



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:29 PM UTC

PDB ID : 8S8H / pdb_00008s8h
EMDB ID : EMD-19805
Title : Structure of a yeast 48S-AUC preinitiation complex in closed conformation (model py48S-AUC-2.2)
Authors : Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on : 2024-03-06
Resolution : 4.00 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:

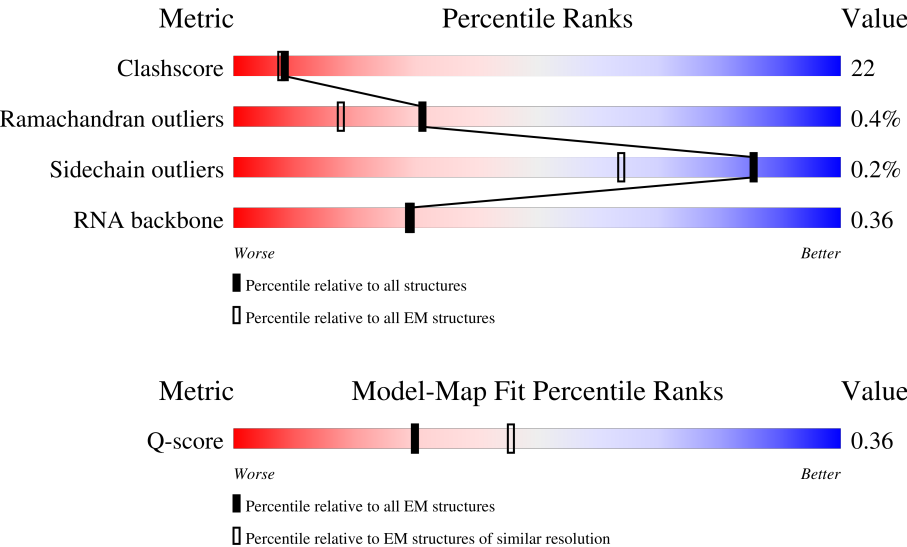
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 4.00 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.



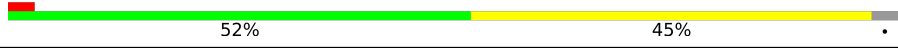
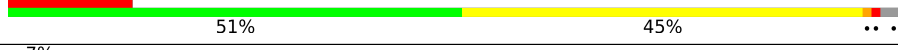
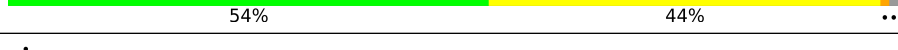
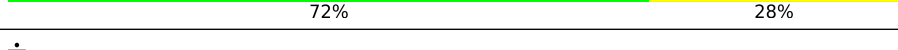
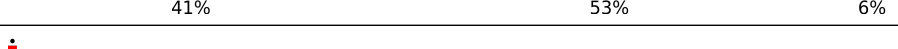
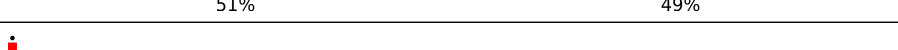
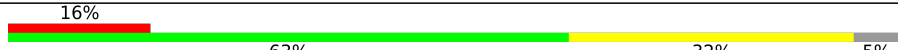
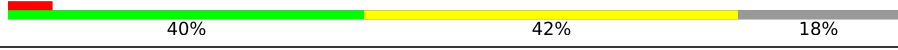
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	7% 21% 57% 21%
2	A	254	5% 47% 39% 14%
3	B	255	6% 45% 41% 12%

