



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:40 AM UTC

PDB ID : 8S8F / pdb_00008s8f
EMDB ID : EMD-19803
Title : Structure of a yeast 48S-AUC preinitiation complex in closed conformation (model py48S-AUC-3.2)
Authors : Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on : 2024-03-06
Resolution : 3.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

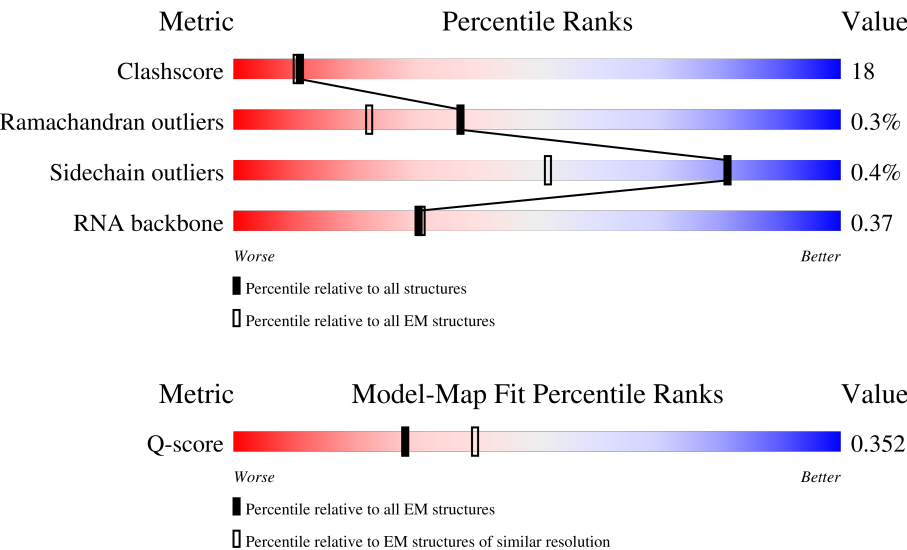
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.95 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.



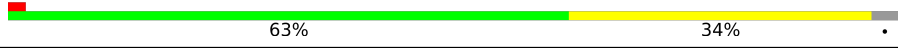
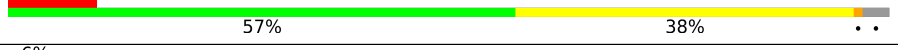
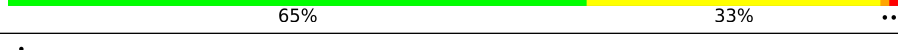
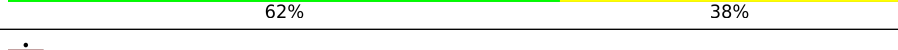
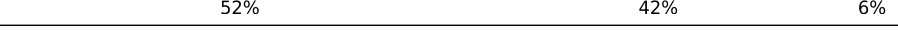
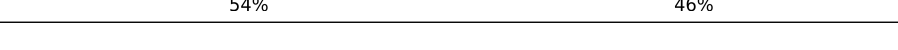
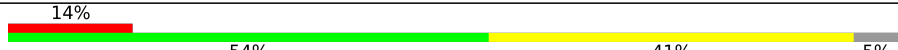
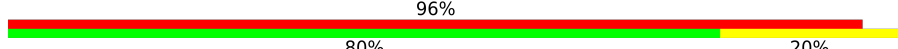
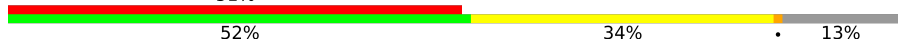
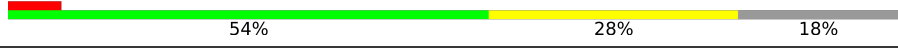
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7707 (3.45 - 4.45)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1798	6% 27% 54% 19% .
2	A	254	52% 35% 14%
3	B	255	5% 54% 34% 12%

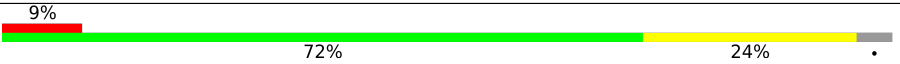
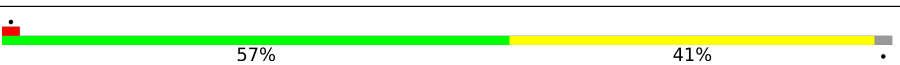
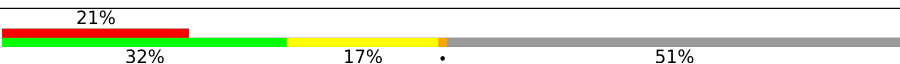
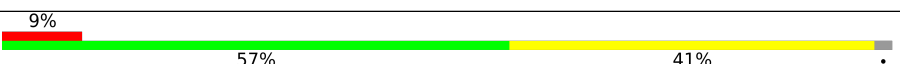
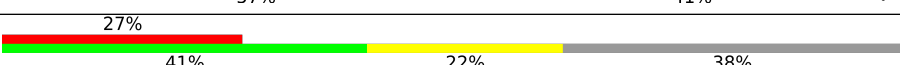
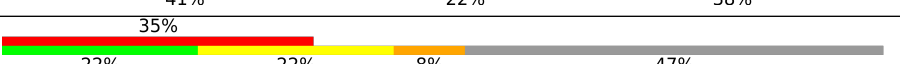
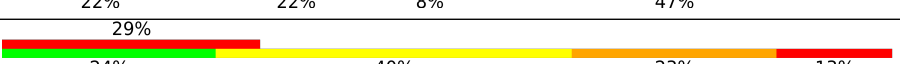
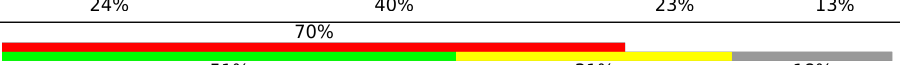
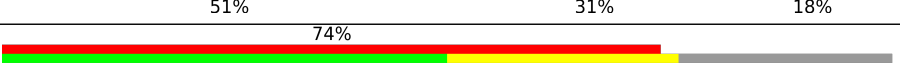
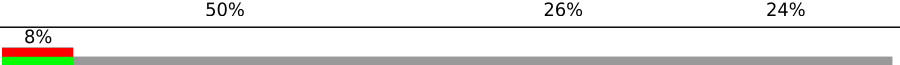
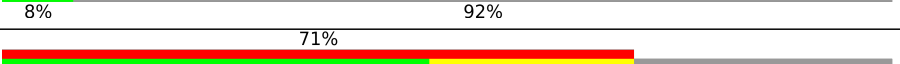
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Mol	Chain	Length	Quality of chain
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	h	25	
21	D	237	
22	F	227	
23	K	106	
24	M	134	
25	P	142	
26	Q	143	
27	R	136	
28	S	146	

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Mol	Chain	Length	Quality of chain
29	T	144	
30	U	117	
31	Z	108	
32	c	67	
33	d	56	
34	f	150	
35	g	326	
36	i	153	
37	3	49	
38	1	75	
39	j	304	
40	k	519	
41	l	285	
42	m	108	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	M2G	1	26	-	-	X	-
38	5MC	1	48	-	-	X	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 85732 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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1789	Total	C	N	O	P	0	0
			38003	16989	6694	12531	1789		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	219	Total	C	N	O	S	0	0
			1702	1085	299	316	2		

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	225	Total	C	N	O	S	0	0
			1796	1135	330	328	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	220	Total	C	N	O	S	0	0
			1648	1053	291	300	4		

- Molecule 5 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 6 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	230	Total	C	N	O	S	0	0
			1832	1146	352	330	4		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 9 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	182	Total	C	N	O	S	0	0
			1464	923	287	253	1		

- Molecule 10 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 11 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	151	Total	C	N	O	S	0	0
			1195	761	224	207	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	129	Total	C	N	O	S	0	0
			955	585	191	176	3		

- Molecule 13 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 15 is a protein called KLLA0B11231p.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 16 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	134	Total	C	N	O	S	0	0
			1061	665	207	189			

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	102	Total	C	N	O	S	0	0
			797	492	168	132	5		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	60	Total	C	N	O	S	0	0
			472	295	96	80	1		

- Molecule 20 is a protein called 40S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	227	Total	C	N	O	S	0	0
			1774	1126	320	323	5		

- Molecule 22 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 23 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	117	Total	C	N	O		0	0
			885	553	161	171			

- Molecule 25 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	117	Total	C	N	O	S	0	0
			923	592	165	161	5		

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	141	Total	C	N	O		0	0
			1105	709	204	192			

- Molecule 27 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	130	Total	C	N	O	S	0	0
			1033	643	194	193	3		

- Molecule 28 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	145	Total	C	N	O	S	0	0
			1189	739	239	209	2		

- Molecule 29 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	143	Total	C	N	O		0	0
			1110	693	210	207			

- Molecule 30 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	78	Total	C	N	O	S	0	0
			594	376	111	106	1		

- Molecule 32 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	64	Total	C	N	O	S	0	0
			499	308	99	91	1		

- Molecule 33 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	55	Total	C	N	O	S	0	0
			461	289	93	78	1		

- Molecule 34 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	74	Total	C	N	O	S	0	0
			584	374	111	95	4		

- Molecule 35 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	320	Total	C	N	O	S	0	0
			2469	1561	432	471	5		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	95	Total	C	N	O	S	0	0
			764	474	142	143	5		

- Molecule 37 is a RNA chain called mRNA (5'-R(P*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	26	Total	C	N	O	P	0	0
			536	242	84	184	26		

- Molecule 38 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	l	23	Total	C	N	O	0	0
			190	124	32	34		

- Molecule 42 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	77	Total	C	N	O	S	0	0
			619	395	109	111	4		

- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
43	2	111	Total	Mg	0
			111	111	
43	S	1	Total	Mg	0
			1	1	
43	T	2	Total	Mg	0
			2	2	
43	i	1	Total	Mg	0
			1	1	
43	k	1	Total	Mg	0
			1	1	

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
44	a	1	Total	Zn	0
			1	1	
44	b	1	Total	Zn	0
			1	1	
44	f	1	Total	Zn	0
			1	1	
44	k	1	Total	Zn	0
			1	1	

- Molecule 45 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
47	2	3	Total 3	O 3	0

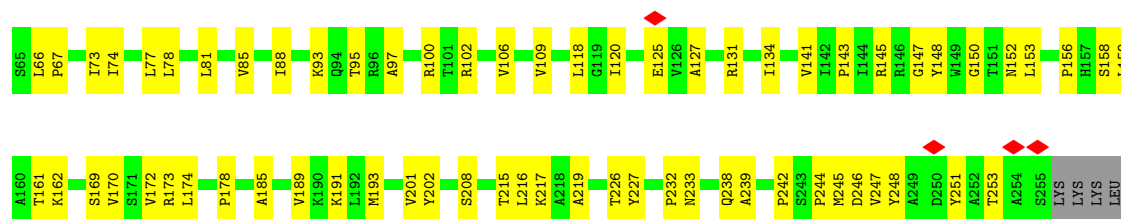
3 Residue-property plots

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

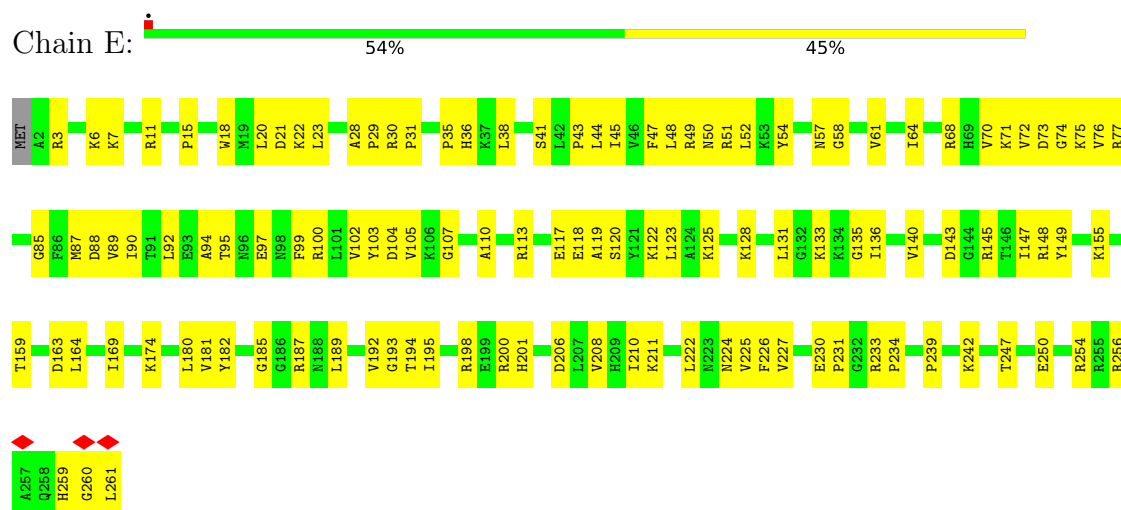
• Molecule 1: 18S ribosomal RNA



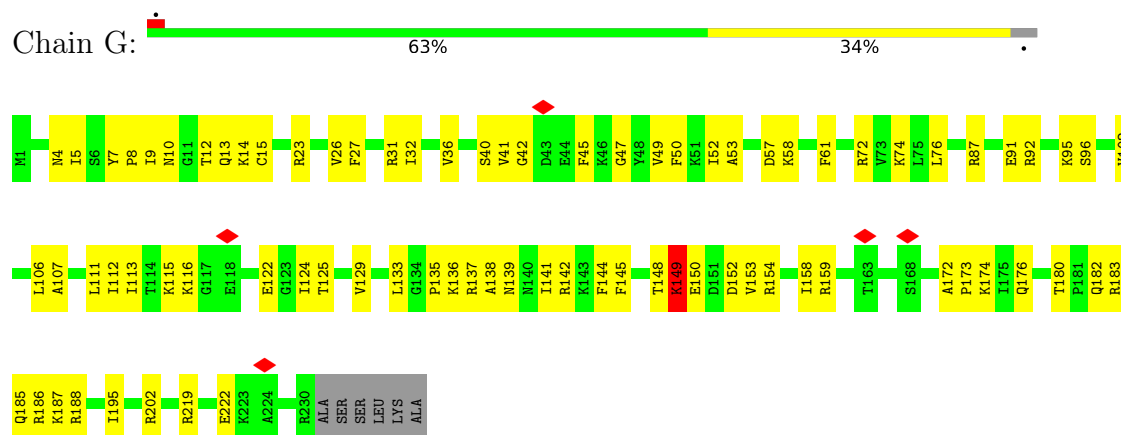
G1539	G1472	C1391	U1259	C1196	A1123	G1052	C989	G924	U859	G796	G732	C671
G1540	A1473	G1392	G1260	G1197	A1124	U1053	G990	A925	U860	C797	A733	G672
A1541	C1474	C1330	G1262	G1198	G1125	U1054	A991	C926	A861	A798	A734	C673
A1542	G1475	C1331	G1263	G1199	G1126	U1055	A992	U927	A862	G801	C735	A674
A1543	G1476	C1332	G1264	G1200	A1131	U1056	G993	A928	U863	A802	C736	C675
A1544	A1477	C1333	U1265	A1201	A1132	U1057	U995	A929	A864	A803	A737	C676
A1545	C1478	U1333	U1266	U1205	A1133	C1058	G996	U931	G865	U804	G738	U676
G1546	C1479	U1334	U1268	C1206	A1137	U1059	A997	A932	G866	A805	G739	G677
G1547	A1480	A1335	G1269	C1207	C1133	U1060	U998	C934	A868	U806	A740	G678
A1548	G1481	C1336	G1270	C1208	U1134	U1061	U999	U935	C939	U807	U679	U680
U1549	A1482	C1337	U1271	C1209	U1135	U1062	A1000	U936	G870	G808	C741	U681
U1552	G1483	U1338	U1272	C1210	A1136	C1065	G1001	A937	G871	G809	U742	U682
A1553	A1484	A1340	U1273	G1211	A1137	C1066	A1002	A938	U872	A810	U743	U683
A1554	A1485	C1343	G1274	G1212	A1142	U1067	U1003	A939	C973	A811	U744	A684
A1555	U1487	A1344	G1276	U1213	U1143	C1075	A1004	A940	G874	U812	U745	A685
A1556	A1488	A1345	C1277	C1214	G1144	C1076	C1005	G941	G875	A813	U746	C686
U1557	C1489	A1346	C1278	G1215	G1145	C1069	C1006	U944	G876	G814	U747	C687
U1558	A1490	U1346	C1279	A1216	A1146	U1070	G1007	U945	G877	G815	U748	G688
U1559	G1491	A1347	G1280	G1217	G1149	C1071	U1008	U946	G878	A816	U749	G689
C1561	C1492	C1350	U1281	A1218	A1150	A1075	U1009	U947	C879	A817	U750	A690
C1562	C1493	U1351	U1282	G1219	A1151	C1076	G1010	U948	A880	G818	U751	A691
C1563	U1494	C1352	C1283	A1220	G1152	C1077	U1011	C948	U881	U819	A752	C692
U1564	A1495	U1353	U1284	C1221	G1153	U1078	A1012	U949	A882	U820	A753	C693
U1565	G1496	C1354	U1285	A1222	C1155	C1079	G1013	C950	G883	U821	A754	U694
C1566	A1497	C1355	U1286	A1223	A1156	A1087	U1014	A951	U885	G822	A755	U695
A1567	C1498	U1356	U1287	U1224	A1157	C1081	C1015	G952	A886	G823	A756	U696
A1568	G1500	C1357	U1288	A1225	C1158	G1082	U1016	G953	U887	U824	A757	C696
C1569	U1501	G1358	G1290	C1226	C1159	A1083	U1019	G956	A888	U825	U758	U698
U1570	G1502	C1359	G1291	G1227	C1160	G1084	C1020	U957	C889	U826	G761	U699
A1571	U1503	U1361	U1292	A1228	A1161	A1085	C1021	U958	A890	U827	A762	C700
C1572	C1504	U1362	G1293	C1229	A1162	A1086	A1022	U959	A891	U828	G763	U701
C1573	U1505	C1363	G1294	A1230	A1163	A1087	U1023	U960	U892	U829	U766	G702
A1574	G1506	G1364	A1295	U1233	G1164	A1091	A1024	C961	U893	U830	U767	G703
A1575	C1507	C1365	G1296	A1234	A1165	U1094	A1025	A962	U895	U831	U768	C704
U1576	U1510	C1366	U1297	C1235	G1166	U1095	A1026	A965	C896	U832	C769	U705
U1577	G1511	G1367	G1298	A1236	U1167	C1096	C1027	A966	A897	U833	A770	A706
A1512	A1513	C1368	U1299	G1237	G1168	U1097	U1028	U967	C898	U834	A771	A707
A1514	U1515	U1369	U1302	U1238	G1169	U1098	A1029	C968	A899	U835	G772	C708
C1516	C1517	G1370	G1304	U1239	A1170	U1099	U1030	U969	G900	G836	G773	C709
U1518	U1519	C1371	U1305	G1240	C1172	G1099	G1031	A970	G901	G837	A774	U710
U1520	G1521	U1373	U1306	A1241	C1173	G1100	C1032	G971	U902	U840	G775	G711
A1522	A1523	C1374	U1307	G1242	U1174	G1101	U1035	A972	C893	U841	G776	G712
A1524	C1527	U1375	G1308	A1243	G1175	U1102	A1036	G975	A904	U842	C777	U713
A1526	U1528	C1376	U1309	G1244	U1181	U1103	C1037	A976	A905	U843	A778	A714
A1528	G1529	U1377	U1312	C1245	A1182	C1104	U1038	A977	U911	G844	A779	C714
A1530	U1531	U1378	U1313	U1246	A1183	U1105	G1039	A978	G912	A845	A780	U715
C1531	G1532	C1381	U1314	C1247	A1184	G1106	G1040	A979	G913	A846	A781	C716
C1532	U1533	G1382	U1315	U1248	U1185	G1107	G1041	G980	A914	C847	G782	C717
A1534	C1535	U1383	G1316	U1249	U1186	G1108	A1042	U981	U915	U848	C783	C718
A1536	U1537	C1384	C1317	C1251	G1187	G1109	U1043	A982	U916	G852	G785	U719
A1538	G1538	G1385	U1318	U1252	A1188	G1110	G1045	A983	U917	U853	G786	G720
U1539	C1539	U1386	A1319	U1253	A1189	G1111	G1046	G984	A918	U854	A787	U721
U1540	A1467	C1387	A1320	G1254	B801190	G1112	G1047	G985	U919	A855	A788	U722
A1542	C1468	C1388	A1321	A1255	U1114	A1113	U1048	G986	U920	A856	A789	G723
A1544	A1469	U1389	C1322	U1256	A1115	G1114	G1049	A987	G921	U857	A790	U724
A1546	C1470	C1390	U1323	U1257	C1194	U1116	G1050	A987	A922	G724	A791	U725
A1548	U1471	U1391	G1323	U1258	A1195	G1117	U1051	U988	A923	G726	A792	C731



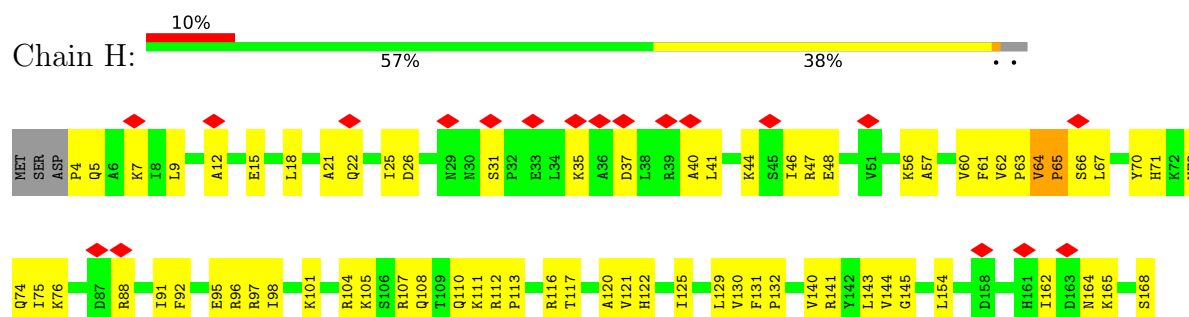
• Molecule 5: 40S ribosomal protein S4



• Molecule 6: Small ribosomal subunit protein eS6

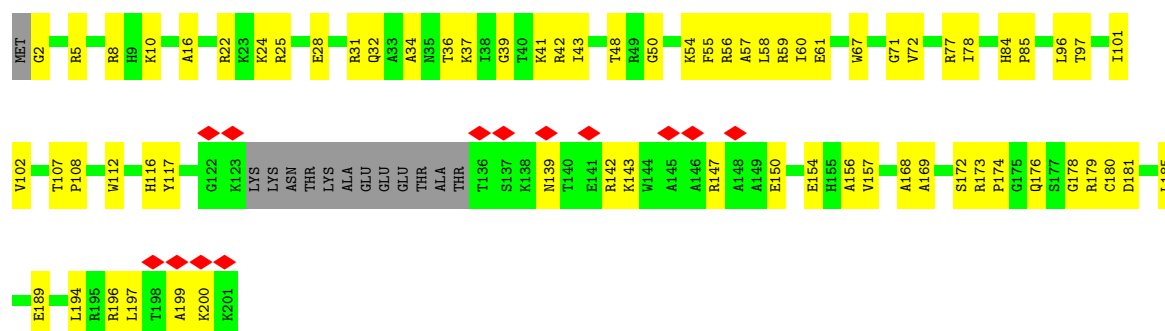


• Molecule 7: 40S ribosomal protein S7

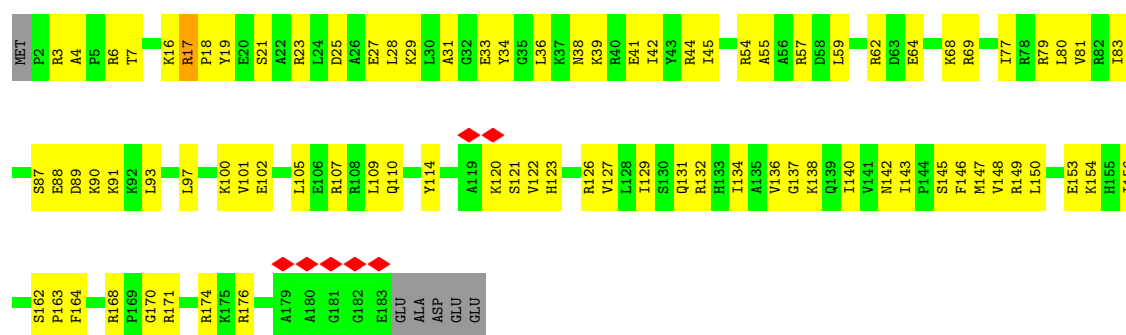




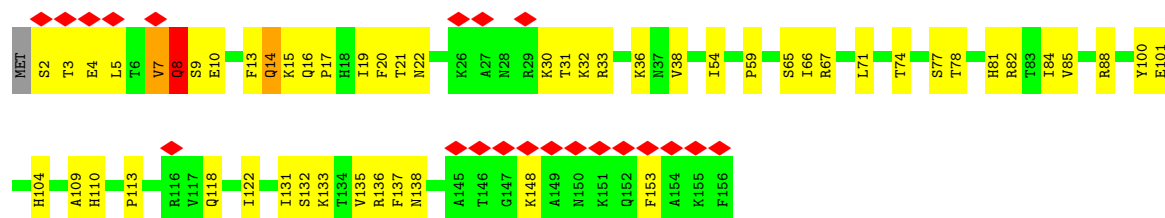
• Molecule 8: 40S ribosomal protein S8



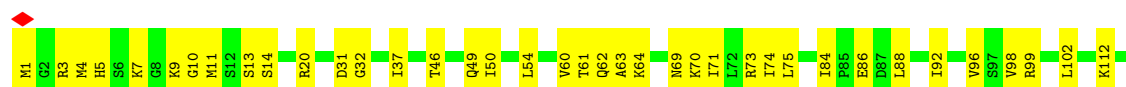
• Molecule 9: KLLA0E23673p



• Molecule 10: KLLA0A10483p

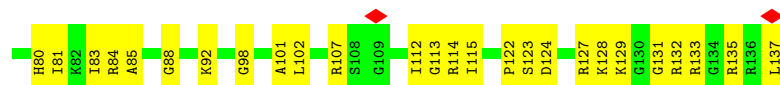


• Molecule 11: KLLA0F18040p

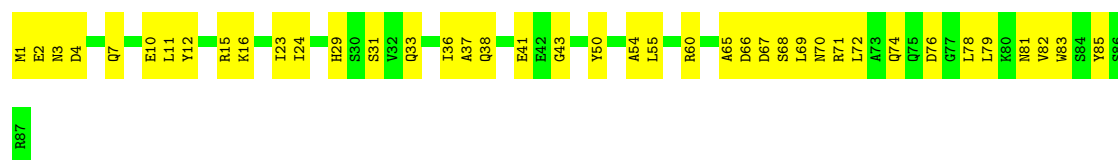




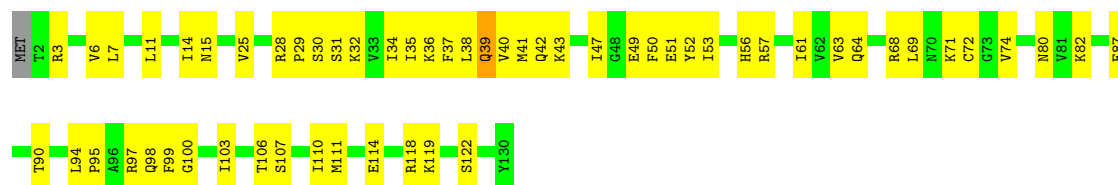
- Molecule 12: Small ribosomal subunit protein uS11



- Molecule 13: 40S ribosomal protein S21



- Molecule 14: Small ribosomal subunit protein uS8

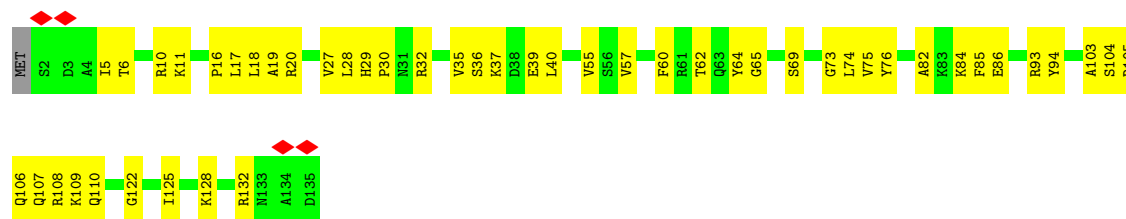


- Molecule 15: KLLA0B11231p

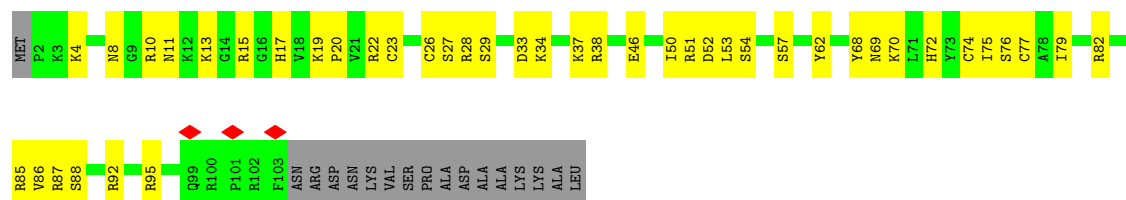


- Molecule 16: 40S ribosomal protein S24





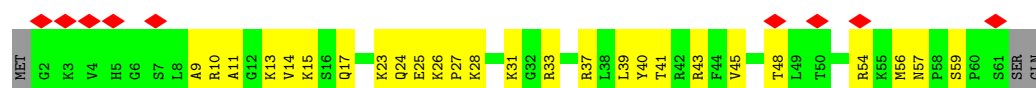
- Molecule 17: 40S ribosomal protein S26



- Molecule 18: 40S ribosomal protein S27



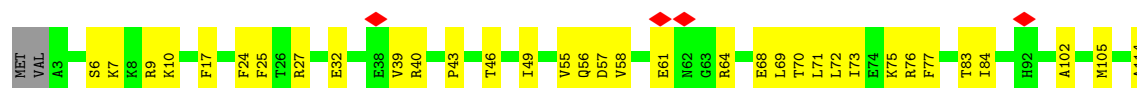
- Molecule 19: 40S ribosomal protein S30

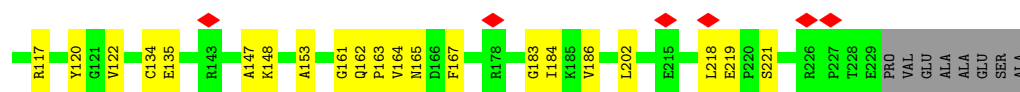


- Molecule 20: 40S ribosomal protein L41-A

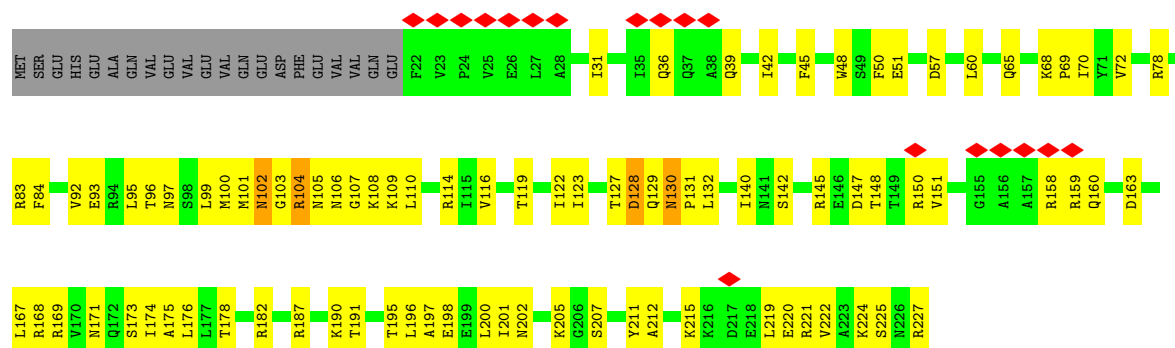


- Molecule 21: 40S ribosomal protein S3

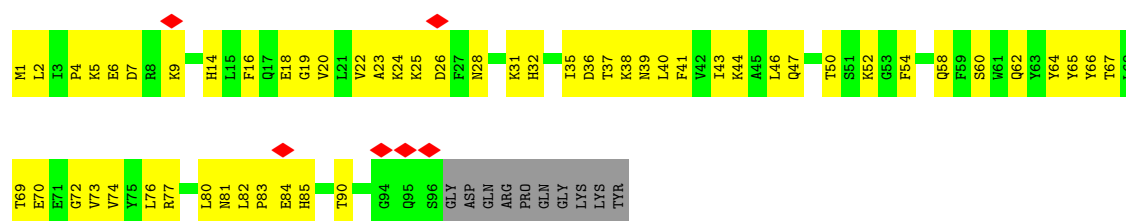




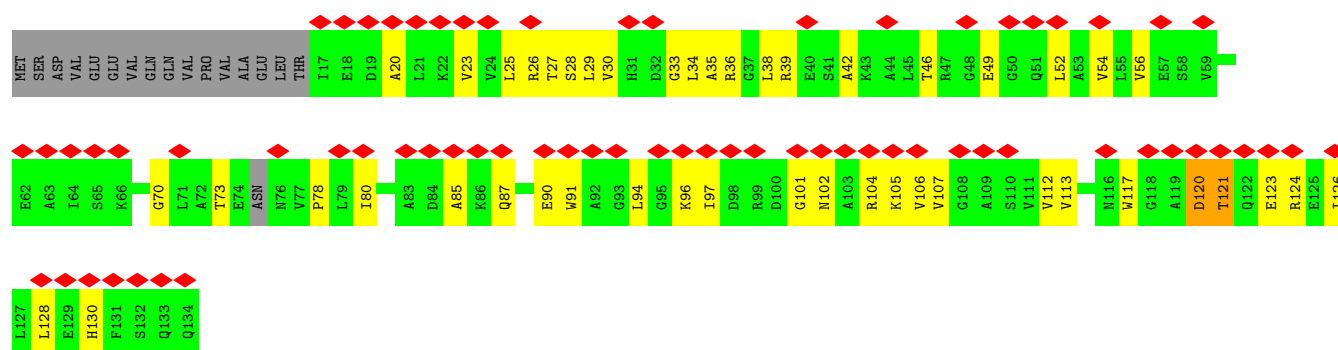
• Molecule 22: KLLA0D10659p



• Molecule 23: KLLA0B08173p

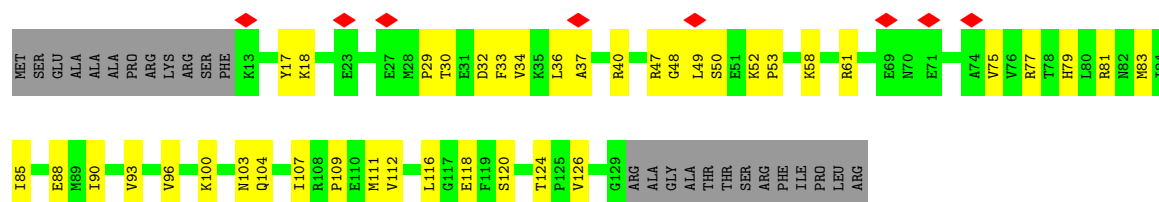


• Molecule 24: 40S ribosomal protein S12

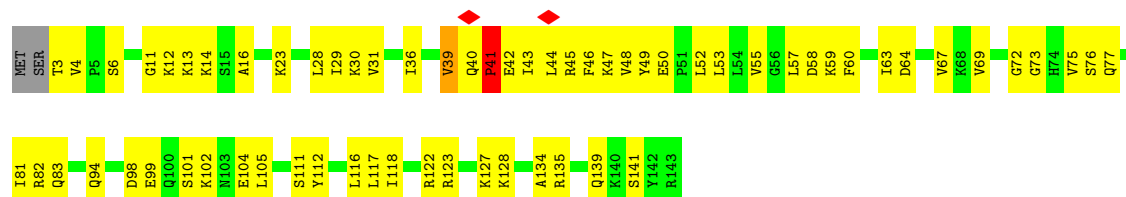


• Molecule 25: KLLA0F07843p

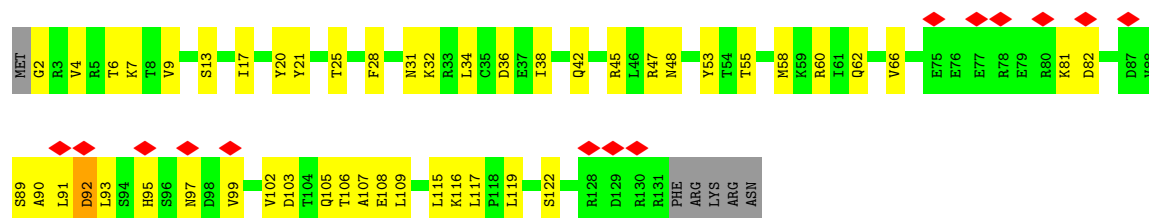




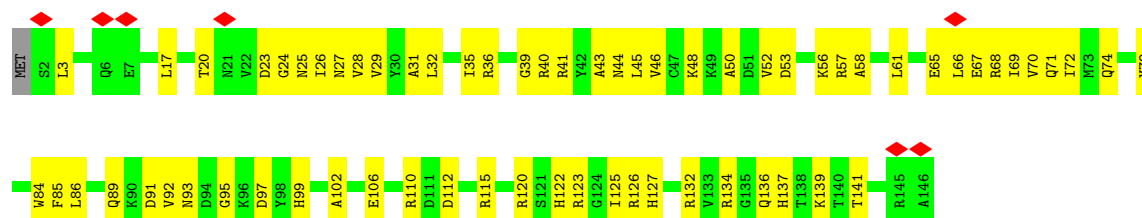
- Molecule 26: Small ribosomal subunit protein uS9



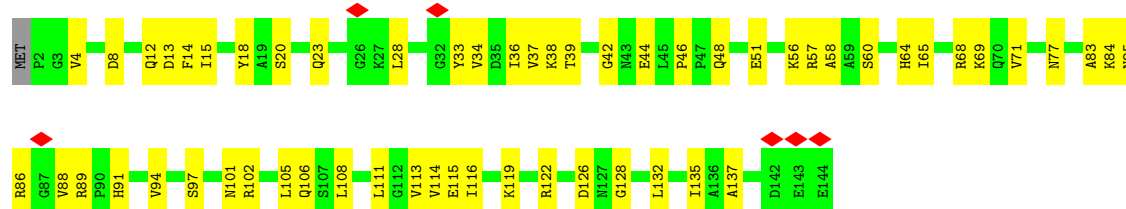
- Molecule 27: KLLA0B01474p



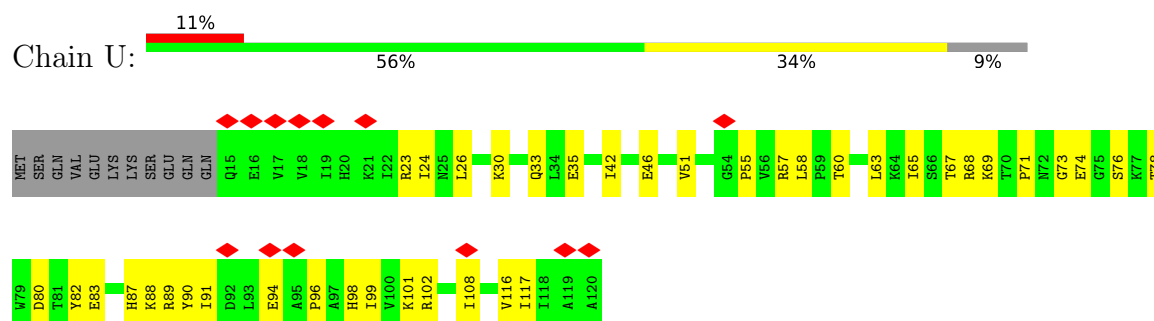
- Molecule 28: KLLA0B01562p



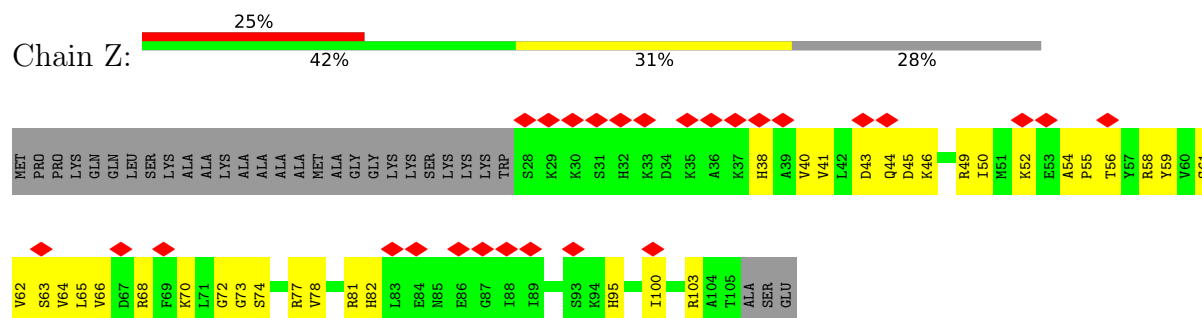
- Molecule 29: KLLA0A07194p



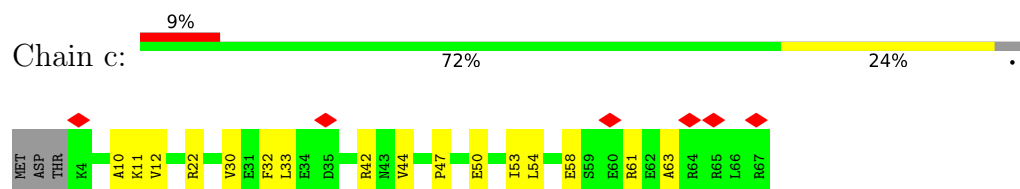
- Molecule 30: Small ribosomal subunit protein uS10



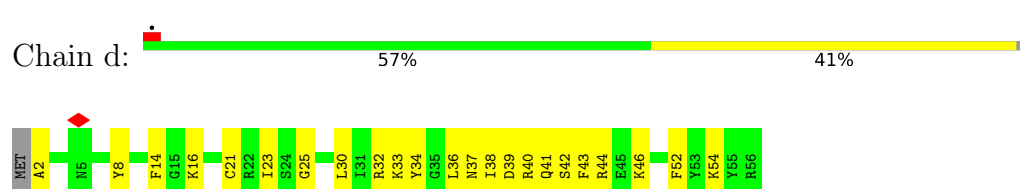
- Molecule 31: 40S ribosomal protein S25



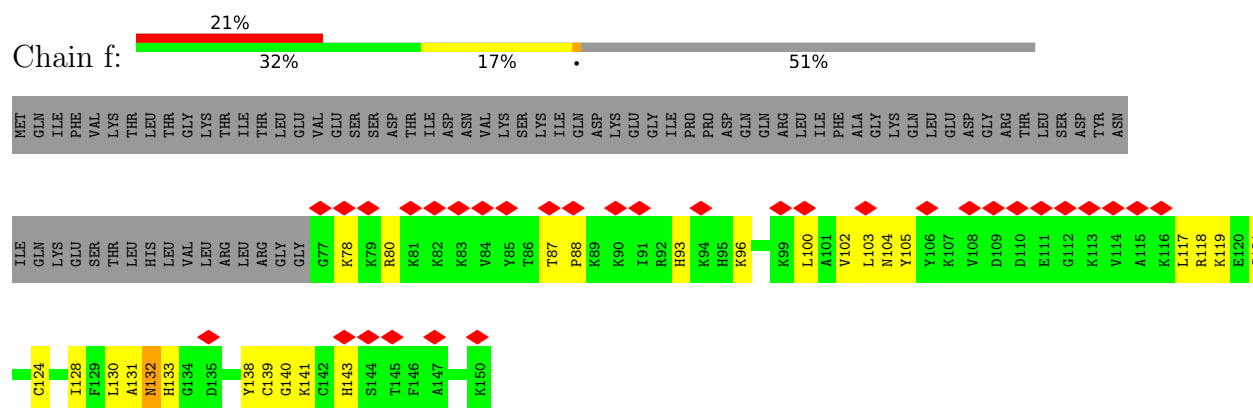
- Molecule 32: Small ribosomal subunit protein eS28



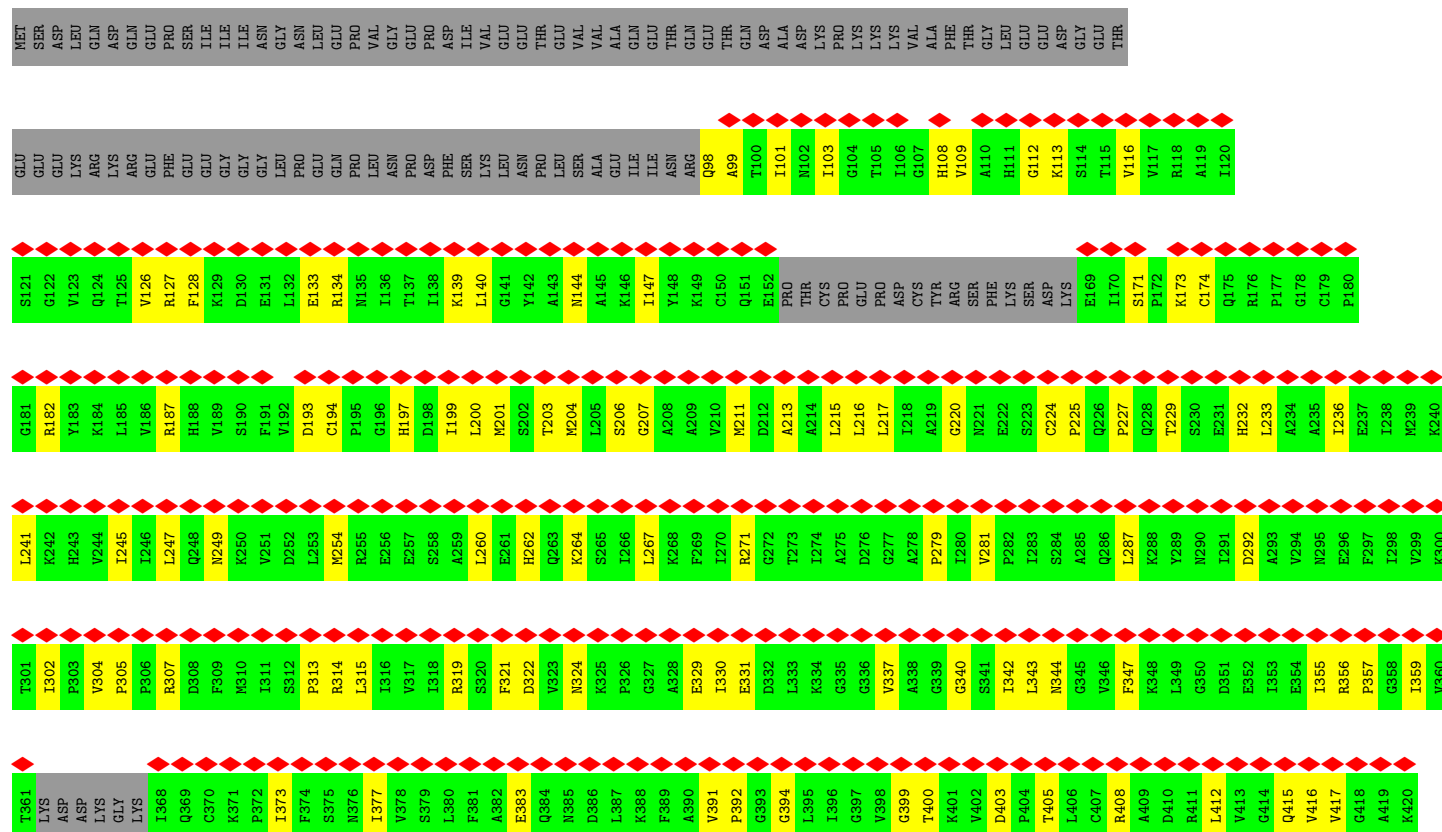
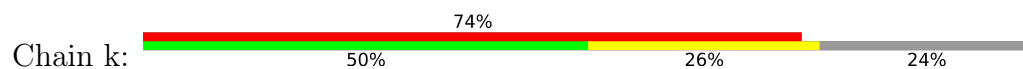
- Molecule 33: Small ribosomal subunit protein uS14

