5	A	2700	G
5	A	2709	U
5	A	2716	U
5	A	2728	U
5	A	2729	G
5	A	2733	A
5	A	2741	G
5	A	2745	G
5	A	2753	U
5	A	2755	U
5	A	2756	G
5	A	2760	A
5	A	2761	C
5	A	2769	G

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Mol	Chain	Res	Type
5	A	2771	G
5	A	2776	A
5	A	2777	A
5	A	2781	U
5	A	2782	C
5	A	2783	U
5	A	2784	A
5	A	2787	C
5	A	2788	A
5	A	2792	A
5	A	2794	C
5	A	2803	A
5	A	2804	G
5	A	2805	A
5	A	2806	U
5	A	2807	G
5	A	2817	A
5	A	2818	A
5	A	2819	C
5	A	2820	U
5	A	2821	U
5	A	2824	G
5	A	2826	U
5	A	2827	A
5	A	2828	U
5	A	2829	A
5	A	2830	A
5	A	2832	A
5	A	2838	C
5	A	2840	A
5	A	2844	U
5	A	2846	A
5	A	2851	G
5	A	2853	U
5	A	2855	A
5	A	2887	G
5	A	2888	A
5	A	2892	G
5	A	2899	A
5	A	2900	C
5	A	2904	U
5	A	2905	C

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Mol	Chain	Res	Type
5	A	2906	G
5	A	2911	A
5	A	2913	G
5	A	2914	A
5	A	2920	U
6	B	3	U
6	B	6	U
6	B	7	G
6	B	8	A
6	B	10	U
6	B	12	U
6	B	13	A
6	B	22	G
6	B	23	U
6	B	24	C
6	B	25	A
6	B	26	C
6	B	30	U
6	B	31	G
6	B	33	U
6	B	35	C
6	B	39	G
6	B	40	C
6	B	41	C
6	B	42	G
6	B	52	G
6	B	54	U
6	B	55	A
6	B	56	A
6	B	58	C
6	B	63	U
6	B	64	A
6	B	65	G
6	B	66	C
6	B	75	U
6	B	85	U
6	B	87	C
6	B	88	G
6	B	102	G
6	B	106	G
6	B	113	G
6	B	114	G

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Mol	Chain	Res	Type
6	B	115	C

All (91) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	69	C
5	A	84	A
5	A	90	A
5	A	161	A
5	A	183	A
5	A	199	A
5	A	202	A
5	A	267	G
5	A	285	U
5	A	291	G
5	A	292	U
5	A	299	U
5	A	327	G
5	A	328	G
5	A	373	A
5	A	403	U
5	A	433	U
5	A	436	A
5	A	502	C
5	A	520	G
5	A	548	A
5	A	576	U
5	A	577	A
5	A	614	U
5	A	657	U
5	A	688	A
5	A	689	A
5	A	698	U
5	A	715	A
5	A	809	A
5	A	890	G
5	A	910	C
5	A	1017	A
5	A	1028	G
5	A	1077	U
5	A	1096	C
5	A	1097	U

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Mol	Chain	Res	Type
5	A	1130	A
5	A	1153	C
5	A	1312	A
5	A	1357	G
5	A	1361	G
5	A	1433	U
5	A	1434	U
5	A	1458	A
5	A	1495	C
5	A	1503	U
5	A	1520	A
5	A	1526	G
5	A	1528	G
5	A	1542	C
5	A	1543	G
5	A	1561	G
5	A	1576	A
5	A	1577	G
5	A	1579	C
5	A	1591	G
5	A	1593	G
5	A	1605	A
5	A	1628	A
5	A	1629	U
5	A	1634	A
5	A	1652	A
5	A	1757	U
5	A	1760	G
5	A	1789	A
5	A	1826	G
5	A	2089	A
5	A	2094	G
5	A	2137	G
5	A	2224	U
5	A	2225	A
5	A	2238	U
5	A	2329	U
5	A	2347	A
5	A	2353	U
5	A	2450	U
5	A	2458	U
5	A	2495	A