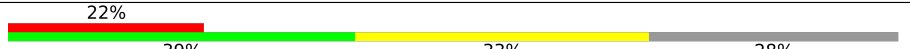
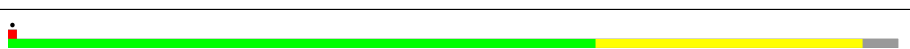
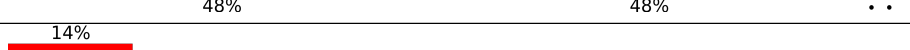
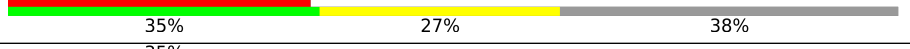
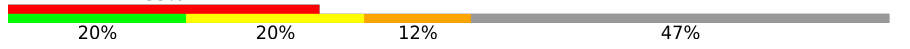
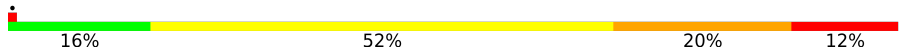
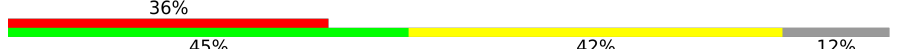
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Mol	Chain	Length	Quality of chain
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	h	25	
21	D	237	
22	F	227	
23	K	106	
24	M	134	
25	P	142	
26	Q	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	527	
41	l	285	

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 86900 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	1798	Total	C	N	O	P	0	0
			38190	17073	6722	12597	1798		

- 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
			1471	929	287	254	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	267	Total	C	N	O	S	0	0
			2145	1369	358	407	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	470	Total	C	N	O	S	0	0
			3596	2279	633	666	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	134	Total	C	N	O	S	0	0
			1083	689	194	193	7		

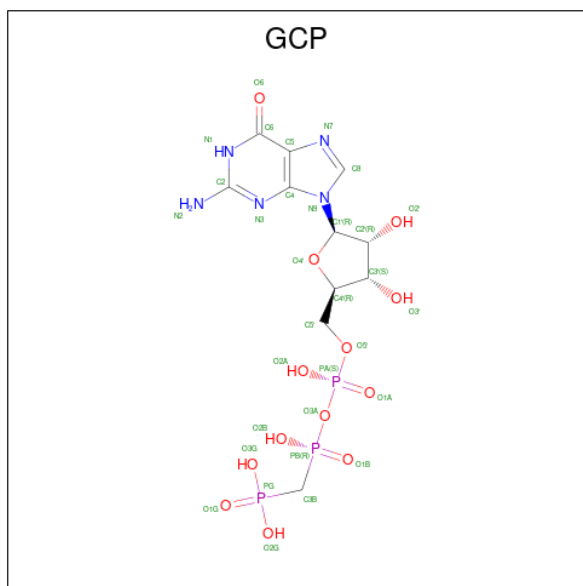
- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
42	2	111	Total	Mg	0
			111	111	
42	N	1	Total	Mg	0
			1	1	
42	Q	1	Total	Mg	0
			1	1	
42	i	1	Total	Mg	0
			1	1	
42	3	1	Total	Mg	0
			1	1	
42	k	1	Total	Mg	0
			1	1	

- Molecule 43 is ZINC ION (CCD ID: ZN) (formula: Zn).

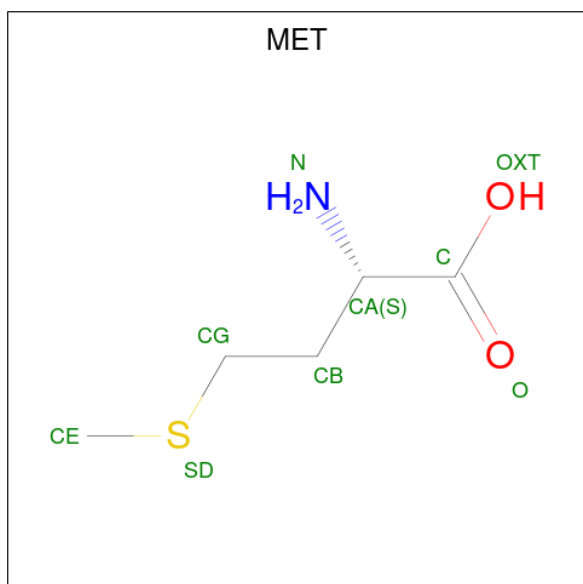
Mol	Chain	Residues	Atoms		AltConf
43	a	1	Total	Zn	0
			1	1	
43	b	1	Total	Zn	0
			1	1	
43	f	1	Total	Zn	0
			1	1	