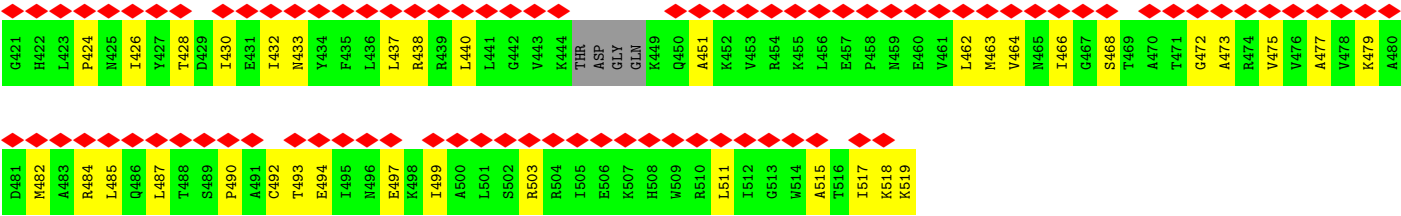


- Molecule 34: Small ribosomal subunit protein eS31

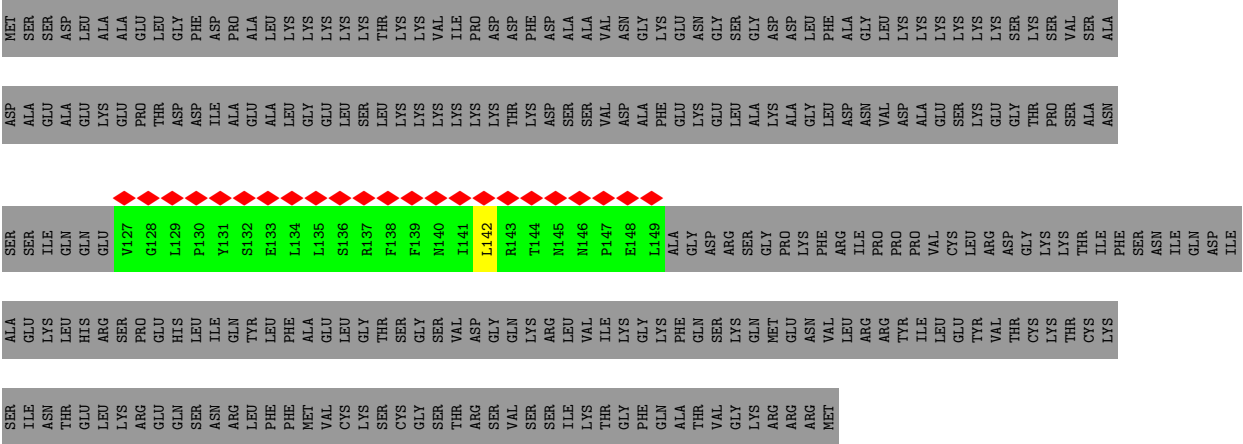


Chain j:

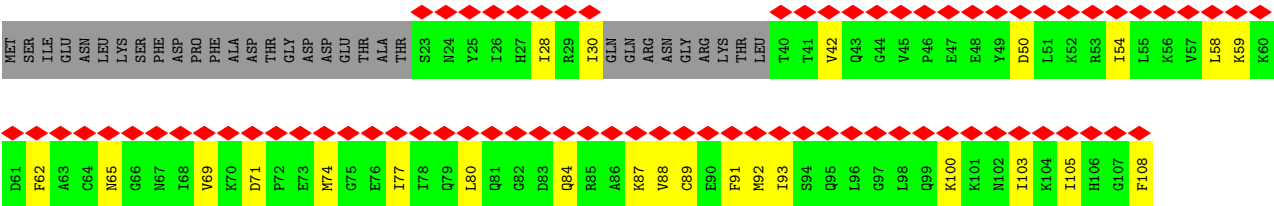




• Molecule 41: Eukaryotic translation initiation factor 2 subunit beta



• Molecule 42: Eukaryotic translation initiation factor eIF-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39886	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.467	Depositor
Minimum map value	-0.252	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, T6A, M2G, PSU, RIA, MG, 7MG, H2U, 5MC, ZN, 1MG, GCP, MA6, B8N, 2MG

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	2	0.14	0/42201	0.32	0/65752
2	A	0.17	0/1742	0.41	0/2383
3	B	0.23	0/1820	0.53	1/2448 (0.0%)
4	C	0.17	0/1678	0.42	0/2277
5	E	0.17	0/2122	0.44	0/2861
6	G	0.16	0/1855	0.41	0/2479
7	H	0.22	0/1507	0.50	0/2028
8	I	0.16	0/1515	0.42	0/2029
9	J	0.24	0/1487	0.64	4/1990 (0.2%)
10	L	0.23	0/1276	0.43	0/1718
11	N	0.17	0/1218	0.42	0/1638
12	O	0.17	0/966	0.47	0/1297
13	V	0.16	0/696	0.40	0/938
14	W	0.21	0/1039	0.47	0/1399
15	X	0.19	0/1137	0.48	0/1516
16	Y	0.17	0/1075	0.44	0/1433
17	a	0.17	0/810	0.47	0/1087
18	b	0.18	0/619	0.46	0/837
19	e	0.19	0/480	0.61	0/640
20	h	0.11	0/234	0.29	0/300
21	D	0.14	0/1800	0.38	0/2421
22	F	0.24	0/1628	0.68	2/2198 (0.1%)
23	K	0.22	0/831	0.62	0/1123
24	M	0.23	0/891	0.52	0/1201
25	P	0.17	0/942	0.51	2/1269 (0.2%)
26	Q	0.26	0/1125	0.59	0/1510
27	R	0.26	0/1044	0.56	0/1402
28	S	0.18	0/1208	0.49	0/1624
29	T	0.17	0/1129	0.40	0/1520
30	U	0.14	0/857	0.38	0/1158
31	Z	0.14	0/603	0.38	0/814
32	c	0.13	0/501	0.39	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.17	0/473	0.49	0/629
34	f	0.16	0/597	0.50	0/795
35	g	0.19	0/2523	0.45	0/3434
36	i	0.15	0/773	0.49	0/1031
37	3	0.08	0/595	0.19	0/920
38	1	0.30	1/1529 (0.1%)	0.57	4/2376 (0.2%)
39	j	0.14	0/2034	0.41	0/2737
40	k	0.13	0/3079	0.41	0/4157
41	l	0.12	0/194	0.33	0/263
42	m	0.13	0/626	0.37	0/835
All	All	0.17	1/90459 (0.0%)	0.40	13/131140 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	26	M2G	O3'-P	7.62	1.72	1.61

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	104	ARG	N-CA-C	-19.00	90.65	111.36
9	J	19	TYR	N-CA-C	10.88	125.12	112.72
22	F	102	ASN	N-CA-C	-10.83	95.90	111.17
38	1	26	M2G	P-O3'-C3'	9.74	134.81	120.20
3	B	190	PRO	CA-N-CD	-9.18	99.15	112.00
38	1	26	M2G	O3'-P-O5'	-8.72	90.92	104.00
9	J	17	ARG	CA-C-N	8.35	128.05	119.19
9	J	17	ARG	C-N-CA	8.35	128.05	119.19
38	1	45	U	N1-C1'-C2'	-6.12	102.82	112.00
38	1	41	C	N1-C1'-C2'	-5.84	103.24	112.00
9	J	21	SER	N-CA-C	5.53	117.31	111.28
25	P	48	GLY	CA-C-N	-5.15	116.31	122.44
25	P	48	GLY	C-N-CA	-5.15	116.31	122.44

There are no chirality outliers.

There are no planarity outliers.

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	2	38003	0	19120	1124	0
2	A	1702	0	1695	86	0
3	B	1796	0	1874	70	0
4	C	1648	0	1727	74	0
5	E	2078	0	2157	108	0
6	G	1832	0	1919	73	0
7	H	1483	0	1579	76	0
8	I	1489	0	1504	53	0
9	J	1464	0	1547	74	0
10	L	1248	0	1311	43	0
11	N	1195	0	1263	43	0
12	O	955	0	987	61	0
13	V	687	0	682	36	0
14	W	1021	0	1056	67	0
15	X	1119	0	1198	60	0
16	Y	1061	0	1111	51	0
17	a	797	0	835	44	0
18	b	609	0	628	19	0
19	e	472	0	508	27	0
20	h	233	0	284	6	0
21	D	1774	0	1855	42	0
22	F	1609	0	1679	102	0
23	K	809	0	810	55	0
24	M	885	0	917	38	0
25	P	923	0	960	38	0
26	Q	1105	0	1170	68	0
27	R	1033	0	1082	46	0
28	S	1189	0	1211	68	0
29	T	1110	0	1124	55	0
30	U	845	0	913	35	0
31	Z	594	0	590	29	0
32	c	499	0	536	14	0
33	d	461	0	448	34	0
34	f	584	0	600	29	0
35	g	2469	0	2403	101	0
36	i	764	0	763	29	0
37	3	536	0	277	5	0
38	l	1639	0	852	94	0
39	j	2006	0	2066	68	0
40	k	3034	0	3195	98	0
41	l	190	0	191	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	m	619	0	646	24	0
43	2	111	0	0	0	0
43	S	1	0	0	0	0
43	T	2	0	0	0	0
43	i	1	0	0	0	0
43	k	1	0	0	0	0
44	a	1	0	0	0	0
44	b	1	0	0	0	0
44	f	1	0	0	0	0
44	k	1	0	0	0	0
45	k	32	0	13	2	0
46	k	8	0	8	1	0
47	2	3	0	0	0	0
All	All	85732	0	67294	2764	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 18.