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Mol	Chain	Res	Type
5	A	2505	A
5	A	2533	U
5	A	2599	A
5	A	2628	C
5	A	2672	G
5	A	2829	A
5	A	2887	G
5	A	2912	A
6	B	22	G
6	B	24	C
6	B	50	A
6	B	63	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	5MU	A	792	5	19,22,23	1.48	5 (26%)	28,32,35	2.24	8 (28%)
5	OMG	A	2278	5	18,26,27	1.06	1 (5%)	19,38,41	1.21	3 (15%)
5	MA6	A	2085	5	18,26,27	1.03	2 (11%)	19,38,41	2.04	5 (26%)
5	2MA	A	2530	32,5	17,25,26	1.07	0	17,37,40	1.29	3 (17%)
5	5MU	A	1966	5	19,22,23	1.66	5 (26%)	28,32,35	2.32	8 (28%)
5	2MG	A	2472	5	18,26,27	1.19	1 (5%)	16,38,41	1.17	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5MU	A	792	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMG	A	2278	5	-	1/5/27/28	0/3/3/3
5	MA6	A	2085	5	-	3/7/29/30	0/3/3/3
5	2MA	A	2530	32,5	-	0/3/25/26	0/3/3/3
5	5MU	A	1966	5	-	0/7/25/26	0/2/2/2
5	2MG	A	2472	5	-	0/5/27/28	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2472	2MG	C6-N1	-3.63	1.32	1.37
5	A	1966	5MU	C4-N3	-3.30	1.32	1.38
5	A	792	5MU	C4-N3	-3.28	1.32	1.38
5	A	1966	5MU	C6-C5	3.11	1.39	1.34
5	A	2278	OMG	C6-N1	-3.07	1.33	1.37
5	A	1966	5MU	C2-N3	-3.01	1.32	1.38
5	A	792	5MU	C6-N1	-2.71	1.33	1.38
5	A	792	5MU	C2-N3	-2.65	1.33	1.38
5	A	1966	5MU	C2-N1	2.57	1.42	1.38
5	A	1966	5MU	C4-C5	2.30	1.48	1.44
5	A	792	5MU	C2-N1	2.16	1.41	1.38
5	A	792	5MU	C6-C5	2.14	1.38	1.34
5	A	2085	MA6	C2'-C1'	-2.02	1.50	1.53
5	A	2085	MA6	C5-C4	2.00	1.46	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1966	5MU	N3-C2-N1	5.86	122.67	114.89
5	A	2085	MA6	C9-N6-C6	-5.78	102.00	119.51
5	A	1966	5MU	C5-C4-N3	5.40	119.92	115.31
5	A	792	5MU	N3-C2-N1	5.31	121.94	114.89
5	A	1966	5MU	C4-N3-C2	-5.12	120.73	127.35
5	A	792	5MU	C4-N3-C2	-5.08	120.77	127.35
5	A	792	5MU	C5-C4-N3	4.05	118.77	115.31
5	A	792	5MU	O4-C4-C5	-3.98	120.29	124.90
5	A	2085	MA6	N3-C2-N1	-3.98	122.46	128.68
5	A	2085	MA6	C10-N6-C9	-3.56	104.66	116.12
5	A	792	5MU	C5-C6-N1	-3.47	119.77	123.34
5	A	1966	5MU	O4-C4-C5	-3.35	121.02	124.90
5	A	1966	5MU	O2-C2-N3	-3.23	115.49	121.50
5	A	792	5MU	C3'-C2'-C1'	3.01	107.15	101.43
5	A	1966	5MU	O4'-C1'-N1	2.86	114.90	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2278	OMG	C5-C6-N1	2.83	118.95	113.95
5	A	2472	2MG	C5-C6-N1	2.82	118.94	113.95
5	A	2085	MA6	C3'-C2'-C1'	2.77	105.15	100.98
5	A	2530	2MA	O4'-C1'-C2'	-2.71	102.97	106.93
5	A	1966	5MU	C6-N1-C2	-2.60	118.66	121.30
5	A	1966	5MU	C5-C6-N1	-2.60	120.66	123.34
5	A	792	5MU	C1'-N1-C2	2.58	122.24	117.57
5	A	2530	2MA	C5-C6-N1	2.56	118.44	114.02
5	A	2472	2MG	C8-N7-C5	2.54	107.83	102.99
5	A	792	5MU	O2-C2-N3	-2.49	116.86	121.50
5	A	2530	2MA	C8-N7-C5	2.39	107.55	102.99
5	A	2085	MA6	C4-C5-N7	-2.20	107.11	109.40
5	A	2278	OMG	O6-C6-C5	-2.19	120.09	124.37
5	A	2278	OMG	C8-N7-C5	2.09	106.97	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2085	MA6	C5-C6-N6-C9
5	A	2085	MA6	C5-C6-N6-C10
5	A	2278	OMG	C1'-C2'-O2'-CM2
5	A	2085	MA6	N1-C6-N6-C9