- Molecule 44 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
44	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 45 is METHIONINE (CCD ID: MET) (formula: $\text{C}_5\text{H}_{11}\text{NO}_2\text{S}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
45	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

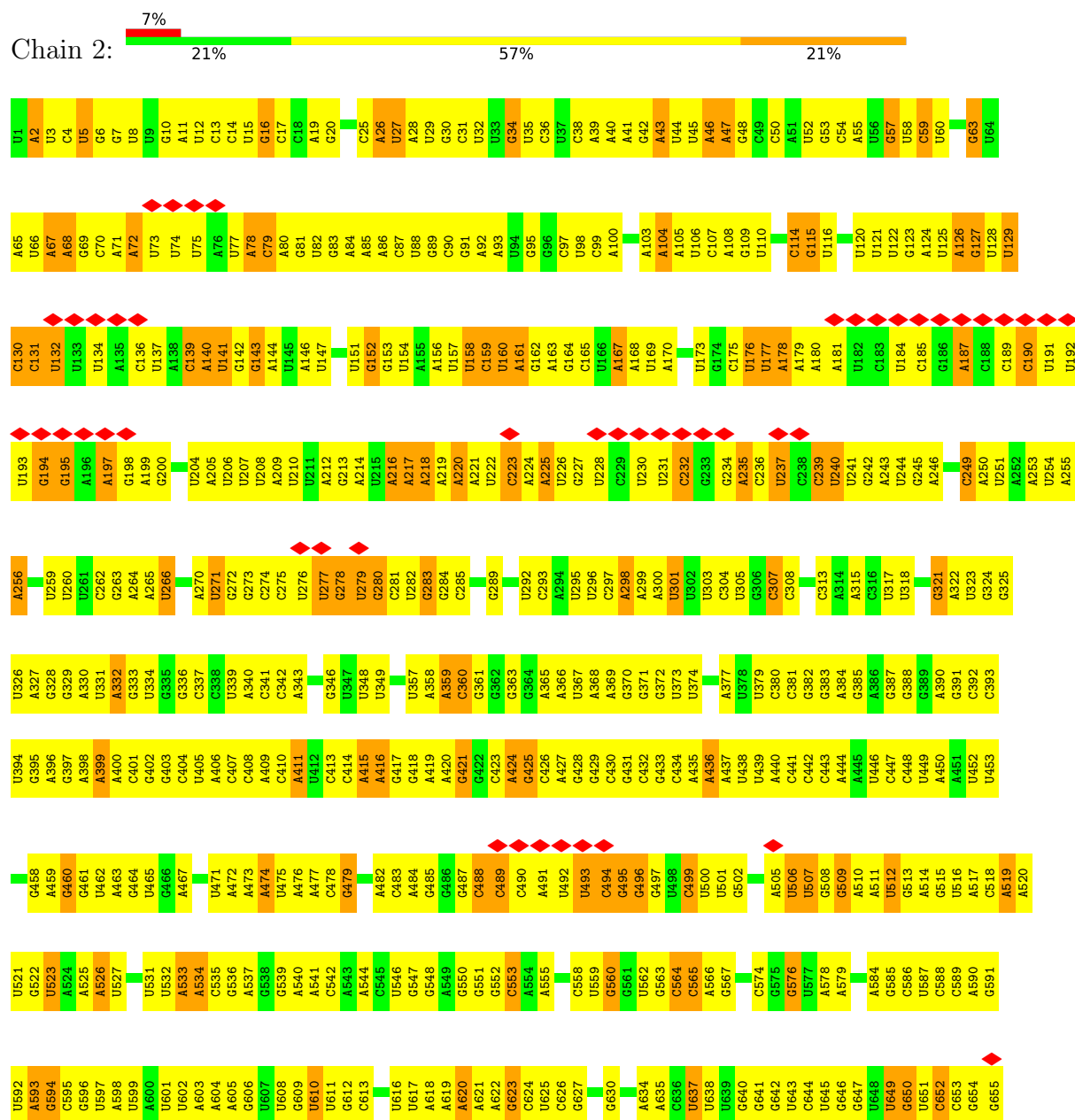
- Molecule 46 is water.