All (2764) 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)
38:1:48:5MC:HM52	38:1:59:A:N1	1.41	1.32
38:1:48:5MC:CM5	38:1:59:A:N1	2.16	1.08
38:1:14:A:C2	38:1:48:5MC:N4	2.24	1.04
17:a:26:CYS:HB3	17:a:77:CYS:SG	2.01	1.01
3:B:144:ARG:HB2	3:B:208:GLN:HB2	1.45	0.98
1:2:654:G:H1	1:2:676:U:H3	0.96	0.94
38:1:25:C:C4	38:1:26:M2G:C8	2.56	0.94
38:1:48:5MC:HM52	38:1:59:A:C2	2.04	0.93
1:2:990:G:H21	1:2:1012:A:H62	1.16	0.91
1:2:1213:U:HO2'	33:d:2:ALA:N	1.67	0.91
38:1:10:2MG:O6	38:1:26:M2G:C2	2.24	0.89
35:g:258:TRP:HB3	35:g:269:ILE:HD11	1.55	0.89
1:2:691:U:C4	1:2:692:C:N4	2.40	0.88
40:k:201:MET:HE1	40:k:511:LEU:HB2	1.55	0.88
38:1:25:C:C4	38:1:26:M2G:N7	2.41	0.88
38:1:10:2MG:C6	38:1:26:M2G:C2	2.62	0.87
15:X:68:ILE:HD12	36:i:82:ARG:HE	1.39	0.87
23:K:82:LEU:HD12	23:K:83:PRO:HD2	1.54	0.87
7:H:61:PHE:HB3	7:H:95:GLU:HB2	1.56	0.86
1:2:22:A:H5''	9:J:18:PRO:HG3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:100:ARG:HH12	4:C:102:ARG:HE	1.23	0.83
40:k:499:ILE:HD11	40:k:517:ILE:HG13	1.61	0.83
1:2:778:G:O6	16:Y:10:ARG:NH1	2.09	0.83
34:f:124:CYS:HB2	34:f:128:ILE:HG21	1.57	0.83
5:E:75:LYS:H	5:E:77:ARG:HH22	1.25	0.83
1:2:1290:G:H1	1:2:1323:G:H22	1.24	0.83
24:M:78:PRO:HB2	24:M:128:LEU:HD22	1.60	0.82
22:F:104:ARG:HG3	22:F:105:ASN:ND2	1.95	0.82
1:2:586:C:H5''	19:e:24:GLN:HE22	1.43	0.82
1:2:1252:U:H5''	34:f:128:ILE:HD11	1.62	0.82
22:F:103:GLY:C	22:F:106:ASN:H	1.87	0.82
1:2:922:A:H2'	1:2:923:A:C8	2.15	0.81
38:1:44:A:O2'	38:1:45:U:C5'	2.28	0.81
9:J:17:ARG:O	9:J:23:ARG:NH2	2.14	0.81
4:C:170:VAL:HG11	4:C:215:THR:HA	1.62	0.80
12:O:60:ALA:HB1	12:O:101:ALA:HB2	1.63	0.80
33:d:41:GLN:HA	33:d:44:ARG:HG2	1.62	0.80
38:1:44:A:O2'	38:1:45:U:O4'	1.98	0.80
9:J:16:LYS:O	9:J:18:PRO:HD3	1.81	0.80
35:g:30:GLN:HE22	35:g:32:ASN:HB2	1.46	0.79
22:F:103:GLY:O	22:F:106:ASN:HB2	1.82	0.79
1:2:586:C:OP1	19:e:26:LYS:NZ	2.15	0.79
22:F:221:ARG:NH2	39:j:45:MET:SD	2.55	0.79
1:2:566:A:OP1	15:X:70:LYS:NZ	2.16	0.79
22:F:101:MET:O	22:F:102:ASN:C	2.25	0.79
1:2:511:A:H5''	9:J:163:PRO:HG3	1.63	0.79
1:2:635:A:H5''	14:W:31:SER:HB2	1.63	0.79
22:F:221:ARG:HH12	39:j:82:TYR:HB3	1.47	0.79
40:k:479:LYS:HD2	40:k:482:MET:HB3	1.63	0.79
1:2:1045:G:OP1	3:B:157:GLN:NE2	2.15	0.79
1:2:1754:A:OP2	36:i:67:LYS:NZ	2.15	0.78
27:R:60:ARG:HE	27:R:66:VAL:HG11	1.48	0.78
1:2:521:U:H5''	16:Y:37:LYS:HG3	1.65	0.78
1:2:554:A:N3	1:2:589:C:O2'	2.16	0.78
1:2:975:G:H1	1:2:1022:A:HO2'	1.27	0.78
22:F:148:THR:HB	22:F:159:ARG:HG2	1.65	0.78
25:P:18:LYS:HB2	25:P:36:LEU:HD21	1.64	0.78
38:1:27:C:O2	38:1:43:G:N2	2.17	0.78
1:2:989:C:H5	1:2:1013:G:H1	1.33	0.77
27:R:28:PHE:HA	27:R:55:THR:HG21	1.65	0.77
24:M:120:ASP:HA	24:M:124:ARG:HD2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:283:G:N7	6:G:188:ARG:NH1	2.31	0.77
1:2:899:A:H3'	1:2:900:G:H21	1.50	0.77
1:2:1345:A:OP2	1:2:1347:A:N6	2.17	0.77
24:M:56:VAL:HG21	24:M:85:ALA:HB2	1.66	0.77
12:O:131:GLY:O	17:a:22:ARG:NH2	2.17	0.77
1:2:761:G:N2	1:2:762:A:N7	2.33	0.77
31:Z:61:SER:H	31:Z:64:VAL:HB	1.50	0.76
4:C:45:LYS:NZ	4:C:253:THR:OG1	2.18	0.76
22:F:150:ARG:HG3	22:F:159:ARG:HH11	1.50	0.76
1:2:1398:A:OP1	27:R:60:ARG:NH2	2.19	0.76
38:1:27:C:N3	38:1:43:G:N1	2.27	0.76
17:a:19:LYS:HD2	17:a:20:PRO:HD2	1.68	0.75
26:Q:94:GLN:HG3	26:Q:102:LYS:HD3	1.65	0.75
38:1:74:C:H4'	38:1:75:C:H5'	1.66	0.75
1:2:310:U:OP2	15:X:20:ARG:NH1	2.19	0.75
1:2:1293:G:H1	1:2:1302:U:H3	1.35	0.75
28:S:56:LYS:NZ	28:S:61:LEU:HB3	2.01	0.75
1:2:620:A:HO2'	1:2:1105:U:HO2'	1.31	0.75
22:F:96:THR:HG22	22:F:116:VAL:HG11	1.68	0.75
1:2:1582:G:N2	1:2:1583:U:O4	2.14	0.75
38:1:25:C:N4	38:1:26:M2G:N7	2.35	0.74
38:1:16:H2U:H2'	38:1:60:A:H1'	1.68	0.74
2:A:183:ARG:NH2	2:A:193:GLN:O	2.20	0.74
5:E:73:ASP:OD2	5:E:145:ARG:NH2	2.19	0.74
1:2:1500:G:N7	29:T:102:ARG:NH2	2.35	0.74
7:H:140:VAL:HB	14:W:52:TYR:HB3	1.70	0.74
9:J:136:VAL:HG22	9:J:156:ILE:HG13	1.70	0.74
1:2:1003:U:O4	42:m:59:LYS:NZ	2.21	0.74
4:C:148:TYR:OH	4:C:153:LEU:O	2.04	0.74
38:1:15:G:H22	38:1:48:5MC:CM5	2.00	0.74
1:2:867:G:H2'	1:2:868:A:H8	1.53	0.74
1:2:1653:A:N6	1:2:1743:G:O2'	2.21	0.74
29:T:64:HIS:CE1	29:T:68:ARG:HH22	2.05	0.74
28:S:84:TRP:HA	28:S:89:GLN:HE22	1.53	0.73
1:2:870:G:H2'	1:2:871:G:C8	2.22	0.73
1:2:65:A:H2	1:2:84:A:H62	1.37	0.73
1:2:1396:U:H3'	1:2:1397:C:H5'	1.68	0.73
5:E:208:VAL:HG21	5:E:225:VAL:HG21	1.70	0.73
34:f:131:ALA:N	34:f:138:TYR:O	2.20	0.73
1:2:142:G:OP2	6:G:139:ASN:ND2	2.21	0.73
1:2:512:U:H2'	1:2:513:G:H8	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:U:63:LEU:O	30:U:83:GLU:HA	1.89	0.73
35:g:14:LEU:HB2	35:g:317:ILE:HB	1.69	0.73
5:E:75:LYS:H	5:E:77:ARG:NH2	1.87	0.73
1:2:1212:G:O2'	1:2:1243:A:N6	2.20	0.72
1:2:809:G:N2	7:H:108:GLN:OE1	2.22	0.72
1:2:897:A:N6	1:2:913:G:O2'	2.22	0.72
1:2:1198:G:O2'	1:2:1199:G:OP2	2.06	0.72
33:d:39:ASP:OD1	33:d:42:SER:OG	2.06	0.72
1:2:553:C:N4	1:2:570:G:O6	2.23	0.72
29:T:84:LYS:HG3	29:T:86:ARG:HG2	1.70	0.72
1:2:1757:C:H2'	1:2:1758:G:H8	1.52	0.72
1:2:337:C:H1'	8:I:5:ARG:HB2	1.71	0.72
1:2:447:C:OP1	5:E:49:ARG:NH2	2.21	0.72
15:X:65:ASN:ND2	15:X:116:ASP:OD2	2.20	0.72
25:P:85:ILE:HG13	25:P:111:MET:HB3	1.72	0.72
2:A:70:PRO:HG3	2:A:185:ARG:HH22	1.55	0.72
35:g:122:LYS:HG2	35:g:188:LEU:HD21	1.71	0.72
1:2:163:A:H5''	6:G:112:ILE:HD11	1.72	0.72
9:J:34:TYR:O	9:J:110:GLN:NE2	2.23	0.72
1:2:139:C:N4	1:2:280:G:OP1	2.22	0.71
1:2:890:A:H2'	1:2:891:A:H8	1.54	0.71
26:Q:94:GLN:NE2	35:g:61:SER:OG	2.23	0.71
21:D:202:LEU:O	27:R:42:GLN:NE2	2.21	0.71
25:P:53:PRO:HB3	25:P:83:MET:HE1	1.72	0.71
6:G:26:VAL:HG11	6:G:40:SER:HB2	1.72	0.71
1:2:353:C:H5''	8:I:16:ALA:HB2	1.72	0.71
39:j:206:LYS:HG3	40:k:331:GLU:HG2	1.71	0.71
1:2:1608:G:H4'	22:F:109:LYS:HD3	1.73	0.71
22:F:101:MET:HB2	22:F:182:ARG:HH22	1.55	0.71
28:S:41:ARG:NH2	29:T:36:ILE:O	2.23	0.71
1:2:855:A:N7	7:H:96:ARG:NH1	2.38	0.71
7:H:143:LEU:HG	7:H:145:GLY:H	1.56	0.71
38:1:26:M2G:HM22	38:1:44:A:C2	2.25	0.71
1:2:142:G:H2'	1:2:143:G:C8	2.24	0.71
1:2:984:G:H1	1:2:1015:C:H5	1.36	0.71
1:2:1099:G:O2'	14:W:74:VAL:O	2.08	0.71
24:M:117:TRP:O	24:M:124:ARG:NH2	2.24	0.71
1:2:887:U:H2'	1:2:888:U:C6	2.26	0.71
1:2:1131:A:H2'	1:2:1132:A:H8	1.55	0.71
1:2:1218:A:H4'	23:K:47:GLN:HE22	1.55	0.70
4:C:95:THR:HG23	4:C:97:ALA:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:17:ALA:HA	12:O:30:VAL:HG22	1.73	0.70
26:Q:28:LEU:HB2	26:Q:64:ASP:HB2	1.71	0.70
1:2:598:A:N3	15:X:47:SER:OG	2.23	0.70
4:C:61:ILE:HG23	4:C:66:LEU:HB2	1.72	0.70
40:k:462:LEU:HD22	40:k:503:ARG:HG2	1.72	0.70
1:2:357:U:H2'	1:2:359:A:H8	1.56	0.70
2:A:84:ARG:NH1	2:A:203:PHE:O	2.24	0.70
25:P:18:LYS:HE3	28:S:95:GLY:HA2	1.73	0.70
35:g:179:MET:HA	35:g:205:TYR:HB2	1.73	0.70
1:2:980:U:H1'	1:2:1123:A:H2	1.57	0.70
28:S:50:ALA:O	28:S:68:ARG:NH2	2.25	0.70
1:2:1353:G:O6	1:2:1368:U:O2	2.10	0.70
1:2:1375:U:O2	1:2:1377:C:N4	2.24	0.70
28:S:28:VAL:HA	28:S:58:ALA:HB2	1.73	0.70
1:2:565:C:OP1	36:i:62:ARG:NH1	2.25	0.70
1:2:917:U:H2'	1:2:918:A:C8	2.27	0.70
1:2:1115:A:H5''	20:h:17:ARG:HH22	1.56	0.70
1:2:106:U:OP1	8:I:8:ARG:NH2	2.25	0.69
40:k:473:ALA:HB2	40:k:487:LEU:HD23	1.72	0.69
1:2:1472:G:H2'	1:2:1473:A:H8	1.57	0.69
14:W:11:LEU:HD12	14:W:72:CYS:HB3	1.73	0.69
40:k:377:ILE:HA	40:k:400:THR:HG22	1.73	0.69
1:2:697:C:OP2	7:H:105:LYS:NZ	2.21	0.69
21:D:218:LEU:HG	21:D:221:SER:HB2	1.74	0.69
35:g:83:SER:OG	35:g:93:TRP:NE1	2.23	0.69
38:1:55:U:OP1	39:j:118:LYS:NZ	2.25	0.69
1:2:990:G:N2	1:2:1012:A:H62	1.89	0.69
1:2:1563:C:OP1	28:S:41:ARG:NH1	2.26	0.69
1:2:1607:U:OP2	26:Q:14:LYS:NZ	2.23	0.69
1:2:1338:C:O2'	1:2:1340:A:N7	2.25	0.69
1:2:1778:G:H2'	1:2:1779:A:C8	2.27	0.69
35:g:117:ASP:OD1	35:g:118:ALA:N	2.26	0.69
39:j:51:LEU:O	39:j:88:ARG:NH1	2.26	0.69
5:E:99:PHE:HE1	5:E:113:ARG:HG3	1.57	0.69
1:2:1219:C:OP1	23:K:52:LYS:NZ	2.24	0.69
1:2:1227:G:H5'	24:M:38:LEU:HD22	1.75	0.69
1:2:1752:A:H2'	36:i:44:ASN:HD22	1.57	0.69
10:L:3:THR:HG21	10:L:7:VAL:HA	1.74	0.69
12:O:112:ILE:HD13	17:a:53:LEU:HD12	1.75	0.69
38:1:58:1MA:H1'	38:1:60:A:H62	1.56	0.69
38:1:72:U:O2'	39:j:223:VAL:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:20:ARG:HH21	14:W:56:HIS:HB3	1.58	0.69
1:2:396:A:H4'	8:I:50:GLY:HA2	1.74	0.68
1:2:1277:G:N2	1:2:1431:G:O6	2.20	0.68
1:2:1545:A:O2'	28:S:89:GLN:O	2.10	0.68
12:O:24:ASN:HA	12:O:55:SER:HB2	1.75	0.68
1:2:99:C:OP2	1:2:377:A:O2'	2.10	0.68
1:2:1488:A:OP1	21:D:9:ARG:NH2	2.26	0.68
5:E:122:LYS:HB2	5:E:164:LEU:HD22	1.74	0.68
15:X:60:GLU:N	15:X:60:GLU:OE2	2.27	0.68
1:2:751:G:H2'	1:2:752:A:H8	1.59	0.68
1:2:928:A:H5''	1:2:930:C:H41	1.57	0.68
24:M:105:LYS:HD2	24:M:106:VAL:HG12	1.75	0.68
6:G:58:LYS:HA	6:G:107:ALA:HB2	1.75	0.68
28:S:56:LYS:HZ2	28:S:61:LEU:HB3	1.59	0.68
39:j:222:LEU:HD21	40:k:324:ASN:HB3	1.74	0.68
40:k:103:ILE:HG12	40:k:213:ALA:HB3	1.74	0.68
1:2:283:G:O6	6:G:188:ARG:NH2	2.25	0.68
1:2:399:A:H5''	8:I:25:ARG:HA	1.74	0.68
1:2:1779:A:O3'	20:h:9:ARG:NH2	2.27	0.68
4:C:232:PRO:O	14:W:68:ARG:NH2	2.26	0.68
21:D:135:GLU:HG2	21:D:153:ALA:HB2	1.75	0.68
1:2:297:C:O3'	5:E:30:ARG:NH2	2.27	0.68
1:2:1456:G:OP2	28:S:139:LYS:NZ	2.25	0.68
5:E:11:ARG:HA	5:E:28:ALA:HB2	1.75	0.68
38:1:44:A:O2'	38:1:45:U:O5'	2.12	0.68
1:2:1085:A:H2'	1:2:1086:A:C8	2.29	0.68
1:2:1406:G:H4'	35:g:18:ASN:HD21	1.57	0.68
7:H:105:LYS:O	7:H:107:ARG:NH2	2.26	0.68
26:Q:49:TYR:HB3	26:Q:53:LEU:HD23	1.76	0.68
1:2:1598:A:H2'	1:2:1599:G:H5''	1.75	0.68
11:N:130:ARG:NH2	11:N:139:TRP:O	2.27	0.68
25:P:18:LYS:HD3	28:S:92:VAL:HG12	1.76	0.68
35:g:249:ALA:H	35:g:262:ALA:HB3	1.57	0.68
39:j:74:LEU:HB3	39:j:75:ARG:HH11	1.58	0.68
1:2:923:A:H2'	1:2:924:G:C8	2.29	0.67
9:J:142:ASN:ND2	16:Y:64:TYR:OH	2.27	0.67
1:2:705:U:H2'	1:2:706:A:H8	1.59	0.67
1:2:760:A:N1	1:2:789:U:C4	2.63	0.67
2:A:30:GLN:NE2	2:A:31:VAL:O	2.27	0.67
15:X:60:GLU:OE1	36:i:60:HIS:NE2	2.25	0.67
28:S:25:ASN:O	28:S:57:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:474:A:OP1	9:J:126:ARG:NH1	2.26	0.67
1:2:905:A:P	12:O:52:ARG:HE	2.17	0.67
1:2:918:A:H1'	12:O:36:ARG:HG2	1.76	0.67
35:g:32:ASN:ND2	35:g:48:LEU:O	2.26	0.67
1:2:512:U:H2'	1:2:513:G:C8	2.30	0.67
1:2:1219:C:H5''	23:K:52:LYS:HD2	1.77	0.67
1:2:1411:U:O2'	1:2:1414:G:OP1	2.09	0.67
1:2:246:A:O2'	10:L:36:LYS:NZ	2.28	0.67
1:2:339:U:H2'	1:2:340:A:H8	1.60	0.67
1:2:357:U:H2'	1:2:359:A:C8	2.30	0.67
1:2:530:C:O2	16:Y:62:THR:OG1	2.13	0.67
1:2:586:C:OP2	19:e:23:LYS:NZ	2.27	0.67
1:2:688:G:OP2	14:W:119:LYS:NZ	2.26	0.67
29:T:97:SER:O	29:T:101:ASN:ND2	2.28	0.67
1:2:22:A:H5''	9:J:18:PRO:CG	2.24	0.67
10:L:8:GLN:HE22	10:L:13:PHE:HA	1.59	0.67
1:2:367:U:O4	1:2:368:A:N6	2.28	0.67
1:2:1564:U:H5''	28:S:39:GLY:H	1.59	0.67
1:2:1677:G:H21	1:2:1720:A:H62	1.42	0.67
1:2:29:U:H2'	1:2:30:G:H8	1.59	0.67
3:B:144:ARG:HB3	3:B:206:PRO:HB2	1.77	0.67
5:E:100:ARG:NH1	5:E:118:GLU:OE1	2.26	0.67
4:C:152:ASN:ND2	13:V:2:GLU:O	2.28	0.67
9:J:81:VAL:HG11	9:J:91:LYS:HE2	1.77	0.67
40:k:305:PRO:HG2	40:k:307:ARG:HD2	1.77	0.67
1:2:1486:G:H3'	1:2:1513:A:H61	1.59	0.66
35:g:92:LEU:HB3	35:g:102:ALA:HB3	1.76	0.66
1:2:165:C:O2'	6:G:133:LEU:O	2.12	0.66
1:2:332:A:H5''	8:I:54:LYS:HE3	1.77	0.66
1:2:1386:A:OP2	27:R:32:LYS:NZ	2.27	0.66
4:C:100:ARG:HH12	4:C:102:ARG:NE	1.91	0.66
7:H:22:GLN:NE2	7:H:26:ASP:OD1	2.29	0.66
11:N:96:VAL:HG11	11:N:150:VAL:HG21	1.75	0.66
1:2:249:C:H2'	1:2:250:A:H8	1.60	0.66
1:2:1640:G:O2'	1:2:1779:A:O2'	2.14	0.66
2:A:76:ILE:HD13	2:A:121:VAL:HG13	1.78	0.66
1:2:654:G:O6	1:2:676:U:O4	2.12	0.66
1:2:893:U:H2'	1:2:894:G:H8	1.60	0.66
1:2:1613:C:H3'	22:F:83:ARG:HD2	1.78	0.66
8:I:43:ILE:HD11	8:I:55:PHE:HB3	1.77	0.66
17:a:22:ARG:NH2	17:a:27:SER:O	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:67:GLU:HA	28:S:70:VAL:HG22	1.78	0.66
7:H:62:VAL:HG21	7:H:67:LEU:HD13	1.77	0.66
8:I:78:ILE:HG21	8:I:96:LEU:HD11	1.76	0.66
11:N:5:HIS:HD2	11:N:121:ARG:HD2	1.59	0.66
42:m:92:MET:HE1	42:m:103:ILE:HG21	1.78	0.66
1:2:902:U:H1'	1:2:905:A:H62	1.60	0.66
2:A:162:CYS:SG	2:A:163:ASN:N	2.69	0.66
38:1:15:G:H22	38:1:48:5MC:HM51	1.61	0.66
38:1:25:C:C5	38:1:26:M2G:C8	2.83	0.66
38:1:48:5MC:CM5	38:1:59:A:C2	2.74	0.66
1:2:865:G:OP1	11:N:1:MET:N	2.23	0.66
1:2:983:G:H2'	1:2:984:G:H8	1.60	0.66
5:E:256:ARG:HA	5:E:259:HIS:HE1	1.60	0.66
11:N:142:GLU:N	11:N:142:GLU:OE2	2.28	0.66
1:2:297:C:H5''	5:E:38:LEU:HD23	1.78	0.66
12:O:127:ARG:HH22	17:a:22:ARG:HG3	1.60	0.66
1:2:703:G:H3'	1:2:704:C:H3'	1.78	0.66
1:2:1170:A:H2'	1:2:1171:G:C8	2.31	0.66
1:2:694:U:H2'	7:H:98:ILE:HG12	1.78	0.65
8:I:116:HIS:O	8:I:147:ARG:NH1	2.29	0.65
21:D:43:PRO:HG3	30:U:108:ILE:HD13	1.78	0.65
22:F:68:LYS:NZ	26:Q:111:SER:O	2.27	0.65
1:2:123:G:OP1	5:E:75:LYS:NZ	2.25	0.65
1:2:152:G:H2'	1:2:153:G:H8	1.61	0.65
1:2:1484:G:H8	1:2:1591:A:H5'	1.61	0.65
4:C:50:VAL:HG21	4:C:73:ILE:HG23	1.77	0.65
1:2:357:U:O2'	1:2:359:A:OP1	2.14	0.65
1:2:371:G:H1'	1:2:611:U:H3	1.61	0.65
25:P:83:MET:HB3	25:P:116:LEU:HD23	1.77	0.65
9:J:28:LEU:HD11	19:e:39:LEU:HD22	1.79	0.65
1:2:1162:A:N3	1:2:1611:U:O2'	2.26	0.65
4:C:93:LYS:HD2	4:C:100:ARG:HH21	1.62	0.65
22:F:31:ILE:HD12	26:Q:57:LEU:HD11	1.77	0.65
39:j:92:SER:HA	39:j:95:ILE:HD12	1.78	0.65
1:2:748:U:OP1	14:W:82:LYS:NZ	2.30	0.65
35:g:161:ASN:OD1	35:g:162:LEU:N	2.30	0.65
1:2:563:G:N2	1:2:576:G:OP1	2.20	0.65
15:X:103:LEU:HD13	15:X:126:LYS:HD3	1.77	0.65
40:k:432:ILE:HG21	40:k:515:ALA:HB1	1.78	0.65
26:Q:13:LYS:HE3	26:Q:14:LYS:HE3	1.79	0.65
40:k:307:ARG:NH2	40:k:342:ILE:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1581:A:OP1	26:Q:135:ARG:NH2	2.30	0.65
35:g:134:VAL:HB	35:g:143:TYR:HB2	1.77	0.65
1:2:1710:A:H2'	1:2:1711:G:H4'	1.79	0.65
39:j:22:VAL:HG12	39:j:36:LEU:HG	1.78	0.65
1:2:207:U:H2'	1:2:208:U:C6	2.32	0.64
1:2:883:A:H2'	1:2:884:G:C8	2.32	0.64
1:2:1170:A:H2'	1:2:1171:G:H8	1.62	0.64
30:U:80:ASP:OD2	33:d:44:ARG:NH1	2.27	0.64
3:B:151:LYS:NZ	3:B:153:THR:O	2.29	0.64
39:j:248:ILE:HG23	39:j:264:ILE:HD13	1.77	0.64
1:2:342:C:H2'	1:2:343:A:H8	1.61	0.64
13:V:11:LEU:HG	13:V:12:TYR:HD1	1.62	0.64
1:2:592:U:H4'	1:2:594:G:H4'	1.80	0.64
35:g:259:LEU:HB2	35:g:272:LEU:HD21	1.79	0.64
1:2:330:A:OP1	8:I:56:ARG:NH2	2.29	0.64
22:F:167:LEU:HG	22:F:171:ASN:HD21	1.63	0.64
42:m:28:ILE:HG12	42:m:42:VAL:HG22	1.78	0.64
14:W:47:ILE:HD11	14:W:63:VAL:HG11	1.79	0.64
30:U:69:LYS:HE2	30:U:78:THR:HG21	1.79	0.64
1:2:1226:A:C6	24:M:36:ARG:HD2	2.33	0.64
21:D:61:GLU:OE2	21:D:64:ARG:NH1	2.30	0.64
26:Q:69:VAL:HG21	26:Q:81:ILE:HD11	1.80	0.64
40:k:432:ILE:HD12	40:k:485:LEU:HD12	1.79	0.64
1:2:1792:A:OP2	17:a:4:LYS:NZ	2.30	0.64
13:V:15:ARG:HH22	13:V:33:GLN:HB2	1.63	0.64
1:2:17:C:H2'	1:2:18:C:H6	1.61	0.63
6:G:7:TYR:HB2	6:G:113:ILE:HD11	1.80	0.63
4:C:178:PRO:HB2	9:J:97:LEU:HD21	1.79	0.63
6:G:122:GLU:OE2	6:G:122:GLU:N	2.25	0.63
6:G:159:ARG:HD2	6:G:172:ALA:HB2	1.80	0.63
7:H:96:ARG:NH2	7:H:116:ARG:HD3	2.14	0.63
10:L:2:SER:HA	10:L:113:PRO:HB3	1.79	0.63
38:1:9:1MG:H4'	38:1:45:U:O2'	1.98	0.63
1:2:862:A:OP1	14:W:57:ARG:NH2	2.29	0.63
1:2:1603:G:OP2	26:Q:127:LYS:NZ	2.29	0.63
8:I:117:TYR:OH	8:I:150:GLU:OE2	2.10	0.63
26:Q:47:LYS:HB3	26:Q:82:ARG:HD3	1.81	0.63
22:F:93:GLU:O	22:F:97:ASN:ND2	2.31	0.63
1:2:339:U:H2'	1:2:340:A:C8	2.33	0.63
1:2:383:G:H2'	1:2:384:A:C8	2.33	0.63
1:2:1021:C:O2'	1:2:1124:A:N1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:16:PRO:HA	16:Y:19:ALA:HA	1.80	0.63
31:Z:78:VAL:HA	31:Z:81:ARG:HE	1.64	0.63
31:Z:78:VAL:HG22	31:Z:81:ARG:HH21	1.63	0.63
1:2:404:C:O2'	6:G:92:ARG:O	2.17	0.63
22:F:190:LYS:HZ3	31:Z:63:SER:HB3	1.63	0.63
1:2:384:A:OP1	8:I:25:ARG:NH1	2.31	0.63
1:2:1086:A:H2'	1:2:1087:A:C8	2.34	0.63
1:2:1673:C:O2'	8:I:32:GLN:NE2	2.32	0.63
3:B:205:PHE:CD1	3:B:206:PRO:HD2	2.34	0.63
1:2:905:A:OP2	12:O:52:ARG:NE	2.28	0.63
1:2:1384:G:H4'	35:g:67:HIS:HE2	1.64	0.63
1:2:1628:U:O2'	1:2:1762:C:O2'	2.17	0.63
3:B:82:ARG:NH2	3:B:103:MET:HE3	2.14	0.63
24:M:90:GLU:HA	24:M:104:ARG:HH12	1.63	0.63
42:m:69:VAL:O	42:m:77:ILE:HB	1.97	0.63
1:2:391:G:OP1	1:2:1727:C:O2'	2.15	0.63
1:2:1765:G:H4'	1:2:1766:G:O5'	1.99	0.63
15:X:6:PRO:HG2	15:X:14:LYS:HG2	1.81	0.63
23:K:5:LYS:HG2	23:K:9:LYS:NZ	2.13	0.63
38:1:26:M2G:HM22	38:1:44:A:N1	2.13	0.63
1:2:403:G:O2'	6:G:91:GLU:OE1	2.16	0.62
1:2:952:G:H2'	1:2:953:G:C8	2.34	0.62
1:2:1556:U:OP1	28:S:122:HIS:ND1	2.31	0.62
9:J:45:ILE:HD13	9:J:105:LEU:HG	1.81	0.62
1:2:326:U:H2'	1:2:327:A:C8	2.33	0.62
1:2:628:U:OP2	1:2:968:C:N4	2.33	0.62
17:a:46:GLU:OE1	17:a:46:GLU:N	2.31	0.62
28:S:136:GLN:N	28:S:136:GLN:OE1	2.30	0.62
1:2:95:G:OP1	5:E:6:LYS:NZ	2.32	0.62
1:2:533:A:H3'	1:2:534:A:H8	1.64	0.62
1:2:559:U:H2'	1:2:560:G:H8	1.65	0.62
1:2:1661:G:N2	1:2:1736:U:O2	2.31	0.62
1:2:1682:U:O2	1:2:1715:G:O6	2.17	0.62
4:C:49:LEU:HD11	4:C:248:TYR:HB3	1.80	0.62
24:M:87:GLN:O	24:M:90:GLU:HG3	1.98	0.62
1:2:418:G:O5'	6:G:72:ARG:NH2	2.32	0.62
1:2:691:U:N3	1:2:692:C:N4	2.47	0.62
25:P:85:ILE:HB	25:P:112:VAL:HA	1.81	0.62
2:A:207:PRO:O	2:A:210:ILE:HG22	2.00	0.62
5:E:182:TYR:N	5:E:226:PHE:O	2.31	0.62
5:E:195:ILE:HG12	5:E:210:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:93:LEU:HB3	19:e:11:ALA:HB1	1.81	0.62
22:F:145:ARG:N	22:F:220:GLU:OE2	2.26	0.62
27:R:60:ARG:NE	27:R:66:VAL:HG11	2.15	0.62
28:S:53:ASP:HB3	28:S:56:LYS:HB2	1.80	0.62
40:k:133:GLU:HB2	40:k:134:ARG:HD2	1.82	0.62
40:k:213:ALA:HB2	40:k:302:ILE:HG21	1.82	0.62
1:2:78:A:O2'	6:G:173:PRO:O	2.17	0.62
1:2:1297:U:O2'	4:C:217:LYS:NZ	2.29	0.62
38:1:10:2MG:O6	38:1:26:M2G:N1	2.31	0.62
1:2:161:A:H3'	1:2:162:G:H21	1.63	0.62
1:2:1472:G:H2'	1:2:1473:A:C8	2.35	0.62
5:E:73:ASP:N	5:E:89:VAL:O	2.32	0.62
8:I:101:ILE:HD12	8:I:185:LEU:HD11	1.82	0.62
1:2:151:U:O2	6:G:4:ASN:ND2	2.32	0.62
1:2:488:C:N3	1:2:489:C:N4	2.48	0.62
1:2:571:C:OP1	15:X:109:ARG:NH1	2.33	0.62
1:2:1253:U:OP2	24:M:39:ARG:NH2	2.32	0.62
1:2:1277:G:H1	1:2:1428:U:H3	1.47	0.62
7:H:56:LYS:HB2	7:H:88:ARG:HG2	1.81	0.62
10:L:131:ILE:HB	10:L:135:VAL:HG13	1.81	0.62
10:L:132:SER:O	10:L:136:ARG:NH1	2.29	0.62
1:2:983:G:H1	1:2:1016:U:H5	1.48	0.62
1:2:1322:C:H2'	1:2:1323:G:C8	2.34	0.62
11:N:64:LYS:HG3	11:N:70:LYS:HZ3	1.65	0.62
25:P:103:ASN:HD21	25:P:120:SER:HA	1.64	0.62
1:2:329:G:OP2	8:I:173:ARG:NH1	2.33	0.62
1:2:1209:C:H2'	1:2:1210:A:H8	1.65	0.62
13:V:1:MET:HA	13:V:10:GLU:HB2	1.80	0.62
9:J:100:LYS:O	9:J:102:GLU:N	2.33	0.61
22:F:197:ALA:O	22:F:201:ILE:HD12	2.00	0.61
23:K:83:PRO:HB2	23:K:85:HIS:CD2	2.35	0.61
1:2:140:A:H61	6:G:187:LYS:HB2	1.65	0.61
15:X:69:ARG:HB3	15:X:86:PHE:HE1	1.64	0.61
39:j:8:PHE:O	39:j:127:TYR:OH	2.14	0.61
1:2:589:C:H5''	19:e:43:ARG:HH21	1.66	0.61
1:2:645:U:O2	1:2:688:G:O6	2.17	0.61
5:E:185:GLY:HA2	5:E:189:LEU:HD12	1.81	0.61
24:M:28:SER:O	24:M:33:GLY:N	2.28	0.61
1:2:154:U:OP2	16:Y:132:ARG:NH2	2.32	0.61
1:2:267:C:OP1	6:G:176:GLN:NE2	2.33	0.61
1:2:697:C:H3'	7:H:105:LYS:HZ3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1064:A:H1'	3:B:146:GLN:HE21	1.65	0.61
1:2:1201:A:N6	1:2:1455:C:OP1	2.33	0.61
1:2:1038:A:O2'	1:2:1039:G:O5'	2.17	0.61
1:2:1580:U:OP1	26:Q:135:ARG:NH1	2.32	0.61
6:G:180:THR:HG23	6:G:183:ARG:H	1.64	0.61
1:2:508:G:H2'	1:2:509:G:C8	2.34	0.61
8:I:32:GLN:OE1	8:I:32:GLN:N	2.29	0.61
22:F:127:THR:HG23	31:Z:58:ARG:HH22	1.64	0.61
29:T:89:ARG:HA	29:T:89:ARG:NE	2.16	0.61
1:2:708:C:O2'	1:2:710:U:OP2	2.16	0.61
4:C:74:ILE:HD11	4:C:78:LEU:HD12	1.83	0.61
10:L:78:THR:HG22	10:L:84:ILE:HD11	1.82	0.61
19:e:41:THR:HA	19:e:45:VAL:HG22	1.82	0.61
39:j:81:GLY:O	39:j:82:TYR:HD1	1.82	0.61
1:2:158:U:O2'	6:G:87:ARG:NE	2.34	0.61
1:2:1590:A:H2'	1:2:1591:A:H8	1.66	0.61
21:D:76:ARG:HG3	21:D:77:PHE:CD1	2.36	0.61
31:Z:45:ASP:O	31:Z:49:ARG:HG2	2.01	0.61
1:2:883:A:H2'	1:2:884:G:H8	1.66	0.61
1:2:1591:A:H2'	1:2:1592:G:H8	1.66	0.61
4:C:118:LEU:HD11	4:C:216:LEU:HB3	1.83	0.61
12:O:83:ILE:H	12:O:83:ILE:HD12	1.66	0.61
34:f:132:ASN:O	34:f:132:ASN:ND2	2.33	0.61
35:g:90:LEU:HD11	35:g:125:SER:HB2	1.83	0.61
1:2:1782:C:H2'	1:2:1783:U:C6	2.36	0.60
9:J:34:TYR:OH	9:J:102:GLU:OE2	2.18	0.60
29:T:51:GLU:OE2	29:T:51:GLU:N	2.32	0.60
1:2:12:U:H2'	1:2:13:C:C6	2.36	0.60
1:2:321:G:O2'	8:I:10:LYS:NZ	2.34	0.60
1:2:1626:U:H2'	1:2:1627:G:H8	1.66	0.60
1:2:1660:G:H2'	1:2:1661:G:H8	1.65	0.60
8:I:36:THR:HG21	8:I:174:PRO:HB2	1.83	0.60
1:2:16:G:H21	1:2:1137:A:H62	1.48	0.60
1:2:443:C:O5'	16:Y:105:ARG:NH1	2.34	0.60
1:2:535:C:H3'	1:2:536:G:H8	1.65	0.60
23:K:16:PHE:HB2	23:K:76:LEU:HD21	1.84	0.60
1:2:129:U:OP1	1:2:131:C:N4	2.34	0.60
1:2:860:U:O2'	14:W:56:HIS:O	2.20	0.60
1:2:1481:A:H2'	1:2:1482:G:C8	2.37	0.60
2:A:191:ARG:HH12	13:V:43:GLY:HA3	1.65	0.60
8:I:67:TRP:O	8:I:71:GLY:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1:16:H2U:H3'	38:1:61:C:OP1	2.00	0.60
1:2:3:U:O2'	9:J:17:ARG:NH2	2.35	0.60
1:2:125:U:O2'	5:E:148:ARG:NH2	2.32	0.60
1:2:965:A:OP2	11:N:124:ARG:NH1	2.35	0.60
2:A:26:ALA:HB2	2:A:48:ILE:HD11	1.83	0.60
10:L:118:GLN:N	10:L:118:GLN:OE1	2.34	0.60
1:2:220:A:H2'	1:2:221:A:C8	2.36	0.60
22:F:103:GLY:HA3	22:F:106:ASN:HB2	1.83	0.60
27:R:21:TYR:OH	27:R:62:GLN:OE1	2.18	0.60
1:2:121:U:H2'	1:2:122:U:C6	2.36	0.60
1:2:917:U:O3'	12:O:18:ARG:NH2	2.34	0.60
1:2:1768:U:H2'	1:2:1769:U:H6	1.67	0.60
2:A:121:VAL:HG23	2:A:141:ILE:HG21	1.84	0.60
7:H:71:HIS:HA	7:H:74:GLN:HB2	1.83	0.60
1:2:234:G:H2'	1:2:235:A:C8	2.37	0.60
2:A:140:ASN:HD21	13:V:29:HIS:HD2	1.49	0.60
7:H:9:LEU:HD21	7:H:21:ALA:HB2	1.84	0.60
10:L:19:ILE:HG23	10:L:32:LYS:HE3	1.84	0.60
34:f:121:CYS:HB3	34:f:128:ILE:HG23	1.82	0.60
42:m:84:GLN:HB3	42:m:87:LYS:HB2	1.82	0.60
1:2:558:C:H5''	19:e:59:SER:HB2	1.84	0.60
14:W:106:THR:OG1	14:W:111:MET:SD	2.53	0.60
15:X:107:PHE:CE2	15:X:114:LYS:HE2	2.37	0.60
17:a:74:CYS:SG	17:a:77:CYS:N	2.66	0.60
34:f:102:VAL:HA	34:f:105:TYR:HD2	1.65	0.60
35:g:34:LEU:O	35:g:45:SER:HA	2.01	0.60
39:j:8:PHE:HE2	39:j:109:HIS:HB2	1.67	0.60
39:j:50:GLU:OE2	39:j:88:ARG:HB2	2.02	0.60
40:k:322:ASP:HB3	40:k:408:ARG:HA	1.84	0.60
1:2:125:U:O4	1:2:290:G:N1	2.32	0.60
1:2:589:C:H2'	1:2:590:A:H8	1.67	0.60
1:2:809:G:N3	7:H:111:LYS:HB2	2.17	0.60
1:2:1431:G:H2'	1:2:1432:U:C6	2.37	0.60
1:2:1457:C:OP2	28:S:126:ARG:NH2	2.29	0.60
1:2:1737:C:H2'	1:2:1738:A:C8	2.37	0.60
3:B:87:ARG:HB2	3:B:101:HIS:HB2	1.82	0.60
3:B:143:THR:HB	3:B:205:PHE:HE2	1.67	0.60
38:1:10:2MG:C6	38:1:26:M2G:N3	2.70	0.60
39:j:186:ALA:HB2	39:j:244:LEU:HD11	1.83	0.60
40:k:359:ILE:HG23	40:k:373:ILE:HD11	1.83	0.60
40:k:463:MET:HA	40:k:472:GLY:HA2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:441:C:O2'	1:2:524:A:N1	2.35	0.59
10:L:30:LYS:HG3	10:L:31:THR:H	1.66	0.59
27:R:116:LYS:HG3	27:R:117:LEU:H	1.67	0.59
3:B:98:THR:H	3:B:232:HIS:HE1	1.50	0.59
24:M:52:LEU:HD12	24:M:128:LEU:HD11	1.84	0.59
16:Y:35:VAL:HG23	16:Y:40:LEU:HD21	1.84	0.59
1:2:25:C:H5''	1:2:26:A:H5''	1.84	0.59
1:2:163:A:H2'	1:2:164:G:C8	2.37	0.59
1:2:1386:A:N6	1:2:1409:A:N7	2.50	0.59
4:C:81:LEU:HD12	4:C:109:VAL:HG22	1.84	0.59
10:L:81:HIS:CE1	10:L:82:ARG:HG3	2.38	0.59
1:2:798:A:O3'	5:E:201:HIS:NE2	2.35	0.59
1:2:1097:U:O2'	14:W:71:LYS:NZ	2.33	0.59
1:2:1733:U:H2'	1:2:1734:G:C8	2.37	0.59
3:B:213:ARG:HD2	3:B:214:LYS:HB2	1.82	0.59
16:Y:122:GLY:HA2	16:Y:125:ILE:HD13	1.84	0.59
26:Q:45:ARG:O	26:Q:48:VAL:HG12	2.02	0.59
30:U:82:TYR:HB3	33:d:52:PHE:HB3	1.82	0.59
1:2:127:G:O6	6:G:202:ARG:NH2	2.28	0.59
1:2:1314:U:OP1	1:2:1327:G:N2	2.33	0.59
1:2:1482:G:N2	1:2:1604:C:O2	2.31	0.59
1:2:1571:A:H4'	1:2:1572:G:O5'	2.02	0.59
3:B:143:THR:HB	3:B:205:PHE:CE2	2.38	0.59
9:J:39:LYS:HA	9:J:42:ILE:HD13	1.83	0.59
26:Q:83:GLN:NE2	26:Q:117:LEU:O	2.35	0.59
28:S:120:ARG:HG3	28:S:125:ILE:HD11	1.83	0.59
30:U:67:THR:OG1	30:U:80:ASP:OD1	2.19	0.59
38:1:25:C:H2'	38:1:26:M2G:O4'	2.03	0.59
1:2:206:U:O2	8:I:179:ARG:NH2	2.36	0.59
1:2:223:C:H2'	1:2:224:A:C8	2.37	0.59
1:2:129:U:H5'	1:2:263:G:H22	1.67	0.59
10:L:77:SER:HB3	10:L:85:VAL:HB	1.85	0.59
14:W:6:VAL:HG13	14:W:34:ILE:HD11	1.85	0.59
23:K:22:VAL:HG23	23:K:23:ALA:H	1.67	0.59
39:j:25:GLN:HG3	39:j:26:GLN:HG2	1.85	0.59
1:2:383:G:H2'	1:2:384:A:H8	1.68	0.59
1:2:1785:C:OP2	12:O:132:ARG:N	2.33	0.59
5:E:104:ASP:HB2	5:E:110:ALA:HB2	1.85	0.59
26:Q:47:LYS:HA	26:Q:50:GLU:HG2	1.83	0.59
28:S:86:LEU:H	28:S:89:GLN:NE2	2.01	0.59
1:2:1590:A:H2'	1:2:1591:A:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1759:U:O2'	37:3:30:U:OP1	2.19	0.58
5:E:122:LYS:NZ	5:E:143:ASP:OD2	2.36	0.58
6:G:47:GLY:O	6:G:115:LYS:NZ	2.34	0.58
11:N:88:LEU:O	11:N:92:ILE:HG12	2.02	0.58
13:V:71:ARG:HE	13:V:72:LEU:HD22	1.67	0.58
22:F:92:VAL:O	22:F:96:THR:HG23	2.03	0.58
40:k:213:ALA:HB1	40:k:302:ILE:HD13	1.84	0.58
1:2:751:G:H2'	1:2:752:A:C8	2.38	0.58
2:A:59:LEU:O	2:A:63:ILE:HG13	2.02	0.58
2:A:84:ARG:NE	27:R:82:ASP:OD1	2.33	0.58
3:B:166:LYS:O	3:B:169:SER:OG	2.14	0.58
9:J:153:GLU:HG2	9:J:154:LYS:HD2	1.84	0.58
14:W:14:ILE:HD12	14:W:25:VAL:HG11	1.85	0.58
28:S:72:ILE:HG23	28:S:79:TYR:HD2	1.67	0.58
35:g:90:LEU:HB2	35:g:104:PHE:HB2	1.86	0.58
39:j:27:ILE:HD11	39:j:63:ILE:HD13	1.85	0.58
1:2:39:A:O2'	1:2:468:C:N4	2.37	0.58
1:2:426:C:H1'	1:2:458:G:H1'	1.84	0.58
1:2:1670:G:H2'	1:2:1671:G:H8	1.68	0.58
7:H:165:LYS:HB3	7:H:169:PHE:CE2	2.38	0.58
27:R:89:SER:N	27:R:92:ASP:OD2	2.34	0.58
1:2:1477:A:OP1	29:T:57:ARG:NE	2.34	0.58
16:Y:10:ARG:HA	16:Y:10:ARG:NE	2.18	0.58
30:U:35:GLU:OE1	30:U:89:ARG:NH1	2.35	0.58
31:Z:58:ARG:HA	31:Z:103:ARG:HD2	1.84	0.58
1:2:5:U:H2'	1:2:6:G:C8	2.38	0.58
1:2:630:G:N2	1:2:1103:U:OP1	2.35	0.58
1:2:771:A:O2'	9:J:6:ARG:NH2	2.36	0.58
2:A:41:ARG:NH1	27:R:103:ASP:OD2	2.36	0.58
16:Y:55:VAL:HG22	16:Y:75:VAL:HG23	1.85	0.58
23:K:77:ARG:O	23:K:81:ASN:N	2.37	0.58
24:M:90:GLU:HB2	24:M:104:ARG:HH22	1.68	0.58
39:j:166:LEU:HD13	39:j:169:LEU:HD12	1.84	0.58
1:2:332:A:OP2	8:I:48:THR:OG1	2.22	0.58
1:2:384:A:H5''	8:I:22:ARG:HG3	1.86	0.58
1:2:1240:G:O2'	1:2:1241:A:O5'	2.20	0.58
1:2:1475:G:OP1	29:T:44:GLU:N	2.32	0.58
3:B:36:SER:HA	3:B:41:ARG:HE	1.67	0.58
4:C:147:GLY:N	4:C:158:SER:O	2.37	0.58
35:g:183:VAL:HB	35:g:199:PHE:HB2	1.86	0.58
38:1:25:C:N3	38:1:26:M2G:C8	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:90:C:O2'	1:2:450:A:H5''	2.04	0.58
1:2:222:U:H2'	1:2:223:C:C6	2.39	0.58
1:2:866:G:O6	1:2:961:C:N4	2.36	0.58
10:L:3:THR:OG1	10:L:82:ARG:NH2	2.37	0.58
24:M:102:ASN:OD1	24:M:104:ARG:NH2	2.37	0.58
26:Q:77:GLN:O	26:Q:81:ILE:HG12	2.04	0.58
35:g:156:ARG:HD3	35:g:210:GLN:HB3	1.84	0.58
1:2:205:A:OP1	5:E:133:LYS:NZ	2.37	0.58
1:2:589:C:H5'	19:e:56:MET:HE1	1.85	0.58
1:2:857:G:OP1	7:H:116:ARG:NH2	2.37	0.58
1:2:1029:A:OP2	17:a:8:ASN:ND2	2.37	0.58
15:X:53:VAL:HG12	15:X:98:GLU:HG2	1.85	0.58
36:i:71:MET:HG2	36:i:77:ILE:HD11	1.86	0.58
1:2:670:G:O2'	1:2:671:C:OP1	2.21	0.58
1:2:1594:C:O2	33:d:32:ARG:NH1	2.36	0.58
1:2:1773:U:OP2	20:h:11:ARG:NH2	2.28	0.58
7:H:117:THR:HG23	7:H:120:ALA:H	1.68	0.58
1:2:627:G:OP1	11:N:124:ARG:NE	2.35	0.58
22:F:48:TRP:CD1	22:F:131:PRO:HD2	2.39	0.58
22:F:190:LYS:HG3	22:F:195:THR:HG22	1.85	0.58
23:K:5:LYS:HG2	23:K:9:LYS:HZ3	1.68	0.58
1:2:245:G:N2	10:L:66:ILE:O	2.29	0.57
1:2:842:U:O4	1:2:843:A:N6	2.37	0.57
1:2:925:A:H2'	1:2:926:C:C6	2.38	0.57
1:2:1069:C:H5''	18:b:17:ARG:HH22	1.69	0.57
11:N:98:VAL:HG12	11:N:115:LEU:HD12	1.86	0.57
38:1:15:G:H22	38:1:48:5MC:HM52	1.68	0.57
1:2:328:G:H2'	1:2:329:G:H8	1.68	0.57
1:2:613:C:OP1	15:X:3:LYS:NZ	2.34	0.57
22:F:50:PHE:HE2	22:F:70:ILE:H	1.51	0.57
22:F:72:VAL:HB	26:Q:47:LYS:HD3	1.87	0.57
35:g:196:GLU:HG3	35:g:197:ALA:H	1.67	0.57
1:2:864:A:P	14:W:3:ARG:HH22	2.27	0.57
1:2:945:U:H5''	3:B:165:ARG:NH1	2.19	0.57
1:2:1553:A:OP2	25:P:47:ARG:NH1	2.37	0.57
6:G:32:ILE:HG23	6:G:53:ALA:HA	1.86	0.57
9:J:36:LEU:HB3	9:J:41:GLU:OE2	2.04	0.57
11:N:7:LYS:O	11:N:9:LYS:NZ	2.36	0.57
14:W:111:MET:HE1	14:W:119:LYS:HD2	1.86	0.57
39:j:24:VAL:HG13	39:j:34:VAL:HG11	1.86	0.57
1:2:392:C:O2'	6:G:92:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1594:C:H3'	33:d:32:ARG:HH12	1.68	0.57
1:2:1626:U:H2'	1:2:1627:G:C8	2.39	0.57
6:G:41:VAL:HG23	6:G:45:PHE:HD2	1.69	0.57
12:O:61:MET:HE1	32:c:61:ARG:HA	1.85	0.57
38:1:44:A:O2'	38:1:45:U:C4'	2.52	0.57
40:k:197:HIS:CD2	40:k:199:ILE:H	2.21	0.57
1:2:74:U:H4'	1:2:75:U:OP1	2.02	0.57
1:2:168:A:OP1	6:G:137:ARG:NH1	2.38	0.57
1:2:188:C:H2'	1:2:189:C:C6	2.39	0.57
5:E:6:LYS:O	5:E:30:ARG:NH1	2.37	0.57
7:H:101:LYS:HD3	7:H:112:ARG:HH12	1.68	0.57
9:J:168:ARG:HB3	9:J:174:ARG:HH21	1.69	0.57
1:2:22:A:C5'	9:J:18:PRO:HG3	2.30	0.57
1:2:1760:A:H1'	1:2:1780:MA6:H2'	1.86	0.57
9:J:42:ILE:H	9:J:42:ILE:HD12	1.69	0.57
21:D:55:VAL:HA	21:D:58:VAL:HG12	1.87	0.57
1:2:1198:G:N2	33:d:30:LEU:O	2.36	0.57
1:2:1573:7MG:HN22	38:1:42:U:H4'	1.70	0.57
3:B:87:ARG:NH1	3:B:89:ASP:OD2	2.37	0.57
12:O:22:SER:OG	12:O:24:ASN:O	2.22	0.57
24:M:126:ILE:HG12	24:M:130:HIS:NE2	2.20	0.57
26:Q:12:LYS:HA	26:Q:16:ALA:O	2.05	0.57
1:2:5:U:O2'	1:2:552:G:H4'	2.04	0.57
3:B:126:THR:HG22	3:B:136:ARG:HE	1.69	0.57
12:O:58:TYR:OH	22:F:227:ARG:NH1	2.37	0.57
12:O:81:ILE:HD13	12:O:102:LEU:HG	1.86	0.57
30:U:80:ASP:HB2	33:d:54:LYS:NZ	2.20	0.57
32:c:44:VAL:HG21	32:c:54:LEU:HD23	1.86	0.57
35:g:172:ILE:HD12	35:g:188:LEU:HD23	1.85	0.57
35:g:206:ILE:HG21	35:g:209:VAL:HG13	1.86	0.57
1:2:735:C:O2'	1:2:736:C:O5'	2.22	0.57
1:2:1427:G:H2'	1:2:1428:U:H6	1.70	0.57
6:G:57:ASP:OD1	6:G:58:LYS:N	2.37	0.57
11:N:135:LEU:HD12	11:N:136:PRO:HD2	1.87	0.57
15:X:68:ILE:HG13	15:X:68:ILE:O	2.05	0.57
1:2:292:U:H2'	1:2:293:C:C6	2.39	0.57
1:2:1589:C:H2'	1:2:1590:A:H8	1.70	0.57
2:A:148:ASP:OD1	2:A:149:LEU:N	2.36	0.57
17:a:23:CYS:SG	17:a:74:CYS:N	2.78	0.57
35:g:176:SER:OG	35:g:186:TRP:NE1	2.34	0.57
1:2:79:C:H1'	6:G:174:LYS:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:685:A:H2'	1:2:686:C:C6	2.40	0.56
19:e:10:ARG:HB2	19:e:13:LYS:HB2	1.86	0.56
26:Q:69:VAL:HG11	26:Q:77:GLN:HG3	1.86	0.56
35:g:52:GLU:OE2	35:g:54:GLN:NE2	2.36	0.56
1:2:163:A:H2'	1:2:164:G:H8	1.69	0.56
1:2:1737:C:H2'	1:2:1738:A:H8	1.70	0.56
1:2:1781:C:H2'	1:2:1782:C:C6	2.40	0.56
1:2:1793:U:OP2	17:a:4:LYS:NZ	2.38	0.56
26:Q:30:LYS:NZ	29:T:8:ASP:OD1	2.38	0.56
26:Q:36:ILE:HD13	26:Q:52:LEU:HD11	1.87	0.56
36:i:39:THR:HG22	36:i:40:LYS:HD3	1.86	0.56
40:k:287:LEU:HD22	41:l:142:LEU:HD12	1.85	0.56
1:2:812:U:H3	10:L:153:PHE:HB2	1.70	0.56
1:2:1035:A:H2'	1:2:1036:C:C6	2.40	0.56
1:2:1528:C:OP2	31:Z:95:HIS:ND1	2.38	0.56
1:2:1640:G:H2'	1:2:1641:U:C6	2.40	0.56
1:2:1675:C:OP1	8:I:42:ARG:NH1	2.36	0.56
3:B:93:GLY:O	3:B:94:LYS:HG3	2.03	0.56
5:E:125:LYS:HB2	5:E:226:PHE:HE1	1.69	0.56
10:L:100:TYR:OH	14:W:80:ASN:ND2	2.38	0.56
11:N:112:LYS:O	11:N:116:ILE:HG12	2.06	0.56
14:W:25:VAL:HG22	14:W:63:VAL:HB	1.86	0.56
18:b:62:VAL:O	18:b:74:SER:OG	2.23	0.56
22:F:42:ILE:HD12	22:F:42:ILE:H	1.70	0.56
22:F:163:ASP:HB2	32:c:44:VAL:HG22	1.87	0.56
27:R:105:GLN:OE1	27:R:105:GLN:N	2.29	0.56
28:S:17:LEU:HD22	28:S:32:LEU:HD11	1.86	0.56
36:i:38:ILE:HD13	36:i:75:ASP:HB2	1.87	0.56
34:f:139:CYS:SG	34:f:140:GLY:N	2.77	0.56
1:2:159:C:O3'	6:G:95:LYS:NZ	2.38	0.56
1:2:1778:G:C8	42:m:59:LYS:HD3	2.40	0.56
2:A:107:PHE:HB2	2:A:135:GLU:HG3	1.86	0.56
6:G:124:ILE:HG23	6:G:125:THR:HG23	1.88	0.56
23:K:38:LYS:HB2	23:K:41:PHE:CE2	2.40	0.56
1:2:29:U:H2'	1:2:30:G:C8	2.38	0.56
1:2:374:U:H5''	15:X:32:ARG:HH12	1.70	0.56
1:2:946:U:H2'	1:2:947:G:H8	1.70	0.56
1:2:1240:G:H2'	1:2:1241:A:C8	2.40	0.56
1:2:1315:G:OP1	27:R:7:LYS:N	2.37	0.56
1:2:1608:G:O2'	22:F:109:LYS:NZ	2.34	0.56
1:2:1787:G:OP2	12:O:132:ARG:NH2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:22:VAL:HG22	2:A:169:SER:HB2	1.86	0.56
9:J:31:ALA:HA	9:J:36:LEU:HD12	1.87	0.56
13:V:3:ASN:OD1	13:V:4:ASP:N	2.37	0.56
17:a:33:ASP:OD1	17:a:34:LYS:N	2.38	0.56
35:g:196:GLU:HG3	35:g:197:ALA:N	2.20	0.56
40:k:464:VAL:HG21	40:k:485:LEU:HD13	1.87	0.56
1:2:802:A:O2'	7:H:104:ARG:NH2	2.38	0.56
5:E:18:TRP:O	5:E:51:ARG:NH2	2.38	0.56
15:X:107:PHE:HE2	15:X:114:LYS:HB3	1.71	0.56
29:T:42:GLY:HA3	29:T:94:VAL:HG21	1.88	0.56
36:i:101:ARG:O	36:i:104:LYS:HG3	2.05	0.56
40:k:307:ARG:HH22	40:k:343:LEU:HD23	1.70	0.56
42:m:93:ILE:HD11	42:m:100:LYS:HE2	1.87	0.56
1:2:1145:G:H2'	1:2:1146:A:C8	2.41	0.56
1:2:1209:C:H2'	1:2:1210:A:C8	2.41	0.56
25:P:90:ILE:HD12	25:P:109:PRO:HA	1.86	0.56
34:f:118:ARG:O	34:f:119:LYS:HB2	2.04	0.56
1:2:162:G:H2'	1:2:163:A:H8	1.70	0.56
1:2:472:A:O3'	9:J:143:ILE:HD11	2.06	0.56
1:2:651:U:H5''	1:2:652:C:H5	1.69	0.56
1:2:893:U:H2'	1:2:894:G:C8	2.39	0.56
1:2:993:G:OP1	1:2:1776:G:O2'	2.24	0.56
10:L:101:GLU:HB2	15:X:12:ALA:HB3	1.88	0.56
22:F:60:LEU:HD11	22:F:169:ARG:HD3	1.86	0.56
25:P:61:ARG:NH2	25:P:88:GLU:OE1	2.39	0.56
1:2:291:U:H2'	1:2:292:U:C6	2.41	0.56
1:2:512:U:C5	9:J:171:ARG:HD3	2.41	0.56
1:2:563:G:N1	1:2:579:A:OP2	2.34	0.56
1:2:788:A:C2	1:2:789:U:H1'	2.41	0.56
1:2:871:G:H2'	1:2:872:U:O4'	2.06	0.56
1:2:1000:A:OP1	38:1:38:A:O2'	2.23	0.56
1:2:1066:C:H5''	3:B:150:VAL:HG12	1.88	0.56
1:2:1213:U:O2'	33:d:2:ALA:N	2.37	0.56
1:2:1241:A:OP2	1:2:1241:A:H8	1.89	0.56
1:2:1427:G:H2'	1:2:1428:U:C6	2.40	0.56
5:E:44:LEU:HD21	5:E:72:VAL:HG21	1.87	0.56
7:H:144:VAL:HA	14:W:42:GLN:HE21	1.71	0.56
10:L:110:HIS:O	10:L:138:ASN:ND2	2.39	0.56
1:2:790:A:H2'	1:2:791:U:C6	2.40	0.55
1:2:1415:A:H2'	1:2:1416:G:O4'	2.05	0.55
1:2:1573:7MG:HN22	38:1:42:U:C4'	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1712:A:H2'	1:2:1713:G:C8	2.40	0.55
1:2:1757:C:H2'	1:2:1758:G:C8	2.37	0.55
4:C:42:PRO:HB2	4:C:48:ARG:HG3	1.88	0.55
5:E:104:ASP:OD1	5:E:105:VAL:N	2.38	0.55
12:O:49:LYS:NZ	22:F:225:SER:O	2.35	0.55
26:Q:127:LYS:NZ	26:Q:128:LYS:O	2.39	0.55
35:g:223:LYS:HA	35:g:246:GLU:HG2	1.86	0.55
1:2:1250:U:H2'	1:2:1251:C:C6	2.41	0.55
4:C:48:ARG:HH11	4:C:253:THR:HA	1.72	0.55
8:I:57:ALA:HB2	8:I:178:GLY:HA2	1.87	0.55
13:V:79:LEU:HD13	13:V:82:VAL:HG11	1.88	0.55
25:P:96:VAL:HG13	25:P:120:SER:HB3	1.88	0.55
26:Q:11:GLY:HA3	26:Q:83:GLN:HB3	1.87	0.55
1:2:1646:A:H2'	1:2:1647:G:C8	2.42	0.55
11:N:132:VAL:HG13	11:N:134:VAL:HG23	1.88	0.55
23:K:64:TYR:HB3	23:K:66:TYR:CZ	2.41	0.55
30:U:98:HIS:HA	30:U:101:LYS:HD2	1.86	0.55
1:2:5:U:H2'	1:2:6:G:H8	1.72	0.55
1:2:1216:A:H5''	23:K:1:MET:HE3	1.87	0.55
1:2:1780:MA6:H8	1:2:1780:MA6:O5'	2.06	0.55
9:J:59:LEU:HD12	9:J:69:ARG:HA	1.88	0.55
17:a:11:ASN:O	17:a:11:ASN:ND2	2.40	0.55
21:D:105:MET:HB3	21:D:122:VAL:HG21	1.89	0.55
35:g:212:SER:OG	35:g:214:ASP:OD1	2.20	0.55
1:2:155:A:H2'	1:2:156:A:O4'	2.06	0.55
1:2:1195:A:H4'	1:2:1196:C:H5''	1.88	0.55
1:2:1589:C:H2'	1:2:1590:A:C8	2.41	0.55
12:O:25:ASP:HA	12:O:54:GLU:HB3	1.89	0.55
14:W:110:ILE:H	14:W:110:ILE:HD12	1.71	0.55
20:h:7:LYS:HD3	20:h:11:ARG:HH21	1.71	0.55
1:2:189:C:O2'	1:2:190:C:O5'	2.25	0.55
1:2:620:A:O2'	1:2:1105:U:O2'	2.08	0.55
1:2:1159:A:H2'	1:2:1160:C:C6	2.41	0.55
2:A:205:ARG:NH2	2:A:213:GLN:HB2	2.21	0.55
4:C:62:PHE:CD2	4:C:143:PRO:HG3	2.41	0.55
16:Y:76:TYR:CE2	16:Y:86:GLU:HG2	2.41	0.55
35:g:112:LEU:HD11	35:g:128:ARG:HG2	1.89	0.55
42:m:28:ILE:HB	42:m:105:ILE:HG23	1.88	0.55
1:2:808:G:H5''	10:L:148:LYS:NZ	2.22	0.55
1:2:843:A:H2'	1:2:844:G:C8	2.42	0.55
1:2:938:A:H2'	1:2:939:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1064:A:H4'	3:B:205:PHE:HD1	1.71	0.55
9:J:109:LEU:HB2	9:J:146:PHE:HB3	1.88	0.55
10:L:14:GLN:HB3	10:L:54:ILE:HG13	1.88	0.55
16:Y:84:LYS:HD3	16:Y:85:PHE:HE1	1.71	0.55
26:Q:44:LEU:HD22	26:Q:47:LYS:HG3	1.88	0.55
40:k:207:GLY:O	40:k:211:MET:HG2	2.06	0.55
40:k:224:CYS:HB2	40:k:225:PRO:HD3	1.89	0.55
1:2:650:G:O6	1:2:684:A:N6	2.40	0.55
4:C:58:ILE:HD12	4:C:62:PHE:CE2	2.42	0.55
1:2:477:A:H2	1:2:509:G:H22	1.54	0.55
1:2:1055:U:N3	1:2:1062:U:O4	2.40	0.55
7:H:41:LEU:HD22	7:H:70:TYR:HE1	1.72	0.55
9:J:140:ILE:HG21	16:Y:65:GLY:HA3	1.89	0.55
29:T:77:ASN:OD1	29:T:101:ASN:ND2	2.39	0.55
39:j:186:ALA:HB3	39:j:230:LEU:HG	1.88	0.55
1:2:70:C:H2'	1:2:71:A:O4'	2.07	0.55
1:2:1413:U:OP1	27:R:45:ARG:NH2	2.35	0.55
8:I:168:ALA:HA	8:I:185:LEU:H	1.72	0.55
22:F:60:LEU:HD22	22:F:140:ILE:HD13	1.89	0.55
27:R:34:LEU:O	27:R:38:ILE:HG12	2.07	0.55
38:1:27:C:N4	38:1:43:G:O6	2.32	0.55
39:j:185:ARG:HG3	39:j:231:THR:HG22	1.89	0.55
40:k:236:ILE:HG23	40:k:241:LEU:HB2	1.89	0.55
42:m:28:ILE:HD12	42:m:105:ILE:HG12	1.89	0.55
1:2:946:U:H2'	1:2:947:G:C8	2.42	0.54
3:B:113:MET:HE3	3:B:209:ASN:ND2	2.23	0.54
10:L:7:VAL:C	10:L:9:SER:H	2.14	0.54
13:V:83:TRP:HH2	13:V:85:TYR:HD1	1.54	0.54
23:K:39:ASN:O	23:K:43:ILE:HG13	2.07	0.54
30:U:96:PRO:HG2	30:U:99:ILE:HD13	1.89	0.54
3:B:67:GLU:OE1	3:B:85:LYS:HG2	2.07	0.54
7:H:141:ARG:HB3	14:W:51:GLU:OE2	2.07	0.54
9:J:145:SER:C	9:J:147:MET:H	2.15	0.54
16:Y:28:LEU:HD23	16:Y:30:PRO:HD3	1.88	0.54
1:2:245:G:H2'	1:2:246:A:C8	2.42	0.54
1:2:399:A:H4'	1:2:400:A:H5''	1.89	0.54
1:2:1159:A:H2'	1:2:1160:C:H6	1.72	0.54
1:2:1357:G:H2'	1:2:1358:C:C6	2.42	0.54
9:J:123:HIS:CE1	19:e:37:ARG:HB2	2.42	0.54
14:W:57:ARG:HD2	18:b:26:GLN:NE2	2.22	0.54
22:F:147:ASP:OD1	22:F:148:THR:N	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:158:ARG:HG3	22:F:160:GLN:OE1	2.06	0.54
33:d:21:CYS:C	33:d:23:ILE:H	2.14	0.54
1:2:928:A:OP2	1:2:930:C:N4	2.39	0.54
1:2:1485:A:H2'	1:2:1486:G:C8	2.42	0.54
5:E:72:VAL:N	5:E:77:ARG:HH21	2.06	0.54
8:I:24:LYS:HB2	8:I:28:GLU:OE2	2.05	0.54
9:J:146:PHE:HD2	9:J:148:VAL:HG22	1.71	0.54
26:Q:49:TYR:HA	26:Q:52:LEU:HD12	1.89	0.54
31:Z:65:LEU:HD12	31:Z:70:LYS:HE3	1.90	0.54
39:j:113:ARG:HG2	39:j:123:LEU:HD11	1.89	0.54
1:2:1250:U:H2'	1:2:1251:C:H6	1.72	0.54
1:2:1672:C:OP1	6:G:92:ARG:NH1	2.41	0.54
2:A:119:ARG:NH2	4:C:245:MET:SD	2.81	0.54
4:C:232:PRO:HG2	14:W:99:PHE:CG	2.42	0.54
11:N:3:ARG:NH1	11:N:10:GLY:O	2.40	0.54
22:F:93:GLU:HG2	22:F:97:ASN:HD21	1.72	0.54
22:F:150:ARG:HG3	22:F:159:ARG:NH1	2.20	0.54
35:g:164:ASP:O	35:g:167:VAL:N	2.41	0.54
1:2:17:C:H2'	1:2:18:C:C6	2.42	0.54
1:2:127:G:O2'	1:2:128:U:H5'	2.07	0.54
1:2:1513:A:O2'	1:2:1514:A:OP1	2.23	0.54
1:2:1775:G:H2'	1:2:1776:G:C8	2.42	0.54
1:2:1788:A:P	17:a:10:ARG:HH12	2.30	0.54
2:A:13:ASP:OD2	2:A:179:ARG:NH2	2.41	0.54
7:H:47:ARG:HG2	7:H:61:PHE:HE2	1.73	0.54
7:H:96:ARG:HH21	7:H:116:ARG:HA	1.73	0.54
11:N:69:ASN:HD22	11:N:74:ILE:HG13	1.73	0.54
11:N:115:LEU:O	11:N:119:GLU:HG3	2.07	0.54
22:F:50:PHE:HD2	22:F:69:PRO:HA	1.73	0.54
26:Q:127:LYS:HA	26:Q:134:ALA:HA	1.89	0.54
38:1:10:2MG:N1	38:1:26:M2G:N3	2.56	0.54
40:k:356:ARG:HB3	40:k:492:CYS:SG	2.48	0.54
1:2:275:C:H1'	1:2:276:U:H5	1.73	0.54
1:2:808:G:H2'	1:2:809:G:C8	2.43	0.54
1:2:1523:A:N3	1:2:1587:C:O2'	2.37	0.54
1:2:1660:G:H2'	1:2:1661:G:C8	2.42	0.54
5:E:64:ILE:HD11	16:Y:18:LEU:HG	1.90	0.54
5:E:87:MET:SD	5:E:123:LEU:HB3	2.48	0.54
5:E:125:LYS:HB2	5:E:226:PHE:CE1	2.43	0.54
24:M:97:ILE:HD12	24:M:101:GLY:HA2	1.90	0.54
27:R:116:LYS:HG3	27:R:117:LEU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1443:G:N2	34:f:88:PRO:O	2.40	0.54
2:A:36:TYR:HB2	2:A:149:LEU:HD21	1.89	0.54
36:i:26:LEU:HD13	36:i:103:LEU:HD21	1.90	0.54
1:2:332:A:H2'	1:2:333:G:C8	2.42	0.54
1:2:431:G:H2'	1:2:432:C:C6	2.43	0.54
1:2:1498:C:OP1	29:T:122:ARG:NH2	2.41	0.54
1:2:1657:A:H2'	1:2:1658:A:C8	2.42	0.54
4:C:40:TRP:HZ3	4:C:51:LYS:HB2	1.72	0.54
9:J:25:ASP:O	9:J:29:LYS:HG2	2.08	0.54
22:F:39:GLN:H	22:F:39:GLN:CD	2.16	0.54
1:2:234:G:H2'	1:2:235:A:H8	1.73	0.54
1:2:448:C:H2'	1:2:449:U:C6	2.43	0.54
1:2:467:A:N1	1:2:593:A:O2'	2.28	0.54
5:E:23:LEU:HD22	9:J:3:ARG:HH21	1.73	0.54
5:E:72:VAL:HG22	5:E:90:ILE:HG12	1.89	0.54
8:I:60:ILE:HD13	8:I:180:CYS:HB2	1.89	0.54
28:S:44:ASN:OD1	28:S:48:LYS:HE2	2.08	0.54
32:c:58:GLU:HG3	32:c:61:ARG:HD3	1.90	0.54
35:g:132:ILE:HD11	35:g:152:VAL:HG21	1.90	0.54
40:k:147:ILE:HB	40:k:187:ARG:O	2.07	0.54
3:B:146:GLN:CD	3:B:206:PRO:HG3	2.33	0.53
4:C:61:ILE:HA	4:C:66:LEU:HD12	1.90	0.53
6:G:50:PHE:CD1	6:G:113:ILE:HG22	2.43	0.53
10:L:132:SER:HB3	10:L:135:VAL:HG12	1.90	0.53
22:F:57:ASP:HB3	22:F:140:ILE:HD12	1.89	0.53
35:g:23:SER:O	35:g:36:SER:HA	2.07	0.53
40:k:127:ARG:NH1	45:k:601:GCP:O2A	2.41	0.53
1:2:331:U:OP1	8:I:31:ARG:NH1	2.42	0.53
1:2:875:G:O6	17:a:15:ARG:NH2	2.41	0.53
1:2:1143:U:H2'	1:2:1144:U:C6	2.43	0.53
1:2:1290:G:H22	1:2:1323:G:N2	2.07	0.53
1:2:1386:A:H5''	27:R:48:ASN:ND2	2.23	0.53
1:2:1430:U:H4'	1:2:1431:G:O5'	2.09	0.53
24:M:49:GLU:OE1	24:M:49:GLU:N	2.41	0.53
39:j:144:ALA:HB1	39:j:154:VAL:HG11	1.88	0.53
40:k:174:CYS:HB2	40:k:182:ARG:HA	1.91	0.53
1:2:115:G:OP2	10:L:65:SER:OG	2.23	0.53
1:2:253:A:H2'	1:2:254:U:C6	2.43	0.53
1:2:445:A:N6	1:2:460:G:H21	2.07	0.53
1:2:905:A:H4'	39:j:53:ARG:HG3	1.90	0.53
1:2:1162:A:O2'	22:F:168:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:93:LYS:HD2	4:C:100:ARG:NH2	2.23	0.53
5:E:230:GLU:HB2	5:E:233:ARG:HB3	1.88	0.53
19:e:25:GLU:OE2	19:e:27:PRO:HD3	2.08	0.53
35:g:21:VAL:HG21	35:g:317:ILE:HG13	1.90	0.53
40:k:329:GLU:HG2	40:k:331:GLU:H	1.73	0.53
1:2:483:C:H2'	1:2:484:A:H8	1.74	0.53
1:2:509:G:H3'	9:J:176:ARG:HH12	1.73	0.53
1:2:706:A:H1'	1:2:734:A:C4	2.43	0.53
1:2:885:U:H3'	1:2:886:A:H8	1.74	0.53
1:2:1040:G:P	2:A:32:HIS:HD1	2.31	0.53
1:2:1254:G:O2'	1:2:1255:A:N7	2.42	0.53
1:2:1443:G:N2	34:f:87:THR:O	2.40	0.53
3:B:179:SER:HB2	3:B:183:GLN:HB2	1.89	0.53
6:G:7:TYR:CE1	6:G:9:ILE:HB	2.43	0.53
11:N:142:GLU:HG2	11:N:143:SER:H	1.73	0.53
15:X:74:VAL:HG11	15:X:104:LEU:HD11	1.90	0.53
28:S:91:ASP:O	28:S:93:ASN:N	2.38	0.53
39:j:218:VAL:HG23	39:j:219:LYS:HG2	1.91	0.53
1:2:638:U:P	7:H:101:LYS:HE3	2.49	0.53
1:2:952:G:H2'	1:2:953:G:H8	1.69	0.53
1:2:1469:A:OP1	22:F:187:ARG:NH2	2.42	0.53
1:2:1577:U:O2'	26:Q:139:GLN:HG3	2.09	0.53
1:2:1670:G:H2'	1:2:1671:G:C8	2.43	0.53
9:J:171:ARG:H	9:J:174:ARG:HD2	1.72	0.53
12:O:88:GLY:HA2	12:O:122:PRO:HD3	1.90	0.53
14:W:7:LEU:HD12	14:W:11:LEU:HD23	1.89	0.53
21:D:105:MET:SD	21:D:184:ILE:HD13	2.49	0.53
29:T:58:ALA:HB1	29:T:108:LEU:HD11	1.89	0.53
1:2:152:G:N7	16:Y:128:LYS:NZ	2.57	0.53
1:2:598:A:H2'	1:2:599:U:C6	2.44	0.53
1:2:891:A:H2'	1:2:892:U:C6	2.44	0.53
1:2:935:G:N7	17:a:15:ARG:NH1	2.57	0.53
1:2:1239:U:H2'	1:2:1241:A:OP2	2.08	0.53
1:2:1640:G:H2'	1:2:1641:U:H6	1.74	0.53
13:V:66:ASP:OD1	13:V:67:ASP:N	2.40	0.53
24:M:29:LEU:HD23	24:M:36:ARG:HH22	1.74	0.53
38:1:9:1MG:OP2	38:1:46:7MG:O3'	2.25	0.53
1:2:586:C:H5''	19:e:24:GLN:NE2	2.19	0.53
1:2:1652:G:N2	1:2:1743:G:H2'	2.24	0.53
4:C:48:ARG:HD2	4:C:253:THR:H	1.73	0.53
1:2:267:C:H41	6:G:186:ARG:HD3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:610:U:O5'	15:X:5:LYS:NZ	2.41	0.53
1:2:801:G:N2	1:2:803:A:H61	2.06	0.53
2:A:77:SER:HB2	2:A:86:VAL:HG21	1.90	0.53
12:O:46:MET:HE3	12:O:46:MET:HA	1.91	0.53
14:W:87:GLU:HA	14:W:90:THR:HG22	1.91	0.53
22:F:198:GLU:O	22:F:202:ASN:ND2	2.42	0.53
26:Q:69:VAL:HG21	26:Q:81:ILE:CD1	2.38	0.53
40:k:321:PHE:HB2	40:k:337:VAL:HG23	1.90	0.53
40:k:355:ILE:HB	40:k:373:ILE:HB	1.91	0.53
42:m:71:ASP:OD1	42:m:74:MET:HE3	2.09	0.53
7:H:31:SER:HA	7:H:35:LYS:HB2	1.91	0.53
9:J:153:GLU:OE2	9:J:153:GLU:N	2.27	0.53
11:N:13:SER:OG	11:N:14:SER:N	2.41	0.53
17:a:54:SER:O	17:a:57:SER:OG	2.24	0.53
38:1:62:C:H2'	38:1:63:G:C8	2.44	0.53
1:2:242:G:H2'	1:2:243:A:C8	2.44	0.53
1:2:853:U:O4	1:2:854:A:N6	2.42	0.53
1:2:1470:C:H4'	1:2:1471:U:O5'	2.09	0.53
6:G:7:TYR:HE1	6:G:9:ILE:HB	1.73	0.53
22:F:105:ASN:HA	22:F:108:LYS:HD2	1.91	0.53
23:K:54:PHE:HB3	23:K:72:GLY:HA2	1.90	0.53
29:T:115:GLU:N	29:T:115:GLU:OE1	2.42	0.53
35:g:123:ILE:O	35:g:134:VAL:HA	2.09	0.53
1:2:923:A:H2'	1:2:924:G:H8	1.73	0.52
2:A:200:ASP:HA	2:A:203:PHE:HD2	1.74	0.52
9:J:129:ILE:HG13	9:J:134:ILE:HD13	1.91	0.52
35:g:86:TRP:HA	35:g:110:ASP:HB2	1.90	0.52
42:m:54:ILE:HG23	42:m:91:PHE:HZ	1.73	0.52
1:2:541:A:OP1	19:e:28:LYS:NZ	2.39	0.52
1:2:609:G:O2'	1:2:612:G:O3'	2.27	0.52
1:2:1564:U:H5''	28:S:39:GLY:N	2.23	0.52
3:B:54:LEU:O	3:B:55:LYS:HB2	2.09	0.52
4:C:64:HIS:CE1	4:C:244:PRO:HD3	2.44	0.52
11:N:71:ILE:O	11:N:75:LEU:HD12	2.09	0.52
16:Y:106:GLN:O	16:Y:110:GLN:HG2	2.09	0.52
34:f:100:LEU:HD13	34:f:103:LEU:HD11	1.91	0.52
38:1:28:A:H2'	38:1:29:G:H8	1.73	0.52
40:k:204:MET:HG2	40:k:232:HIS:CE1	2.44	0.52
40:k:357:PRO:HB2	40:k:415:GLN:HE21	1.74	0.52
1:2:326:U:H2'	1:2:327:A:H8	1.74	0.52
1:2:694:U:H3	1:2:695:U:H5	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1131:A:H2'	1:2:1132:A:C8	2.40	0.52
1:2:1219:C:H2'	1:2:1220:A:C8	2.44	0.52
4:C:227:TYR:OH	13:V:11:LEU:O	2.13	0.52
5:E:31:PRO:HG3	5:E:43:PRO:HG3	1.91	0.52
5:E:89:VAL:HG21	5:E:119:ALA:HB1	1.91	0.52
22:F:119:THR:HA	22:F:122:ILE:HD12	1.90	0.52
23:K:44:LYS:HA	23:K:47:GLN:HG3	1.90	0.52
27:R:107:ALA:HB1	27:R:119:LEU:HD21	1.91	0.52
32:c:12:VAL:HG13	32:c:50:GLU:HA	1.92	0.52
1:2:568:C:H41	15:X:69:ARG:HH12	1.57	0.52
1:2:786:G:H2'	1:2:787:A:C8	2.45	0.52
1:2:1389:A:H2'	1:2:1390:U:C6	2.44	0.52
5:E:52:LEU:HB3	5:E:54:TYR:HD1	1.74	0.52
9:J:87:SER:OG	9:J:89:ASP:OD1	2.24	0.52
27:R:47:ARG:HD2	27:R:47:ARG:C	2.35	0.52
39:j:195:TYR:HE1	40:k:373:ILE:HA	1.73	0.52
1:2:141:U:P	6:G:139:ASN:HD21	2.32	0.52
1:2:400:A:O2'	1:2:401:C:H4'	2.10	0.52
12:O:58:TYR:O	12:O:62:LEU:HG	2.10	0.52
14:W:37:PHE:HE1	14:W:103:ILE:HG13	1.73	0.52
21:D:69:LEU:O	21:D:73:ILE:HG23	2.09	0.52
29:T:13:ASP:OD1	29:T:14:PHE:N	2.42	0.52
1:2:649:U:O2'	1:2:650:G:OP1	2.25	0.52
1:2:1787:G:OP1	17:a:17:HIS:NE2	2.39	0.52
4:C:162:LYS:NZ	14:W:95:PRO:HA	2.24	0.52
5:E:18:TRP:HB3	5:E:20:LEU:HD13	1.92	0.52
25:P:50:SER:OG	25:P:53:PRO:HD2	2.10	0.52
35:g:62:TYR:HB3	35:g:93:TRP:CZ3	2.45	0.52
35:g:226:GLN:NE2	35:g:242:ASP:OD1	2.42	0.52
35:g:257:PHE:CD2	35:g:272:LEU:HB2	2.45	0.52
42:m:62:PHE:HZ	42:m:88:VAL:HA	1.75	0.52
1:2:700:C:O2'	1:2:701:U:OP1	2.24	0.52
1:2:888:U:H2'	1:2:889:C:C6	2.45	0.52
2:A:53:THR:HG22	2:A:161:PRO:HG2	1.90	0.52
2:A:205:ARG:HH22	2:A:213:GLN:HB2	1.73	0.52
15:X:5:LYS:O	15:X:7:ARG:HG3	2.10	0.52
28:S:36:ARG:HB2	28:S:102:ALA:HA	1.92	0.52
36:i:58:MET:HE1	36:i:60:HIS:CE1	2.45	0.52
38:1:36:U:H2'	38:1:37:T6A:C8	2.45	0.52
40:k:216:LEU:HD22	40:k:233:LEU:HD13	1.92	0.52
1:2:11:A:N3	1:2:1299:A:O2'	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:443:C:H6	16:Y:105:ARG:HH12	1.58	0.52
1:2:586:C:H2'	1:2:587:U:C6	2.45	0.52
1:2:677:G:H2'	1:2:678:G:C8	2.45	0.52
1:2:841:C:H2'	1:2:842:U:C6	2.44	0.52
1:2:1206:C:O2'	1:2:1207:A:OP2	2.22	0.52
2:A:183:ARG:HG3	2:A:188:LEU:HD23	1.92	0.52
4:C:159:LEU:HD22	4:C:226:THR:HG21	1.92	0.52
5:E:15:PRO:HG2	5:E:18:TRP:CD1	2.45	0.52
6:G:219:ARG:O	6:G:222:GLU:HG3	2.10	0.52
15:X:100:ASP:OD1	15:X:101:GLU:N	2.43	0.52
16:Y:6:THR:CG2	16:Y:28:LEU:HB3	2.40	0.52
19:e:17:GLN:OE1	19:e:17:GLN:N	2.43	0.52
21:D:46:THR:HB	21:D:84:ILE:HG13	1.91	0.52
35:g:62:TYR:HB3	35:g:93:TRP:CE3	2.45	0.52
1:2:13:C:H1'	1:2:1298:G:H21	1.74	0.52
1:2:79:C:H2'	1:2:80:A:O4'	2.10	0.52
1:2:369:A:H3'	1:2:370:G:H8	1.75	0.52
1:2:589:C:H2'	1:2:590:A:C8	2.45	0.52
1:2:1275:U:H5'	21:D:147:ALA:HB2	1.92	0.52
1:2:1423:A:O2'	1:2:1424:C:H5'	2.10	0.52
15:X:43:PHE:O	15:X:45:GLY:N	2.42	0.52
17:a:82:ARG:HD3	17:a:85:ARG:HD3	1.92	0.52
19:e:43:ARG:O	19:e:54:ARG:NH1	2.43	0.52
22:F:50:PHE:CD2	22:F:69:PRO:HA	2.45	0.52
28:S:65:GLU:O	28:S:69:ILE:HD12	2.10	0.52
28:S:137:HIS:O	28:S:141:THR:OG1	2.24	0.52
35:g:188:LEU:HA	35:g:193:TYR:HA	1.91	0.52
1:2:806:A:H2'	1:2:807:U:C6	2.45	0.52
1:2:1188:A:O2'	1:2:1189:C:OP1	2.20	0.52
1:2:1280:G:O3'	30:U:76:SER:OG	2.27	0.52
1:2:1381:G:O5'	30:U:89:ARG:NH2	2.42	0.52
1:2:1398:A:H2'	1:2:1399:A:C8	2.45	0.52
1:2:1405:U:H2'	1:2:1406:G:H8	1.75	0.52
7:H:154:LEU:O	7:H:186:PRO:HD2	2.11	0.52
35:g:171:ARG:HA	35:g:188:LEU:O	2.10	0.52
1:2:97:C:H2'	1:2:98:U:C6	2.45	0.51
1:2:590:A:H2'	1:2:591:G:C8	2.45	0.51
1:2:976:A:N7	1:2:1023:U:O4	2.43	0.51
1:2:1367:G:H5''	29:T:69:LYS:HG2	1.91	0.51
1:2:1488:A:H2'	1:2:1488:A:OP2	2.11	0.51
5:E:52:LEU:HB3	5:E:54:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:42:ASN:ND2	18:b:57:GLU:OE2	2.41	0.51
28:S:35:ILE:HG23	28:S:102:ALA:HB2	1.90	0.51
33:d:33:LYS:HG2	33:d:34:TYR:CD2	2.46	0.51
34:f:132:ASN:C	34:f:132:ASN:HD22	2.16	0.51
1:2:543:A:O3'	19:e:31:LYS:NZ	2.43	0.51
1:2:693:U:H5'	1:2:695:U:H5''	1.91	0.51
1:2:1077:C:H2'	1:2:1078:U:C6	2.45	0.51
6:G:184:LEU:O	6:G:188:ARG:HG2	2.10	0.51
24:M:70:GLY:O	24:M:73:THR:OG1	2.22	0.51
40:k:108:HIS:HB2	40:k:229:THR:HG23	1.92	0.51
1:2:327:A:H2'	1:2:328:G:H8	1.75	0.51
1:2:1070:U:H2'	1:2:1071:C:C6	2.45	0.51
1:2:1711:G:H3'	1:2:1712:A:C8	2.46	0.51
1:2:1711:G:H3'	1:2:1712:A:H8	1.75	0.51
8:I:39:GLY:HA2	8:I:61:GLU:HB3	1.91	0.51
10:L:21:THR:HG23	10:L:32:LYS:H	1.74	0.51
14:W:31:SER:H	14:W:34:ILE:HD13	1.75	0.51
22:F:101:MET:O	22:F:102:ASN:O	2.28	0.51
35:g:83:SER:HG	35:g:93:TRP:HE1	1.55	0.51
1:2:14:C:H5'	4:C:169:SER:OG	2.11	0.51
1:2:1001:G:O2'	42:m:65:ASN:OD1	2.27	0.51
1:2:1086:A:OP2	1:2:1086:A:H8	1.93	0.51
1:2:1741:U:H2'	1:2:1742:A:C8	2.45	0.51
3:B:99:ASN:OD1	3:B:100:PHE:N	2.43	0.51
4:C:158:SER:OG	4:C:159:LEU:N	2.43	0.51
1:2:97:C:H2'	1:2:98:U:H6	1.75	0.51
1:2:638:U:H2'	7:H:101:LYS:HG3	1.93	0.51
1:2:709:C:H2'	1:2:710:U:H4'	1.92	0.51
1:2:1657:A:H2'	1:2:1658:A:H8	1.75	0.51
15:X:107:PHE:HA	15:X:123:LYS:HG3	1.91	0.51
40:k:260:LEU:HG	40:k:264:LYS:HE2	1.93	0.51
1:2:66:U:OP1	6:G:136:LYS:NZ	2.44	0.51
1:2:603:A:H2'	1:2:604:A:O4'	2.11	0.51
1:2:861:A:P	11:N:20:ARG:HH12	2.34	0.51
1:2:917:U:H2'	1:2:918:A:H8	1.75	0.51
1:2:1647:G:H2'	1:2:1648:U:C6	2.45	0.51
1:2:1768:U:H2'	1:2:1769:U:C6	2.45	0.51
10:L:20:PHE:HE1	10:L:22:ASN:HB3	1.76	0.51
25:P:49:LEU:HG	25:P:50:SER:H	1.76	0.51
25:P:118:GLU:O	28:S:122:HIS:N	2.38	0.51
38:1:1:A:H2'	38:1:2:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1405:U:H2'	1:2:1406:G:C8	2.46	0.51
2:A:200:ASP:HA	2:A:203:PHE:CD2	2.45	0.51
3:B:27:LYS:HB3	3:B:47:LEU:HD11	1.93	0.51
27:R:25:THR:O	27:R:58:MET:HG2	2.11	0.51
29:T:88:VAL:HG12	29:T:89:ARG:HH21	1.76	0.51
40:k:220:GLY:HA2	40:k:262:HIS:CE1	2.46	0.51
40:k:356:ARG:HG3	40:k:424:PRO:HG2	1.91	0.51
1:2:494:C:H3'	1:2:495:G:C8	2.46	0.51
1:2:1754:A:N6	36:i:66:ARG:O	2.42	0.51
5:E:45:ILE:HA	5:E:61:VAL:HG11	1.92	0.51
5:E:68:ARG:NH1	5:E:76:VAL:HG11	2.26	0.51
18:b:20:LYS:HG3	18:b:21:LEU:HG	1.91	0.51
38:1:16:H2U:C2'	38:1:60:A:H1'	2.40	0.51
1:2:863:U:H3'	14:W:28:ARG:HH21	1.76	0.51
1:2:1279:C:H4'	30:U:69:LYS:HG2	1.92	0.51
1:2:1582:G:O2'	1:2:1583:U:OP2	2.29	0.51
1:2:1771:C:H2'	1:2:1772:G:H8	1.75	0.51
3:B:140:ILE:HD11	3:B:213:ARG:CZ	2.40	0.51
34:f:140:GLY:HA2	34:f:143:HIS:HB3	1.92	0.51
38:1:16:H2U:H61	38:1:60:A:O3'	2.11	0.51
1:2:22:A:C5'	9:J:18:PRO:CG	2.89	0.51
1:2:525:A:OP2	16:Y:93:ARG:NH2	2.39	0.51
1:2:1276:G:O3'	21:D:183:GLY:HA3	2.11	0.51
1:2:1332:C:H2'	1:2:1333:U:H6	1.75	0.51
5:E:49:ARG:NE	5:E:50:ASN:OD1	2.35	0.51
8:I:36:THR:HA	8:I:58:LEU:HA	1.92	0.51
9:J:147:MET:HE2	9:J:147:MET:HA	1.92	0.51
12:O:16:VAL:HG12	12:O:80:HIS:HB2	1.93	0.51
29:T:38:LYS:O	29:T:39:THR:OG1	2.25	0.51
40:k:215:LEU:HB3	40:k:247:LEU:HD11	1.92	0.51
1:2:463:A:C2	1:2:464:G:C8	2.99	0.50
1:2:1582:G:N7	26:Q:14:LYS:HE2	2.27	0.50
2:A:183:ARG:CZ	2:A:191:ARG:HA	2.40	0.50
5:E:256:ARG:HA	5:E:259:HIS:CE1	2.42	0.50
12:O:127:ARG:HH12	17:a:22:ARG:HD3	1.75	0.50
16:Y:10:ARG:HE	16:Y:11:LYS:H	1.58	0.50
22:F:95:LEU:HA	22:F:174:ILE:HD11	1.92	0.50
31:Z:78:VAL:HA	31:Z:81:ARG:NE	2.24	0.50
38:1:47:H2U:H5''	38:1:47:H2U:H61	1.93	0.50
40:k:313:PRO:HB2	40:k:347:PHE:HE1	1.76	0.50
1:2:1:U:O4'	9:J:54:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:890:A:H2'	1:2:891:A:C8	2.41	0.50
2:A:120:LEU:HD21	2:A:144:ILE:HD12	1.93	0.50
5:E:88:ASP:OD1	5:E:122:LYS:NZ	2.33	0.50
5:E:100:ARG:HG2	5:E:102:VAL:HG13	1.91	0.50
7:H:122:HIS:HA	7:H:125:ILE:HG22	1.92	0.50
12:O:71:CYS:HA	12:O:74:VAL:HG22	1.92	0.50
22:F:123:ILE:HB	22:F:131:PRO:HB3	1.92	0.50
27:R:102:VAL:O	27:R:122:SER:OG	2.28	0.50
35:g:304:ASP:OD1	35:g:305:GLY:N	2.44	0.50
36:i:30:GLU:HB2	36:i:33:GLN:HE22	1.75	0.50
40:k:204:MET:O	40:k:204:MET:HE3	2.11	0.50
40:k:267:LEU:O	40:k:271:ARG:HG3	2.11	0.50
40:k:430:ILE:HA	40:k:519:LYS:HE2	1.93	0.50
1:2:961:C:H2'	1:2:962:A:O4'	2.12	0.50
5:E:94:ALA:O	5:E:95:THR:OG1	2.25	0.50
9:J:83:ILE:O	9:J:107:ARG:NH1	2.45	0.50
11:N:61:THR:OG1	11:N:62:GLN:OE1	2.23	0.50
12:O:15:GLY:O	12:O:80:HIS:N	2.45	0.50
24:M:23:VAL:O	24:M:27:THR:HG23	2.11	0.50
32:c:42:ARG:HA	32:c:63:ALA:HB3	1.92	0.50
38:1:26:M2G:C6	38:1:44:A:N6	2.79	0.50
39:j:27:ILE:HG12	39:j:32:ALA:HB2	1.94	0.50
39:j:44:GLY:HA2	39:j:83:ILE:HB	1.93	0.50
1:2:31:C:O2'	1:2:546:U:OP1	2.29	0.50
1:2:1107:G:H4'	1:2:1108:G:H5''	1.93	0.50
7:H:15:GLU:HA	7:H:18:LEU:HD23	1.93	0.50
9:J:88:GLU:OE1	9:J:88:GLU:N	2.45	0.50
14:W:11:LEU:HD11	14:W:41:MET:HE1	1.93	0.50
36:i:59:ALA:HA	36:i:89:CYS:O	2.11	0.50
39:j:104:LYS:HB3	39:j:140:HIS:NE2	2.26	0.50
1:2:340:A:H2'	1:2:341:C:C6	2.46	0.50
1:2:709:C:H42	1:2:730:G:H2'	1.77	0.50
1:2:1794:C:O2'	17:a:95:ARG:NH1	2.45	0.50
2:A:210:ILE:HG13	27:R:81:LYS:HZ3	1.77	0.50
38:1:12:G:H1'	42:m:74:MET:HE2	1.94	0.50
40:k:477:ALA:HB3	40:k:484:ARG:HB2	1.92	0.50
1:2:160:U:OP2	6:G:87:ARG:NH2	2.45	0.50
1:2:1511:G:O2'	1:2:1513:A:N3	2.43	0.50
1:2:1532:G:O2'	31:Z:72:GLY:O	2.25	0.50
5:E:117:GLU:OE2	5:E:117:GLU:N	2.30	0.50
7:H:141:ARG:HB3	14:W:51:GLU:CD	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:3:ARG:HD2	9:J:4:ALA:N	2.26	0.50
23:K:77:ARG:NH1	23:K:84:GLU:HG2	2.27	0.50
24:M:54:VAL:HG22	24:M:80:ILE:HB	1.93	0.50
29:T:33:TYR:HD2	29:T:37:VAL:HG21	1.77	0.50
36:i:61:ILE:HG13	36:i:61:ILE:O	2.11	0.50
38:1:11:C:H2'	38:1:12:G:C8	2.47	0.50
38:1:28:A:H2'	38:1:29:G:C8	2.46	0.50
1:2:1522:A:H2'	1:2:1523:A:C8	2.47	0.50
5:E:147:ILE:HG21	5:E:169:ILE:HG23	1.93	0.50
18:b:26:GLN:H	18:b:26:GLN:CD	2.20	0.50
28:S:45:LEU:HD11	29:T:36:ILE:HD13	1.94	0.50
33:d:40:ARG:HG3	33:d:41:GLN:N	2.26	0.50
35:g:302:SER:OG	35:g:304:ASP:OD1	2.27	0.50
1:2:753:A:H8	5:E:187:ARG:HH12	1.58	0.50
1:2:864:A:OP1	14:W:28:ARG:NH2	2.43	0.50
3:B:205:PHE:CG	3:B:206:PRO:HD2	2.47	0.50
5:E:233:ARG:NH1	5:E:234:PRO:O	2.44	0.50
8:I:143:LYS:HE2	8:I:143:LYS:HA	1.94	0.50
9:J:132:ARG:HG2	9:J:140:ILE:HD11	1.94	0.50
24:M:120:ASP:HA	24:M:124:ARG:CD	2.40	0.50
35:g:109:GLY:H	35:g:129:ASP:HB3	1.76	0.50
35:g:301:TRP:CE2	35:g:308:LEU:HD13	2.47	0.50
1:2:86:A:H2'	1:2:87:C:H6	1.77	0.50
1:2:242:G:H2'	1:2:243:A:H8	1.75	0.50
1:2:706:A:C5	1:2:707:A:H1'	2.47	0.50
1:2:771:A:H5''	9:J:7:THR:HG23	1.94	0.50
1:2:888:U:H2'	1:2:889:C:H6	1.77	0.50
1:2:990:G:H21	1:2:1012:A:N6	1.98	0.50
1:2:1661:G:H1	1:2:1736:U:H3	1.57	0.50
5:E:75:LYS:HB2	5:E:77:ARG:NH1	2.27	0.50
23:K:54:PHE:HB3	23:K:72:GLY:CA	2.41	0.50
26:Q:16:ALA:HB2	26:Q:72:GLY:HA3	1.92	0.50
26:Q:60:PHE:HB2	26:Q:63:ILE:HD13	1.93	0.50
1:2:408:C:H2'	1:2:409:A:H8	1.76	0.49
1:2:1241:A:O2'	25:P:52:LYS:NZ	2.30	0.49
1:2:1584:A:H2'	1:2:1585:A:O4'	2.12	0.49
9:J:114:TYR:HE2	9:J:121:SER:H	1.59	0.49
14:W:97:ARG:HG2	14:W:97:ARG:HH11	1.77	0.49
22:F:110:LEU:HD12	26:Q:43:ILE:HG13	1.94	0.49
31:Z:62:VAL:O	31:Z:66:VAL:HG23	2.11	0.49
35:g:184:ARG:HD2	35:g:195:ILE:HD11	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:271:ASP:OD2	35:g:274:ASN:HB2	2.12	0.49
40:k:315:LEU:HD11	40:k:340:GLY:HA3	1.94	0.49
1:2:894:G:H22	1:2:916:U:H3	1.60	0.49
1:2:1480:C:H2'	1:2:1481:A:H5''	1.93	0.49
11:N:54:LEU:HB3	11:N:60:VAL:HB	1.94	0.49
14:W:11:LEU:O	14:W:14:ILE:HG22	2.12	0.49
16:Y:103:ALA:O	16:Y:108:ARG:NH2	2.45	0.49
18:b:54:VAL:HG12	18:b:64:CYS:SG	2.52	0.49
35:g:285:PHE:HE1	35:g:318:ARG:HH21	1.59	0.49
39:j:224:ALA:HB3	39:j:227:LEU:HB2	1.93	0.49
1:2:1064:A:H4'	3:B:205:PHE:CD1	2.47	0.49
1:2:1658:A:H2'	1:2:1659:U:C6	2.47	0.49
2:A:18:LEU:HD12	2:A:23:HIS:CD2	2.48	0.49
4:C:232:PRO:HG2	14:W:99:PHE:CD2	2.47	0.49
15:X:91:GLY:H	15:X:136:TRP:NE1	2.10	0.49
15:X:100:ASP:OD2	15:X:144:ARG:NH2	2.44	0.49
22:F:50:PHE:CE2	22:F:70:ILE:HG22	2.47	0.49
27:R:105:GLN:O	27:R:108:GLU:HG3	2.13	0.49
30:U:69:LYS:HG3	33:d:44:ARG:NH2	2.26	0.49
35:g:84:ALA:HB2	35:g:114:VAL:HB	1.94	0.49
40:k:112:GLY:O	40:k:249:ASN:ND2	2.43	0.49
40:k:113:LYS:NZ	40:k:193:ASP:OD1	2.29	0.49
1:2:107:C:H5''	1:2:382:G:O2'	2.12	0.49
1:2:161:A:H3'	1:2:162:G:N2	2.26	0.49
1:2:271:U:O2'	1:2:283:G:N2	2.44	0.49
1:2:1063:G:O2'	3:B:204:ILE:O	2.30	0.49
1:2:1350:G:H2'	1:2:1351:U:C6	2.48	0.49
1:2:1554:A:H2'	25:P:40:ARG:NH2	2.27	0.49
5:E:75:LYS:N	5:E:77:ARG:HH22	2.04	0.49
5:E:180:LEU:HB2	5:E:231:PRO:HA	1.93	0.49
7:H:5:GLN:HE22	7:H:22:GLN:N	2.11	0.49
14:W:114:GLU:OE2	14:W:118:ARG:NE	2.38	0.49
23:K:28:ASN:HB3	33:d:8:TYR:CE2	2.48	0.49
23:K:46:LEU:HD13	23:K:66:TYR:HD2	1.77	0.49
26:Q:73:GLY:N	26:Q:76:SER:OG	2.46	0.49
38:1:63:G:N2	38:1:64:RIA:O2X	2.43	0.49
1:2:448:C:O2'	1:2:449:U:H5'	2.13	0.49
1:2:1460:G:H2'	1:2:1461:C:C6	2.47	0.49
1:2:1677:G:N2	1:2:1720:A:H62	2.07	0.49
1:2:1783:U:P	12:O:133:ARG:HH22	2.35	0.49
6:G:27:PHE:HE1	6:G:36:VAL:HG11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:87:ARG:HD2	17:a:92:ARG:HA	1.94	0.49
23:K:4:PRO:HG2	23:K:7:ASP:HB2	1.94	0.49
29:T:86:ARG:HB2	29:T:89:ARG:HB2	1.94	0.49
39:j:27:ILE:HD11	39:j:63:ILE:HG21	1.94	0.49
40:k:144:ASN:CG	40:k:383:GLU:HG2	2.37	0.49
1:2:14:C:OP1	4:C:169:SER:N	2.33	0.49
1:2:349:U:H4'	1:2:350:C:H5''	1.94	0.49
1:2:520:A:H2'	1:2:521:U:C6	2.48	0.49
1:2:594:G:H2'	1:2:595:C:C6	2.46	0.49
1:2:945:U:H2'	1:2:946:U:C6	2.48	0.49
1:2:1585:A:H1'	22:F:106:ASN:ND2	2.27	0.49
2:A:139:VAL:HG13	2:A:141:ILE:CD1	2.41	0.49
23:K:31:LYS:HG2	23:K:36:ASP:HA	1.93	0.49
25:P:107:ILE:HA	25:P:111:MET:HG3	1.94	0.49
28:S:56:LYS:HZ1	28:S:61:LEU:HB3	1.74	0.49
35:g:189:ASN:HB2	35:g:192:SER:HB3	1.94	0.49
40:k:101:ILE:HD12	40:k:304:VAL:HA	1.95	0.49
1:2:476:A:H2'	1:2:477:A:H8	1.78	0.49
1:2:576:G:O6	37:3:34:U:H5''	2.13	0.49
1:2:918:A:P	12:O:18:ARG:HH22	2.36	0.49
1:2:1319:U:O2'	1:2:1321:A:OP1	2.21	0.49
1:2:1477:A:H5'	29:T:56:LYS:HG2	1.94	0.49
1:2:1540:G:H5''	29:T:88:VAL:HG22	1.95	0.49
1:2:1613:C:C4	22:F:83:ARG:HA	2.48	0.49
1:2:1683:G:H2'	1:2:1684:C:C6	2.48	0.49
21:D:24:PHE:HE1	23:K:65:TYR:CG	2.30	0.49
22:F:51:GLU:OE1	22:F:51:GLU:N	2.43	0.49
25:P:90:ILE:HD11	25:P:112:VAL:HG23	1.94	0.49
1:2:2:A:C8	4:C:202:TYR:CD2	3.01	0.49
1:2:305:U:H2'	1:2:306:G:H8	1.78	0.49
1:2:867:G:H22	1:2:959:U:H3	1.59	0.49
1:2:932:A:OP2	17:a:37:LYS:HE3	2.13	0.49
1:2:1252:U:H2'	1:2:1253:U:C6	2.47	0.49
1:2:1682:U:H2'	1:2:1683:G:C8	2.48	0.49
5:E:92:LEU:HD13	16:Y:17:LEU:HD21	1.95	0.49
6:G:23:ARG:HE	6:G:42:GLY:HA2	1.78	0.49
7:H:64:VAL:N	7:H:65:PRO:HD3	2.28	0.49
15:X:136:TRP:NE1	19:e:15:LYS:HE2	2.28	0.49
22:F:39:GLN:HE21	26:Q:53:LEU:CD1	2.26	0.49
31:Z:59:TYR:HE1	31:Z:100:ILE:HG23	1.78	0.49
38:1:27:C:H2'	38:1:28:A:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:430:ILE:HG22	40:k:432:ILE:HG13	1.94	0.49
1:2:53:G:O3'	16:Y:110:GLN:NE2	2.40	0.49
1:2:403:G:H2'	1:2:404:C:C6	2.48	0.49
1:2:855:A:H62	7:H:96:ARG:NE	2.11	0.49
1:2:1173:C:OP1	28:S:136:GLN:HB3	2.12	0.49
1:2:1467:A:H2'	1:2:1468:C:C6	2.48	0.49
1:2:1490:A:O2'	1:2:1491:A:O4'	2.26	0.49
1:2:1513:A:O2'	1:2:1515:U:OP2	2.30	0.49
1:2:1542:U:O3'	28:S:132:ARG:NH1	2.40	0.49
1:2:1592:G:N2	1:2:1598:A:H61	2.11	0.49
1:2:1712:A:H2'	1:2:1713:G:H8	1.78	0.49
2:A:198:MET:HE3	2:A:199:PRO:HD2	1.95	0.49
8:I:194:LEU:HA	8:I:197:LEU:HD12	1.95	0.49
9:J:120:LYS:O	9:J:121:SER:OG	2.31	0.49
28:S:23:ASP:OD1	28:S:24:GLY:N	2.46	0.49
1:2:108:A:H2'	1:2:109:G:C8	2.47	0.49
1:2:141:U:OP2	6:G:139:ASN:ND2	2.45	0.49
1:2:754:A:H2	1:2:792:A:H3'	1.78	0.49
1:2:815:G:H21	7:H:110:GLN:HE22	1.58	0.49
1:2:863:U:O2'	11:N:11:MET:SD	2.65	0.49
2:A:158:VAL:HG22	13:V:69:LEU:HD23	1.94	0.49
22:F:104:ARG:HG3	22:F:105:ASN:N	2.28	0.49
1:2:97:C:O2	1:2:424:A:O2'	2.28	0.48
1:2:1230:U:H5'	1:2:1258:U:H1'	1.95	0.48
1:2:1786:G:H3'	12:O:132:ARG:HH12	1.77	0.48
2:A:76:ILE:HG13	2:A:98:ILE:HB	1.95	0.48
8:I:41:LYS:HA	8:I:59:ARG:O	2.13	0.48
12:O:21:ALA:HB2	12:O:98:GLY:HA3	1.95	0.48
15:X:36:THR:O	15:X:40:SER:OG	2.29	0.48
30:U:65:ILE:HD11	33:d:43:PHE:CZ	2.47	0.48
1:2:220:A:H2'	1:2:221:A:H8	1.75	0.48
1:2:271:U:N3	6:G:182:GLN:OE1	2.44	0.48
1:2:305:U:H2'	1:2:306:G:C8	2.47	0.48
1:2:783:C:H2'	1:2:784:U:O4'	2.13	0.48
1:2:1194:C:N4	26:Q:141:SER:OG	2.47	0.48
1:2:1195:A:N6	1:2:1599:G:O2'	2.46	0.48
14:W:69:LEU:HD11	14:W:72:CYS:SG	2.53	0.48
15:X:70:LYS:HG2	15:X:93:LEU:HD22	1.95	0.48
16:Y:10:ARG:HE	16:Y:11:LYS:N	2.11	0.48
17:a:74:CYS:SG	17:a:76:SER:N	2.86	0.48
21:D:27:ARG:HB3	23:K:58:GLN:NE2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:99:LEU:O	22:F:182:ARG:NH2	2.46	0.48
23:K:32:HIS:CE1	23:K:35:ILE:HD12	2.48	0.48
38:1:9:1MG:H4'	38:1:45:U:C2'	2.43	0.48
40:k:220:GLY:HA3	40:k:254:MET:HE3	1.94	0.48
1:2:819:U:N3	1:2:820:U:O2'	2.45	0.48
1:2:1563:C:H2'	1:2:1564:U:H6	1.78	0.48
5:E:11:ARG:HD3	5:E:21:ASP:O	2.13	0.48
8:I:77:ARG:NH1	8:I:78:ILE:O	2.46	0.48
11:N:84:ILE:HD11	11:N:149:LEU:HD22	1.95	0.48
12:O:51:ASP:C	12:O:52:ARG:HD2	2.37	0.48
25:P:81:ARG:NH2	25:P:120:SER:O	2.45	0.48
35:g:252:PHE:CE1	35:g:259:LEU:HD12	2.48	0.48
38:1:15:G:N2	38:1:48:5MC:HM52	2.27	0.48
40:k:315:LEU:HB3	40:k:417:VAL:HB	1.94	0.48
1:2:645:U:H2'	1:2:646:G:H8	1.78	0.48
1:2:653:C:H2'	1:2:654:G:H8	1.78	0.48
1:2:842:U:H2'	1:2:843:A:C8	2.49	0.48
1:2:1667:U:H3'	1:2:1668:G:H8	1.77	0.48
3:B:111:ARG:HB3	17:a:68:TYR:HD2	1.78	0.48
4:C:161:THR:HG23	14:W:95:PRO:HB2	1.96	0.48
6:G:138:ALA:HA	6:G:141:ILE:HD12	1.95	0.48
21:D:32:GLU:HG2	21:D:57:ASP:HB3	1.96	0.48
1:2:164:G:H2'	1:2:165:C:C6	2.48	0.48
1:2:299:A:H2'	1:2:300:A:C8	2.49	0.48
1:2:1175:G:H1'	1:2:1194:C:O2'	2.12	0.48
1:2:1198:G:P	33:d:40:ARG:HH12	2.36	0.48
1:2:1355:U:H3	1:2:1366:G:H1	1.61	0.48
1:2:1368:U:OP1	29:T:119:LYS:NZ	2.40	0.48
1:2:1390:U:H2'	1:2:1391:C:C6	2.48	0.48