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	792	5MU	1	0
5	A	2278	OMG	1	0
5	A	2085	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	A1D6G	A	3000	32	70,73,73	2.33	22 (31%)	96,107,107	1.60	20 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	A1D6G	A	3000	32	-	8/82/113/113	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	3000	A1D6G	C65-N64	8.42	1.45	1.33
31	A	3000	A1D6G	C11-N13	7.17	1.50	1.34
31	A	3000	A1D6G	O10-C11	5.47	1.44	1.35
31	A	3000	A1D6G	O67-C65	4.56	1.43	1.36
31	A	3000	A1D6G	C22-C21	4.54	1.55	1.44
31	A	3000	A1D6G	O67-C68	-4.23	1.41	1.47
31	A	3000	A1D6G	O04-C03	-3.90	1.39	1.46
31	A	3000	A1D6G	O04-C05	3.69	1.42	1.34
31	A	3000	A1D6G	C19-C20	3.43	1.56	1.47
31	A	3000	A1D6G	C28-C29	3.42	1.54	1.48
31	A	3000	A1D6G	C25-C26	-3.23	1.42	1.48
31	A	3000	A1D6G	O42-C41	2.84	1.49	1.41
31	A	3000	A1D6G	C35-N33	-2.80	1.34	1.40
31	A	3000	A1D6G	C50-C46	-2.60	1.48	1.53
31	A	3000	A1D6G	C63-N64	-2.48	1.41	1.45
31	A	3000	A1D6G	C25-C35	-2.28	1.37	1.41
31	A	3000	A1D6G	C45-C46	-2.14	1.49	1.53
31	A	3000	A1D6G	O60-C59	-2.13	1.18	1.21
31	A	3000	A1D6G	C56-C52	2.10	1.55	1.52
31	A	3000	A1D6G	C46-N47	2.10	1.52	1.48
31	A	3000	A1D6G	O27-C26	-2.08	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	3000	A1D6G	C21-C20	2.00	1.22	1.19

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	3000	A1D6G	O10-C11-N13	4.78	119.50	111.11
31	A	3000	A1D6G	C44-C43-C45	-3.79	107.44	113.40
31	A	3000	A1D6G	C02-C03-C68	-3.71	110.11	115.23
31	A	3000	A1D6G	O12-C11-N13	-3.58	119.48	124.96
31	A	3000	A1D6G	O42-C43-C45	3.40	114.34	109.14
31	A	3000	A1D6G	O67-C65-O66	3.39	125.57	121.66
31	A	3000	A1D6G	O66-C65-N64	-3.25	125.43	129.22
31	A	3000	A1D6G	C52-C39-C37	-3.09	108.87	113.61
31	A	3000	A1D6G	O30-C29-C28	2.78	122.76	115.83
31	A	3000	A1D6G	O30-C29-O31	-2.49	117.90	123.61
31	A	3000	A1D6G	C41-O42-C43	2.49	116.85	112.91
31	A	3000	A1D6G	C14-N13-C11	-2.47	117.93	121.89
31	A	3000	A1D6G	C56-C52-C39	-2.38	107.37	110.25
31	A	3000	A1D6G	O10-C11-O12	-2.33	121.02	124.53
31	A	3000	A1D6G	O04-C05-C07	2.32	116.64	111.56
31	A	3000	A1D6G	O67-C68-C69	2.21	110.82	106.93
31	A	3000	A1D6G	C56-C57-C59	-2.13	109.66	113.32
31	A	3000	A1D6G	C69-C68-C63	-2.13	113.43	116.42
31	A	3000	A1D6G	C28-C32-N33	-2.10	120.27	123.16
31	A	3000	A1D6G	C45-C46-N47	-2.06	109.84	115.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