1:2:1563:C:H2'	1:2:1564:U:C6	2.48	0.48
1:2:1645:U:H2'	1:2:1646:A:C8	2.48	0.48
2:A:56:LYS:HZ2	13:V:70:ASN:HD21	1.62	0.48
23:K:25:LYS:HD3	23:K:64:TYR:CE2	2.49	0.48
29:T:38:LYS:HG3	29:T:46:PRO:HA	1.94	0.48
38:1:60:A:H2'	38:1:61:C:H5	1.78	0.48
1:2:748:U:O2'	14:W:122:SER:O	2.27	0.48
1:2:1035:A:H2'	1:2:1036:C:H6	1.78	0.48
1:2:1617:C:H2'	1:2:1618:C:H6	1.77	0.48
5:E:131:LEU:HD12	5:E:135:GLY:HA2	1.95	0.48
6:G:148:THR:O	6:G:150:GLU:N	2.46	0.48
35:g:296:ALA:HA	35:g:312:TYR:HD1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:394:U:H3	1:2:398:A:H62	1.61	0.48
1:2:883:A:H5''	3:B:136:ARG:CZ	2.43	0.48
1:2:1046:G:H1	1:2:1070:U:H3	1.61	0.48
1:2:1067:C:H2'	1:2:1068:A:H8	1.78	0.48
1:2:1398:A:O2'	1:2:1399:A:O4'	2.24	0.48
1:2:1745:G:H2'	1:2:1746:G:H8	1.79	0.48
2:A:181:VAL:O	2:A:185:ARG:HG3	2.14	0.48
8:I:139:ASN:ND2	8:I:142:ARG:HH22	2.12	0.48
21:D:76:ARG:HG2	23:K:65:TYR:OH	2.14	0.48
22:F:148:THR:OG1	22:F:159:ARG:NE	2.45	0.48
26:Q:99:GLU:N	26:Q:99:GLU:OE1	2.47	0.48
35:g:223:LYS:HA	35:g:246:GLU:HA	1.96	0.48
36:i:101:ARG:HD3	36:i:101:ARG:N	2.29	0.48
1:2:107:C:H2'	1:2:108:A:H8	1.79	0.48
1:2:349:U:O2'	1:2:969:A:N1	2.45	0.48
1:2:423:C:O2'	1:2:425:G:OP1	2.19	0.48
1:2:1426:2MG:N2	30:U:74:GLU:OE2	2.46	0.48
1:2:1530:U:O4'	29:T:48:GLN:NE2	2.46	0.48
6:G:74:LYS:HA	6:G:96:SER:HA	1.96	0.48
10:L:74:THR:HG22	10:L:122:ILE:HG22	1.96	0.48
12:O:127:ARG:HE	12:O:128:LYS:N	2.12	0.48
12:O:135:ARG:N	17:a:26:CYS:O	2.41	0.48
27:R:31:ASN:HD22	27:R:55:THR:HG22	1.78	0.48
30:U:24:ILE:HD12	30:U:116:VAL:HG12	1.96	0.48
39:j:198:ILE:HG22	39:j:202:LYS:HE2	1.94	0.48
40:k:499:ILE:HB	40:k:515:ALA:HB3	1.96	0.48
1:2:82:U:H2'	1:2:83:G:O4'	2.13	0.48
1:2:1252:U:H2'	1:2:1253:U:H6	1.79	0.48
1:2:1332:C:H2'	1:2:1333:U:C6	2.49	0.48
1:2:1577:U:H2'	1:2:1578:C:C6	2.49	0.48
11:N:142:GLU:HG2	11:N:143:SER:N	2.29	0.48
15:X:95:PHE:HA	15:X:142:LYS:HZ3	1.78	0.48
22:F:36:GLN:HG3	26:Q:57:LEU:HD12	1.96	0.48
22:F:84:PHE:CE1	22:F:167:LEU:HD22	2.49	0.48
22:F:103:GLY:C	22:F:105:ASN:N	2.66	0.48
27:R:13:SER:O	27:R:17:ILE:HG12	2.13	0.48
35:g:41:LYS:HB3	35:g:65:HIS:O	2.13	0.48
1:2:208:U:N3	1:2:209:A:N7	2.62	0.48
1:2:1487:U:OP2	1:2:1513:A:N6	2.46	0.48
27:R:31:ASN:ND2	27:R:55:THR:HG22	2.29	0.48
1:2:199:A:H2'	1:2:200:G:C8	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:217:A:O2'	1:2:218:A:OP1	2.30	0.47
1:2:584:A:H2'	1:2:585:G:H8	1.78	0.47
1:2:804:U:OP1	14:W:32:LYS:NZ	2.43	0.47
5:E:163:ASP:OD1	5:E:164:LEU:N	2.47	0.47
6:G:61:PHE:HD2	6:G:72:ARG:HD2	1.79	0.47
11:N:31:ASP:OD1	11:N:32:GLY:N	2.47	0.47
28:S:57:ARG:HH12	31:Z:40:VAL:HG21	1.78	0.47
1:2:589:C:H5''	19:e:43:ARG:NH2	2.27	0.47
1:2:1445:C:O4'	34:f:80:ARG:NH2	2.47	0.47
1:2:1554:A:H5''	25:P:40:ARG:HH21	1.79	0.47
1:2:1664:U:H2'	1:2:1665:A:O4'	2.13	0.47
2:A:48:ILE:HG13	2:A:149:LEU:HD11	1.95	0.47
7:H:48:GLU:CD	7:H:56:LYS:HB3	2.38	0.47
9:J:77:ILE:HD11	9:J:93:LEU:HG	1.95	0.47
39:j:144:ALA:HB1	39:j:154:VAL:HG21	1.97	0.47
39:j:147:LEU:O	39:j:151:ASP:N	2.41	0.47
1:2:396:A:H2'	1:2:397:G:O4'	2.14	0.47
1:2:400:A:O3'	5:E:3:ARG:NH1	2.47	0.47
1:2:473:A:N6	1:2:594:G:OP1	2.47	0.47
1:2:638:U:OP1	7:H:101:LYS:HE3	2.14	0.47
1:2:867:G:P	11:N:121:ARG:HH21	2.37	0.47
1:2:1278:C:O2'	30:U:71:PRO:HG3	2.14	0.47
2:A:60:ALA:O	2:A:64:ILE:HD12	2.13	0.47
2:A:210:ILE:HD11	27:R:81:LYS:HG3	1.96	0.47
5:E:36:HIS:ND1	5:E:85:GLY:HA3	2.30	0.47
6:G:148:THR:C	6:G:150:GLU:N	2.71	0.47
13:V:76:ASP:HB3	13:V:78:LEU:HD23	1.97	0.47
22:F:70:ILE:HD12	26:Q:112:TYR:CE2	2.50	0.47
23:K:43:ILE:HD13	23:K:64:TYR:CE2	2.48	0.47
26:Q:39:VAL:O	26:Q:45:ARG:NH2	2.47	0.47
26:Q:47:LYS:O	26:Q:50:GLU:HB2	2.13	0.47
29:T:105:LEU:HD12	29:T:122:ARG:HD2	1.97	0.47
38:1:1:A:N1	38:1:75:C:N4	2.61	0.47
1:2:387:G:C6	1:2:409:A:C6	3.02	0.47
1:2:1350:G:H2'	1:2:1351:U:H6	1.78	0.47
1:2:1581:A:H5'	26:Q:135:ARG:HH21	1.78	0.47
1:2:1582:G:O2'	1:2:1608:G:O6	2.25	0.47
1:2:1758:G:H1'	1:2:1779:A:N1	2.29	0.47
9:J:126:ARG:HG2	19:e:33:ARG:HD3	1.97	0.47
15:X:75:GLN:NE2	15:X:80:GLY:HA2	2.29	0.47
15:X:107:PHE:CE2	15:X:114:LYS:HB3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:79:ILE:HD11	17:a:86:VAL:HG23	1.96	0.47
1:2:216:A:O2'	1:2:217:A:OP1	2.29	0.47
1:2:550:G:H2'	1:2:551:G:H8	1.79	0.47
1:2:1165:A:H2'	1:2:1166:G:O4'	2.14	0.47
1:2:1319:U:H2'	1:2:1321:A:H5'	1.97	0.47
1:2:1506:U:H2'	1:2:1507:C:C6	2.50	0.47
1:2:1543:A:P	28:S:132:ARG:HH12	2.37	0.47
1:2:1786:G:H3'	12:O:132:ARG:NH1	2.30	0.47
4:C:57:SER:HA	4:C:77:LEU:HD12	1.96	0.47
28:S:43:ALA:HA	28:S:46:VAL:HG12	1.96	0.47
29:T:12:GLN:O	29:T:15:ILE:HG22	2.15	0.47
40:k:139:LYS:HB3	40:k:319:ARG:NH1	2.30	0.47
40:k:171:SER:OG	40:k:173:LYS:O	2.26	0.47
1:2:326:U:O2'	10:L:10:GLU:OE2	2.33	0.47
1:2:752:A:H2	1:2:796:G:H22	1.60	0.47
1:2:958:U:H2'	1:2:958:U:O2	2.14	0.47
1:2:1040:G:H2'	1:2:1041:G:C8	2.49	0.47
1:2:1422:A:H2'	1:2:1423:A:O4'	2.14	0.47
1:2:1449:C:H5'	33:d:8:TYR:H	1.79	0.47
1:2:1595:A:C8	33:d:14:PHE:HD2	2.32	0.47
2:A:36:TYR:CE2	2:A:56:LYS:HD2	2.50	0.47
14:W:6:VAL:HG23	14:W:29:PRO:HG2	1.96	0.47
25:P:75:VAL:HA	25:P:93:VAL:O	2.15	0.47
31:Z:43:ASP:OD1	31:Z:44:GLN:N	2.48	0.47
31:Z:77:ARG:HH11	31:Z:77:ARG:HG3	1.79	0.47
38:1:53:G:H2'	38:1:54:A:C8	2.50	0.47
40:k:247:LEU:HD23	40:k:281:VAL:HB	1.96	0.47
1:2:142:G:H2'	1:2:143:G:H8	1.76	0.47
1:2:497:G:N2	1:2:498:U:O4	2.42	0.47
1:2:588:C:H1'	19:e:57:ASN:HD22	1.79	0.47
1:2:601:U:H2'	1:2:602:U:C6	2.49	0.47
1:2:782:G:N7	16:Y:10:ARG:NH2	2.61	0.47
1:2:1293:G:H2'	1:2:1294:G:H8	1.79	0.47
1:2:1475:G:O2'	29:T:48:GLN:N	2.36	0.47
1:2:1600:C:H2'	1:2:1601:U:C6	2.50	0.47
1:2:1658:A:H2'	1:2:1659:U:H6	1.80	0.47
1:2:1711:G:H2'	1:2:1711:G:N3	2.28	0.47
3:B:185:THR:O	3:B:189:ILE:HG12	2.15	0.47
14:W:11:LEU:HA	14:W:14:ILE:HG22	1.96	0.47
18:b:46:VAL:HG22	18:b:54:VAL:HG11	1.96	0.47
18:b:54:VAL:HG13	18:b:54:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:224:LYS:HD2	22:F:227:ARG:NH2	2.30	0.47
28:S:3:LEU:HB3	31:Z:82:HIS:ND1	2.28	0.47
28:S:89:GLN:C	28:S:91:ASP:H	2.22	0.47
28:S:97:ASP:N	28:S:97:ASP:OD1	2.47	0.47
35:g:91:ARG:HE	35:g:103:ARG:HG3	1.80	0.47
35:g:240:ASN:OD1	35:g:241:PHE:N	2.48	0.47
35:g:267:ILE:HB	35:g:281:LEU:HB2	1.95	0.47
39:j:7:ARG:HD2	39:j:12:LYS:HG3	1.97	0.47
1:2:221:A:H2'	1:2:222:U:O4'	2.15	0.47
1:2:328:G:H2'	1:2:329:G:C8	2.48	0.47
1:2:356:G:H2'	1:2:357:U:C6	2.50	0.47
1:2:406:A:H2'	1:2:407:C:C6	2.49	0.47
1:2:1233:A:O2'	34:f:138:TYR:OH	2.33	0.47
1:2:1336:A:O5'	26:Q:123:ARG:NH1	2.39	0.47
1:2:1480:C:H5	1:2:1523:A:H62	1.61	0.47
1:2:1531:C:H4'	1:2:1537:G:O6	2.14	0.47
1:2:1753:A:OP2	15:X:63:GLN:NE2	2.48	0.47
2:A:4:PRO:HG3	13:V:41:GLU:HA	1.96	0.47
3:B:124:ASN:OD1	3:B:125:VAL:N	2.48	0.47
8:I:84:HIS:HE2	8:I:97:THR:HB	1.80	0.47
9:J:55:ALA:O	9:J:59:LEU:HD23	2.14	0.47
11:N:61:THR:OG1	11:N:62:GLN:N	2.48	0.47
15:X:107:PHE:HD1	15:X:123:LYS:HG3	1.80	0.47
16:Y:20:ARG:NE	16:Y:76:TYR:HE1	2.13	0.47
18:b:8:LEU:C	18:b:10:PRO:HD3	2.40	0.47
21:D:102:ALA:HB2	21:D:186:VAL:HG11	1.96	0.47
24:M:25:LEU:HD22	24:M:34:LEU:HD11	1.96	0.47
35:g:6:ILE:HD11	35:g:322:VAL:HG13	1.95	0.47
38:1:48:5MC:HM53	38:1:59:A:N1	2.20	0.47
1:2:255:A:H2'	1:2:256:A:C8	2.50	0.47
1:2:393:C:H2'	1:2:394:U:C6	2.49	0.47
1:2:437:A:H1'	1:2:464:G:H22	1.80	0.47
1:2:590:A:H2'	1:2:591:G:H8	1.79	0.47
1:2:801:G:O2'	14:W:107:SER:HB2	2.15	0.47
1:2:1112:A:OP1	1:2:1114:U:H1'	2.14	0.47
1:2:1532:G:O2'	31:Z:73:GLY:HA3	2.15	0.47
3:B:144:ARG:HB2	3:B:208:GLN:CB	2.33	0.47
5:E:136:ILE:HG23	5:E:149:TYR:CE1	2.49	0.47
8:I:37:LYS:H	8:I:59:ARG:H	1.61	0.47
8:I:154:GLU:OE2	8:I:157:VAL:HG23	2.15	0.47
9:J:109:LEU:N	9:J:145:SER:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:129:GLN:O	22:F:130:ASN:C	2.58	0.47
23:K:6:GLU:OE2	23:K:6:GLU:N	2.37	0.47
24:M:121:THR:C	24:M:123:GLU:H	2.22	0.47
28:S:123:ARG:HG2	28:S:127:HIS:CE1	2.50	0.47
36:i:29:LYS:N	36:i:35:TYR:OH	2.47	0.47
38:1:62:C:H2'	38:1:63:G:H8	1.80	0.47
39:j:22:VAL:HG11	39:j:85:LEU:HD11	1.96	0.47
1:2:610:U:H5''	15:X:15:LEU:HD11	1.96	0.47
1:2:867:G:H2'	1:2:868:A:C8	2.42	0.47
1:2:918:A:H2'	1:2:919:U:C6	2.49	0.47
1:2:1134:U:H2'	1:2:1135:U:C6	2.50	0.47
1:2:1448:U:H2'	1:2:1449:C:C6	2.50	0.47
1:2:1497:G:H2'	1:2:1498:C:C6	2.49	0.47
4:C:64:HIS:HA	13:V:15:ARG:HH11	1.80	0.47
11:N:37:ILE:HG23	11:N:50:ILE:HG21	1.96	0.47
23:K:74:VAL:HG22	23:K:77:ARG:NH2	2.30	0.47
1:2:1537:G:H4'	28:S:40:ARG:CZ	2.45	0.46
3:B:35:PRO:HA	3:B:232:HIS:CD2	2.50	0.46
4:C:162:LYS:HZ3	14:W:95:PRO:HA	1.80	0.46
4:C:242:PRO:HB3	13:V:50:TYR:OH	2.15	0.46
5:E:120:SER:O	5:E:164:LEU:HB3	2.15	0.46
28:S:17:LEU:O	28:S:20:THR:OG1	2.24	0.46
28:S:69:ILE:HA	28:S:72:ILE:HD12	1.97	0.46
28:S:84:TRP:HA	28:S:89:GLN:NE2	2.25	0.46
29:T:34:VAL:O	29:T:36:ILE:HG12	2.15	0.46
30:U:98:HIS:O	30:U:102:ARG:HG2	2.14	0.46
31:Z:68:ARG:HB2	31:Z:70:LYS:HE2	1.98	0.46
38:1:28:A:C4	38:1:43:G:N2	2.83	0.46
1:2:1067:C:H2'	1:2:1068:A:C8	2.49	0.46
1:2:1182:A:C4	25:P:100:LYS:HE2	2.50	0.46
1:2:1741:U:H2'	1:2:1742:A:H8	1.79	0.46
9:J:107:ARG:HH22	9:J:150:LEU:HD13	1.80	0.46
10:L:13:PHE:CE2	10:L:15:LYS:HB3	2.51	0.46
13:V:7:GLN:OE1	13:V:7:GLN:N	2.48	0.46
31:Z:59:TYR:CE2	31:Z:61:SER:HB3	2.50	0.46
35:g:23:SER:HB2	35:g:37:GLY:H	1.81	0.46
37:3:39:U:H2'	37:3:40:C:H4'	1.96	0.46
38:1:10:2MG:N1	38:1:26:M2G:C4	2.83	0.46
38:1:16:H2U:H52	38:1:60:A:H4'	1.97	0.46
40:k:140:LEU:O	40:k:319:ARG:NH1	2.46	0.46
1:2:107:C:H2'	1:2:108:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:280:G:H2'	1:2:281:C:C6	2.51	0.46
1:2:1499:C:OP2	29:T:106:GLN:NE2	2.47	0.46
1:2:1779:A:H2'	1:2:1780:MA6:C8	2.45	0.46
2:A:198:MET:SD	2:A:199:PRO:HD2	2.55	0.46
8:I:107:THR:N	8:I:108:PRO:HD2	2.31	0.46
13:V:83:TRP:CH2	13:V:85:TYR:HD1	2.32	0.46
14:W:49:GLU:O	14:W:64:GLN:HB2	2.16	0.46
28:S:35:ILE:H	28:S:35:ILE:HD12	1.80	0.46
28:S:112:ASP:OD1	28:S:115:ARG:NH2	2.49	0.46
36:i:63:GLY:O	36:i:64:LYS:HB3	2.15	0.46
46:k:604:MET:SD	46:k:604:MET:N	2.88	0.46
42:m:100:LYS:HA	42:m:103:ILE:HD13	1.97	0.46
1:2:2:A:C8	1:2:369:A:H1'	2.51	0.46
1:2:29:U:O3'	15:X:126:LYS:NZ	2.41	0.46
1:2:369:A:C4	1:2:370:G:C8	3.03	0.46
1:2:495:G:H2'	1:2:496:G:C8	2.51	0.46
1:2:748:U:H2'	1:2:749:U:H6	1.80	0.46
1:2:1483:C:H1'	1:2:1604:C:H4'	1.98	0.46
5:E:36:HIS:CE1	5:E:85:GLY:HA3	2.51	0.46
7:H:96:ARG:NH1	7:H:97:ARG:H	2.13	0.46
11:N:119:GLU:HA	11:N:122:ILE:HG22	1.97	0.46
16:Y:5:ILE:H	16:Y:5:ILE:HD12	1.81	0.46
25:P:30:THR:O	25:P:34:VAL:HG23	2.15	0.46
34:f:119:LYS:HD2	34:f:130:LEU:HD12	1.97	0.46
35:g:174:PHE:CE2	35:g:186:TRP:HB2	2.51	0.46
37:3:33:C:H5'	37:3:34:U:C5	2.50	0.46
39:j:188:VAL:HG22	39:j:264:ILE:HG12	1.96	0.46
1:2:72:A:N3	1:2:73:U:N3	2.63	0.46
1:2:175:C:H2'	1:2:176:U:C6	2.50	0.46
1:2:267:C:N4	6:G:186:ARG:HD3	2.30	0.46
1:2:707:A:N7	1:2:708:C:N4	2.63	0.46
1:2:809:G:C4	7:H:111:LYS:HB2	2.50	0.46
1:2:867:G:P	11:N:121:ARG:NH2	2.87	0.46
1:2:966:A:H2'	1:2:967:U:C6	2.50	0.46
1:2:1171:G:H2'	1:2:1172:C:C6	2.50	0.46
16:Y:57:VAL:N	16:Y:94:TYR:OH	2.49	0.46
17:a:38:ARG:HA	17:a:38:ARG:HD3	1.66	0.46
22:F:103:GLY:CA	22:F:106:ASN:H	2.29	0.46
24:M:87:GLN:O	24:M:91:TRP:CD1	2.68	0.46
24:M:96:LYS:H	24:M:104:ARG:HG2	1.80	0.46
35:g:19:GLY:HA3	35:g:39:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:219:ALA:HB3	35:g:250:LEU:HD13	1.97	0.46
36:i:52:PHE:CE2	36:i:109:LEU:HD23	2.50	0.46
38:1:28:A:C5	38:1:43:G:N2	2.84	0.46
40:k:113:LYS:HZ3	40:k:194:CYS:C	2.23	0.46
40:k:197:HIS:HD2	40:k:199:ILE:H	1.62	0.46
1:2:405:U:C2	1:2:406:A:C8	3.04	0.46
1:2:778:G:H1	16:Y:10:ARG:HD3	1.80	0.46
1:2:977:A:C4	1:2:978:A:C8	3.04	0.46
1:2:1412:U:OP1	27:R:2:GLY:N	2.49	0.46
4:C:145:ARG:HB2	4:C:227:TYR:CD1	2.50	0.46
5:E:206:ASP:HB2	5:E:222:LEU:HB3	1.97	0.46
7:H:44:LYS:HE3	7:H:63:PRO:HB3	1.97	0.46
13:V:16:LYS:HG2	13:V:23:ILE:HA	1.96	0.46
22:F:191:THR:O	22:F:195:THR:HG23	2.15	0.46
25:P:29:PRO:HG2	25:P:32:ASP:HB2	1.98	0.46
26:Q:128:LYS:NZ	26:Q:134:ALA:O	2.45	0.46
31:Z:54:ALA:HB3	31:Z:55:PRO:HD3	1.96	0.46
35:g:136:ASN:HD22	35:g:138:VAL:H	1.63	0.46
35:g:266:GLY:HA3	35:g:281:LEU:O	2.15	0.46
39:j:15:GLU:HG3	39:j:18:ASP:HB3	1.97	0.46
1:2:122:U:N3	1:2:123:G:N7	2.64	0.46
1:2:157:U:O2'	1:2:159:C:OP2	2.30	0.46
1:2:781:A:O2'	1:2:782:G:OP1	2.25	0.46
1:2:852:G:H2'	1:2:853:U:C6	2.51	0.46
1:2:899:A:OP1	12:O:43:THR:OG1	2.24	0.46
1:2:924:G:H2'	1:2:925:A:H8	1.80	0.46
1:2:1144:U:O2'	4:C:93:LYS:HE2	2.15	0.46
2:A:49:ASN:O	2:A:53:THR:HG23	2.15	0.46
22:F:42:ILE:HB	22:F:69:PRO:HB2	1.97	0.46
22:F:114:ARG:NH2	26:Q:43:ILE:HA	2.31	0.46
22:F:196:LEU:HD23	22:F:200:LEU:HD13	1.98	0.46
35:g:300:ALA:HB3	35:g:309:PHE:HB2	1.98	0.46
40:k:403:ASP:OD1	40:k:405:THR:OG1	2.23	0.46
40:k:426:ILE:HG23	40:k:490:PRO:HB2	1.98	0.46
1:2:350:C:O4'	15:X:13:ARG:NH1	2.48	0.46
1:2:445:A:H62	1:2:460:G:H21	1.63	0.46
1:2:627:G:N1	1:2:969:A:OP2	2.34	0.46
1:2:969:A:H2'	1:2:970:A:H5'	1.97	0.46
1:2:1216:A:C5	23:K:40:LEU:HD11	2.51	0.46
3:B:34:ALA:HB1	3:B:38:PHE:HD2	1.81	0.46
9:J:83:ILE:HD12	9:J:149:ARG:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:32:ASP:OD1	12:O:32:ASP:N	2.49	0.46
14:W:28:ARG:HB3	14:W:29:PRO:HD3	1.97	0.46
16:Y:29:HIS:ND1	16:Y:32:ARG:O	2.46	0.46
29:T:65:ILE:HD13	29:T:114:VAL:HG21	1.98	0.46
35:g:140:ASP:OD1	35:g:141:CYS:N	2.48	0.46
38:1:10:2MG:HN2	38:1:26:M2G:H1'	1.80	0.46
40:k:109:VAL:HG11	40:k:197:HIS:ND1	2.31	0.46
1:2:623:G:H2'	1:2:624:C:C6	2.51	0.46
1:2:965:A:C6	1:2:966:A:N6	2.83	0.46
1:2:1220:A:H2'	1:2:1221:C:C6	2.51	0.46
1:2:1335:A:H2'	1:2:1336:A:O4'	2.16	0.46
4:C:74:ILE:HD13	4:C:141:VAL:HG11	1.96	0.46
13:V:15:ARG:HH21	13:V:54:ALA:HB2	1.81	0.46
27:R:13:SER:OG	27:R:53:TYR:HD2	1.98	0.46
27:R:91:LEU:O	27:R:93:LEU:N	2.48	0.46
40:k:139:LYS:HB3	40:k:319:ARG:HH11	1.80	0.46
42:m:50:ASP:OD1	42:m:50:ASP:N	2.49	0.46
1:2:16:G:N2	1:2:1137:A:H62	2.12	0.46
1:2:275:C:O2'	1:2:276:U:O5'	2.32	0.46
1:2:786:G:O2'	1:2:787:A:H5'	2.16	0.46
1:2:901:G:H22	12:O:52:ARG:NH2	2.13	0.46
1:2:978:A:H4'	1:2:1784:G:H21	1.81	0.46
1:2:1038:A:O2'	1:2:1039:G:H8	1.98	0.46
2:A:63:ILE:HG12	13:V:36:ILE:HD12	1.98	0.46
2:A:195:TRP:CZ2	2:A:197:ILE:HD11	2.51	0.46
3:B:31:ASP:OD1	3:B:32:ILE:N	2.49	0.46
5:E:76:VAL:HG23	5:E:77:ARG:N	2.31	0.46
7:H:101:LYS:HD3	7:H:112:ARG:HH22	1.80	0.46
21:D:162:GLN:NE2	21:D:165:ASN:HD22	2.13	0.46
26:Q:98:ASP:OD1	26:Q:99:GLU:N	2.49	0.46
29:T:89:ARG:NE	29:T:89:ARG:CA	2.78	0.46
35:g:104:PHE:CE2	35:g:139:GLY:HA2	2.51	0.46
40:k:98:GLN:HE22	40:k:391:VAL:N	2.14	0.46
40:k:433:ASN:HB2	40:k:518:LYS:HD3	1.97	0.46
1:2:14:C:H2'	1:2:15:U:C6	2.52	0.45
1:2:38:C:H4'	9:J:6:ARG:HH12	1.80	0.45
1:2:54:C:H5'	16:Y:110:GLN:OE1	2.15	0.45
1:2:71:A:H1'	1:2:81:G:N2	2.31	0.45
1:2:650:G:C6	1:2:684:A:N6	2.84	0.45
1:2:1187:G:C6	1:2:1197:G:C6	3.04	0.45
6:G:76:LEU:HD21	6:G:92:ARG:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:102:VAL:HA	6:G:106:LEU:HD11	1.98	0.45
6:G:185:GLN:HA	6:G:188:ARG:NE	2.30	0.45
9:J:39:LYS:HA	9:J:42:ILE:CD1	2.46	0.45
11:N:139:TRP:C	11:N:140:LYS:HD2	2.41	0.45
12:O:45:GLY:HA2	12:O:54:GLU:HG2	1.97	0.45
25:P:17:TYR:CD2	25:P:18:LYS:HG2	2.50	0.45
29:T:15:ILE:HD11	29:T:60:SER:N	2.31	0.45
35:g:124:ILE:HG22	35:g:134:VAL:HG22	1.97	0.45
35:g:257:PHE:CE2	35:g:272:LEU:HB2	2.50	0.45
38:1:19:G:OP1	38:1:57:G:N2	2.49	0.45
39:j:29:GLU:OE2	39:j:30:MET:HG3	2.16	0.45
1:2:236:C:H4'	1:2:237:U:C6	2.51	0.45
1:2:732:G:O2'	1:2:734:A:N6	2.49	0.45
1:2:989:C:H5	1:2:1013:G:N1	2.08	0.45
1:2:1651:C:H2'	1:2:1652:G:O4'	2.16	0.45
1:2:1791:G:C6	17:a:75:ILE:HG21	2.51	0.45
3:B:129:THR:HG21	3:B:133:TYR:HB2	1.98	0.45
22:F:45:PHE:HB2	22:F:48:TRP:CZ3	2.51	0.45
22:F:99:LEU:HA	22:F:178:THR:OG1	2.16	0.45
25:P:93:VAL:HG13	25:P:104:GLN:NE2	2.30	0.45
27:R:20:TYR:CE2	27:R:38:ILE:HD12	2.51	0.45
27:R:90:ALA:HA	27:R:95:HIS:CE1	2.51	0.45
28:S:17:LEU:HD11	28:S:66:LEU:HD11	1.98	0.45
29:T:18:TYR:CD1	29:T:135:ILE:HG21	2.51	0.45
29:T:42:GLY:HA2	29:T:84:LYS:HB2	1.98	0.45
36:i:83:ASP:OD1	36:i:83:ASP:N	2.48	0.45
38:1:28:A:C6	38:1:43:G:N1	2.84	0.45
38:1:44:A:O2'	38:1:45:U:H5''	2.12	0.45
39:j:6:CYS:SG	39:j:127:TYR:HB3	2.56	0.45
39:j:23:ASN:HA	39:j:67:LYS:O	2.16	0.45
42:m:58:LEU:HD13	42:m:80:LEU:HD11	1.98	0.45
1:2:27:U:H2'	1:2:28:A:C8	2.50	0.45
1:2:366:A:H2'	1:2:367:U:O4'	2.17	0.45
1:2:743:U:C4	1:2:808:G:C2	3.04	0.45
1:2:987:A:H2'	1:2:988:U:C6	2.51	0.45
1:2:1182:A:H2'	1:2:1183:A:C8	2.51	0.45
1:2:1605:G:H2'	1:2:1606:U:C6	2.51	0.45
1:2:1679:A:N6	1:2:1718:G:O2'	2.34	0.45
5:E:185:GLY:HA3	5:E:224:ASN:HD21	1.81	0.45
12:O:84:ARG:HG2	12:O:85:ALA:O	2.17	0.45
12:O:133:ARG:HG2	17:a:28:ARG:HH12	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:51:ARG:O	17:a:54:SER:N	2.49	0.45
28:S:71:GLN:O	28:S:74:GLN:HG2	2.16	0.45
31:Z:46:LYS:HA	31:Z:46:LYS:HD3	1.71	0.45
38:1:47:H2U:H2'	38:1:50:U:OP1	2.16	0.45
1:2:69:G:H2'	1:2:70:C:C6	2.51	0.45
1:2:90:C:N4	1:2:91:G:O6	2.50	0.45
1:2:129:U:O4'	1:2:263:G:N1	2.50	0.45
1:2:225:A:H3'	1:2:226:U:H5'	1.99	0.45
1:2:989:C:H2'	1:2:990:G:O4'	2.16	0.45
1:2:1234:C:C2	1:2:1235:A:C8	3.04	0.45
1:2:1462:G:H2'	1:2:1463:C:C6	2.51	0.45
1:2:1671:G:H2'	1:2:1672:C:C6	2.52	0.45
11:N:63:ALA:HB3	11:N:71:ILE:HD11	1.97	0.45
1:2:71:A:H2'	1:2:72:A:C4	2.52	0.45
1:2:432:C:H2'	1:2:433:G:O4'	2.16	0.45
1:2:1485:A:H2'	1:2:1486:G:H8	1.81	0.45
2:A:62:ARG:HH21	13:V:38:GLN:HA	1.81	0.45
2:A:89:TYR:HD1	2:A:178:ALA:HB2	1.82	0.45
4:C:100:ARG:NH1	4:C:102:ARG:HE	2.03	0.45
6:G:148:THR:O	6:G:149:LYS:C	2.58	0.45
7:H:62:VAL:C	7:H:64:VAL:H	2.24	0.45
12:O:81:ILE:HB	12:O:115:ILE:HG22	1.99	0.45
18:b:34:ASP:HB2	18:b:43:ILE:HD11	1.98	0.45
22:F:78:ARG:HE	26:Q:122:ARG:HG2	1.80	0.45
22:F:103:GLY:C	22:F:106:ASN:HB2	2.42	0.45
26:Q:44:LEU:O	26:Q:47:LYS:HB2	2.17	0.45
27:R:115:LEU:HB2	27:R:117:LEU:HD13	1.98	0.45
29:T:84:LYS:HD2	29:T:85:ASN:N	2.32	0.45
1:2:36:C:H2'	1:2:37:U:C6	2.52	0.45
1:2:182:U:H2'	1:2:183:C:H6	1.81	0.45
1:2:848:C:H2'	1:2:849:A:C8	2.51	0.45
1:2:1334:U:O2	1:2:1414:G:N2	2.50	0.45
1:2:1343:A:H2'	1:2:1344:A:C8	2.52	0.45
1:2:1464:G:O2'	1:2:1600:C:OP1	2.20	0.45
1:2:1788:A:O5'	17:a:10:ARG:NH1	2.50	0.45
3:B:146:GLN:O	3:B:149:GLN:HG2	2.16	0.45
5:E:54:TYR:OH	5:E:97:GLU:OE2	2.28	0.45
5:E:247:THR:HB	5:E:250:GLU:HG2	1.98	0.45
10:L:88:ARG:O	10:L:104:HIS:HA	2.16	0.45
14:W:40:VAL:O	14:W:43:LYS:HG2	2.17	0.45
22:F:45:PHE:HB2	22:F:48:TRP:HZ3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Q:101:SER:O	26:Q:105:LEU:HD23	2.16	0.45
28:S:27:ASN:HA	28:S:57:ARG:HD3	1.98	0.45
29:T:116:ILE:HD13	29:T:122:ARG:HG2	1.98	0.45
38:1:28:A:C5	38:1:43:G:C2	3.05	0.45
1:2:460:G:H2'	1:2:461:G:C8	2.52	0.45
1:2:752:A:O5'	5:E:187:ARG:NH2	2.50	0.45
1:2:1357:G:H5'	29:T:126:ASP:OD1	2.16	0.45
1:2:1601:U:H2'	1:2:1602:U:C6	2.51	0.45
1:2:1613:C:O2'	1:2:1614:G:OP2	2.26	0.45
2:A:80:THR:HA	2:A:83:GLN:OE1	2.17	0.45
6:G:135:PRO:HD2	6:G:158:ILE:HD12	1.98	0.45
24:M:42:ALA:O	24:M:46:THR:HG23	2.17	0.45
24:M:56:VAL:HG11	24:M:85:ALA:HA	1.98	0.45
26:Q:28:LEU:O	26:Q:29:ILE:HD13	2.17	0.45
32:c:11:LYS:HB2	32:c:53:ILE:HG22	1.97	0.45
34:f:124:CYS:SG	34:f:141:LYS:HB3	2.56	0.45
42:m:84:GLN:O	42:m:88:VAL:HG23	2.17	0.45
1:2:137:U:H2'	1:2:138:A:C8	2.52	0.45
1:2:236:C:O2'	1:2:238:C:N4	2.49	0.45
1:2:544:A:H2'	19:e:31:LYS:HD3	1.98	0.45
1:2:743:U:P	7:H:108:GLN:H	2.40	0.45
1:2:748:U:H2'	1:2:749:U:C6	2.52	0.45
1:2:773:C:P	5:E:22:LYS:HG2	2.56	0.45
1:2:1330:A:OP1	27:R:45:ARG:NH1	2.49	0.45
1:2:1598:A:C2'	1:2:1599:G:H5''	2.45	0.45
1:2:1647:G:H2'	1:2:1648:U:H6	1.82	0.45
2:A:90:ALA:HA	2:A:95:ALA:HB3	1.99	0.45
2:A:119:ARG:HH22	4:C:246:ASP:HA	1.82	0.45
5:E:45:ILE:HG13	5:E:61:VAL:HG11	1.97	0.45
5:E:75:LYS:O	5:E:77:ARG:NH2	2.50	0.45
17:a:74:CYS:SG	17:a:75:ILE:N	2.90	0.45
18:b:30:SER:OG	18:b:31:HIS:N	2.50	0.45
21:D:148:LYS:HD3	37:3:37:U:H3	1.80	0.45
35:g:214:ASP:OD1	35:g:215:GLY:N	2.50	0.45
38:1:28:A:C6	38:1:43:G:C2	3.04	0.45
1:2:16:G:H2'	1:2:17:C:C6	2.51	0.45
1:2:19:A:OP1	15:X:110:LYS:NZ	2.50	0.45
1:2:341:C:H2'	1:2:342:C:C6	2.52	0.45
1:2:446:U:H2'	1:2:447:C:O4'	2.17	0.45
1:2:762:A:OP1	9:J:79:ARG:NH2	2.36	0.45
1:2:1183:A:O3'	1:2:1185:U:H5''	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1229:A:O2'	1:2:1258:U:O2	2.34	0.45
1:2:1240:G:OP1	25:P:77:ARG:NE	2.47	0.45
1:2:1390:U:H2'	1:2:1391:C:H6	1.80	0.45
2:A:23:HIS:CE1	27:R:106:THR:HG21	2.52	0.45
4:C:58:ILE:HD12	4:C:62:PHE:HE2	1.79	0.45
11:N:64:LYS:HG3	11:N:70:LYS:NZ	2.32	0.45
22:F:130:ASN:O	22:F:132:LEU:N	2.50	0.45
23:K:80:LEU:HG	23:K:82:LEU:HB2	1.98	0.45
27:R:47:ARG:NE	27:R:48:ASN:OD1	2.50	0.45
40:k:466:ILE:HA	40:k:499:ILE:HG12	1.99	0.45
1:2:8:U:O2	1:2:1137:A:H3'	2.17	0.45
1:2:277:U:H4'	1:2:278:G:O5'	2.17	0.45
1:2:445:A:O3'	5:E:57:ASN:ND2	2.35	0.45
1:2:569:A:N6	15:X:116:ASP:OD1	2.50	0.45
1:2:1077:C:H2'	1:2:1078:U:H6	1.81	0.45
1:2:1096:U:H1'	4:C:173:ARG:HH11	1.82	0.45
3:B:53:GLY:HA2	3:B:56:ASN:OD1	2.17	0.45
7:H:41:LEU:HD22	7:H:70:TYR:CE1	2.49	0.45
9:J:23:ARG:HH11	9:J:27:GLU:CD	2.24	0.45
9:J:89:ASP:OD1	9:J:90:LYS:N	2.50	0.45
12:O:92:LYS:NZ	12:O:122:PRO:HD2	2.31	0.45
14:W:94:LEU:HD22	14:W:100:GLY:HA3	1.99	0.45
16:Y:27:VAL:HG21	16:Y:35:VAL:HG21	1.98	0.45
18:b:53:ALA:HB1	18:b:62:VAL:HG23	1.98	0.45
23:K:81:ASN:HD21	24:M:30:VAL:CG1	2.30	0.45
38:1:19:G:N3	38:1:20:A:N6	2.65	0.45
1:2:220:A:C6	1:2:840:U:C4	3.04	0.44
1:2:274:C:H5''	1:2:275:C:OP2	2.17	0.44
1:2:809:G:N3	7:H:108:GLN:NE2	2.60	0.44
1:2:1233:A:H4'	34:f:143:HIS:CE1	2.52	0.44
2:A:30:GLN:OE1	2:A:149:LEU:HB3	2.17	0.44
3:B:114:VAL:O	3:B:114:VAL:HG13	2.17	0.44
3:B:142:PHE:O	3:B:208:GLN:N	2.50	0.44
3:B:184:LEU:O	3:B:188:LEU:HG	2.17	0.44
4:C:152:ASN:O	4:C:153:LEU:HD23	2.16	0.44
4:C:189:VAL:O	4:C:193:MET:HG2	2.17	0.44
5:E:70:VAL:HG22	5:E:92:LEU:HD21	1.98	0.44
8:I:34:ALA:HB2	8:I:56:ARG:HE	1.81	0.44
8:I:154:GLU:OE2	8:I:156:ALA:HB3	2.17	0.44
12:O:80:HIS:HA	12:O:113:GLY:O	2.16	0.44
12:O:114:ARG:HA	17:a:62:TYR:OH	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:58:LYS:HD2	25:P:58:LYS:HA	1.85	0.44
28:S:84:TRP:O	28:S:85:PHE:HB2	2.17	0.44
35:g:249:ALA:O	35:g:262:ALA:N	2.39	0.44
40:k:99:ALA:HB3	40:k:394:GLY:HA3	1.99	0.44
1:2:437:A:H1'	1:2:464:G:N2	2.32	0.44
1:2:643:U:H2'	1:2:644:C:H6	1.80	0.44
1:2:824:U:C2	1:2:825:U:C5	3.05	0.44
1:2:1125:G:H2'	1:2:1126:G:H8	1.82	0.44
1:2:1679:A:O2'	6:G:31:ARG:NH1	2.50	0.44
2:A:84:ARG:NH1	2:A:205:ARG:HB2	2.32	0.44
2:A:110:TYR:HB2	4:C:43:VAL:HG11	1.98	0.44
7:H:46:ILE:HG12	7:H:60:VAL:HG12	1.98	0.44
14:W:34:ILE:O	14:W:38:LEU:HD23	2.17	0.44
21:D:83:THR:HB	21:D:84:ILE:HD12	1.99	0.44
22:F:65:GLN:HE22	22:F:68:LYS:HB3	1.82	0.44
22:F:119:THR:O	22:F:123:ILE:HG12	2.17	0.44
23:K:60:SER:HB3	23:K:65:TYR:HE2	1.83	0.44
30:U:24:ILE:HB	30:U:91:ILE:HG13	1.99	0.44
38:1:36:U:H2'	38:1:37:T6A:H8	1.83	0.44
38:1:70:G:H2'	38:1:71:C:C6	2.52	0.44
42:m:62:PHE:CZ	42:m:88:VAL:HA	2.52	0.44
1:2:566:A:N3	19:e:14:VAL:HG21	2.32	0.44
1:2:765:G:H1'	1:2:768:C:OP1	2.17	0.44
1:2:1296:G:H5'	1:2:1297:U:OP2	2.17	0.44
1:2:1726:U:H2'	1:2:1727:C:C6	2.51	0.44
3:B:209:ASN:OD1	3:B:211:HIS:HD2	2.00	0.44
4:C:162:LYS:HA	4:C:174:LEU:O	2.18	0.44
4:C:172:VAL:HG11	4:C:219:ALA:HA	2.00	0.44
10:L:2:SER:C	10:L:4:GLU:H	2.25	0.44
29:T:114:VAL:HG22	29:T:122:ARG:HB3	1.99	0.44
30:U:58:LEU:HD21	30:U:90:TYR:CD2	2.53	0.44
38:1:15:G:H1	38:1:48:5MC:N4	2.15	0.44
38:1:74:C:C5	40:k:128:PHE:HB2	2.52	0.44
39:j:242:GLU:HA	39:j:245:GLU:HG2	1.99	0.44
40:k:113:LYS:HB3	40:k:217:LEU:HD11	1.99	0.44
40:k:475:VAL:HG22	40:k:485:LEU:HD22	1.98	0.44
1:2:252:A:H2'	1:2:253:A:C8	2.52	0.44
1:2:304:C:H2'	1:2:305:U:C6	2.53	0.44
1:2:327:A:H2'	1:2:328:G:C8	2.52	0.44
1:2:450:A:N6	1:2:452:U:O2	2.43	0.44
1:2:641:G:O6	1:2:642:G:O6	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1102:U:OP1	15:X:8:GLY:N	2.51	0.44
1:2:1353:G:O6	1:2:1368:U:C2	2.69	0.44
1:2:1478:G:N7	1:2:1479:C:N4	2.65	0.44
1:2:1789:A:H4'	1:2:1790:G:H21	1.81	0.44
7:H:60:VAL:HG22	7:H:92:PHE:HA	1.99	0.44
7:H:131:PHE:N	7:H:132:PRO:HD2	2.33	0.44
9:J:62:ARG:NH1	9:J:68:LYS:HD3	2.33	0.44
12:O:107:ARG:HG2	17:a:52:ASP:OD2	2.18	0.44
22:F:176:LEU:HD21	22:F:215:LYS:HB2	1.98	0.44
24:M:25:LEU:HD12	24:M:91:TRP:CZ3	2.52	0.44
24:M:26:ARG:HH11	24:M:30:VAL:HG21	1.82	0.44
28:S:26:ILE:HB	28:S:31:ALA:HB2	2.00	0.44
28:S:52:VAL:HG13	28:S:68:ARG:HH22	1.82	0.44
39:j:27:ILE:HG23	39:j:31:GLY:O	2.18	0.44
1:2:72:A:OP1	1:2:72:A:H4'	2.17	0.44
1:2:112:A:HO2'	10:L:67:ARG:HE	1.60	0.44
1:2:182:U:H2'	1:2:183:C:C6	2.51	0.44
1:2:1053:U:H2'	1:2:1054:U:C6	2.53	0.44
1:2:1243:A:H2'	1:2:1243:A:N3	2.32	0.44
1:2:1351:U:H2'	1:2:1352:U:O4'	2.17	0.44
1:2:1362:U:H5''	1:2:1363:G:H8	1.82	0.44
1:2:1646:A:H2'	1:2:1647:G:H8	1.82	0.44
1:2:1754:A:P	36:i:67:LYS:HZ1	2.38	0.44
2:A:139:VAL:HG23	4:C:67:PRO:HG2	2.00	0.44
5:E:35:PRO:HB3	5:E:143:ASP:O	2.17	0.44
6:G:14:LYS:NZ	6:G:15:CYS:H	2.16	0.44
15:X:70:LYS:HE3	36:i:84:PHE:CZ	2.52	0.44
22:F:211:TYR:CE1	22:F:215:LYS:HE2	2.52	0.44
23:K:2:LEU:HD23	23:K:2:LEU:H	1.82	0.44
26:Q:55:VAL:HG12	26:Q:59:LYS:HB3	1.98	0.44
26:Q:101:SER:HA	26:Q:104:GLU:HG2	1.98	0.44
29:T:28:LEU:H	29:T:111:LEU:HD21	1.81	0.44
34:f:102:VAL:HA	34:f:105:TYR:CD2	2.50	0.44
40:k:245:ILE:HG12	40:k:279:PRO:HG2	2.00	0.44
1:2:163:A:H1'	6:G:13:GLN:NE2	2.33	0.44
1:2:180:A:H2'	1:2:181:A:C8	2.52	0.44
1:2:398:A:H4'	5:E:3:ARG:HB3	2.00	0.44
1:2:1065:C:H4'	3:B:149:GLN:OE1	2.17	0.44
2:A:195:TRP:CH2	2:A:197:ILE:HD11	2.53	0.44
3:B:125:VAL:HG22	3:B:127:VAL:HG13	2.00	0.44
4:C:148:TYR:CE2	4:C:156:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:33:GLU:OE2	19:e:40:TYR:OH	2.20	0.44
14:W:36:LYS:O	14:W:39:GLN:HG3	2.18	0.44
15:X:48:HIS:CD2	15:X:105:ALA:HB2	2.52	0.44
30:U:51:VAL:HG23	30:U:94:GLU:HB3	2.00	0.44
35:g:39:ARG:HE	35:g:68:ILE:HD12	1.82	0.44
35:g:91:ARG:HB3	35:g:93:TRP:NE1	2.32	0.44
35:g:151:TRP:O	35:g:178:GLY:HA3	2.18	0.44
1:2:91:G:H2'	1:2:92:A:O4'	2.17	0.44
1:2:350:C:O2'	10:L:104:HIS:NE2	2.41	0.44
1:2:394:U:O4	1:2:398:A:N7	2.51	0.44
1:2:464:G:H2'	1:2:465:PSU:H6	1.83	0.44
1:2:773:C:H5''	5:E:21:ASP:OD1	2.18	0.44
1:2:926:C:H1'	12:O:124:ASP:O	2.17	0.44
1:2:1094:U:OP1	1:2:1095:C:H2'	2.18	0.44
1:2:1201:A:H3'	1:2:1201:A:N3	2.32	0.44
1:2:1220:A:H2'	1:2:1221:C:H6	1.82	0.44
1:2:1297:U:H2'	1:2:1298:G:O4'	2.18	0.44
1:2:1746:G:H2'	1:2:1747:A:C8	2.52	0.44
2:A:166:GLY:O	2:A:167:LYS:HB3	2.16	0.44
5:E:250:GLU:O	5:E:254:ARG:HG3	2.17	0.44
8:I:72:VAL:HG11	8:I:112:TRP:CZ2	2.52	0.44
8:I:78:ILE:HG23	8:I:102:VAL:HG21	2.00	0.44
14:W:53:ILE:HD11	18:b:8:LEU:HD22	2.00	0.44
16:Y:73:GLY:C	16:Y:74:LEU:HD12	2.42	0.44
25:P:96:VAL:CG1	25:P:120:SER:HB3	2.47	0.44
29:T:37:VAL:HG12	29:T:39:THR:H	1.82	0.44
30:U:23:ARG:HB3	30:U:117:ILE:HG13	2.00	0.44
31:Z:55:PRO:O	31:Z:56:THR:OG1	2.29	0.44
40:k:314:ARG:HE	40:k:494:GLU:HG2	1.83	0.44
1:2:71:A:H3'	1:2:72:A:C5'	2.47	0.44
1:2:865:G:H2'	1:2:866:G:H8	1.82	0.44
1:2:1246:U:H5'	34:f:93:HIS:HB2	2.00	0.44
3:B:104:ASP:OD1	3:B:214:LYS:HA	2.17	0.44
15:X:62:LYS:HG2	15:X:63:GLN:H	1.83	0.44
32:c:22:ARG:HD3	32:c:22:ARG:HA	1.76	0.44
35:g:204:ASN:HD21	35:g:223:LYS:HD2	1.83	0.44
38:1:9:1MG:P	38:1:46:7MG:H1'	2.58	0.44
39:j:67:LYS:HG2	39:j:68:ASN:H	1.83	0.44
1:2:1116:U:H2'	1:2:1117:G:H8	1.83	0.44
1:2:1650:C:H2'	1:2:1651:C:C6	2.53	0.44
7:H:162:ILE:HG23	7:H:165:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:169:ALA:HB2	8:I:185:LEU:HD21	1.99	0.44
16:Y:32:ARG:NH2	16:Y:39:GLU:OE1	2.51	0.44
21:D:68:GLU:OE2	23:K:67:THR:OG1	2.36	0.44
23:K:22:VAL:HG23	23:K:23:ALA:N	2.31	0.44
23:K:25:LYS:NZ	23:K:64:TYR:OH	2.20	0.44
23:K:62:GLN:HE22	33:d:23:ILE:C	2.24	0.44
26:Q:40:GLN:O	26:Q:41:PRO:C	2.61	0.44
28:S:41:ARG:HG3	28:S:85:PHE:HE1	1.83	0.44
31:Z:40:VAL:HG13	31:Z:41:VAL:HG23	2.00	0.44
38:1:5:C:H2'	38:1:6:C:H6	1.83	0.44
1:2:393:C:H2'	1:2:394:U:H6	1.83	0.43
1:2:533:A:H3'	1:2:534:A:C8	2.47	0.43
1:2:845:G:H3'	1:2:846:A:H8	1.82	0.43
1:2:870:G:C6	1:2:956:G:C6	3.06	0.43
1:2:970:A:C2	1:2:971:G:H1'	2.53	0.43
1:2:979:G:H4'	1:2:1774:A:H4'	1.99	0.43
1:2:1106:G:H2'	1:2:1107:G:N3	2.33	0.43
1:2:1710:A:C5	1:2:1711:G:H1'	2.52	0.43
1:2:1770:C:OP2	20:h:2:ARG:NH1	2.51	0.43
4:C:193:MET:HE2	4:C:201:VAL:HG11	2.00	0.43
5:E:180:LEU:HD12	5:E:193:GLY:O	2.18	0.43
6:G:102:VAL:HG13	6:G:106:LEU:HD12	2.00	0.43
10:L:38:VAL:HG11	10:L:59:PRO:HB2	2.00	0.43
18:b:15:GLU:O	18:b:29:ARG:NH2	2.51	0.43
23:K:46:LEU:O	23:K:50:THR:HG23	2.18	0.43
25:P:77:ARG:H	25:P:77:ARG:HG2	1.60	0.43
39:j:13:TYR:HB3	39:j:78:LYS:HG2	2.00	0.43
39:j:140:HIS:CG	39:j:141:ALA:N	2.85	0.43
40:k:112:GLY:HA3	45:k:601:GCP:H8	2.00	0.43
1:2:71:A:H3'	1:2:72:A:H5''	1.99	0.43
1:2:262:C:H2'	1:2:263:G:C8	2.53	0.43
1:2:330:A:H2'	1:2:331:U:C6	2.53	0.43
1:2:705:U:H2'	1:2:706:A:C8	2.45	0.43
2:A:78:SER:OG	2:A:129:ASP:OD1	2.24	0.43
2:A:92:HIS:ND1	2:A:202:TYR:OH	2.49	0.43
7:H:162:ILE:O	7:H:164:ASN:N	2.50	0.43
15:X:48:HIS:HB3	15:X:103:LEU:HD21	2.01	0.43
22:F:100:MET:HE1	22:F:107:GLY:H	1.83	0.43
22:F:119:THR:HG21	22:F:196:LEU:HD22	1.99	0.43
23:K:24:LYS:HG2	23:K:26:ASP:H	1.84	0.43
28:S:132:ARG:HH21	28:S:136:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:104:PHE:CD2	35:g:139:GLY:HA2	2.53	0.43
1:2:67:A:C6	1:2:84:A:C8	3.06	0.43
1:2:328:G:C4	1:2:329:G:C8	3.05	0.43
1:2:987:A:H2'	1:2:988:U:H6	1.82	0.43
1:2:1188:A:H2'	1:2:1193:A:H1'	1.99	0.43
1:2:1240:G:P	1:2:1240:G:H21	2.41	0.43
1:2:1270:G:H5''	34:f:78:LYS:H	1.84	0.43
1:2:1314:U:H1'	27:R:4:VAL:HG21	2.00	0.43
1:2:1386:A:H61	1:2:1407:G:H21	1.66	0.43
1:2:1391:C:H2'	1:2:1392:G:H8	1.83	0.43
12:O:127:ARG:NH1	17:a:22:ARG:HH11	2.16	0.43
14:W:34:ILE:HD12	14:W:34:ILE:H	1.84	0.43
17:a:88:SER:O	17:a:92:ARG:HG3	2.17	0.43
27:R:42:GLN:H	27:R:42:GLN:CD	2.19	0.43
33:d:23:ILE:HG13	33:d:38:ILE:HG23	2.00	0.43
35:g:10:LEU:HD11	35:g:318:ARG:HB3	2.01	0.43
1:2:19:A:H2'	1:2:20:G:H8	1.82	0.43
1:2:57:G:C6	1:2:91:G:N1	2.87	0.43
1:2:476:A:OP1	19:e:31:LYS:N	2.42	0.43
1:2:674:A:H2'	1:2:674:A:N3	2.32	0.43
1:2:687:C:OP1	14:W:119:LYS:HE2	2.18	0.43
1:2:740:A:H2'	1:2:741:C:O4'	2.18	0.43
4:C:106:VAL:HG13	4:C:120:ILE:HG22	2.00	0.43
5:E:36:HIS:HB3	5:E:41:SER:HB3	2.00	0.43
5:E:254:ARG:HB3	5:E:254:ARG:NH1	2.34	0.43
7:H:40:ALA:O	7:H:41:LEU:HD23	2.19	0.43
8:I:189:GLU:OE1	8:I:189:GLU:N	2.33	0.43
15:X:54:LEU:HD12	15:X:73:ARG:HH21	1.83	0.43
16:Y:18:LEU:O	16:Y:20:ARG:HG3	2.18	0.43
21:D:163:PRO:HB3	21:D:167:PHE:CD2	2.53	0.43
28:S:3:LEU:HD22	31:Z:82:HIS:HB3	2.00	0.43
29:T:132:LEU:HA	29:T:135:ILE:HG22	2.01	0.43
33:d:23:ILE:HG12	33:d:38:ILE:HD12	1.99	0.43
1:2:309:C:N3	1:2:356:G:N1	2.67	0.43
1:2:535:C:H3'	1:2:536:G:C8	2.51	0.43
1:2:624:C:H2'	1:2:625:U:H6	1.84	0.43
1:2:778:G:H2'	1:2:779:A:N7	2.33	0.43
1:2:989:C:O3'	12:O:129:LYS:HA	2.18	0.43
1:2:1623:C:H2'	1:2:1624:U:H6	1.82	0.43
2:A:200:ASP:OD2	27:R:89:SER:HA	2.18	0.43
5:E:174:LYS:HD2	5:E:174:LYS:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:13:PHE:HE2	10:L:15:LYS:HB3	1.83	0.43
23:K:14:HIS:CD2	23:K:35:ILE:HG12	2.54	0.43
23:K:60:SER:HB3	23:K:65:TYR:CE2	2.52	0.43
24:M:20:ALA:CB	24:M:123:GLU:HB3	2.48	0.43
27:R:36:ASP:OD1	27:R:47:ARG:HG3	2.18	0.43
30:U:55:PRO:HA	30:U:91:ILE:HG22	2.00	0.43
39:j:18:ASP:OD1	39:j:73:VAL:HB	2.18	0.43
40:k:307:ARG:NH2	40:k:343:LEU:HA	2.33	0.43
40:k:412:LEU:HD23	40:k:415:GLN:OE1	2.18	0.43
1:2:637:U:OP2	14:W:32:LYS:HD3	2.17	0.43
1:2:1145:G:H2'	1:2:1146:A:H8	1.81	0.43
1:2:1613:C:OP2	32:c:47:PRO:HB3	2.18	0.43
2:A:122:ILE:HD13	2:A:144:ILE:HB	1.99	0.43
4:C:178:PRO:HG3	9:J:57:ARG:HD3	2.00	0.43
5:E:242:LYS:HE3	5:E:242:LYS:HB3	1.82	0.43
6:G:152:ASP:OD1	6:G:154:ARG:NH1	2.51	0.43
7:H:66:SER:O	7:H:67:LEU:C	2.61	0.43
8:I:84:HIS:HA	8:I:85:PRO:HD3	1.90	0.43
16:Y:32:ARG:HE	16:Y:35:VAL:HG12	1.84	0.43
22:F:65:GLN:NE2	22:F:68:LYS:H	2.17	0.43
26:Q:58:ASP:N	26:Q:58:ASP:OD1	2.51	0.43
29:T:113:VAL:HG12	29:T:128:GLY:HA2	2.01	0.43
32:c:33:LEU:HD23	32:c:33:LEU:HA	1.93	0.43
34:f:96:LYS:HB2	34:f:96:LYS:HE2	1.88	0.43
35:g:210:GLN:HG3	35:g:250:LEU:HD12	2.01	0.43
1:2:369:A:H3'	1:2:370:G:C8	2.52	0.43
1:2:483:C:H2'	1:2:484:A:C8	2.52	0.43
1:2:1181:U:H4'	25:P:124:THR:OG1	2.19	0.43
1:2:1187:G:O2'	1:2:1428:U:OP1	2.32	0.43
1:2:1196:C:O2'	30:U:73:GLY:O	2.33	0.43
1:2:1293:G:N2	1:2:1302:U:O2	2.45	0.43
1:2:1463:C:OP1	26:Q:139:GLN:NE2	2.52	0.43
1:2:1522:A:N3	1:2:1588:G:O2'	2.42	0.43
1:2:1689:A:H2'	1:2:1690:G:C4	2.54	0.43
2:A:168:HIS:HA	2:A:203:PHE:HE1	1.84	0.43
3:B:58:SER:O	3:B:62:LYS:HG2	2.18	0.43
5:E:181:VAL:HG22	5:E:182:TYR:H	1.84	0.43
9:J:137:GLY:O	9:J:138:LYS:HG2	2.19	0.43
10:L:3:THR:O	10:L:4:GLU:HB2	2.18	0.43
10:L:20:PHE:O	10:L:32:LYS:HE2	2.19	0.43
11:N:69:ASN:OD1	11:N:73:ARG:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:W:32:LYS:HA	14:W:35:ILE:HD12	1.99	0.43
16:Y:20:ARG:HG2	16:Y:76:TYR:CD1	2.54	0.43
17:a:13:LYS:HE2	17:a:13:LYS:HB2	1.85	0.43
22:F:142:SER:OG	22:F:173:SER:HB2	2.18	0.43
28:S:45:LEU:HD12	28:S:45:LEU:HA	1.82	0.43
30:U:60:THR:HG22	30:U:87:HIS:CD2	2.54	0.43
35:g:259:LEU:O	35:g:269:ILE:HD12	2.18	0.43
42:m:30:ILE:HB	42:m:108:PHE:HD2	1.84	0.43
1:2:239:C:H4'	1:2:240:U:OP2	2.19	0.43
1:2:273:G:H2'	1:2:274:C:C6	2.53	0.43
1:2:638:U:OP2	7:H:117:THR:OG1	2.37	0.43
1:2:700:C:H2'	1:2:701:U:C6	2.54	0.43
1:2:833:G:H2'	1:2:834:U:O4'	2.18	0.43
1:2:1200:G:N2	1:2:1598:A:N3	2.66	0.43
1:2:1249:U:O2'	34:f:133:HIS:HA	2.19	0.43
1:2:1304:U:H5''	1:2:1305:C:C5	2.54	0.43
11:N:141:TYR:CE1	11:N:146:ALA:HB2	2.54	0.43
15:X:73:ARG:HG2	15:X:84:THR:HG22	1.99	0.43
17:a:46:GLU:O	17:a:50:ILE:HG23	2.19	0.43
22:F:176:LEU:HG	22:F:212:ALA:HA	2.01	0.43
40:k:437:LEU:HG	40:k:438:ARG:H	1.84	0.43
1:2:14:C:H5''	4:C:208:SER:HB2	2.01	0.43
1:2:72:A:H1'	1:2:73:U:C5	2.54	0.43
1:2:406:A:H2'	1:2:407:C:H6	1.83	0.43
1:2:824:U:H2'	1:2:825:U:C6	2.54	0.43
1:2:1009:C:H2'	1:2:1010:G:O4'	2.19	0.43
1:2:1598:A:OP1	1:2:1598:A:H4'	2.18	0.43
2:A:56:LYS:NZ	13:V:70:ASN:HD21	2.17	0.43
3:B:39:GLU:HB3	3:B:74:GLN:HA	2.00	0.43
3:B:103:MET:O	3:B:215:VAL:N	2.51	0.43
5:E:47:PHE:HD2	5:E:48:LEU:HD22	1.84	0.43
5:E:182:TYR:HD1	5:E:192:VAL:HG22	1.83	0.43
7:H:73:VAL:O	7:H:73:VAL:HG12	2.18	0.43
24:M:121:THR:H	24:M:124:ARG:HD2	1.84	0.43
26:Q:13:LYS:HG2	26:Q:76:SER:HA	1.99	0.43
35:g:85:SER:OG	35:g:87:ASP:OD1	2.29	0.43
36:i:66:ARG:HG3	36:i:67:LYS:H	1.84	0.43
38:1:14:A:H2'	38:1:15:G:C4	2.53	0.43
38:1:60:A:H2'	38:1:61:C:C5	2.53	0.43
39:j:230:LEU:HD11	39:j:244:LEU:HG	2.01	0.43
1:2:18:C:C2	1:2:19:A:C8	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:697:C:H3'	7:H:105:LYS:NZ	2.32	0.43
1:2:697:C:H5''	7:H:105:LYS:NZ	2.34	0.43
1:2:975:G:N2	1:2:1023:U:OP2	2.51	0.43
1:2:1343:A:H4'	1:2:1344:A:OP1	2.19	0.43
1:2:1482:G:H2'	1:2:1483:C:C6	2.53	0.43
1:2:1617:C:O2	32:c:22:ARG:NH1	2.52	0.43
1:2:1771:C:H2'	1:2:1772:G:C8	2.52	0.43
2:A:92:HIS:CE1	2:A:202:TYR:HH	2.36	0.43
7:H:48:GLU:OE2	7:H:57:ALA:N	2.52	0.43
12:O:17:ALA:HB3	12:O:81:ILE:HG12	2.01	0.43
21:D:40:ARG:HD3	21:D:49:ILE:HD11	2.00	0.43
29:T:4:VAL:HG11	29:T:137:ALA:HB2	2.01	0.43
1:2:40:A:H3'	1:2:41:A:H8	1.84	0.42
1:2:86:A:H2'	1:2:87:C:C6	2.54	0.42
1:2:269:C:H2'	1:2:270:A:H8	1.83	0.42
1:2:522:G:N1	1:2:527:U:OP2	2.42	0.42
1:2:653:C:H2'	1:2:654:G:C8	2.54	0.42
1:2:862:A:P	14:W:57:ARG:HH21	2.40	0.42
1:2:874:G:OP1	3:B:158:SER:N	2.42	0.42
1:2:1557:A:C5	28:S:134:ARG:HD2	2.54	0.42
4:C:233:ASN:HB2	13:V:1:MET:HE2	2.01	0.42
9:J:42:ILE:HA	9:J:45:ILE:HG22	2.01	0.42
12:O:92:LYS:HB3	17:a:69:ASN:HD21	1.82	0.42
16:Y:36:SER:O	16:Y:36:SER:OG	2.31	0.42
22:F:151:VAL:HG12	22:F:160:GLN:HE21	1.83	0.42
38:1:9:1MG:OP2	38:1:46:7MG:H1'	2.19	0.42
42:m:62:PHE:CD2	42:m:80:LEU:HD13	2.54	0.42
1:2:157:U:C4	1:2:419:A:H4'	2.55	0.42
1:2:472:A:OP1	9:J:44:ARG:NE	2.52	0.42
1:2:870:G:C6	1:2:956:G:N1	2.87	0.42
1:2:947:G:H2'	1:2:948:C:H6	1.85	0.42
1:2:1064:A:OP1	3:B:160:HIS:NE2	2.52	0.42
1:2:1144:U:H2'	1:2:1145:G:H8	1.85	0.42
1:2:1241:A:H4'	25:P:52:LYS:HZ2	1.84	0.42
1:2:1456:G:H21	25:P:126:VAL:HG11	1.83	0.42
1:2:1683:G:C6	1:2:1715:G:C6	3.07	0.42
4:C:85:VAL:HG21	4:C:88:ILE:HD11	2.02	0.42
6:G:32:ILE:HD13	6:G:52:ILE:HG12	2.01	0.42
6:G:49:VAL:HG12	6:G:115:LYS:HB3	2.01	0.42
10:L:71:LEU:HD12	10:L:137:PHE:HE2	1.84	0.42
11:N:86:GLU:OE1	11:N:86:GLU:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:99:ARG:HG2	11:N:115:LEU:HD11	2.01	0.42
12:O:42:VAL:HG23	12:O:46:MET:HG3	2.01	0.42
12:O:135:ARG:HG2	12:O:137:LEU:HD23	2.00	0.42
15:X:141:GLU:HA	15:X:141:GLU:OE1	2.18	0.42
21:D:56:GLN:H	21:D:56:GLN:CD	2.27	0.42
22:F:39:GLN:OE1	22:F:39:GLN:N	2.52	0.42
22:F:219:LEU:HA	22:F:222:VAL:HG12	2.00	0.42
23:K:69:THR:HG23	23:K:72:GLY:H	1.85	0.42
23:K:69:THR:O	23:K:73:VAL:HG23	2.19	0.42
26:Q:82:ARG:HH12	26:Q:116:LEU:HD23	1.84	0.42
33:d:21:CYS:C	33:d:23:ILE:N	2.76	0.42
35:g:156:ARG:HD3	35:g:210:GLN:CB	2.48	0.42
1:2:199:A:H2'	1:2:200:G:H8	1.85	0.42
1:2:313:C:N3	1:2:354:G:C6	2.88	0.42
1:2:414:C:H2'	1:2:416:A:C5	2.54	0.42
1:2:433:G:N2	1:2:435:A:H3'	2.34	0.42
1:2:454:C:H3'	1:2:455:A:H8	1.84	0.42
1:2:871:G:N2	1:2:1046:G:H4'	2.35	0.42
1:2:1019:A:H2'	1:2:1020:C:O4'	2.19	0.42
1:2:1594:C:OP1	33:d:16:LYS:NZ	2.46	0.42
1:2:1667:U:H2'	1:2:1668:G:O4'	2.19	0.42
1:2:1671:G:H2'	1:2:1672:C:H6	1.85	0.42
2:A:166:GLY:C	2:A:168:HIS:H	2.26	0.42
10:L:109:ALA:HA	10:L:135:VAL:HG23	2.00	0.42
12:O:29:HIS:CD2	12:O:41:ARG:HG2	2.55	0.42
12:O:132:ARG:HD2	17:a:29:SER:OG	2.19	0.42
13:V:68:SER:O	13:V:72:LEU:HD23	2.20	0.42
23:K:52:LYS:HB3	23:K:54:PHE:CE2	2.54	0.42
24:M:54:VAL:HB	24:M:112:VAL:HG23	2.00	0.42
24:M:97:ILE:HG23	24:M:101:GLY:HA2	2.00	0.42
26:Q:31:VAL:HG12	26:Q:67:VAL:HB	2.02	0.42
35:g:208:VAL:HG21	35:g:250:LEU:H	1.84	0.42
35:g:253:SER:HB2	35:g:256:ARG:O	2.19	0.42
35:g:254:PRO:HG2	35:g:302:SER:O	2.20	0.42
36:i:63:GLY:C	36:i:65:LEU:H	2.26	0.42
38:1:27:C:H2'	38:1:28:A:C8	2.55	0.42
39:j:10:GLU:OE1	39:j:136:ARG:NH2	2.52	0.42
1:2:434:C:H2'	1:2:435:A:O4'	2.19	0.42
1:2:514:A:H62	1:2:536:G:H21	1.66	0.42
1:2:564:C:H4'	1:2:565:C:C5	2.53	0.42
1:2:608:U:O2'	15:X:23:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:884:G:N2	12:O:123:SER:OG	2.52	0.42
1:2:977:A:H2'	1:2:978:A:O4'	2.20	0.42
1:2:1282:U:OP2	1:2:1283:C:O2'	2.26	0.42
1:2:1293:G:H2'	1:2:1294:G:C8	2.55	0.42
1:2:1586:G:H1	1:2:1606:U:H3	1.66	0.42
1:2:1595:A:C8	33:d:14:PHE:CD2	3.07	0.42
3:B:38:PHE:HB3	3:B:73:LEU:HD12	2.00	0.42
5:E:107:GLY:HA2	5:E:189:LEU:HD22	2.01	0.42
5:E:155:LYS:HA	5:E:155:LYS:HD3	1.88	0.42
5:E:159:THR:OG1	5:E:227:VAL:HB	2.20	0.42
6:G:149:LYS:HD3	6:G:149:LYS:HA	1.35	0.42
9:J:16:LYS:C	9:J:18:PRO:HD3	2.42	0.42
11:N:46:THR:OG1	11:N:49:GLN:HG3	2.19	0.42
14:W:90:THR:OG1	14:W:94:LEU:HD12	2.19	0.42
22:F:175:ALA:HA	22:F:178:THR:HG22	2.02	0.42
33:d:33:LYS:O	33:d:36:LEU:HD23	2.20	0.42
35:g:185:SER:O	35:g:196:GLU:HB3	2.18	0.42
38:1:15:G:N1	38:1:48:5MC:N4	2.67	0.42
39:j:14:PRO:O	39:j:78:LYS:NZ	2.39	0.42
39:j:218:VAL:O	39:j:219:LYS:HE2	2.18	0.42
40:k:292:ASP:N	40:k:292:ASP:OD1	2.52	0.42
1:2:387:G:O6	1:2:409:A:N6	2.52	0.42
1:2:1003:U:H5'	1:2:1004:A:H5''	2.02	0.42
1:2:1173:C:O2'	1:2:1195:A:N6	2.51	0.42
1:2:1389:A:H2'	1:2:1390:U:H6	1.82	0.42
1:2:1563:C:H4'	28:S:85:PHE:HA	2.01	0.42
1:2:1582:G:H22	1:2:1609:A:P	2.43	0.42
2:A:56:LYS:HD3	2:A:161:PRO:HD3	2.01	0.42
2:A:93:THR:HG23	2:A:95:ALA:H	1.83	0.42
3:B:129:THR:HA	3:B:176:VAL:HG12	2.00	0.42
4:C:54:LYS:HE3	4:C:251:TYR:CE2	2.54	0.42
6:G:7:TYR:HA	6:G:8:PRO:HD3	1.91	0.42
9:J:170:GLY:H	9:J:174:ARG:HG3	1.85	0.42
17:a:70:LYS:HE2	17:a:72:HIS:HE1	1.83	0.42
21:D:71:LEU:HD13	23:K:90:THR:HG22	2.01	0.42
22:F:107:GLY:HA2	22:F:109:LYS:HZ2	1.84	0.42
23:K:32:HIS:N	23:K:37:THR:O	2.34	0.42
23:K:62:GLN:NE2	33:d:23:ILE:O	2.38	0.42
29:T:115:GLU:O	29:T:122:ARG:HA	2.20	0.42
31:Z:52:LYS:O	31:Z:55:PRO:HD2	2.18	0.42
34:f:138:TYR:OH	34:f:143:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:189:GLU:HG2	39:j:227:LEU:HD23	2.02	0.42
1:2:164:G:H2'	1:2:165:C:H6	1.85	0.42
1:2:512:U:O2'	1:2:513:G:O4'	2.27	0.42
1:2:775:G:H2'	1:2:776:G:H8	1.85	0.42
1:2:810:A:N6	7:H:113:PRO:HD3	2.34	0.42
1:2:894:G:H1'	12:O:36:ARG:O	2.20	0.42
1:2:1040:G:H2'	1:2:1041:G:H8	1.84	0.42
1:2:1561:C:H2'	1:2:1562:U:H6	1.85	0.42
2:A:59:LEU:HD22	13:V:79:LEU:HD11	2.00	0.42
2:A:84:ARG:HA	2:A:87:LEU:HD12	2.01	0.42
5:E:206:ASP:OD2	5:E:222:LEU:HD13	2.20	0.42
8:I:173:ARG:HE	8:I:176:GLN:HG3	1.84	0.42
11:N:4:MET:SD	11:N:5:HIS:CD2	3.13	0.42
23:K:32:HIS:HD1	23:K:35:ILE:HB	1.84	0.42
36:i:64:LYS:C	36:i:65:LEU:HD12	2.44	0.42
38:1:9:1MG:O3'	38:1:45:U:O2'	2.37	0.42
40:k:108:HIS:CE1	40:k:227:PRO:HD2	2.55	0.42
42:m:89:CYS:O	42:m:92:MET:HG2	2.20	0.42
1:2:212:A:H2'	1:2:213:G:O4'	2.19	0.42
1:2:269:C:H2'	1:2:270:A:C8	2.54	0.42
1:2:633:G:C6	1:2:965:A:N6	2.88	0.42
1:2:811:A:N6	1:2:857:G:H2'	2.35	0.42
1:2:932:A:C5	1:2:934:U:C2	3.08	0.42
1:2:940:A:O2'	1:2:976:A:O4'	2.30	0.42
1:2:1295:A:OP1	2:A:138:TYR:OH	2.28	0.42
1:2:1386:A:C6	1:2:1409:A:N7	2.88	0.42
1:2:1424:C:H3'	1:2:1425:A:H4'	2.01	0.42
1:2:1486:G:H3'	1:2:1513:A:N6	2.31	0.42
1:2:1751:A:H2'	1:2:1752:A:O4'	2.20	0.42
4:C:247:VAL:HG23	4:C:248:TYR:HD2	1.84	0.42
29:T:65:ILE:HG12	29:T:71:VAL:HG22	2.02	0.42
30:U:68:ARG:NH1	30:U:78:THR:H	2.18	0.42
32:c:10:ALA:HB2	32:c:32:PHE:CD1	2.54	0.42
39:j:115:CYS:SG	39:j:165:VAL:HB	2.59	0.42
40:k:313:PRO:HA	40:k:344:ASN:O	2.20	0.42
40:k:428:THR:HG22	40:k:490:PRO:HB3	2.01	0.42
42:m:62:PHE:HD2	42:m:80:LEU:HD13	1.84	0.42
42:m:89:CYS:HA	42:m:92:MET:SD	2.60	0.42
1:2:447:C:O5'	5:E:29:PRO:HG3	2.19	0.42
1:2:523:U:H1'	1:2:526:A:N7	2.34	0.42
1:2:640:G:H2'	1:2:641:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:928:A:H3'	1:2:929:A:H8	1.84	0.42
1:2:947:G:H2'	1:2:948:C:C6	2.55	0.42
1:2:995:U:H2'	1:2:996:G:C8	2.54	0.42
1:2:1252:U:C2	1:2:1253:U:C5	3.07	0.42
1:2:1527:C:H2'	1:2:1528:C:C6	2.54	0.42
1:2:1575:A:H2'	1:2:1576:U:O4'	2.20	0.42
3:B:103:MET:HE1	3:B:188:LEU:HB3	2.00	0.42
5:E:71:LYS:HG2	5:E:74:GLY:H	1.85	0.42
5:E:102:VAL:HG23	5:E:239:PRO:HG3	2.01	0.42
5:E:208:VAL:CG2	5:E:225:VAL:HG21	2.45	0.42
6:G:27:PHE:CE1	6:G:36:VAL:HG11	2.54	0.42
6:G:148:THR:HG22	6:G:150:GLU:H	1.84	0.42
22:F:105:ASN:O	22:F:106:ASN:C	2.61	0.42
26:Q:3:THR:HB	26:Q:4:VAL:H	1.68	0.42
30:U:30:LYS:HD2	30:U:33:GLN:HG3	2.01	0.42
38:l:18:G:N1	39:j:110:SER:HB2	2.34	0.42
40:k:200:LEU:HD11	40:k:203:THR:HG23	2.02	0.42
40:k:357:PRO:HD3	40:k:416:VAL:O	2.20	0.42
1:2:157:U:O2'	1:2:158:U:H5'	2.20	0.42
1:2:384:A:H2'	1:2:385:G:C8	2.54	0.42
1:2:525:A:OP1	16:Y:93:ARG:NE	2.50	0.42
1:2:624:C:H2'	1:2:625:U:C6	2.55	0.42
1:2:760:A:C2	1:2:761:G:H1'	2.55	0.42
1:2:978:A:H4'	1:2:1784:G:N2	2.35	0.42
1:2:1046:G:H2'	1:2:1047:G:C8	2.55	0.42
2:A:122:ILE:HG21	2:A:174:TRP:CH2	2.55	0.42
3:B:61:LEU:HA	3:B:64:ARG:HH11	1.85	0.42
4:C:127:ALA:O	4:C:131:ARG:HG3	2.20	0.42
5:E:71:LYS:HG3	5:E:75:LYS:O	2.20	0.42
6:G:7:TYR:HD1	6:G:10:ASN:H	1.65	0.42
14:W:25:VAL:CG2	14:W:63:VAL:HB	2.48	0.42
15:X:131:SER:O	15:X:135:LEU:HG	2.20	0.42
16:Y:57:VAL:HB	16:Y:60:PHE:HE2	1.85	0.42
21:D:46:THR:O	21:D:84:ILE:HG23	2.19	0.42
21:D:72:LEU:HD12	23:K:65:TYR:HD1	1.85	0.42
32:c:10:ALA:HB1	32:c:30:VAL:HB	2.02	0.42
1:2:410:C:H2'	1:2:411:A:O4'	2.19	0.42
1:2:646:G:C6	1:2:688:G:C6	3.08	0.42
1:2:996:G:H2'	1:2:997:A:H8	1.84	0.42
1:2:1167:U:C2	1:2:1168:G:C8	3.08	0.42
1:2:1228:G:H21	1:2:1255:A:H62	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1240:G:C2	25:P:79:HIS:CE1	3.08	0.42
1:2:1262:G:H2'	1:2:1263:G:O4'	2.19	0.42
1:2:1497:G:H2'	1:2:1498:C:H6	1.85	0.42
1:2:1749:C:H2'	1:2:1750:U:C6	2.55	0.42
3:B:187:LYS:HG2	3:B:193:ILE:HD11	2.02	0.42
3:B:213:ARG:HD2	3:B:214:LYS:CB	2.50	0.42
7:H:75:ILE:HG13	7:H:76:LYS:N	2.35	0.42
8:I:196:ARG:O	8:I:200:LYS:HG2	2.20	0.42
14:W:37:PHE:CD1	14:W:103:ILE:HG21	2.55	0.42
14:W:50:PHE:HB2	14:W:63:VAL:HG22	2.01	0.42
22:F:93:GLU:O	22:F:96:THR:OG1	2.27	0.42
26:Q:127:LYS:HG2	26:Q:128:LYS:N	2.35	0.42
29:T:12:GLN:HA	29:T:15:ILE:HG22	2.02	0.42
30:U:80:ASP:HB2	33:d:54:LYS:HZ1	1.82	0.42
32:c:10:ALA:HB2	32:c:32:PHE:HD1	1.85	0.42
39:j:147:LEU:HA	39:j:150:ILE:HG12	2.01	0.42
1:2:443:C:H6	16:Y:105:ARG:NH1	2.18	0.41
1:2:594:G:H2'	1:2:595:C:H6	1.85	0.41
1:2:690:A:H2'	1:2:691:U:O4'	2.20	0.41
1:2:760:A:N1	1:2:788:A:N6	2.67	0.41
1:2:780:A:H4'	1:2:781:A:C5	2.55	0.41
1:2:1482:G:H1	1:2:1589:C:H1'	1.85	0.41
1:2:1493:C:O2'	1:2:1517:U:O2	2.31	0.41
1:2:1656:G:C6	1:2:1742:A:C6	3.08	0.41
1:2:1777:U:H2'	1:2:1779:A:OP2	2.20	0.41
7:H:130:VAL:HG22	7:H:169:PHE:CE1	2.54	0.41
10:L:7:VAL:C	10:L:9:SER:N	2.78	0.41
17:a:23:CYS:HB2	17:a:74:CYS:HB3	2.01	0.41
21:D:6:SER:O	21:D:10:LYS:N	2.50	0.41
22:F:72:VAL:HG11	26:Q:44:LEU:HD23	2.02	0.41
24:M:94:LEU:HB3	24:M:107:VAL:HG21	2.02	0.41
27:R:36:ASP:HB2	27:R:47:ARG:HH11	1.83	0.41
31:Z:38:HIS:HB3	31:Z:72:GLY:HA2	2.01	0.41
33:d:42:SER:O	33:d:46:LYS:HG2	2.20	0.41
38:1:22:G:H2'	38:1:22:G:N3	2.35	0.41
1:2:129:U:H5'	1:2:263:G:N2	2.34	0.41
1:2:392:C:H2'	1:2:393:C:C6	2.54	0.41
1:2:457:G:OP2	16:Y:105:ARG:NH2	2.52	0.41
1:2:1024:A:H2'	1:2:1026:A:OP1	2.20	0.41
1:2:1101:G:H2'	1:2:1102:U:O4'	2.20	0.41
1:2:1233:A:O2'	34:f:143:HIS:ND1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1340:A:O2'	35:g:103:ARG:NH2	2.53	0.41
1:2:1548:A:H2'	1:2:1549:U:C6	2.55	0.41
1:2:1588:G:H5'	29:T:91:HIS:O	2.20	0.41
2:A:162:CYS:SG	2:A:169:SER:OG	2.58	0.41
4:C:150:GLY:HA2	14:W:98:GLN:NE2	2.34	0.41
4:C:191:LYS:HE2	4:C:191:LYS:HB2	1.85	0.41
5:E:88:ASP:HA	5:E:122:LYS:HE3	2.02	0.41
5:E:128:LYS:HB3	5:E:140:VAL:HB	2.02	0.41
5:E:198:ARG:HE	5:E:200:ARG:CZ	2.33	0.41
10:L:17:PRO:O	10:L:19:ILE:HD12	2.20	0.41
13:V:12:TYR:CD2	13:V:12:TYR:O	2.73	0.41
21:D:70:THR:O	21:D:73:ILE:HG12	2.19	0.41
22:F:119:THR:HG21	22:F:196:LEU:CD2	2.51	0.41
27:R:20:TYR:CD2	27:R:38:ILE:HD12	2.55	0.41
28:S:106:GLU:O	28:S:110:ARG:HG3	2.20	0.41
34:f:104:ASN:O	34:f:117:LEU:HD22	2.20	0.41
35:g:72:VAL:HG22	35:g:83:SER:HA	2.01	0.41
39:j:24:VAL:HB	39:j:65:VAL:HA	2.01	0.41
40:k:330:ILE:H	40:k:330:ILE:HD12	1.85	0.41
40:k:357:PRO:HG2	40:k:415:GLN:HG2	2.01	0.41
1:2:103:A:H4'	1:2:105:A:C8	2.55	0.41
1:2:119:A:H1'	1:2:396:A:C5	2.56	0.41
1:2:1182:A:C2	1:2:1209:C:H1'	2.55	0.41
1:2:1248:U:H3'	1:2:1249:U:C6	2.56	0.41
1:2:1312:A:N6	27:R:4:VAL:HG22	2.35	0.41
1:2:1607:U:H5''	26:Q:75:VAL:HG22	2.02	0.41
2:A:179:ARG:HD3	2:A:183:ARG:CZ	2.51	0.41
5:E:57:ASN:OD1	5:E:58:GLY:N	2.52	0.41
5:E:95:THR:OG1	5:E:97:GLU:HG3	2.20	0.41
7:H:162:ILE:C	7:H:164:ASN:H	2.28	0.41
9:J:143:ILE:HG23	9:J:146:PHE:HB2	2.02	0.41
12:O:58:TYR:CZ	22:F:227:ARG:HG3	2.55	0.41
14:W:30:SER:HB2	14:W:61:ILE:HG13	2.01	0.41
15:X:61:SER:OG	15:X:62:LYS:N	2.54	0.41
21:D:75:LYS:NZ	23:K:20:VAL:O	2.53	0.41
21:D:105:MET:HE2	21:D:105:MET:HB2	1.95	0.41
21:D:134:CYS:SG	21:D:135:GLU:N	2.92	0.41
22:F:103:GLY:HA3	22:F:106:ASN:CB	2.48	0.41
22:F:147:ASP:CG	22:F:148:THR:H	2.24	0.41
23:K:54:PHE:O	23:K:69:THR:HG22	2.20	0.41
27:R:105:GLN:O	27:R:109:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1:25:C:C2	38:1:26:M2G:C8	3.08	0.41
38:1:49:5MC:HN41	38:1:65:G:H1	1.68	0.41
39:j:198:ILE:HD11	40:k:403:ASP:HA	2.02	0.41
40:k:126:VAL:HG12	40:k:128:PHE:HB3	2.03	0.41
1:2:392:C:OP2	8:I:2:GLY:N	2.53	0.41
1:2:473:A:N6	1:2:593:A:H5'	2.35	0.41
1:2:902:U:O2'	1:2:904:A:N7	2.47	0.41
1:2:1222:A:C4	1:2:1223:A:C8	3.08	0.41
2:A:74:VAL:HG22	2:A:96:THR:HB	2.03	0.41
3:B:166:LYS:O	3:B:170:GLU:OE1	2.39	0.41
3:B:185:THR:HA	3:B:188:LEU:HD12	2.01	0.41
5:E:7:LYS:O	5:E:7:LYS:HD3	2.20	0.41
6:G:142:ARG:NE	6:G:153:VAL:HB	2.35	0.41
6:G:195:ILE:HD13	6:G:195:ILE:HA	1.94	0.41
9:J:80:LEU:HA	9:J:83:ILE:HG22	2.01	0.41
16:Y:57:VAL:O	16:Y:94:TYR:OH	2.37	0.41
18:b:47:PHE:HE2	18:b:49:HIS:HB2	1.86	0.41
33:d:21:CYS:HB3	33:d:25:GLY:H	1.85	0.41
35:g:48:LEU:HD21	35:g:309:PHE:HZ	1.85	0.41
39:j:166:LEU:O	39:j:170:LYS:HG3	2.20	0.41
40:k:337:VAL:HG12	40:k:399:GLY:HA3	2.03	0.41
40:k:440:LEU:HD12	40:k:451:ALA:H	1.84	0.41
1:2:388:G:H2'	1:2:389:G:O4'	2.20	0.41
1:2:414:C:O2'	1:2:417:G:O6	2.35	0.41
1:2:716:C:N4	1:2:723:G:N3	2.69	0.41
1:2:736:C:O2'	1:2:737:A:O5'	2.38	0.41
1:2:1733:U:H2'	1:2:1734:G:H8	1.82	0.41
5:E:103:TYR:N	5:E:182:TYR:OH	2.51	0.41
7:H:96:ARG:HH11	7:H:97:ARG:H	1.69	0.41
15:X:70:LYS:CG	15:X:93:LEU:HD22	2.49	0.41
40:k:307:ARG:HB3	40:k:392:PRO:HG2	2.03	0.41
40:k:493:THR:HA	40:k:497:GLU:OE1	2.20	0.41
1:2:106:U:H2'	1:2:107:C:O4'	2.20	0.41
1:2:210:U:H5''	10:L:20:PHE:CE2	2.56	0.41
1:2:945:U:H5''	3:B:165:ARG:CZ	2.51	0.41
1:2:1155:C:H2'	1:2:1156:A:H8	1.86	0.41
1:2:1650:C:H2'	1:2:1651:C:H6	1.86	0.41
4:C:134:ILE:HD13	4:C:134:ILE:HA	1.90	0.41
11:N:102:LEU:HD21	11:N:112:LYS:HA	2.02	0.41
18:b:7:LEU:O	18:b:24:LEU:HD11	2.21	0.41
18:b:14:SER:HA	18:b:17:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:33:PHE:CE2	25:P:37:ALA:HB2	2.55	0.41
28:S:86:LEU:HA	28:S:99:HIS:ND1	2.35	0.41
28:S:110:ARG:HB3	28:S:110:ARG:HH11	1.85	0.41
33:d:30:LEU:HD11	33:d:37:ASN:C	2.45	0.41
35:g:104:PHE:HB3	35:g:135:TRP:CE3	2.56	0.41
36:i:97:LEU:HD12	36:i:101:ARG:HH21	1.85	0.41
39:j:50:GLU:HG2	39:j:86:SER:HB2	2.02	0.41
40:k:337:VAL:HG12	40:k:399:GLY:CA	2.51	0.41
1:2:126:A:N1	1:2:262:C:O2'	2.50	0.41
1:2:373:U:H2'	1:2:374:U:H6	1.86	0.41
1:2:623:G:H2'	1:2:624:C:H6	1.86	0.41
1:2:643:U:H2'	1:2:644:C:C6	2.54	0.41
1:2:691:U:H5'	1:2:692:C:OP2	2.21	0.41
1:2:743:U:OP1	7:H:108:GLN:N	2.53	0.41
1:2:819:U:H2'	1:2:820:U:O3'	2.21	0.41
1:2:899:A:O2'	1:2:915:U:O2'	2.35	0.41
1:2:1315:G:OP1	27:R:6:THR:OG1	2.32	0.41
1:2:1373:U:H2'	1:2:1374:C:C6	2.55	0.41
1:2:1540:G:O3'	1:2:1541:A:H8	2.04	0.41
4:C:125:GLU:OE1	21:D:120:TYR:OH	2.32	0.41
6:G:9:ILE:H	6:G:9:ILE:HD12	1.85	0.41
7:H:168:SER:O	7:H:172:VAL:HG23	2.20	0.41
8:I:172:SER:OG	8:I:181:ASP:HB2	2.19	0.41
9:J:38:ASN:CG	9:J:39:LYS:H	2.28	0.41
22:F:211:TYR:HE1	22:F:215:LYS:HE2	1.85	0.41
26:Q:6:SER:HB3	26:Q:23:LYS:HG2	2.03	0.41
26:Q:94:GLN:HG2	26:Q:99:GLU:HG3	2.01	0.41
28:S:50:ALA:HB1	28:S:68:ARG:HH21	1.85	0.41
35:g:208:VAL:HG21	35:g:249:ALA:HA	2.01	0.41
35:g:275:GLU:O	35:g:275:GLU:CD	2.64	0.41
38:1:53:G:H2'	38:1:54:A:H8	1.85	0.41
39:j:21:MET:HG2	39:j:70:VAL:HA	2.02	0.41
1:2:985:G:H3'	1:2:986:G:H8	1.84	0.41
1:2:1182:A:H2	1:2:1209:C:H1'	1.86	0.41
1:2:1309:U:O2'	1:2:1400:G:O2'	2.38	0.41
1:2:1386:A:H4'	1:2:1387:C:O4'	2.20	0.41
1:2:1531:C:P	31:Z:74:SER:HB2	2.60	0.41
1:2:1678:G:N2	1:2:1718:G:H2'	2.35	0.41
3:B:57:ALA:O	3:B:61:LEU:HD23	2.21	0.41
3:B:170:GLU:O	3:B:174:ARG:HG3	2.21	0.41
6:G:5:ILE:HD13	6:G:111:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:35:LYS:C	7:H:37:ASP:H	2.29	0.41
13:V:24:ILE:HD12	13:V:31:SER:OG	2.21	0.41
13:V:55:LEU:HD23	13:V:65:ALA:HB1	2.03	0.41
15:X:107:PHE:CD1	15:X:123:LYS:HG3	2.55	0.41
15:X:125:VAL:C	15:X:132:LEU:HD23	2.46	0.41
26:Q:40:GLN:O	26:Q:42:GLU:N	2.53	0.41
28:S:27:ASN:O	28:S:31:ALA:N	2.54	0.41
28:S:29:VAL:HG11	28:S:44:ASN:HA	2.03	0.41
34:f:139:CYS:HB3	34:f:143:HIS:HA	2.02	0.41
36:i:33:GLN:HG3	36:i:78:LEU:HD11	2.03	0.41
38:1:47:H2U:H2'	38:1:50:U:P	2.60	0.41
40:k:116:VAL:HG21	40:k:249:ASN:OD1	2.20	0.41
1:2:32:U:O2'	1:2:593:A:N1	2.50	0.41
1:2:194:G:O2'	1:2:195:G:H5'	2.21	0.41
1:2:248:U:H3'	1:2:249:C:H5'	2.02	0.41
1:2:279:U:H1'	1:2:280:G:OP2	2.20	0.41
1:2:374:U:H2'	1:2:375:C:C6	2.55	0.41
1:2:442:C:P	16:Y:105:ARG:HG3	2.61	0.41
1:2:502:G:H2'	1:2:503:U:C6	2.56	0.41
1:2:517:A:H2'	1:2:518:C:H5''	2.02	0.41
1:2:552:G:H2'	1:2:553:C:C6	2.55	0.41
1:2:744:U:H2'	1:2:745:U:O4'	2.21	0.41
1:2:769:A:H2'	1:2:770:A:H8	1.85	0.41
1:2:878:G:H2'	1:2:879:C:C6	2.56	0.41
1:2:1163:G:P	22:F:168:ARG:HH22	2.43	0.41
1:2:1172:C:N3	1:2:1173:C:C4	2.89	0.41
1:2:1205:U:OP2	1:2:1206:C:O2'	2.38	0.41
1:2:1467:A:H2'	1:2:1468:C:H6	1.86	0.41
1:2:1521:G:N7	29:T:68:ARG:NH2	2.68	0.41
1:2:1552:U:H2'	1:2:1553:A:O4'	2.20	0.41
1:2:1568:A:H2'	1:2:1569:C:O4'	2.21	0.41
1:2:1760:A:C2	1:2:1761:A:C8	3.09	0.41
2:A:53:THR:O	2:A:57:ILE:HG13	2.20	0.41
2:A:55:GLU:O	2:A:58:VAL:HG12	2.21	0.41
2:A:129:ASP:HB3	2:A:132:ALA:HB3	2.03	0.41
2:A:157:ASP:O	2:A:158:VAL:C	2.64	0.41
3:B:157:GLN:O	3:B:161:ILE:HD12	2.21	0.41
4:C:185:ALA:HB1	4:C:189:VAL:HB	2.02	0.41
4:C:227:TYR:OH	13:V:10:GLU:OE1	2.39	0.41
5:E:194:THR:N	5:E:211:LYS:O	2.53	0.41
7:H:162:ILE:HG23	7:H:165:LYS:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:64:GLU:HG2	9:J:69:ARG:NH1	2.36	0.41
9:J:127:VAL:O	9:J:131:GLN:N	2.51	0.41
14:W:11:LEU:HA	14:W:11:LEU:HD13	1.91	0.41
14:W:36:LYS:O	14:W:40:VAL:HG23	2.21	0.41
15:X:93:LEU:HD12	15:X:96:VAL:HG21	2.03	0.41
18:b:30:SER:HB2	18:b:49:HIS:ND1	2.36	0.41
21:D:17:PHE:HE2	21:D:39:VAL:HG11	1.85	0.41
21:D:24:PHE:HD2	21:D:25:PHE:HD1	1.68	0.41
23:K:18:GLU:HG2	23:K:19:GLY:N	2.36	0.41
25:P:75:VAL:HG22	25:P:93:VAL:HG12	2.03	0.41
28:S:56:LYS:HD3	28:S:56:LYS:C	2.46	0.41
30:U:63:LEU:HA	30:U:63:LEU:HD12	1.82	0.41
35:g:36:SER:O	35:g:43:LEU:HA	2.20	0.41
35:g:68:ILE:HB	35:g:86:TRP:CE3	2.55	0.41
35:g:115:ALA:HB3	35:g:124:ILE:HD11	2.02	0.41
38:l:10:2MG:HM23	38:l:11:C:H1'	2.02	0.41
39:j:218:VAL:N	39:j:232:THR:HG23	2.36	0.41
1:2:54:C:O3'	16:Y:109:LYS:HD3	2.21	0.41
1:2:72:A:H1'	1:2:73:U:C4	2.55	0.41
1:2:114:C:N4	1:2:246:A:N7	2.69	0.41
1:2:613:C:H2'	1:2:614:A:H8	1.86	0.41
1:2:756:A:C4	1:2:757:A:C8	3.09	0.41
1:2:880:A:N1	1:2:947:G:C6	2.89	0.41
1:2:1244:G:H4'	1:2:1245:C:H5'	2.03	0.41
1:2:1408:A:H3'	26:Q:118:ILE:HD11	2.03	0.41
1:2:1423:A:H2'	1:2:1424:C:C6	2.56	0.41
1:2:1513:A:OP2	21:D:7:LYS:HG3	2.20	0.41
3:B:93:GLY:C	3:B:95:ASN:H	2.29	0.41
3:B:129:THR:HG23	3:B:131:ASP:H	1.85	0.41
4:C:238:GLN:HG3	4:C:239:ALA:N	2.36	0.41
5:E:36:HIS:CG	5:E:85:GLY:HA3	2.55	0.41
7:H:4:PRO:HA	7:H:7:LYS:NZ	2.36	0.41
7:H:98:ILE:HG22	7:H:121:VAL:HG11	2.03	0.41
8:I:43:ILE:HD12	8:I:56:ARG:O	2.21	0.41
8:I:196:ARG:O	8:I:199:ALA:HB3	2.21	0.41
10:L:132:SER:OG	10:L:133:LYS:N	2.54	0.41
12:O:63:ALA:O	12:O:67:VAL:HG23	2.21	0.41
13:V:74:GLN:HE22	13:V:81:ASN:H	1.67	0.41
16:Y:76:TYR:CE2	16:Y:82:ALA:HA	2.55	0.41
16:Y:104:SER:OG	16:Y:107:GLN:HG2	2.21	0.41
21:D:114:ALA:HB3	21:D:117:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:57:ARG:HD3	28:S:57:ARG:HA	1.94	0.41
30:U:26:LEU:O	30:U:88:LYS:HA	2.21	0.41
30:U:42:ILE:O	30:U:46:GLU:HG2	2.21	0.41
31:Z:46:LYS:O	31:Z:50:ILE:HG13	2.21	0.41
39:j:33:TYR:HA	39:j:45:MET:HA	2.03	0.41
39:j:55:ARG:NH2	39:j:57:ARG:HH11	2.20	0.41
39:j:195:TYR:CE1	40:k:373:ILE:HA	2.55	0.41
1:2:325:G:N1	1:2:342:C:N3	2.68	0.40
1:2:326:U:O4	1:2:327:A:N6	2.54	0.40
1:2:342:C:C2	1:2:343:A:C8	3.10	0.40
1:2:454:C:H3'	1:2:455:A:C8	2.55	0.40
1:2:521:U:H2'	1:2:522:G:O4'	2.21	0.40
1:2:567:G:H4'	15:X:90:ASP:OD1	2.20	0.40
1:2:917:U:O3'	12:O:18:ARG:NH1	2.53	0.40
1:2:1115:A:H2'	1:2:1116:U:O4'	2.21	0.40
1:2:1135:U:OP2	15:X:113:ALA:HB3	2.21	0.40
1:2:1166:G:C4	1:2:1167:U:C5	3.09	0.40
1:2:1173:C:N3	1:2:1464:G:C2	2.90	0.40
1:2:1247:C:OP2	34:f:93:HIS:ND1	2.31	0.40
1:2:1251:C:O4'	34:f:131:ALA:HB2	2.21	0.40
1:2:1475:G:C6	1:2:1529:G:C6	3.09	0.40
2:A:92:HIS:HE1	2:A:202:TYR:HE1	1.67	0.40
2:A:157:ASP:CG	13:V:60:ARG:HH21	2.29	0.40
4:C:49:LEU:HD12	4:C:54:LYS:HB2	2.02	0.40
7:H:46:ILE:H	7:H:46:ILE:HG13	1.61	0.40
12:O:20:PHE:HD2	12:O:27:PHE:HB2	1.85	0.40
12:O:80:HIS:ND1	12:O:113:GLY:O	2.54	0.40
24:M:35:ALA:HB3	24:M:113:VAL:HB	2.02	0.40
26:Q:46:PHE:O	26:Q:49:TYR:HB2	2.21	0.40
35:g:62:TYR:CE1	35:g:98:GLY:HA2	2.55	0.40
38:1:9:1MG:O2'	38:1:45:U:O2	2.34	0.40
1:2:278:G:C6	1:2:280:G:C6	3.08	0.40
1:2:447:C:C2	1:2:448:C:C5	3.09	0.40
1:2:509:G:H3'	9:J:176:ARG:NH1	2.34	0.40
1:2:645:U:H2'	1:2:646:G:C8	2.55	0.40
1:2:1470:C:H5'	1:2:1472:G:O4'	2.22	0.40
1:2:1564:U:H2'	1:2:1565:U:C6	2.56	0.40
1:2:1645:U:H2'	1:2:1646:A:H8	1.86	0.40
2:A:147:THR:CG2	2:A:159:ALA:HB1	2.51	0.40
2:A:163:ASN:O	2:A:169:SER:OG	2.40	0.40
5:E:76:VAL:HG23	5:E:77:ARG:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:101:LYS:HD3	7:H:101:LYS:HA	1.76	0.40
10:L:16:GLN:HE22	10:L:33:ARG:HA	1.84	0.40
14:W:50:PHE:HB2	14:W:63:VAL:HA	2.03	0.40
15:X:68:ILE:HD11	19:e:9:ALA:HB2	2.03	0.40
15:X:75:GLN:HE21	15:X:80:GLY:HA2	1.86	0.40
16:Y:29:HIS:ND1	16:Y:29:HIS:O	2.54	0.40
30:U:57:ARG:HE	30:U:89:ARG:CZ	2.34	0.40
33:d:54:LYS:HD3	33:d:54:LYS:HA	1.81	0.40
35:g:67:HIS:ND1	35:g:87:ASP:HA	2.35	0.40
38:1:5:C:H2'	38:1:6:C:C6	2.56	0.40
1:2:739:G:H2'	1:2:740:A:C8	2.56	0.40
1:2:1238:U:H2'	1:2:1239:U:O4'	2.21	0.40
1:2:1449:C:H5'	33:d:8:TYR:N	2.37	0.40
2:A:66:ALA:HA	13:V:37:ALA:HB2	2.03	0.40
4:C:67:PRO:HG3	13:V:29:HIS:CD2	2.55	0.40
6:G:12:THR:HG22	6:G:129:VAL:HG23	2.04	0.40
6:G:115:LYS:NZ	6:G:116:LYS:O	2.39	0.40
7:H:4:PRO:HG2	7:H:25:ILE:HD13	2.03	0.40
7:H:143:LEU:O	14:W:42:GLN:NE2	2.54	0.40
16:Y:27:VAL:CG1	16:Y:69:SER:HB2	2.52	0.40
22:F:39:GLN:HE21	26:Q:53:LEU:HD11	1.86	0.40
23:K:70:GLU:N	23:K:70:GLU:OE1	2.55	0.40
29:T:20:SER:O	29:T:23:GLN:HB3	2.22	0.40
29:T:33:TYR:CD2	29:T:37:VAL:HG21	2.56	0.40
35:g:86:TRP:CA	35:g:110:ASP:HB2	2.51	0.40
35:g:269:ILE:HG22	35:g:279:ASP:O	2.21	0.40
36:i:97:LEU:HA	36:i:101:ARG:HH21	1.86	0.40
38:1:48:5MC:C5	38:1:59:A:C2	3.09	0.40
40:k:206:SER:HA	40:k:468:SER:HA	2.03	0.40
1:2:28:A:O2'	1:2:434:C:H1'	2.21	0.40
1:2:208:U:C2	1:2:209:A:C8	3.10	0.40
1:2:250:A:N3	5:E:131:LEU:HD21	2.36	0.40
1:2:327:A:C4	1:2:328:G:C8	3.09	0.40
1:2:483:C:H6	1:2:483:C:O5'	2.05	0.40
1:2:737:A:O2'	1:2:738:G:H8	2.04	0.40
1:2:832:U:H5'	1:2:833:G:C5'	2.52	0.40
1:2:919:U:H5'	1:2:920:U:OP2	2.21	0.40
1:2:1253:U:H2'	1:2:1254:G:C8	2.56	0.40
1:2:1286:A:H2'	1:2:1312:A:H4'	2.02	0.40
1:2:1723:U:H2'	1:2:1724:G:O4'	2.21	0.40
2:A:179:ARG:HD2	2:A:183:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:113:MET:HG3	3:B:142:PHE:CD2	2.56	0.40
6:G:144:PHE:HD2	6:G:145:PHE:CD1	2.40	0.40
7:H:12:ALA:HB1	7:H:18:LEU:HD21	2.04	0.40
8:I:41:LYS:N	8:I:61:GLU:OE1	2.36	0.40
21:D:76:ARG:O	21:D:76:ARG:NH1	2.36	0.40
21:D:161:GLY:O	21:D:164:VAL:HG22	2.21	0.40
22:F:190:LYS:HG3	22:F:195:THR:CG2	2.50	0.40
24:M:87:GLN:O	24:M:91:TRP:HD1	2.04	0.40
25:P:49:LEU:O	25:P:50:SER:HB3	2.22	0.40
27:R:6:THR:O	27:R:9:VAL:HG12	2.21	0.40
29:T:83:ALA:HB1	29:T:91:HIS:HB3	2.03	0.40
30:U:63:LEU:HD11	33:d:34:TYR:CE2	2.56	0.40
38:1:63:G:H21	38:1:64:RIA:P'	2.44	0.40
1:2:371:G:H1'	1:2:611:U:N3	2.34	0.40
1:2:379:U:H5'	1:2:380:C:H5	1.86	0.40
1:2:471:U:O2'	1:2:769:A:N3	2.52	0.40
1:2:515:G:C6	1:2:516:U:C5	3.09	0.40
1:2:1031:G:H2'	1:2:1032:C:H6	1.86	0.40
1:2:1125:G:H5'	20:h:11:ARG:HD3	2.04	0.40
1:2:1170:A:O2'	1:2:1568:A:N3	2.44	0.40
1:2:1215:C:H4'	1:2:1216:A:C2	2.56	0.40
1:2:1254:G:H8	1:2:1254:G:OP2	2.05	0.40
1:2:1268:U:H5''	1:2:1430:U:OP2	2.22	0.40
1:2:1424:C:O2'	1:2:1426:2MG:H8	2.04	0.40
3:B:180:THR:HG22	3:B:183:GLN:OE1	2.22	0.40
5:E:260:GLY:C	5:E:261:LEU:HD12	2.47	0.40
7:H:91:ILE:HG21	7:H:129:LEU:HD12	2.03	0.40
19:e:48:THR:H	19:e:54:ARG:HH22	1.69	0.40
21:D:219:GLU:O	35:g:201:GLY:HA2	2.22	0.40
22:F:95:LEU:CA	22:F:174:ILE:HD11	2.51	0.40
22:F:205:LYS:HG3	22:F:207:SER:HB2	2.03	0.40
29:T:88:VAL:CG1	29:T:89:ARG:HH21	2.33	0.40
30:U:60:THR:HG22	30:U:87:HIS:NE2	2.36	0.40
36:i:38:ILE:HD12	36:i:38:ILE:H	1.87	0.40
39:j:88:ARG:O	39:j:90:VAL:N	2.52	0.40
39:j:131:ALA:HA	39:j:134:LEU:HB3	2.04	0.40
39:j:255:ILE:HG12	39:j:262:CYS:SG	2.61	0.40
40:k:319:ARG:HD2	40:k:321:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
2	A	217/254 (85%)	195 (90%)	22 (10%)	0	100	100
3	B	221/255 (87%)	197 (89%)	22 (10%)	2 (1%)	14	48
4	C	218/259 (84%)	201 (92%)	16 (7%)	1 (0%)	24	60
5	E	258/261 (99%)	232 (90%)	26 (10%)	0	100	100
6	G	228/236 (97%)	217 (95%)	10 (4%)	1 (0%)	30	65
7	H	182/190 (96%)	160 (88%)	21 (12%)	1 (0%)	24	60
8	I	184/201 (92%)	162 (88%)	22 (12%)	0	100	100
9	J	180/188 (96%)	156 (87%)	22 (12%)	2 (1%)	11	44
10	L	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	18	53
11	N	149/151 (99%)	142 (95%)	7 (5%)	0	100	100
12	O	127/137 (93%)	114 (90%)	13 (10%)	0	100	100
13	V	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
14	W	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
15	X	142/145 (98%)	125 (88%)	17 (12%)	0	100	100
16	Y	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
17	a	100/119 (84%)	82 (82%)	18 (18%)	0	100	100
18	b	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
19	e	58/63 (92%)	48 (83%)	10 (17%)	0	100	100
20	h	23/25 (92%)	23 (100%)	0	0	100	100
21	D	225/237 (95%)	215 (96%)	10 (4%)	0	100	100
22	F	204/227 (90%)	181 (89%)	21 (10%)	2 (1%)	12	45
23	K	94/106 (89%)	77 (82%)	17 (18%)	0	100	100
24	M	113/134 (84%)	94 (83%)	19 (17%)	0	100	100
25	P	115/142 (81%)	95 (83%)	20 (17%)	0	100	100
26	Q	139/143 (97%)	125 (90%)	13 (9%)	1 (1%)	18	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	R	128/136 (94%)	104 (81%)	21 (16%)	3 (2%)	5	31
28	S	143/146 (98%)	125 (87%)	18 (13%)	0	100	100
29	T	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
30	U	104/117 (89%)	96 (92%)	8 (8%)	0	100	100
31	Z	76/108 (70%)	70 (92%)	6 (8%)	0	100	100
32	c	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
33	d	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
34	f	72/150 (48%)	58 (81%)	14 (19%)	0	100	100
35	g	314/326 (96%)	289 (92%)	24 (8%)	1 (0%)	36	69
36	i	93/153 (61%)	81 (87%)	12 (13%)	0	100	100
39	j	243/304 (80%)	221 (91%)	22 (9%)	0	100	100
40	k	388/519 (75%)	352 (91%)	36 (9%)	0	100	100
41	l	21/285 (7%)	21 (100%)	0	0	100	100
42	m	73/108 (68%)	68 (93%)	5 (7%)	0	100	100
All	All	5664/6682 (85%)	5090 (90%)	559 (10%)	15 (0%)	37	69

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	65	PRO
9	J	101	VAL
10	L	8	GLN
3	B	221	PRO
6	G	149	LYS
27	R	97	ASN
35	g	119	ASN
22	F	128	ASP
4	C	45	LYS
27	R	92	ASP
26	Q	41	PRO
27	R	99	VAL
22	F	130	ASN
9	J	122	VAL
3	B	3	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
2	A	180/211 (85%)	180 (100%)	0	100	100
3	B	202/228 (89%)	200 (99%)	2 (1%)	68	76
4	C	177/203 (87%)	177 (100%)	0	100	100
5	E	223/224 (100%)	223 (100%)	0	100	100
6	G	192/200 (96%)	191 (100%)	1 (0%)	81	82
7	H	164/170 (96%)	163 (99%)	1 (1%)	78	81
8	I	147/159 (92%)	147 (100%)	0	100	100
9	J	152/158 (96%)	150 (99%)	2 (1%)	61	72
10	L	136/137 (99%)	132 (97%)	4 (3%)	37	58
11	N	128/128 (100%)	128 (100%)	0	100	100
12	O	97/104 (93%)	97 (100%)	0	100	100
13	V	73/73 (100%)	73 (100%)	0	100	100
14	W	110/111 (99%)	108 (98%)	2 (2%)	51	67
15	X	119/120 (99%)	119 (100%)	0	100	100
16	Y	108/109 (99%)	108 (100%)	0	100	100
17	a	83/100 (83%)	83 (100%)	0	100	100
18	b	71/72 (99%)	71 (100%)	0	100	100
19	e	51/55 (93%)	51 (100%)	0	100	100
20	h	23/23 (100%)	23 (100%)	0	100	100
21	D	188/196 (96%)	188 (100%)	0	100	100
22	F	174/194 (90%)	173 (99%)	1 (1%)	78	81
23	K	88/96 (92%)	88 (100%)	0	100	100
24	M	93/109 (85%)	91 (98%)	2 (2%)	45	64
25	P	99/119 (83%)	99 (100%)	0	100	100
26	Q	117/119 (98%)	115 (98%)	2 (2%)	53	68
27	R	116/124 (94%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	S	127/129 (98%)	127 (100%)	0	100	100
29	T	117/118 (99%)	117 (100%)	0	100	100
30	U	96/107 (90%)	96 (100%)	0	100	100
31	Z	59/88 (67%)	59 (100%)	0	100	100
32	c	55/59 (93%)	55 (100%)	0	100	100
33	d	47/48 (98%)	47 (100%)	0	100	100
34	f	60/133 (45%)	59 (98%)	1 (2%)	53	68
35	g	264/272 (97%)	263 (100%)	1 (0%)	84	84
36	i	80/130 (62%)	80 (100%)	0	100	100
39	j	224/274 (82%)	224 (100%)	0	100	100
40	k	332/443 (75%)	332 (100%)	0	100	100
41	l	22/246 (9%)	22 (100%)	0	100	100
42	m	69/96 (72%)	69 (100%)	0	100	100
All	All	4863/5685 (86%)	4844 (100%)	19 (0%)	81	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	3	VAL
3	B	5	LYS
6	G	149	LYS
7	H	64	VAL
9	J	162	SER
9	J	164	PHE
10	L	5	LEU
10	L	7	VAL
10	L	8	GLN
10	L	14	GLN
14	W	15	ASN
14	W	39	GLN
22	F	128	ASP
24	M	120	ASP
24	M	121	THR
26	Q	39	VAL
26	Q	41	PRO
34	f	132	ASN
35	g	122	LYS