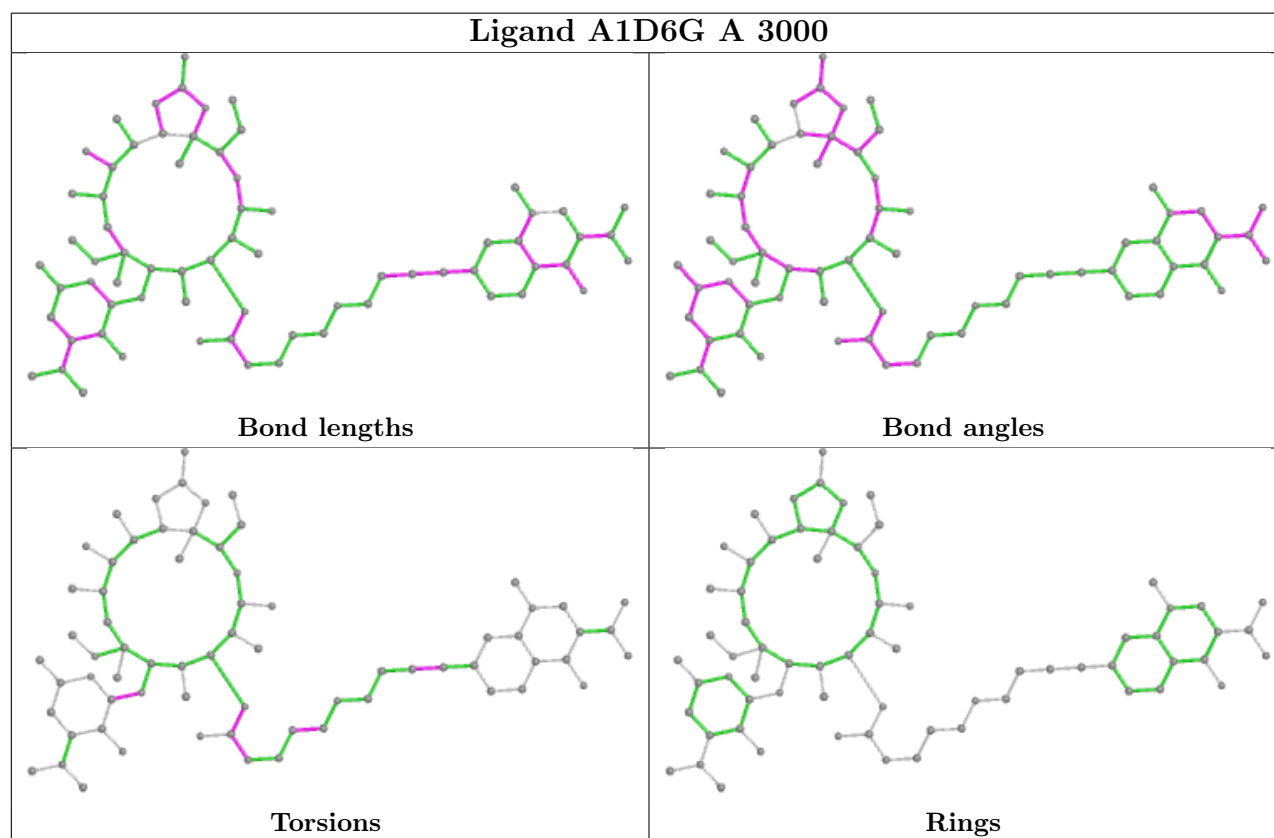
Mol	Chain	Res	Type	Atoms
31	A	3000	A1D6G	O10-C11-N13-C14
31	A	3000	A1D6G	O12-C11-N13-C14
31	A	3000	A1D6G	C19-C20-C21-C22
31	A	3000	A1D6G	N13-C11-O10-C09
31	A	3000	A1D6G	O42-C41-O40-C39
31	A	3000	A1D6G	O12-C11-O10-C09
31	A	3000	A1D6G	C50-C41-O40-C39
31	A	3000	A1D6G	C14-C15-C16-O17

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	3000	A1D6G	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.