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

Mol	Chain	Res	Type
2	A	131	GLN
3	B	49	ASN
3	B	146	GLN
3	B	157	GLN
3	B	163	GLN
3	B	194	ASN
3	B	211	HIS
4	C	80	ASN
4	C	115	HIS
5	E	216	ASN
5	E	259	HIS
6	G	34	GLN
6	G	190	GLN
7	H	71	HIS
7	H	110	GLN
7	H	161	HIS
8	I	139	ASN
8	I	176	GLN
9	J	142	ASN
10	L	8	GLN
10	L	81	HIS
11	N	5	HIS
11	N	36	GLN
13	V	21	ASN
13	V	29	HIS
13	V	70	ASN
14	W	42	GLN
14	W	80	ASN
21	D	162	GLN
21	D	195	ASN
22	F	36	GLN
22	F	65	GLN
22	F	97	ASN
22	F	102	ASN
22	F	106	ASN
22	F	141	ASN
23	K	28	ASN
23	K	39	ASN
23	K	47	GLN
23	K	85	HIS
24	M	130	HIS

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Mol	Chain	Res	Type
26	Q	32	ASN
26	Q	40	GLN
27	R	74	GLN
28	S	19	ASN
28	S	71	GLN
28	S	89	GLN
29	T	64	HIS
29	T	101	ASN
30	U	44	ASN
33	d	37	ASN
33	d	41	GLN
34	f	132	ASN
35	g	18	ASN
35	g	321	GLN
36	i	44	ASN
36	i	85	GLN
39	j	23	ASN
39	j	41	ASN
39	j	103	GLN
40	k	144	ASN
40	k	226	GLN
40	k	286	GLN
40	k	376	ASN
40	k	465	ASN
42	m	79	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1787/1798 (99%)	570 (31%)	26 (1%)
37	3	25/49 (51%)	13 (52%)	0
38	1	72/75 (96%)	31 (43%)	7 (9%)
All	All	1884/1922 (98%)	614 (32%)	33 (1%)

All (614) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	23	G
1	2	26	A

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Mol	Chain	Res	Type
1	2	27	U
1	2	34	G
1	2	43	A
1	2	47	A
1	2	50	C
1	2	54	C
1	2	57	G
1	2	59	C
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	104	A
1	2	111	U
1	2	114	C
1	2	115	G
1	2	116	U
1	2	124	A
1	2	125	U
1	2	127	G
1	2	128	U
1	2	130	C
1	2	132	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	140	A
1	2	146	A
1	2	152	G
1	2	158	U
1	2	160	U
1	2	161	A
1	2	167	A
1	2	168	A
1	2	173	U
1	2	176	U
1	2	177	U
1	2	184	U
1	2	185	C

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Mol	Chain	Res	Type
1	2	187	A
1	2	190	C
1	2	191	U
1	2	192	U
1	2	193	U
1	2	194	G
1	2	195	G
1	2	198	G
1	2	199	A
1	2	210	U
1	2	214	A
1	2	217	A
1	2	218	A
1	2	220	A
1	2	223	C
1	2	225	A
1	2	226	U
1	2	227	G
1	2	228	U
1	2	230	U
1	2	231	U
1	2	232	C
1	2	234	G
1	2	235	A
1	2	237	U
1	2	239	C
1	2	240	U
1	2	248	U
1	2	249	C
1	2	256	A
1	2	259	U
1	2	260	U
1	2	264	A
1	2	266	U
1	2	267	C
1	2	271	U
1	2	274	C
1	2	275	C
1	2	276	U
1	2	278	G
1	2	280	G
1	2	281	C

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Mol	Chain	Res	Type
1	2	289	G
1	2	298	A
1	2	300	A
1	2	301	U
1	2	307	C
1	2	311	A
1	2	313	C
1	2	315	A
1	2	321	G
1	2	332	A
1	2	336	G
1	2	337	C
1	2	338	C
1	2	350	C
1	2	358	A
1	2	359	A
1	2	360	C
1	2	389	G
1	2	399	A
1	2	400	A
1	2	401	C
1	2	403	G
1	2	411	A
1	2	415	A
1	2	416	A
1	2	421	G
1	2	422	G
1	2	423	C
1	2	424	A
1	2	425	G
1	2	433	G
1	2	434	C
1	2	436	A
1	2	438	U
1	2	439	U
1	2	440	A
1	2	443	C
1	2	446	U
1	2	447	C
1	2	449	U
1	2	453	U
1	2	457	G

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Mol	Chain	Res	Type
1	2	459	A
1	2	460	G
1	2	467	A
1	2	468	C
1	2	473	A
1	2	474	A
1	2	475	U
1	2	476	A
1	2	479	G
1	2	481	U
1	2	482	A
1	2	485	G
1	2	488	C
1	2	489	C
1	2	490	C
1	2	491	A
1	2	492	U
1	2	493	U
1	2	494	C
1	2	495	G
1	2	496	G
1	2	499	C
1	2	502	G
1	2	505	A
1	2	506	U
1	2	507	U
1	2	509	G
1	2	516	U
1	2	518	C
1	2	519	A
1	2	526	A
1	2	527	U
1	2	533	A
1	2	534	A
1	2	535	C
1	2	537	A
1	2	539	G
1	2	540	A
1	2	541	A
1	2	542	C
1	2	543	A
1	2	545	C

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Mol	Chain	Res	Type
1	2	553	C
1	2	554	A
1	2	557	U
1	2	558	C
1	2	564	C
1	2	565	C
1	2	567	G
1	2	583	C
1	2	584	A
1	2	587	U
1	2	593	A
1	2	594	G
1	2	597	U
1	2	605	A
1	2	610	U
1	2	616	U
1	2	618	A
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	G
1	2	634	A
1	2	637	U
1	2	638	U
1	2	641	G
1	2	647	G
1	2	650	G
1	2	652	C
1	2	653	C
1	2	657	C
1	2	671	C
1	2	673	C
1	2	675	C
1	2	676	U
1	2	679	U
1	2	680	U
1	2	681	U
1	2	684	A
1	2	685	A
1	2	686	C
1	2	688	G

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Mol	Chain	Res	Type
1	2	693	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	701	U
1	2	702	G
1	2	704	C
1	2	705	U
1	2	709	C
1	2	710	U
1	2	711	G
1	2	712	U
1	2	713	A
1	2	714	C
1	2	715	U
1	2	716	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G
1	2	727	C
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	737	A
1	2	738	G
1	2	741	C
1	2	742	U
1	2	745	U
1	2	761	G
1	2	765	G
1	2	766	PSU
1	2	774	A
1	2	778	G
1	2	779	A
1	2	780	A
1	2	781	A

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Mol	Chain	Res	Type
1	2	782	G
1	2	783	C
1	2	787	A
1	2	788	A
1	2	789	U
1	2	792	A
1	2	793	U
1	2	811	A
1	2	813	A
1	2	817	C
1	2	819	U
1	2	820	U
1	2	821	U
1	2	822	G
1	2	826	C
1	2	827	U
1	2	828	A
1	2	829	U
1	2	830	U
1	2	832	U
1	2	833	G
1	2	836	G
1	2	837	G
1	2	840	U
1	2	845	G
1	2	855	A
1	2	856	U
1	2	859	U
1	2	862	A
1	2	872	U
1	2	875	G
1	2	876	G
1	2	885	U
1	2	895	U
1	2	897	A
1	2	904	A
1	2	905	A
1	2	911	U
1	2	913	G
1	2	914	A
1	2	915	U
1	2	916	U

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Mol	Chain	Res	Type
1	2	917	U
1	2	918	A
1	2	919	U
1	2	920	U
1	2	928	A
1	2	932	A
1	2	934	U
1	2	941	G
1	2	944	U
1	2	950	A
1	2	958	U
1	2	959	U
1	2	965	A
1	2	968	C
1	2	969	A
1	2	970	A
1	2	972	A
1	2	982	A
1	2	986	G
1	2	987	A
1	2	991	A
1	2	998	PSU
1	2	1003	U
1	2	1008	U
1	2	1011	U
1	2	1015	C
1	2	1020	C
1	2	1022	A
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1030	U
1	2	1031	G
1	2	1035	A
1	2	1038	A
1	2	1039	G
1	2	1042	A
1	2	1049	G
1	2	1050	G
1	2	1051	U
1	2	1052	G
1	2	1055	U

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Mol	Chain	Res	Type
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1075	A
1	2	1081	C
1	2	1082	G
1	2	1084	G
1	2	1085	A
1	2	1086	A
1	2	1091	A
1	2	1095	C
1	2	1096	U
1	2	1099	G
1	2	1103	U
1	2	1108	G
1	2	1110	G
1	2	1113	G
1	2	1118	G
1	2	1125	G
1	2	1137	A
1	2	1142	A
1	2	1146	A
1	2	1149	G
1	2	1150	A
1	2	1154	G
1	2	1157	C
1	2	1158	C
1	2	1163	G
1	2	1166	G
1	2	1184	U
1	2	1185	U
1	2	1187	G
1	2	1189	C
1	2	1190	B8N
1	2	1193	A
1	2	1195	A
1	2	1198	G
1	2	1199	G
1	2	1201	A
1	2	1207	A
1	2	1211	G
1	2	1216	A

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Mol	Chain	Res	Type
1	2	1217	G
1	2	1224	U
1	2	1227	G
1	2	1228	G
1	2	1229	A
1	2	1230	U
1	2	1236	G
1	2	1237	A
1	2	1240	G
1	2	1241	A
1	2	1243	A
1	2	1244	G
1	2	1247	C
1	2	1249	U
1	2	1250	U
1	2	1251	C
1	2	1254	G
1	2	1255	A
1	2	1256	U
1	2	1258	U
1	2	1259	U
1	2	1260	G
1	2	1265	U
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1284	U
1	2	1292	U
1	2	1296	G
1	2	1305	C
1	2	1307	G
1	2	1313	U
1	2	1314	U
1	2	1315	G
1	2	1317	G
1	2	1320	A
1	2	1321	A
1	2	1323	G
1	2	1336	A
1	2	1337	C
1	2	1339	U
1	2	1343	A

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Mol	Chain	Res	Type
1	2	1344	A
1	2	1345	A
1	2	1346	U
1	2	1347	A
1	2	1353	G
1	2	1355	U
1	2	1358	C
1	2	1361	U
1	2	1362	U
1	2	1363	G
1	2	1364	C
1	2	1366	G
1	2	1369	U
1	2	1370	G
1	2	1378	U
1	2	1380	A
1	2	1383	G
1	2	1388	U
1	2	1389	A
1	2	1390	U
1	2	1396	U
1	2	1397	C
1	2	1398	A
1	2	1400	G
1	2	1401	C
1	2	1408	A
1	2	1409	A
1	2	1410	G
1	2	1411	U
1	2	1413	U
1	2	1416	G
1	2	1424	C
1	2	1425	A
1	2	1426	2MG
1	2	1431	G
1	2	1434	A
1	2	1442	A
1	2	1444	A
1	2	1455	C
1	2	1456	G
1	2	1457	C
1	2	1464	G

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Mol	Chain	Res	Type
1	2	1469	A
1	2	1470	C
1	2	1471	U
1	2	1476	G
1	2	1479	C
1	2	1481	A
1	2	1482	G
1	2	1483	C
1	2	1484	G
1	2	1488	A
1	2	1489	C
1	2	1490	A
1	2	1491	A
1	2	1494	U
1	2	1498	C
1	2	1499	C
1	2	1504	G
1	2	1510	G
1	2	1511	G
1	2	1512	U
1	2	1514	A
1	2	1518	U
1	2	1521	G
1	2	1522	A
1	2	1523	A
1	2	1533	U
1	2	1535	C
1	2	1538	G
1	2	1540	G
1	2	1544	G
1	2	1547	C
1	2	1555	U
1	2	1557	A
1	2	1558	U
1	2	1566	C
1	2	1571	A
1	2	1572	G
1	2	1573	7MG
1	2	1588	G
1	2	1595	A
1	2	1597	C
1	2	1598	A

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Mol	Chain	Res	Type
1	2	1599	G
1	2	1614	G
1	2	1617	C
1	2	1620	G
1	2	1632	C
1	2	1633	A
1	2	1637	5MC
1	2	1640	G
1	2	1648	U
1	2	1655	U
1	2	1656	G
1	2	1662	C
1	2	1677	G
1	2	1678	G
1	2	1679	A
1	2	1683	G
1	2	1685	U
1	2	1686	U
1	2	1687	A
1	2	1688	G
1	2	1689	A
1	2	1692	A
1	2	1693	G
1	2	1694	G
1	2	1695	G
1	2	1697	G
1	2	1698	C
1	2	1699	A
1	2	1700	A
1	2	1702	U
1	2	1703	C
1	2	1704	C
1	2	1705	A
1	2	1707	C
1	2	1708	U
1	2	1709	C
1	2	1710	A
1	2	1711	G
1	2	1712	A
1	2	1725	G
1	2	1734	G
1	2	1742	A

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Mol	Chain	Res	Type
1	2	1743	G
1	2	1748	A
1	2	1749	C
1	2	1753	A
1	2	1754	A
1	2	1755	G
1	2	1758	G
1	2	1764	A
1	2	1766	G
1	2	1767	U
1	2	1768	U
1	2	1778	G
1	2	1781	C
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1793	U
1	2	1794	C
1	2	1797	U
1	2	1798	A
37	3	16	U
37	3	18	U
37	3	22	U
37	3	24	U
37	3	25	A
37	3	26	A
37	3	32	U
37	3	33	C
37	3	35	C
37	3	36	U
37	3	37	U
37	3	39	U
37	3	40	C
38	1	4	G
38	1	8	U
38	1	9	1MG
38	1	10	2MG
38	1	14	A
38	1	15	G
38	1	16	H2U
38	1	18	G
38	1	19	G

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Mol	Chain	Res	Type
38	1	20	A
38	1	21	A
38	1	22	G
38	1	23	C
38	1	26	M2G
38	1	42	U
38	1	43	G
38	1	44	A
38	1	45	U
38	1	46	7MG
38	1	47	H2U
38	1	48	5MC
38	1	49	5MC
38	1	52	G
38	1	58	1MA
38	1	59	A
38	1	60	A
38	1	61	C
38	1	71	C
38	1	73	A
38	1	75	C
38	1	76	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	74	U
1	2	216	A
1	2	217	A
1	2	226	U
1	2	239	C
1	2	277	U
1	2	279	U
1	2	649	U
1	2	670	G
1	2	695	U
1	2	700	C
1	2	781	A
1	2	828	A
1	2	1188	A
1	2	1198	G
1	2	1206	C

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Mol	Chain	Res	Type
1	2	1343	A
1	2	1430	U
1	2	1455	C
1	2	1470	C
1	2	1513	A
1	2	1571	A
1	2	1573	7MG
1	2	1613	C
1	2	1765	G
1	2	1797	U
38	1	8	U
38	1	42	U
38	1	43	G
38	1	44	A
38	1	45	U
38	1	58	1MA
38	1	74	C

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

23 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	$\# Z > 2$
1	2MG	2	1570	1	23,26,27	2.91	8 (34%)	33,38,41	2.19	11 (33%)
1	MA6	2	1780	1	23,26,27	1.39	4 (17%)	33,38,41	3.28	12 (36%)
38	2MG	1	10	38	23,26,27	2.94	8 (34%)	33,38,41	2.17	11 (33%)
38	7MG	1	46	38	23,26,27	3.64	11 (47%)	27,39,42	2.18	9 (33%)
38	H2U	1	16	38	18,21,22	3.15	4 (22%)	19,30,33	1.49	4 (21%)
1	PSU	2	1289	1	18,21,22	4.46	7 (38%)	21,30,33	1.81	5 (23%)
1	5MC	2	1006	1	19,22,23	3.78	8 (42%)	26,32,35	1.15	2 (7%)
38	M2G	1	26	38	24,27,28	2.68	8 (33%)	33,40,43	1.70	7 (21%)
38	1MA	1	58	38	21,25,26	3.14	6 (28%)	30,37,40	2.30	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	5MC	1	49	38	19,22,23	3.95	8 (42%)	26,32,35	1.00	1 (3%)
1	2MG	2	1426	1,43	23,26,27	2.90	8 (34%)	33,38,41	2.18	9 (27%)
38	RIA	1	64	38	35,38,39	4.61	14 (40%)	50,57,60	2.00	13 (26%)
1	B8N	2	1190	1	25,29,30	3.38	7 (28%)	28,42,45	2.00	7 (25%)
1	PSU	2	766	1	18,21,22	4.48	8 (44%)	21,30,33	2.07	6 (28%)
1	PSU	2	998	1	18,21,22	4.38	8 (44%)	21,30,33	1.91	4 (19%)
38	T6A	1	37	38	31,34,35	1.78	7 (22%)	43,49,52	2.09	15 (34%)
38	H2U	1	47	38	18,21,22	3.15	4 (22%)	19,30,33	1.45	4 (21%)
1	7MG	2	1573	1	23,26,27	3.59	10 (43%)	27,39,42	2.29	9 (33%)
1	5MC	2	1637	1	19,22,23	3.86	8 (42%)	26,32,35	1.11	2 (7%)
38	1MG	1	9	38	23,26,27	3.32	7 (30%)	33,39,42	2.33	8 (24%)
1	PSU	2	465	1	18,21,22	4.41	7 (38%)	21,30,33	1.91	5 (23%)
38	5MC	1	48	38	19,22,23	3.99	9 (47%)	26,32,35	1.71	5 (19%)
1	PSU	2	120	1	18,21,22	4.50	7 (38%)	21,30,33	1.89	6 (28%)

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
1	2MG	2	1570	1	-	0/9/27/28	0/3/3/3
1	MA6	2	1780	1	-	3/11/29/30	0/3/3/3
38	2MG	1	10	38	-	2/9/27/28	0/3/3/3
38	7MG	1	46	38	-	1/7/37/38	0/3/3/3
38	H2U	1	16	38	-	3/7/38/39	0/2/2/2
1	PSU	2	1289	1	-	3/7/25/26	0/2/2/2
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
38	M2G	1	26	38	-	3/11/29/30	0/3/3/3
38	1MA	1	58	38	-	1/7/25/26	0/3/3/3
38	5MC	1	49	38	-	3/7/25/26	0/2/2/2
1	2MG	2	1426	1,43	-	1/9/27/28	0/3/3/3
38	RIA	1	64	38	-	9/17/51/52	0/4/4/4
1	B8N	2	1190	1	-	5/16/34/35	0/2/2/2
1	PSU	2	766	1	-	2/7/25/26	0/2/2/2
1	PSU	2	998	1	-	3/7/25/26	0/2/2/2
38	T6A	1	37	38	-	6/23/41/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	H2U	1	47	38	-	3/7/38/39	0/2/2/2
1	7MG	2	1573	1	-	2/7/37/38	0/3/3/3
1	5MC	2	1637	1	-	3/7/25/26	0/2/2/2
38	1MG	1	9	38	-	2/7/25/26	0/3/3/3
1	PSU	2	465	1	-	0/7/25/26	0/2/2/2
38	5MC	1	48	38	-	3/7/25/26	0/2/2/2
1	PSU	2	120	1	-	2/7/25/26	0/2/2/2

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	64	RIA	C1'-C2'	-16.12	1.32	1.52
1	2	120	PSU	C6-C5	11.94	1.48	1.35
1	2	1289	PSU	C6-C5	11.79	1.48	1.35
1	2	465	PSU	C6-C5	11.74	1.48	1.35
1	2	766	PSU	C6-C5	11.72	1.48	1.35
1	2	998	PSU	C6-C5	11.58	1.48	1.35
38	1	64	RIA	O1'-C1'	10.92	1.60	1.41
1	2	120	PSU	C2-N1	10.14	1.49	1.36
1	2	766	PSU	C2-N1	10.01	1.49	1.36
1	2	1289	PSU	C2-N1	9.94	1.49	1.36
38	1	16	H2U	C2-N1	9.88	1.49	1.35
38	1	47	H2U	C2-N1	9.86	1.49	1.35
1	2	465	PSU	C2-N1	9.81	1.49	1.36
1	2	998	PSU	C2-N1	9.71	1.49	1.36
38	1	58	1MA	C2-N3	9.65	1.48	1.30
38	1	64	RIA	C2A-C1A	-9.55	1.29	1.53
38	1	49	5MC	C6-C5	9.36	1.49	1.34
38	1	9	1MG	C2-N2	9.25	1.50	1.34
38	1	48	5MC	C6-C5	9.25	1.49	1.34
1	2	1637	5MC	C6-C5	9.19	1.49	1.34
38	1	64	RIA	O4'-C1A	9.17	1.63	1.42
1	2	1006	5MC	C6-C5	9.10	1.49	1.34
1	2	1573	7MG	C8-N9	8.83	1.51	1.45
38	1	46	7MG	C8-N9	8.59	1.51	1.45
1	2	1190	B8N	C6-N1	8.51	1.57	1.36
1	2	766	PSU	C2-N3	7.79	1.50	1.37
38	1	10	2MG	C2-N3	7.75	1.46	1.32
1	2	1289	PSU	C2-N3	7.70	1.50	1.37
1	2	1570	2MG	C2-N3	7.66	1.46	1.32
1	2	1426	2MG	C2-N3	7.64	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1190	B8N	C4-N3	-7.63	1.26	1.40
1	2	998	PSU	C2-N3	7.62	1.50	1.37
1	2	120	PSU	C2-N3	7.61	1.50	1.37
1	2	465	PSU	C2-N3	7.57	1.49	1.37
1	2	1190	B8N	C4-C5	7.46	1.64	1.47
38	1	48	5MC	C5-C4	7.37	1.49	1.44
38	1	58	1MA	C4-N3	7.19	1.50	1.35
38	1	46	7MG	C5-N7	7.11	1.44	1.35
38	1	49	5MC	C4-N3	7.05	1.45	1.34
38	1	48	5MC	C4-N3	7.03	1.45	1.34
38	1	9	1MG	C2-N3	6.96	1.44	1.33
38	1	49	5MC	C5-C4	6.89	1.49	1.44
38	1	26	M2G	C4-N3	6.80	1.49	1.34
1	2	1637	5MC	C4-N3	6.74	1.44	1.34
38	1	10	2MG	C4-N3	6.70	1.49	1.34
1	2	1570	2MG	C4-N3	6.68	1.49	1.34
38	1	26	M2G	C2-N2	6.64	1.47	1.35
38	1	64	RIA	O1'-C4'	-6.64	1.30	1.45
1	2	1006	5MC	C4-N3	6.62	1.44	1.34
1	2	1426	2MG	C4-N3	6.62	1.49	1.34
1	2	1637	5MC	C5-C4	6.60	1.49	1.44
38	1	47	H2U	C2-N3	6.55	1.49	1.38
38	1	16	H2U	C2-N3	6.54	1.49	1.38
1	2	1573	7MG	C5-N7	6.48	1.43	1.35
38	1	9	1MG	C4-N3	6.48	1.49	1.34
38	1	49	5MC	C2-N3	6.38	1.49	1.36
1	2	1006	5MC	C5-C4	6.30	1.48	1.44
1	2	1637	5MC	C2-N3	6.21	1.48	1.36
1	2	1573	7MG	C2-N3	6.12	1.48	1.33
1	2	1006	5MC	C2-N3	6.09	1.48	1.36
38	1	26	M2G	C2-N3	5.99	1.46	1.32
38	1	46	7MG	C2-N3	5.99	1.47	1.33
38	1	48	5MC	C2-N3	5.97	1.48	1.36
1	2	1573	7MG	C4-N3	5.93	1.47	1.34
38	1	64	RIA	C6-N6	5.92	1.49	1.34
38	1	64	RIA	O4'-C4A	-5.91	1.31	1.45
38	1	46	7MG	C4-N3	5.88	1.47	1.34
38	1	10	2MG	C2-N2	5.84	1.45	1.33
1	2	1190	B8N	C2-N1	5.83	1.56	1.39
1	2	1570	2MG	C2-N2	5.83	1.45	1.33
1	2	1426	2MG	C2-N2	5.80	1.45	1.33
1	2	1573	7MG	C4-N9	5.48	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	120	PSU	C6-N1	5.45	1.45	1.36
38	1	9	1MG	C2-N1	5.43	1.47	1.37
38	1	46	7MG	C4-N9	5.35	1.44	1.37
1	2	1289	PSU	C6-N1	5.30	1.45	1.36
1	2	766	PSU	C6-N1	5.25	1.44	1.36
1	2	465	PSU	C6-N1	5.23	1.44	1.36
1	2	1190	B8N	C6-C5	5.22	1.42	1.35
38	1	37	T6A	C10-N6	5.16	1.48	1.37
38	1	47	H2U	C4-N3	5.08	1.46	1.37
1	2	998	PSU	C6-N1	5.05	1.44	1.36
38	1	46	7MG	C2-N2	5.03	1.46	1.34
38	1	37	T6A	C10-N11	5.02	1.49	1.35
38	1	16	H2U	C4-N3	5.01	1.46	1.37
1	2	1426	2MG	C2-N1	4.95	1.44	1.36
38	1	58	1MA	C2-N1	4.94	1.45	1.35
1	2	1570	2MG	C2-N1	4.93	1.44	1.36
38	1	10	2MG	C2-N1	4.85	1.44	1.36
1	2	1573	7MG	C2-N2	4.80	1.45	1.34
38	1	49	5MC	C6-N1	4.76	1.46	1.38
1	2	1637	5MC	C2-N1	4.62	1.49	1.40
38	1	48	5MC	C4-N4	4.58	1.45	1.34
1	2	1637	5MC	C6-N1	4.55	1.45	1.38
38	1	48	5MC	C6-N1	4.50	1.45	1.38
38	1	49	5MC	C4-N4	4.49	1.45	1.34
1	2	1006	5MC	C6-N1	4.47	1.45	1.38
1	2	1637	5MC	C4-N4	4.46	1.45	1.34
1	2	1006	5MC	C4-N4	4.43	1.45	1.34
38	1	49	5MC	C2-N1	4.43	1.49	1.40
1	2	1006	5MC	C2-N1	4.37	1.49	1.40
1	2	1190	B8N	C1'-C5	-4.30	1.40	1.50
38	1	48	5MC	C2-N1	4.23	1.48	1.40
38	1	58	1MA	C5-C6	4.06	1.54	1.43
38	1	46	7MG	C2-N1	3.91	1.47	1.37
1	2	1289	PSU	C4-N3	3.89	1.46	1.38
1	2	465	PSU	C4-N3	3.84	1.46	1.38
1	2	1780	MA6	C6-N6	3.83	1.47	1.36
1	2	120	PSU	C4-N3	3.81	1.46	1.38
1	2	766	PSU	C4-N3	3.80	1.46	1.38
38	1	46	7MG	C5-C6	3.73	1.52	1.43
38	1	9	1MG	O6-C6	-3.67	1.15	1.23
1	2	998	PSU	C4-N3	3.64	1.45	1.38
1	2	1573	7MG	C2-N1	3.62	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	26	M2G	C2-N1	3.59	1.44	1.36
38	1	9	1MG	C5-C6	3.46	1.54	1.45
1	2	1573	7MG	C5-C6	3.43	1.52	1.43
38	1	46	7MG	C6-N1	3.31	1.45	1.38
38	1	9	1MG	C5-N7	-3.28	1.32	1.39
38	1	48	5MC	O4'-C4'	-3.12	1.38	1.45
38	1	64	RIA	O3A-C3A	-3.12	1.35	1.43
38	1	64	RIA	O2'-C2'	3.05	1.50	1.43
1	2	1573	7MG	O6-C6	-3.01	1.17	1.23
38	1	58	1MA	C5-N7	-2.97	1.33	1.39
1	2	1426	2MG	C5-N7	-2.96	1.33	1.39
38	1	64	RIA	O2A-C2A	2.93	1.51	1.43
1	2	1570	2MG	C5-N7	-2.91	1.33	1.39
38	1	10	2MG	C5-N7	-2.90	1.33	1.39
1	2	1780	MA6	C5-C4	-2.88	1.33	1.39
38	1	64	RIA	C5-N7	-2.85	1.33	1.39
38	1	26	M2G	C6-N1	2.84	1.44	1.38
1	2	1573	7MG	C6-N1	2.79	1.44	1.38
38	1	48	5MC	O2-C2	-2.78	1.18	1.23
38	1	26	M2G	C5-C6	2.75	1.54	1.44
1	2	1006	5MC	O2-C2	-2.74	1.18	1.23
1	2	1637	5MC	O2-C2	-2.74	1.18	1.23
38	1	49	5MC	O2-C2	-2.69	1.18	1.23
38	1	26	M2G	C5-N7	-2.64	1.33	1.39
38	1	16	H2U	O2-C2	-2.61	1.18	1.23
38	1	37	T6A	C5-N7	-2.58	1.34	1.39
38	1	47	H2U	O2-C2	-2.53	1.18	1.23
1	2	998	PSU	O4-C4	-2.52	1.18	1.23
1	2	1570	2MG	C5-C6	2.50	1.53	1.44
38	1	46	7MG	O6-C6	-2.50	1.18	1.23
1	2	1426	2MG	O6-C6	-2.47	1.18	1.23
38	1	10	2MG	C6-N1	2.47	1.43	1.38
1	2	120	PSU	O4-C4	-2.45	1.18	1.23
38	1	10	2MG	C5-C6	2.45	1.53	1.44
1	2	766	PSU	O4-C4	-2.45	1.18	1.23
1	2	1289	PSU	O4-C4	-2.45	1.18	1.23
1	2	1780	MA6	C5-N7	-2.44	1.34	1.39
1	2	1426	2MG	C5-C6	2.44	1.53	1.44
1	2	1570	2MG	C6-N1	2.42	1.43	1.38
1	2	766	PSU	O4'-C1'	-2.42	1.40	1.43
1	2	1570	2MG	O6-C6	-2.42	1.19	1.23
38	1	10	2MG	O6-C6	-2.41	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	465	PSU	O4-C4	-2.38	1.19	1.23
38	1	64	RIA	O3'-C3'	-2.37	1.37	1.43
1	2	1426	2MG	C6-N1	2.36	1.43	1.38
38	1	37	T6A	C6-N6	2.32	1.44	1.39
38	1	37	T6A	ODA-C13	2.29	1.28	1.22
38	1	37	T6A	C2-N1	2.28	1.38	1.33
38	1	64	RIA	C2-N1	2.19	1.37	1.33
1	2	998	PSU	O2-C2	-2.19	1.18	1.23
38	1	64	RIA	P'-O5'	2.18	1.67	1.60
1	2	998	PSU	O4'-C1'	-2.15	1.40	1.43
38	1	26	M2G	O6-C6	-2.14	1.19	1.23
1	2	766	PSU	O2-C2	-2.14	1.18	1.23
38	1	58	1MA	CM1-N1	-2.14	1.42	1.46
1	2	465	PSU	O2-C2	-2.11	1.18	1.23
38	1	37	T6A	C5-C4	-2.10	1.35	1.39
1	2	1289	PSU	O2-C2	-2.09	1.18	1.23
1	2	120	PSU	O2-C2	-2.07	1.19	1.23
38	1	46	7MG	C5-C4	2.07	1.44	1.37
1	2	1190	B8N	O4'-C1'	-2.06	1.41	1.43
1	2	1780	MA6	C8-N9	-2.06	1.34	1.37

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	N1-C6-N6	-12.07	102.15	116.86
1	2	1780	MA6	C5-C6-N6	7.95	137.92	125.33
38	1	9	1MG	C1'-N9-C4	-6.77	106.48	126.49
1	2	1570	2MG	C2-N3-C4	6.46	120.09	112.00
38	1	10	2MG	C2-N3-C4	6.46	120.08	112.00
1	2	1426	2MG	C2-N3-C4	6.46	120.08	112.00
38	1	9	1MG	C1'-N9-C8	6.36	144.81	126.73
38	1	48	5MC	O4'-C4'-C5'	-6.12	89.74	109.33
38	1	58	1MA	C1'-N9-C8	-6.10	109.40	126.73
38	1	37	T6A	N3-C2-N1	-5.94	119.59	128.58
38	1	64	RIA	N3-C2-N1	-5.66	120.01	128.58
1	2	1780	MA6	N1-C2-N3	-5.48	120.28	128.58
1	2	1426	2MG	C5-C4-N3	-5.35	119.87	128.39
38	1	64	RIA	C5-C4-N3	-5.34	119.37	126.72
38	1	10	2MG	C5-C4-N3	-5.31	119.94	128.39
1	2	1573	7MG	C5-C6-N1	5.30	120.27	110.94
1	2	1190	B8N	C5-C4-N3	5.28	125.75	116.15
38	1	26	M2G	C5-C4-N3	-5.27	120.01	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	58	1MA	N1-C2-N3	-5.26	119.74	126.00
1	2	1570	2MG	C5-C4-N3	-5.25	120.04	128.39
38	1	58	1MA	C1'-N9-C4	5.06	141.43	126.49
38	1	9	1MG	C5-C4-N3	-5.05	120.36	128.39
38	1	46	7MG	C5-C6-N1	5.01	119.76	110.94
1	2	1780	MA6	C5-C4-N3	-5.00	119.84	126.72
1	2	766	PSU	C4-N3-C2	-4.76	119.82	126.37
38	1	64	RIA	N6-C6-N1	-4.74	107.81	118.38
1	2	120	PSU	C4-N3-C2	-4.69	119.90	126.37
1	2	465	PSU	C4-N3-C2	-4.63	120.00	126.37
38	1	46	7MG	C2-N3-C4	4.62	120.25	112.30
1	2	1573	7MG	C5-C4-N3	-4.57	119.55	128.13
38	1	58	1MA	C5-C4-N3	-4.55	120.57	127.27
38	1	37	T6A	C5-C4-N3	-4.55	120.46	126.72
1	2	766	PSU	N1-C2-N3	4.52	119.93	115.17
1	2	1190	B8N	C4-N3-C2	-4.50	120.08	125.62
1	2	1289	PSU	C4-N3-C2	-4.45	120.25	126.37
1	2	1573	7MG	C2-N3-C4	4.44	119.95	112.30
1	2	998	PSU	C4-N3-C2	-4.44	120.26	126.37
1	2	465	PSU	N1-C2-N3	4.39	119.80	115.17
38	1	26	M2G	C2-N3-C4	4.31	120.48	112.51
1	2	998	PSU	N1-C2-N3	4.26	119.67	115.17
1	2	1573	7MG	C4-C5-N7	4.20	110.34	105.38
38	1	46	7MG	C5-C4-N3	-4.20	120.25	128.13
1	2	120	PSU	N1-C2-N3	4.20	119.59	115.17
38	1	37	T6A	N6-C10-N11	4.19	119.53	113.77
1	2	1426	2MG	C2-N1-C6	-4.16	119.52	124.55
1	2	1780	MA6	C4-C5-C6	4.16	120.21	115.91
38	1	37	T6A	N9-C8-N7	-4.16	108.04	113.94
38	1	64	RIA	N9-C8-N7	-4.15	108.04	113.94
1	2	1780	MA6	N9-C8-N7	-4.13	108.08	113.94
1	2	1570	2MG	C2-N1-C6	-4.05	119.66	124.55
1	2	1289	PSU	N1-C2-N3	4.03	119.42	115.17
38	1	10	2MG	C2-N1-C6	-4.01	119.70	124.55
38	1	37	T6A	C4-C5-C6	3.91	120.03	116.78
1	2	998	PSU	C6-N1-C2	-3.87	119.10	122.69
38	1	46	7MG	C4-C5-N7	3.79	109.86	105.38
38	1	58	1MA	C2-N3-C4	3.79	119.96	112.53
1	2	1190	B8N	C1'-C5-C4	3.79	123.35	117.61
1	2	766	PSU	C6-C5-C4	3.63	120.62	118.17
1	2	1006	5MC	C5-C6-N1	-3.59	119.41	123.31
38	1	16	H2U	N3-C2-N1	3.57	120.24	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	9	1MG	C2-N3-C4	3.54	119.93	111.98
38	1	48	5MC	C5-C6-N1	-3.53	119.48	123.31
38	1	64	RIA	C2-N3-C4	3.53	120.46	111.83
38	1	64	RIA	N3-C4-N9	3.52	133.15	127.17
38	1	64	RIA	C5-C6-N6	3.47	131.88	123.29
38	1	58	1MA	N9-C8-N7	-3.47	106.97	113.40
1	2	1426	2MG	N1-C2-N2	3.45	120.08	116.56
1	2	1570	2MG	N1-C2-N2	3.41	120.04	116.56
1	2	465	PSU	C6-N1-C2	-3.33	119.60	122.69
1	2	766	PSU	C6-N1-C2	-3.32	119.61	122.69
1	2	1190	B8N	N3-C2-N1	3.32	120.77	116.72
1	2	1780	MA6	C2-N3-C4	3.30	119.88	111.83
1	2	1573	7MG	N9-C4-N3	3.29	130.29	125.46
38	1	47	H2U	N3-C2-N1	3.29	119.95	116.65
1	2	1780	MA6	C2-N1-C6	3.28	119.85	111.83
38	1	37	T6A	C2-N3-C4	3.26	119.80	111.83
38	1	10	2MG	N9-C4-N3	3.23	132.42	125.95
38	1	9	1MG	N9-C8-N7	-3.22	107.42	113.40
38	1	64	RIA	C1'-O2A-C2A	-3.20	110.40	117.98
1	2	1573	7MG	C2-N1-C6	-3.17	119.36	125.11
38	1	46	7MG	C5-C4-N9	3.17	110.39	106.33
1	2	1570	2MG	N9-C4-N3	3.15	132.26	125.95
38	1	9	1MG	N9-C4-N3	3.15	132.26	125.95
1	2	1289	PSU	C6-N1-C2	-3.15	119.77	122.69
1	2	1426	2MG	N9-C4-N3	3.14	132.23	125.95
38	1	37	T6A	C12-N11-C10	3.10	127.15	121.99
38	1	64	RIA	C1'-C2'-C3'	3.08	106.12	102.29
1	2	120	PSU	C6-N1-C2	-3.04	119.87	122.69
1	2	1780	MA6	N3-C4-N9	3.02	132.30	127.17
1	2	1573	7MG	C5-C4-N9	2.99	110.16	106.33
38	1	64	RIA	C5-N7-C8	2.98	108.13	103.45
38	1	10	2MG	N1-C2-N2	2.97	119.59	116.56
1	2	1190	B8N	O4-C4-N3	-2.96	115.18	119.99
38	1	47	H2U	C5-C6-N1	2.96	120.47	111.52
38	1	47	H2U	C5-C4-N3	2.91	119.78	116.69
38	1	16	H2U	C5-C4-N3	2.90	119.77	116.69
38	1	37	T6A	C5-N7-C8	2.88	107.97	103.45
1	2	1637	5MC	C5-C6-N1	-2.87	120.20	123.31
1	2	1570	2MG	N9-C8-N7	-2.86	108.09	113.40
38	1	10	2MG	N9-C8-N7	-2.85	108.11	113.40
38	1	26	M2G	N9-C4-N3	2.85	131.65	125.95
1	2	1780	MA6	C5-N7-C8	2.85	107.93	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	16	H2U	C5-C6-N1	2.84	120.12	111.52
1	2	1573	7MG	O6-C6-C5	-2.83	120.68	127.62
1	2	998	PSU	O2-C2-N1	-2.80	119.90	122.79
38	1	26	M2G	N9-C8-N7	-2.80	108.21	113.40
1	2	766	PSU	O2-C2-N1	-2.79	119.91	122.79
38	1	46	7MG	C2-N1-C6	-2.78	120.06	125.11
38	1	46	7MG	O6-C6-C5	-2.77	120.82	127.62
38	1	49	5MC	C5-C6-N1	-2.71	120.37	123.31
38	1	16	H2U	O2-C2-N1	-2.70	119.85	123.10
38	1	9	1MG	C5-C6-N1	2.69	119.99	115.02
1	2	1426	2MG	N9-C8-N7	-2.67	108.44	113.40
38	1	46	7MG	N9-C4-N3	2.66	129.36	125.46
1	2	465	PSU	O2-C2-N1	-2.65	120.05	122.79
38	1	48	5MC	CM5-C5-C6	-2.63	119.30	122.85
1	2	120	PSU	C6-C5-C4	2.61	119.94	118.17
1	2	1570	2MG	C5-C6-N1	2.61	119.91	113.25
1	2	1426	2MG	C5-C6-N1	2.60	119.88	113.25
38	1	10	2MG	C5-C6-N1	2.60	119.87	113.25
38	1	37	T6A	O10-C10-N6	-2.55	119.10	123.64
1	2	1289	PSU	C6-C5-C4	2.54	119.89	118.17
38	1	37	T6A	N3-C4-N9	2.54	131.48	127.17
38	1	47	H2U	O2-C2-N1	-2.53	120.06	123.10
38	1	26	M2G	C5-C6-N1	2.53	119.69	113.25
1	2	1426	2MG	O6-C6-C5	-2.51	119.90	126.53
1	2	1570	2MG	O6-C6-C5	-2.48	120.00	126.53
38	1	10	2MG	O6-C6-C5	-2.47	120.01	126.53
38	1	48	5MC	O4'-C4'-C3'	2.46	110.05	105.15
1	2	465	PSU	C6-C5-C4	2.46	119.83	118.17
1	2	1573	7MG	N9-C8-N7	2.42	106.81	103.37
38	1	46	7MG	N9-C8-N7	2.41	106.79	103.37
1	2	1190	B8N	O4'-C1'-C2'	2.40	108.47	105.15
38	1	58	1MA	C8-N7-C5	2.38	108.50	104.26
1	2	1289	PSU	O2-C2-N1	-2.36	120.36	122.79
1	2	1637	5MC	O2-C2-N3	-2.32	118.67	122.33
38	1	58	1MA	N9-C4-N3	2.29	132.12	126.90
38	1	37	T6A	C4-C5-N7	-2.28	107.97	110.58
38	1	9	1MG	C8-N7-C5	2.28	108.32	104.26
38	1	64	RIA	C4-N9-C8	2.27	108.12	105.74
1	2	120	PSU	O2-C2-N1	-2.20	120.51	122.79
38	1	26	M2G	C8-N7-C5	2.19	108.16	104.26
1	2	1570	2MG	C1'-N9-C4	-2.18	120.04	126.49
38	1	48	5MC	C5-C4-N3	-2.18	119.52	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	26	M2G	O6-C6-C5	-2.16	120.84	126.53
38	1	10	2MG	N1-C2-N3	-2.14	120.08	123.68
1	2	1780	MA6	C4-N9-C8	2.14	107.98	105.74
1	2	1780	MA6	C4-C5-N7	-2.13	108.15	110.58
38	1	10	2MG	C1'-N9-C4	-2.13	120.21	126.49
38	1	37	T6A	C13-C12-N11	-2.12	105.53	110.17
38	1	37	T6A	C4-N9-C8	2.12	107.96	105.74
1	2	1570	2MG	N1-C2-N3	-2.11	120.12	123.68
1	2	1006	5MC	C5-C4-N3	-2.10	119.60	121.75
38	1	64	RIA	C6-C5-C4	2.08	120.02	117.18
1	2	1570	2MG	C8-N7-C5	2.07	107.95	104.26
38	1	64	RIA	C4-C5-N7	-2.07	108.22	110.58
38	1	37	T6A	C5-C4-N9	2.07	108.06	105.81
38	1	10	2MG	C8-N7-C5	2.06	107.93	104.26
1	2	1426	2MG	N1-C2-N3	-2.05	120.23	123.68
1	2	766	PSU	O4'-C1'-C2'	2.03	107.96	105.15
1	2	120	PSU	O4'-C1'-C2'	2.03	107.96	105.15
1	2	1190	B8N	O4-C4-C5	-2.03	119.07	122.58
38	1	37	T6A	N6-C6-N1	2.02	122.76	117.54

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	998	PSU	C2'-C1'-C5-C4
1	2	998	PSU	C2'-C1'-C5-C6
1	2	1190	B8N	O4'-C4'-C5'-O5'
1	2	1573	7MG	O4'-C4'-C5'-O5'
1	2	1637	5MC	O4'-C4'-C5'-O5'
1	2	1780	MA6	C5-C6-N6-C10
1	2	1780	MA6	N1-C6-N6-C10
38	1	9	1MG	O4'-C4'-C5'-O5'
38	1	16	H2U	C4'-C5'-O5'-P
38	1	37	T6A	C14-C12-N11-C10
38	1	37	T6A	C13-C12-C14-O14
38	1	37	T6A	C13-C12-C14-C15
38	1	47	H2U	C4'-C5'-O5'-P
38	1	64	RIA	C5'-O5'-P'-O1X
38	1	64	RIA	C5'-O5'-P'-O2X
38	1	64	RIA	C5'-O5'-P'-O3X
1	2	1190	B8N	C3'-C4'-C5'-O5'
1	2	1289	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2	1289	PSU	O4'-C4'-C5'-O5'
1	2	1573	7MG	C3'-C4'-C5'-O5'
1	2	1637	5MC	C3'-C4'-C5'-O5'
38	1	9	1MG	C3'-C4'-C5'-O5'
38	1	16	H2U	C3'-C4'-C5'-O5'
38	1	26	M2G	C3'-C4'-C5'-O5'
38	1	47	H2U	C3'-C4'-C5'-O5'
38	1	48	5MC	C3'-C4'-C5'-O5'
38	1	37	T6A	C13-C12-N11-C10
1	2	120	PSU	O4'-C4'-C5'-O5'
38	1	16	H2U	O4'-C4'-C5'-O5'
38	1	26	M2G	O4'-C4'-C5'-O5'
38	1	48	5MC	O4'-C4'-C5'-O5'
38	1	64	RIA	C3'-C4'-C5'-O5'
38	1	64	RIA	C3A-C4A-C5A-O5A
1	2	766	PSU	C3'-C4'-C5'-O5'
38	1	10	2MG	O4'-C4'-C5'-O5'
38	1	10	2MG	C3'-C4'-C5'-O5'
38	1	49	5MC	O4'-C4'-C5'-O5'
38	1	64	RIA	O1'-C4'-C5'-O5'
38	1	47	H2U	O4'-C4'-C5'-O5'
38	1	64	RIA	O4'-C4A-C5A-O5A
38	1	64	RIA	C4A-C5A-O5A-P
38	1	37	T6A	N11-C12-C14-C15
1	2	1780	MA6	C5-C6-N6-C9
1	2	766	PSU	O4'-C4'-C5'-O5'
1	2	1289	PSU	C4'-C5'-O5'-P
38	1	46	7MG	C4'-C5'-O5'-P
38	1	48	5MC	C4'-C5'-O5'-P
38	1	58	1MA	C4'-C5'-O5'-P
1	2	1190	B8N	O4'-C1'-C5-C4
1	2	1190	B8N	N34-C33-C34-O36
1	2	998	PSU	C4'-C5'-O5'-P
38	1	37	T6A	N11-C12-C14-O14
1	2	120	PSU	C3'-C4'-C5'-O5'
38	1	26	M2G	C4'-C5'-O5'-P
38	1	49	5MC	C3'-C4'-C5'-O5'
38	1	49	5MC	C4'-C5'-O5'-P
1	2	1637	5MC	C2'-C1'-N1-C2
38	1	64	RIA	C3A-C2A-O2A-C1'
1	2	1426	2MG	C4'-C5'-O5'-P
1	2	1190	B8N	N34-C33-C34-O35

There are no ring outliers.

15 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1780	MA6	3	0
38	1	10	2MG	8	0
38	1	46	7MG	3	0
38	1	16	H2U	5	0
38	1	26	M2G	17	0
38	1	58	1MA	1	0
38	1	49	5MC	1	0
1	2	1426	2MG	2	0
38	1	64	RIA	2	0
38	1	37	T6A	2	0
38	1	47	H2U	3	0
1	2	1573	7MG	2	0
38	1	9	1MG	7	0
1	2	465	PSU	1	0
38	1	48	5MC	13	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 122 ligands modelled in this entry, 120 are monoatomic - leaving 2 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	$\# Z > 2$
46	MET	k	604	-	6,7,8	0.50	0	2,7,9	0.18	0
45	GCP	k	601	-	32,34,34	3.21	12 (37%)	49,54,54	1.64	9 (18%)

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
46	MET	k	604	-	-	0/5/6/8	-
45	GCP	k	601	-	-	2/19/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	k	601	GCP	O4'-C1'	8.73	1.62	1.42
45	k	601	GCP	C2'-C1'	-7.17	1.31	1.53
45	k	601	GCP	PB-O3A	6.32	1.65	1.58
45	k	601	GCP	O4'-C4'	-6.25	1.31	1.45
45	k	601	GCP	PA-O3A	5.58	1.65	1.59
45	k	601	GCP	C2-N2	4.82	1.45	1.34
45	k	601	GCP	C6-N1	-3.25	1.32	1.38
45	k	601	GCP	O2'-C2'	2.78	1.49	1.43
45	k	601	GCP	O3'-C3'	-2.78	1.36	1.43
45	k	601	GCP	O6-C6	-2.51	1.18	1.23
45	k	601	GCP	C5-N7	-2.36	1.34	1.39
45	k	601	GCP	PB-O2B	-2.04	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	k	601	GCP	C5-C4-N3	-5.38	119.82	128.39
45	k	601	GCP	C2-N3-C4	4.46	119.99	112.30
45	k	601	GCP	N9-C4-N3	3.20	132.35	125.95
45	k	601	GCP	C2-N1-C6	-2.84	119.96	125.11
45	k	601	GCP	N9-C8-N7	-2.70	108.39	113.40
45	k	601	GCP	C5-C6-N1	2.62	119.93	113.25
45	k	601	GCP	O6-C6-C5	-2.47	120.03	126.53
45	k	601	GCP	PB-O3A-PA	-2.19	125.21	132.37
45	k	601	GCP	C3'-C2'-C1'	2.15	105.54	101.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

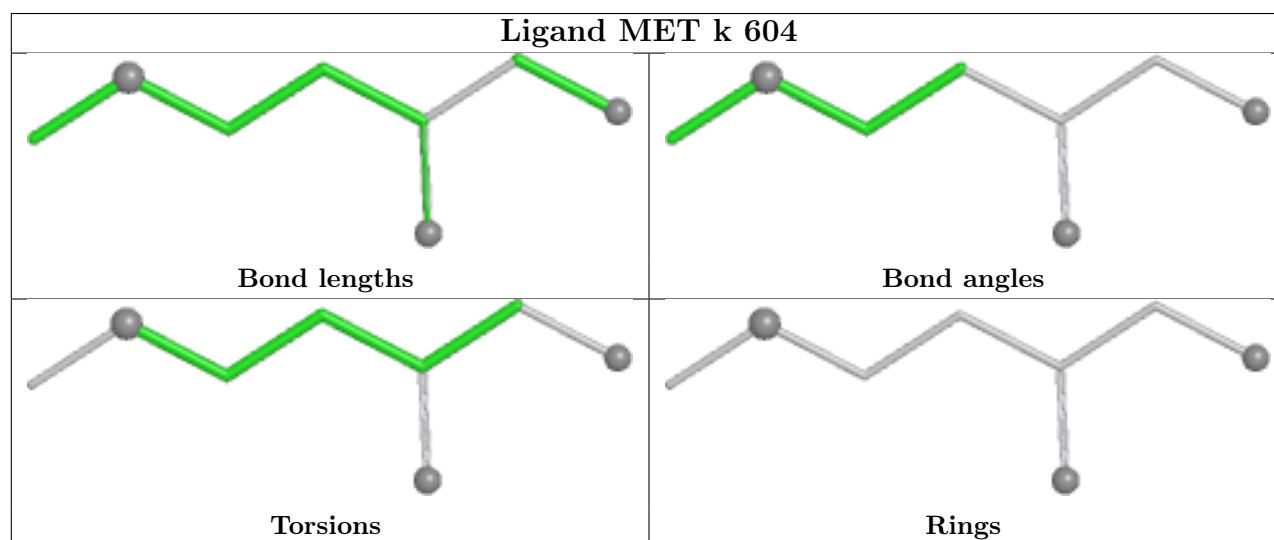
Mol	Chain	Res	Type	Atoms
45	k	601	GCP	O4'-C4'-C5'-O5'
45	k	601	GCP	C3'-C4'-C5'-O5'

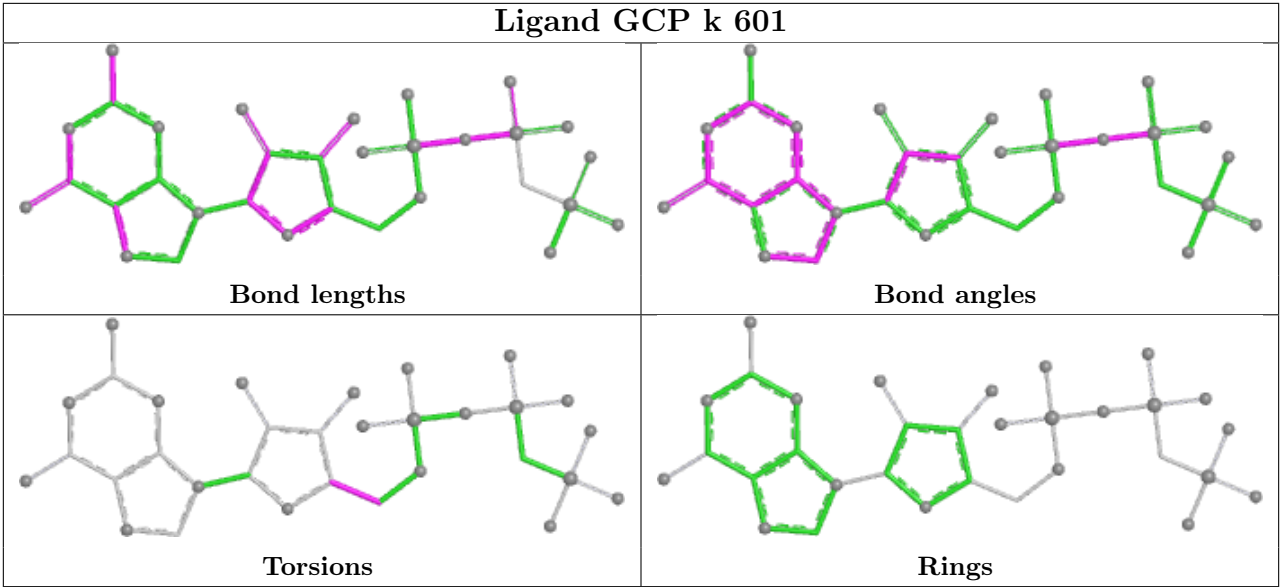
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	k	604	MET	1	0
45	k	601	GCP	2	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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	64:RIA	O3'	65:G	P	7.48
1	1	63:G	O3'	64:RIA	P	5.09
1	1	16:H2U	O3'	18:G	P	3.37

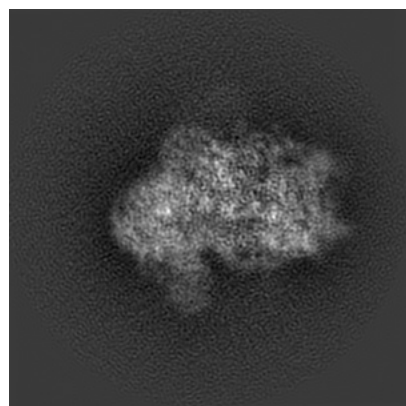
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19803. These allow visual inspection of the internal detail of the map and identification of artifacts.

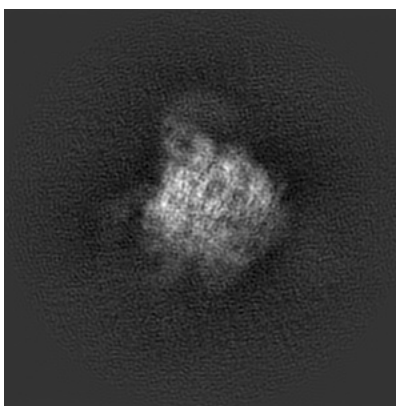
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

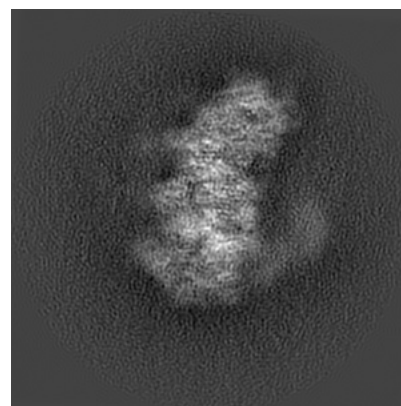
6.1.1 Primary map



X

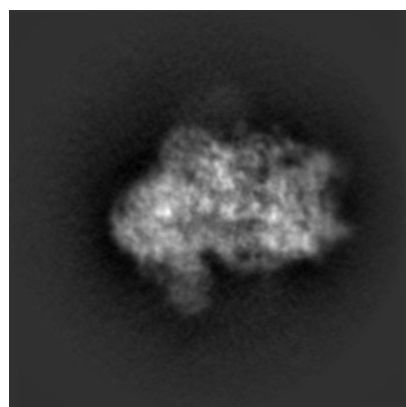


Y

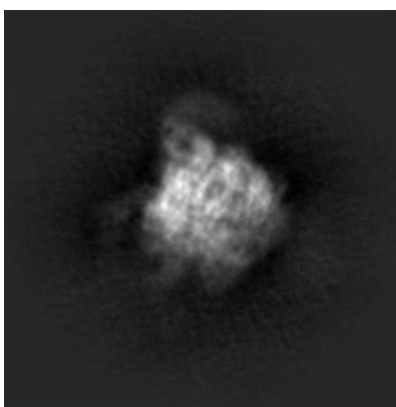


Z

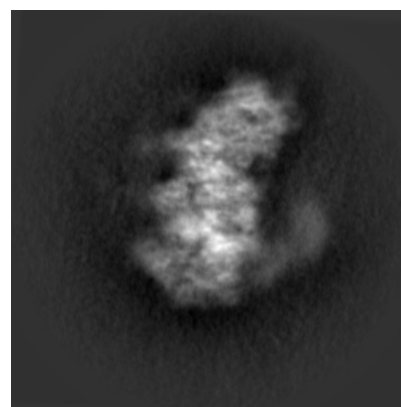
6.1.2 Raw map



X



Y

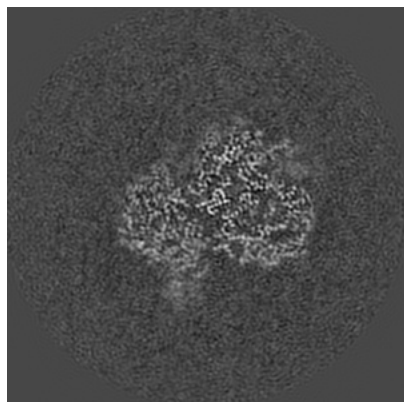


Z

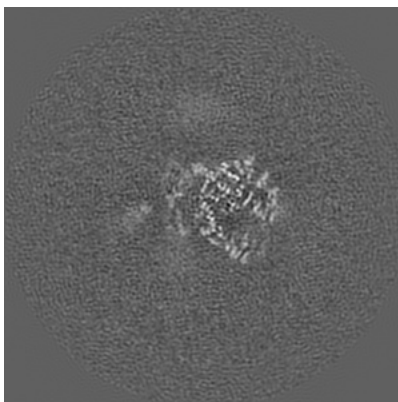
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

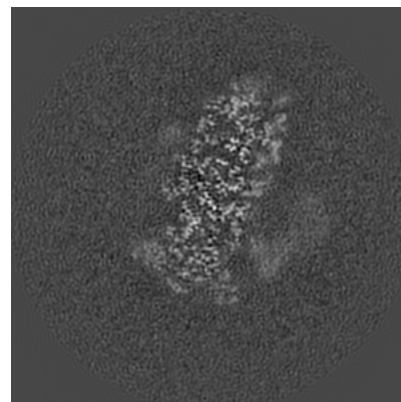
6.2.1 Primary map



X Index: 150

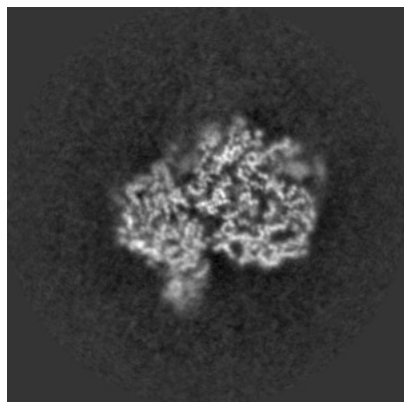


Y Index: 150

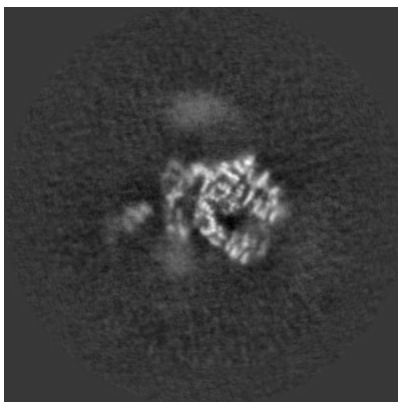


Z Index: 150

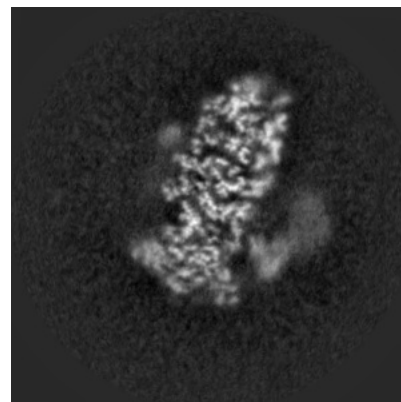
6.2.2 Raw map



X Index: 150



Y Index: 150

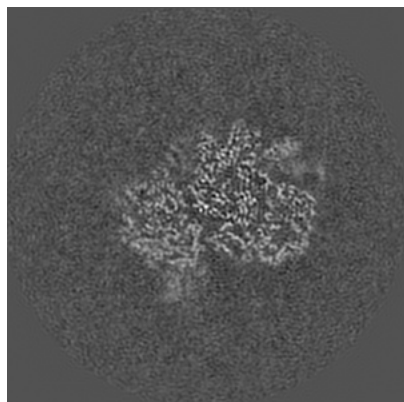


Z Index: 150

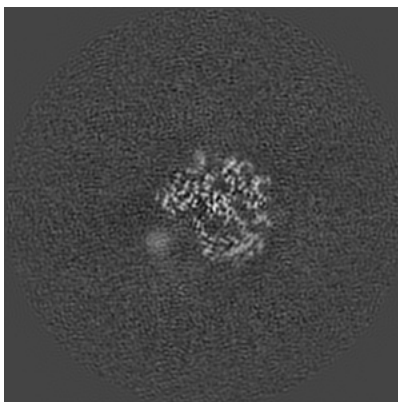
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

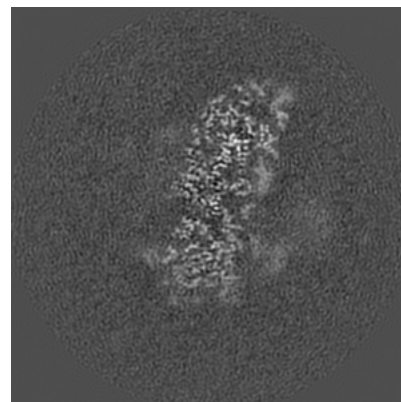
6.3.1 Primary map



X Index: 152

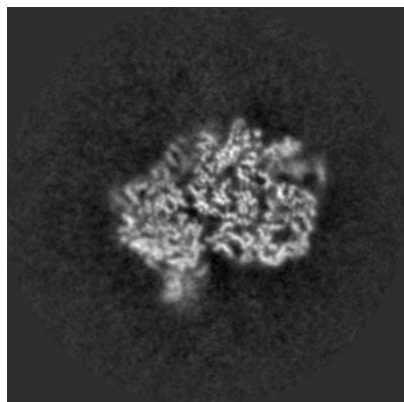


Y Index: 162

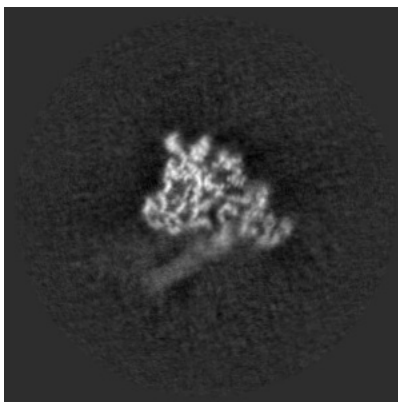


Z Index: 146

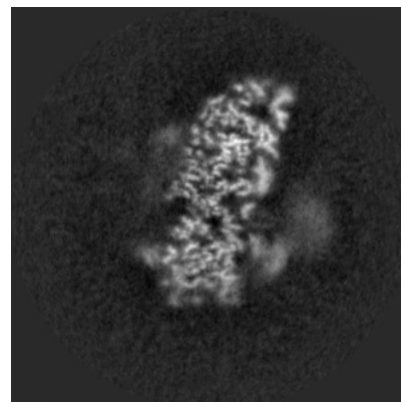
6.3.2 Raw map



X Index: 152



Y Index: 198

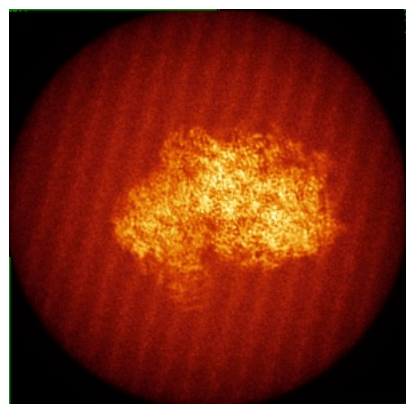


Z Index: 146

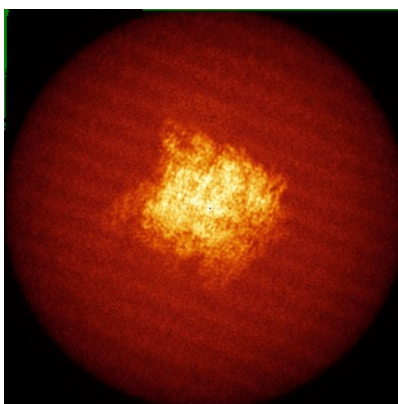
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

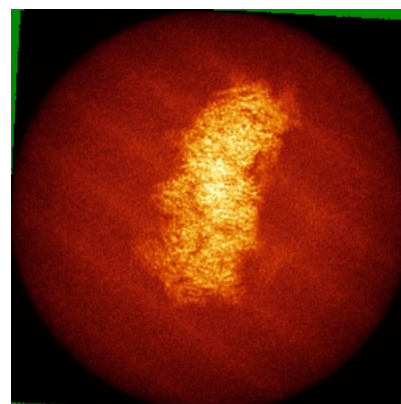
6.4.1 Primary map



X

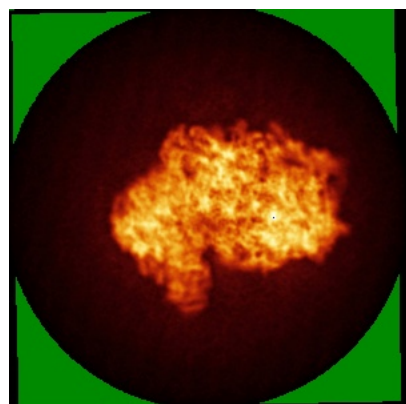


Y

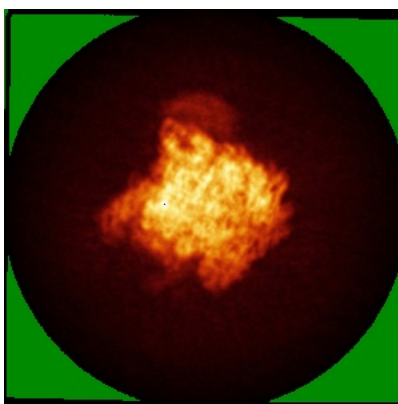


Z

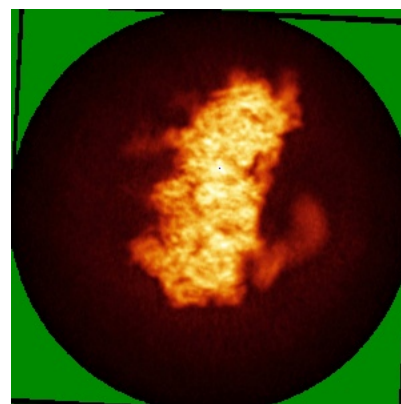
6.4.2 Raw map



X



Y

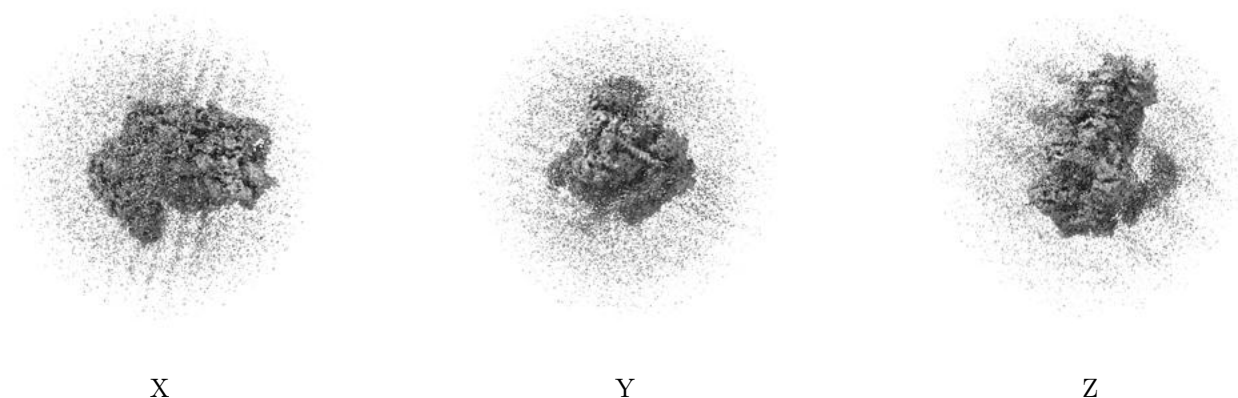


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

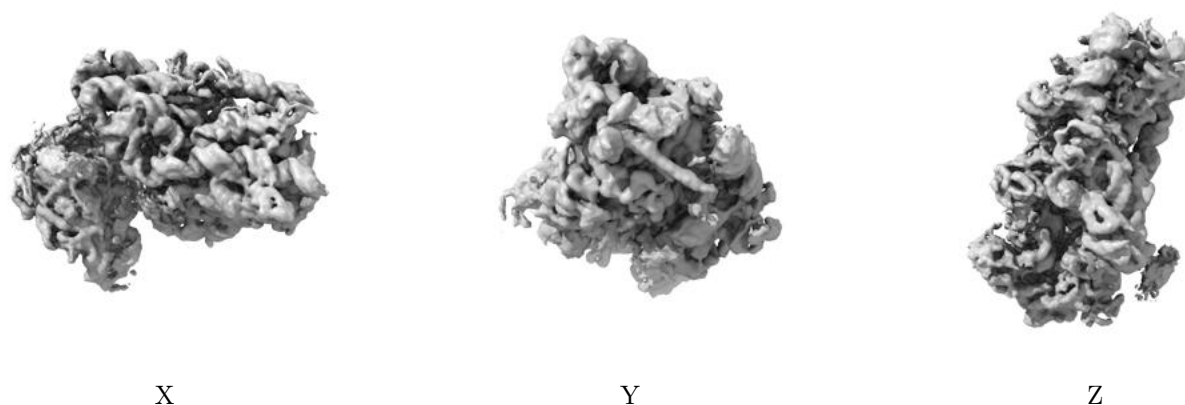
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

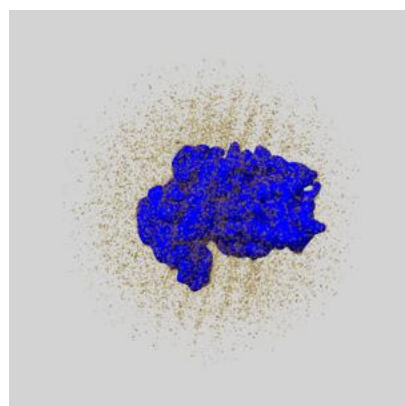
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

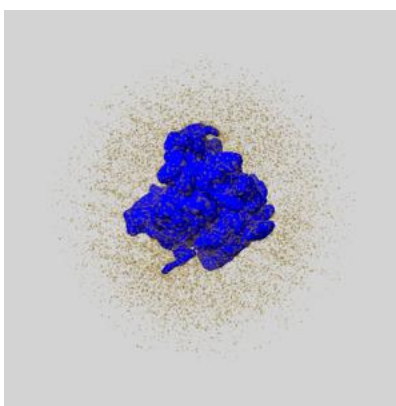
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

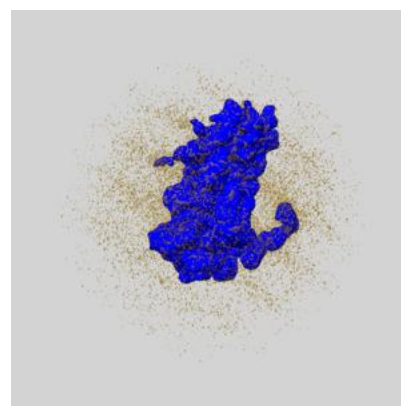
6.6.1 emd_19803_msk_1.map [i](#)



X



Y

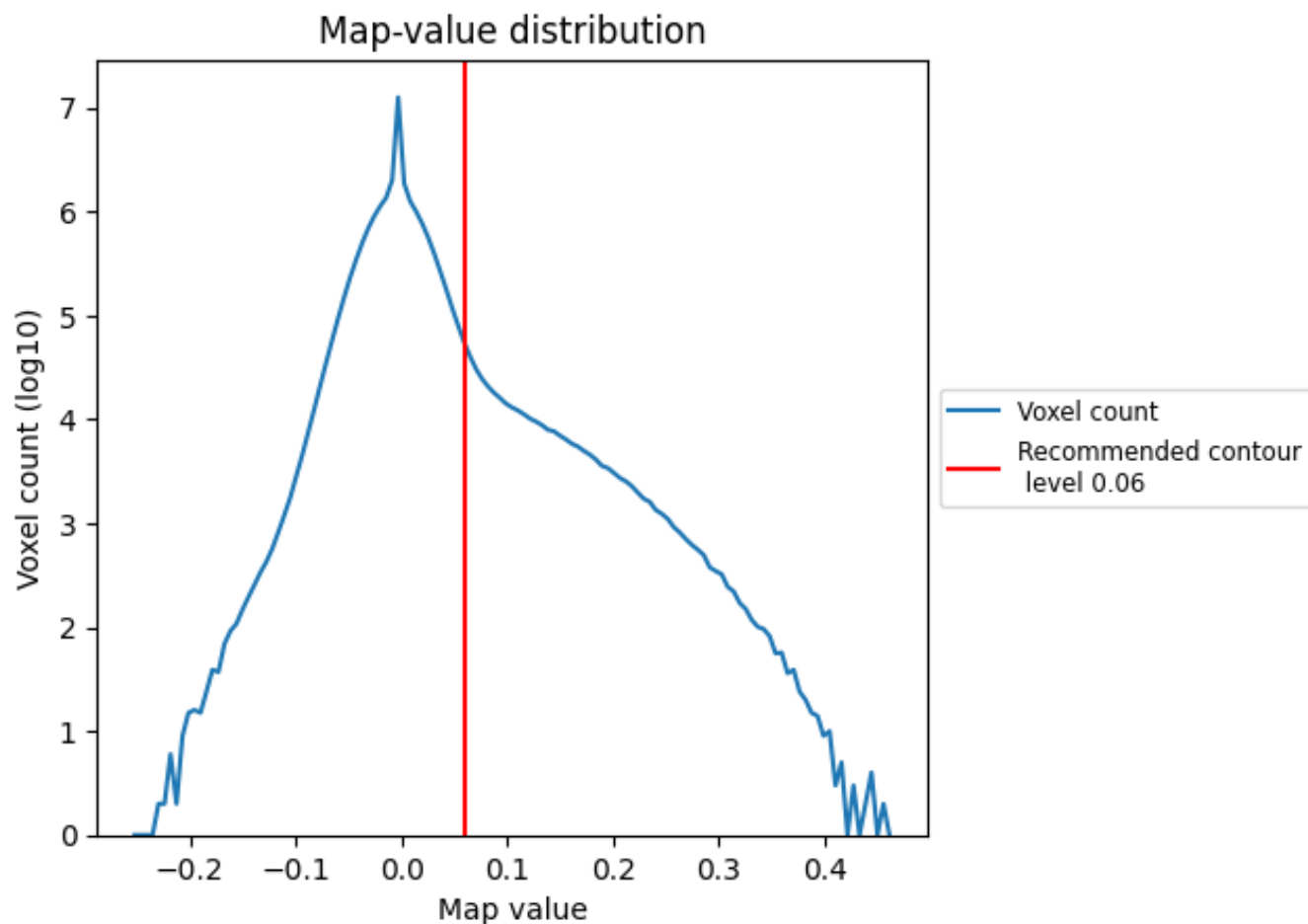


Z

7 Map analysis [i](#)

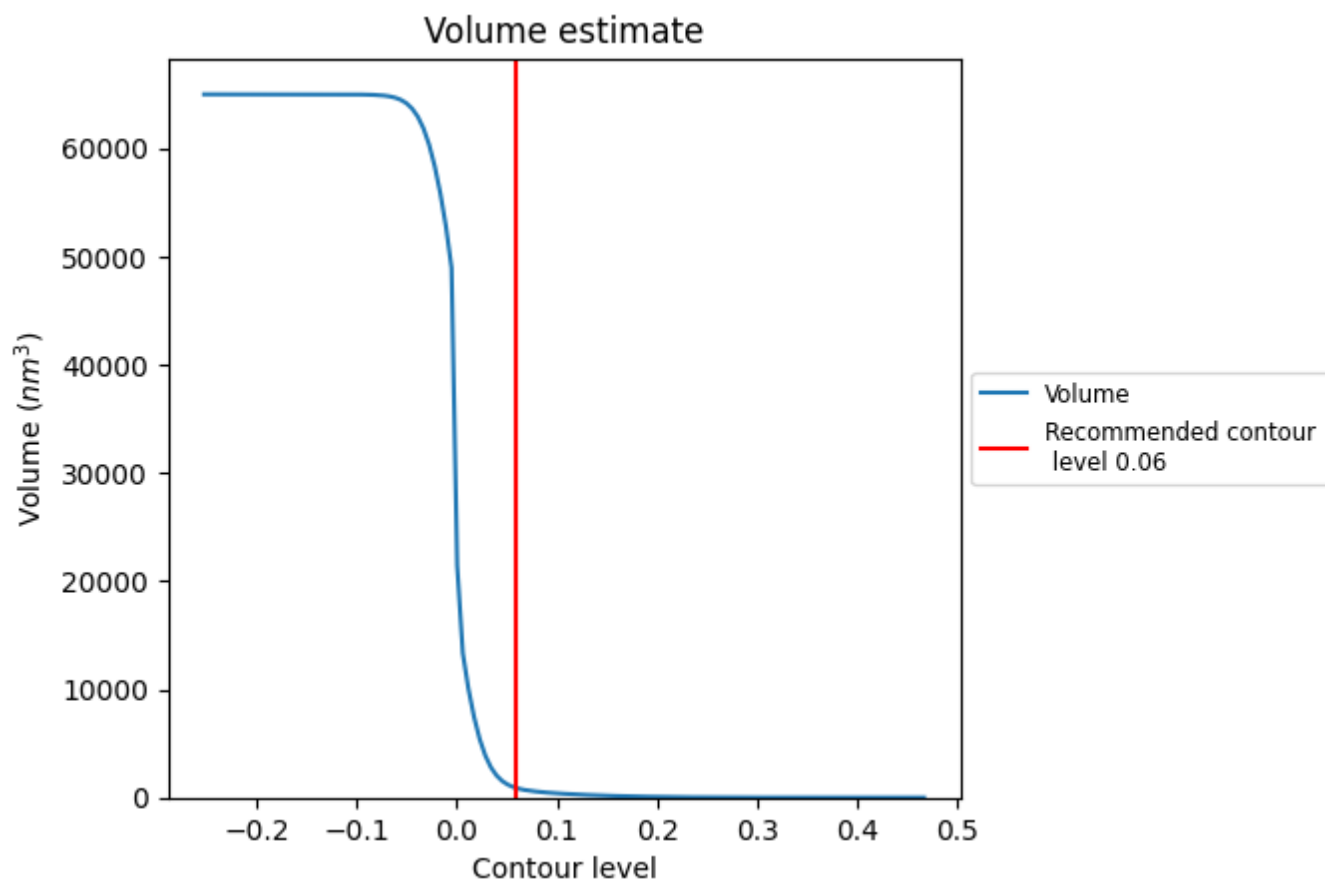
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

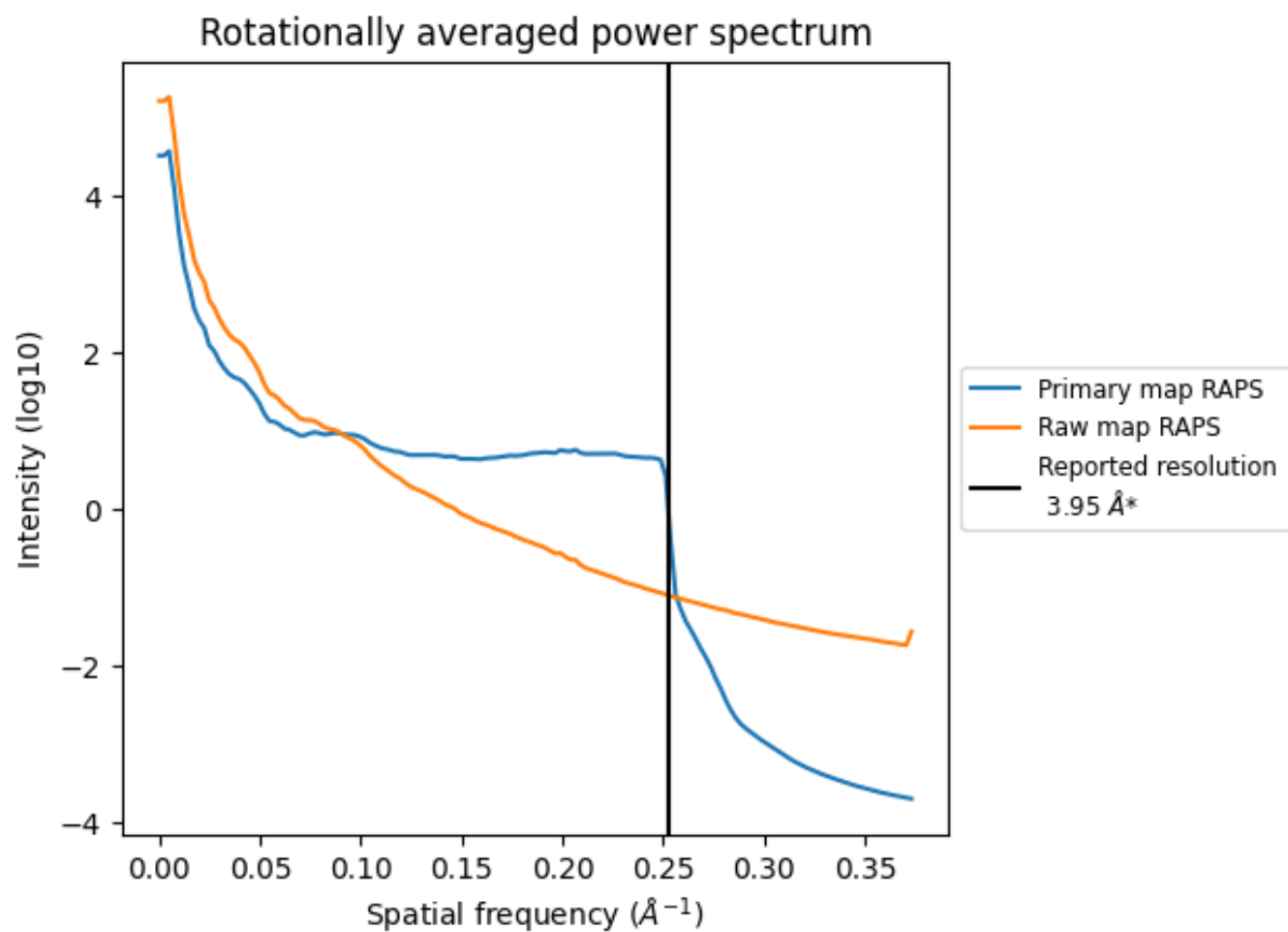
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 878 nm³; this corresponds to an approximate mass of 793 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

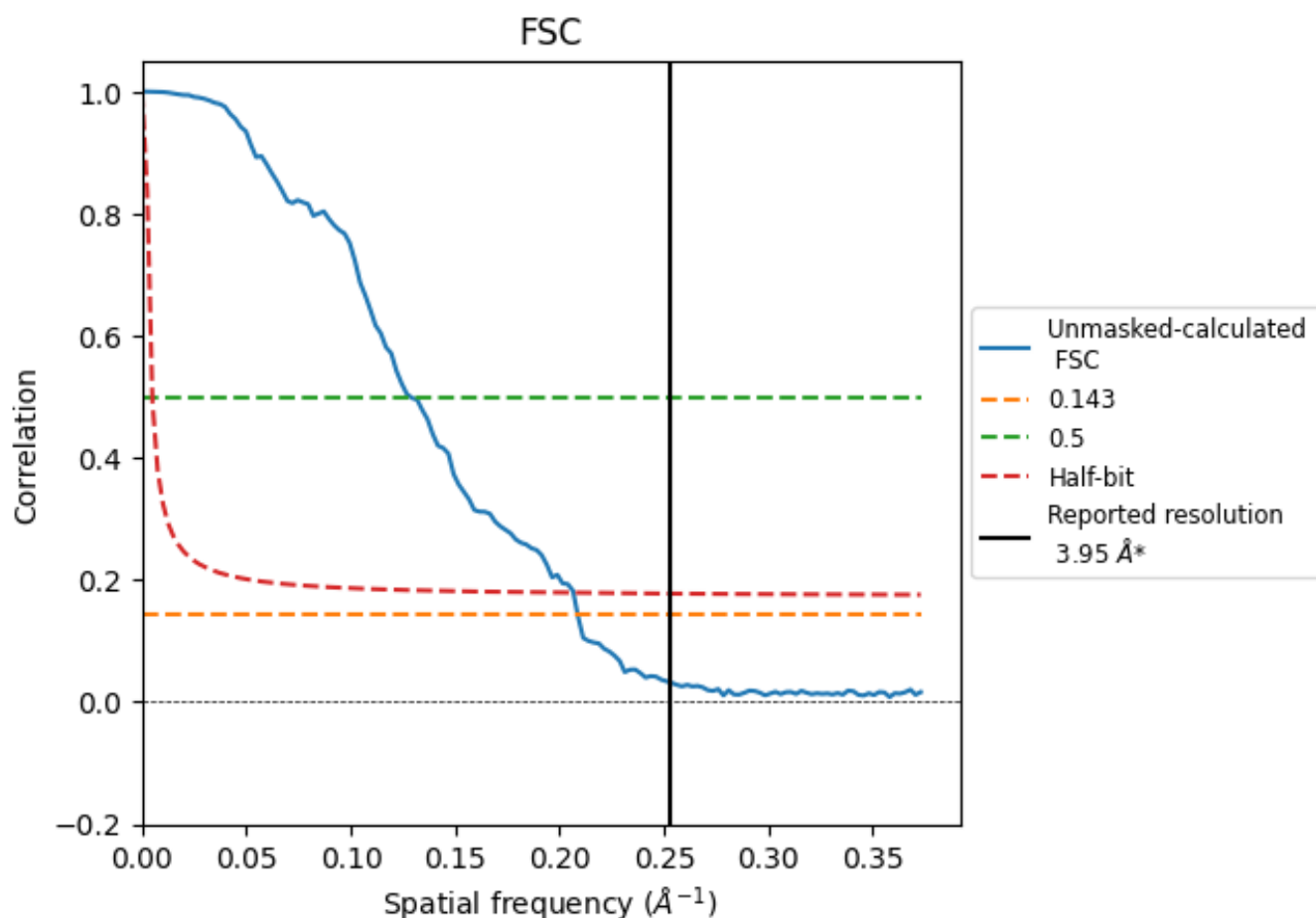


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.253 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

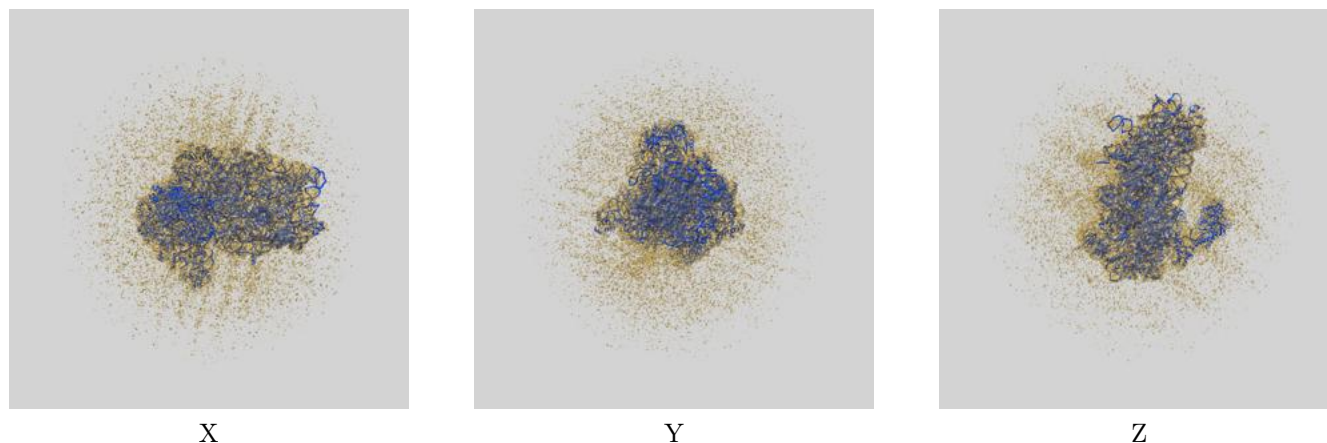
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.79	7.78	4.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.79 differs from the reported value 3.95 by more than 10 %

9 Map-model fit [i](#)

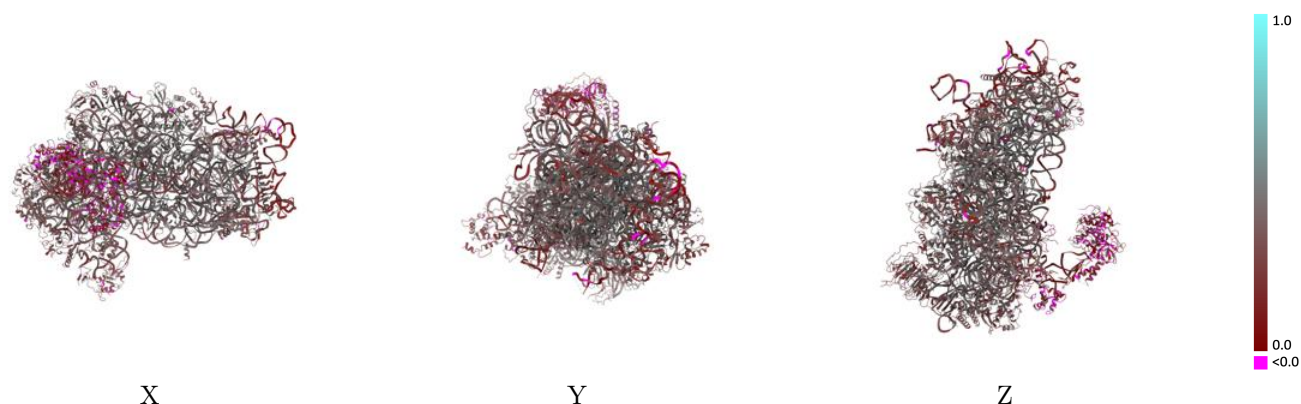
This section contains information regarding the fit between EMDB map EMD-19803 and PDB model 8S8F. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



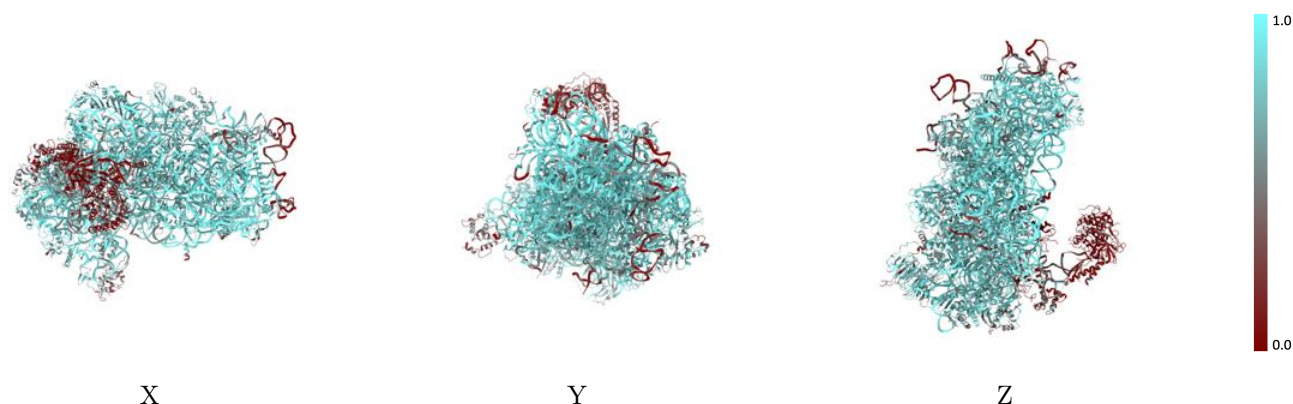
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



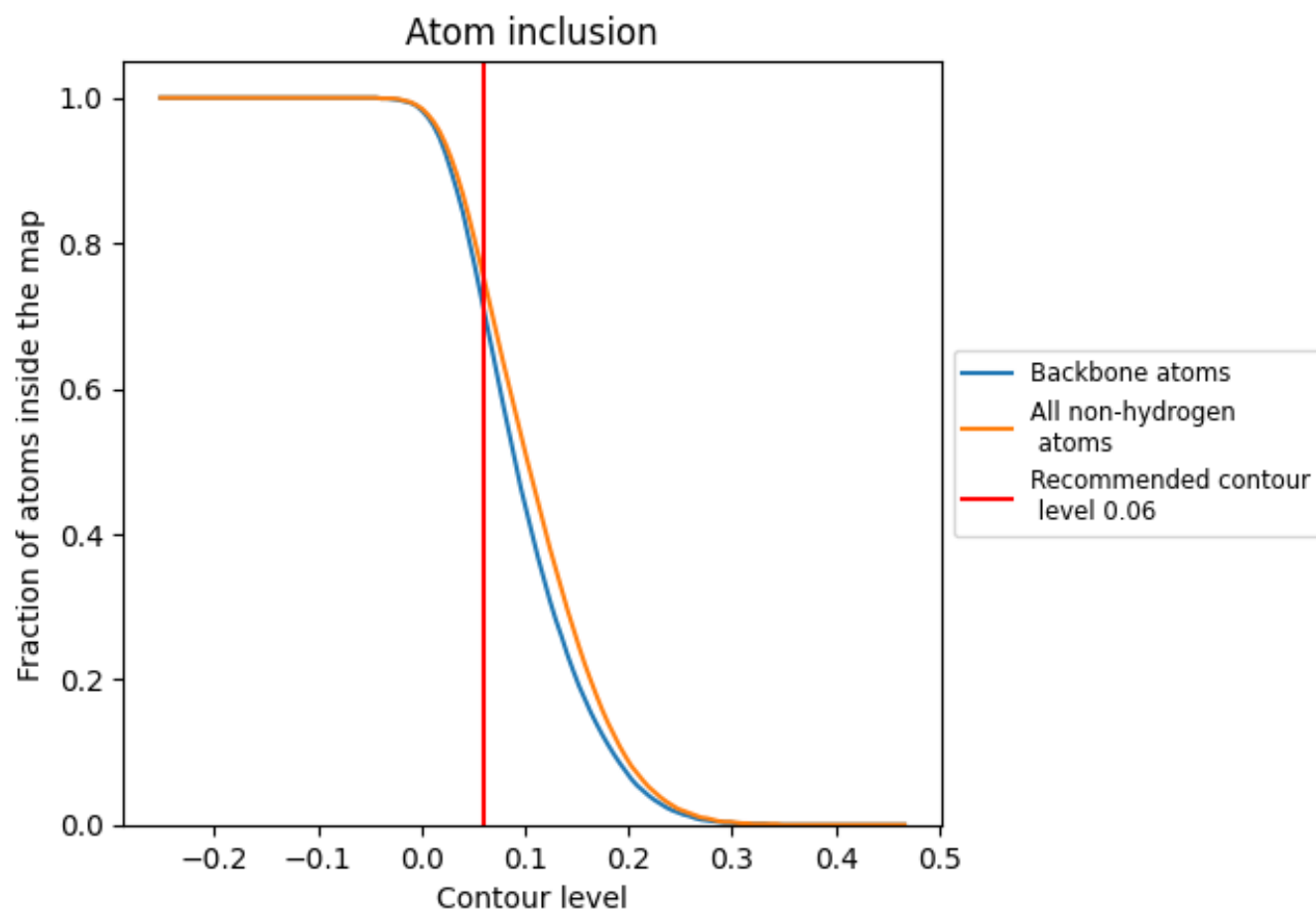
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.3520
1	 0.5570	 0.2260
2	 0.8740	 0.3620
3	 0.3470	 0.2790
A	 0.8160	 0.3950
B	 0.7740	 0.3740
C	 0.8090	 0.4270
D	 0.7620	 0.3810
E	 0.8430	 0.4260
F	 0.7390	 0.3810
G	 0.8070	 0.3530
H	 0.6840	 0.3430
I	 0.8030	 0.4060
J	 0.7890	 0.4000
K	 0.7570	 0.3290
L	 0.7540	 0.4000
M	 0.3430	 0.2270
N	 0.8310	 0.4110
O	 0.7930	 0.3800
P	 0.7710	 0.3190
Q	 0.8040	 0.3840
R	 0.7090	 0.3610
S	 0.7670	 0.3370
T	 0.8300	 0.3570
U	 0.6870	 0.3540
V	 0.8700	 0.4020
W	 0.8170	 0.4360
X	 0.8260	 0.4390
Y	 0.8370	 0.3940
Z	 0.5230	 0.3140
a	 0.8220	 0.4370
b	 0.8060	 0.4130
c	 0.7660	 0.4360
d	 0.8510	 0.4150
e	 0.7210	 0.3820



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Chain	Atom inclusion	Q-score
f	 0.4890	 0.2520
g	 0.7360	 0.3310
h	 0.1790	 0.3130
i	 0.4460	 0.3480
j	 0.1700	 0.1730
k	 0.0850	 0.1480
l	 0.0590	 0.0490
m	 0.0520	 0.1940