Mol	Chain	Residues	Atoms		AltConf
46	2	3	Total 3	O 3	0

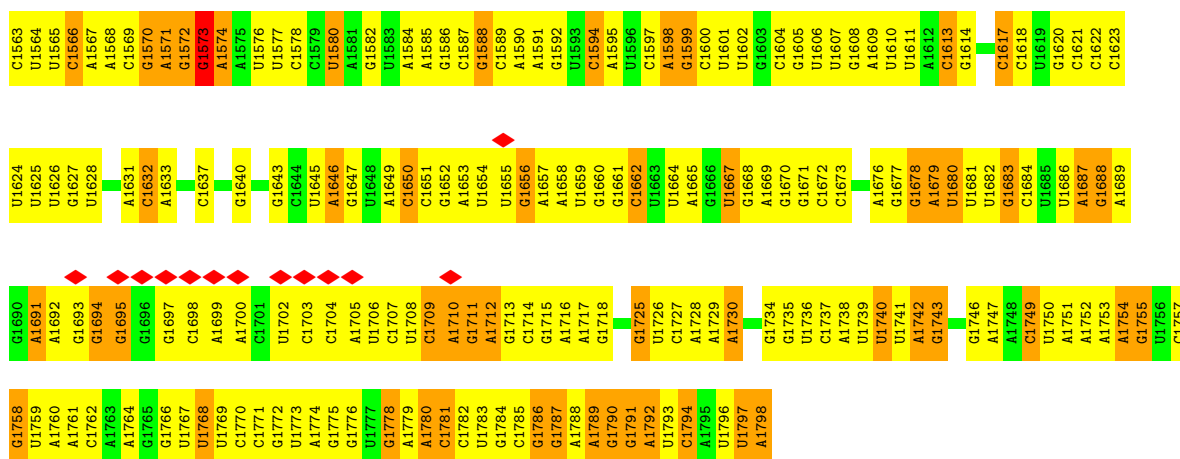
3 Residue-property plots

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.

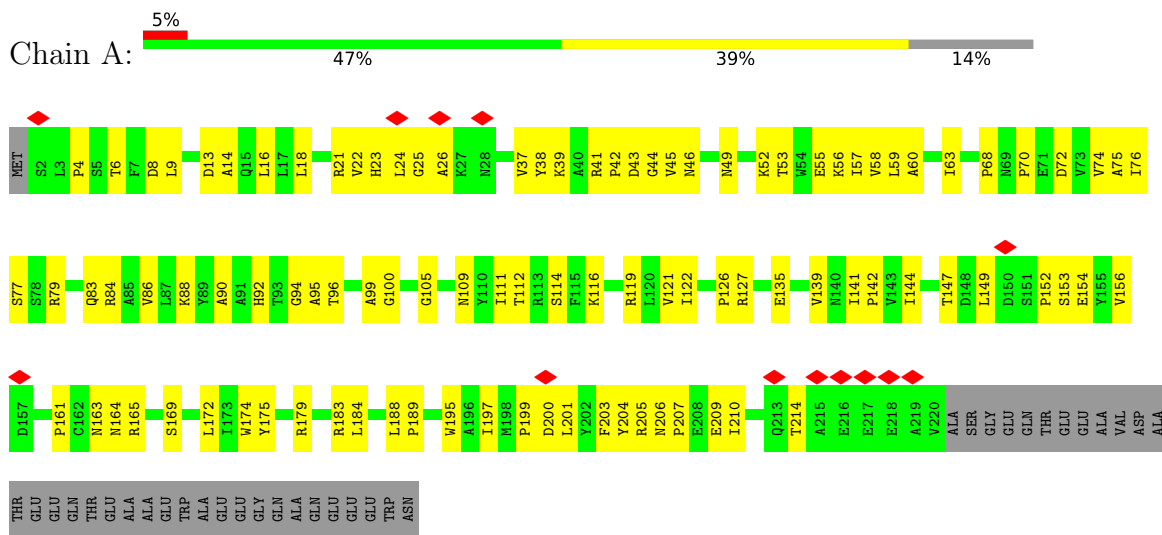
• Molecule 1: 18S ribosomal RNA



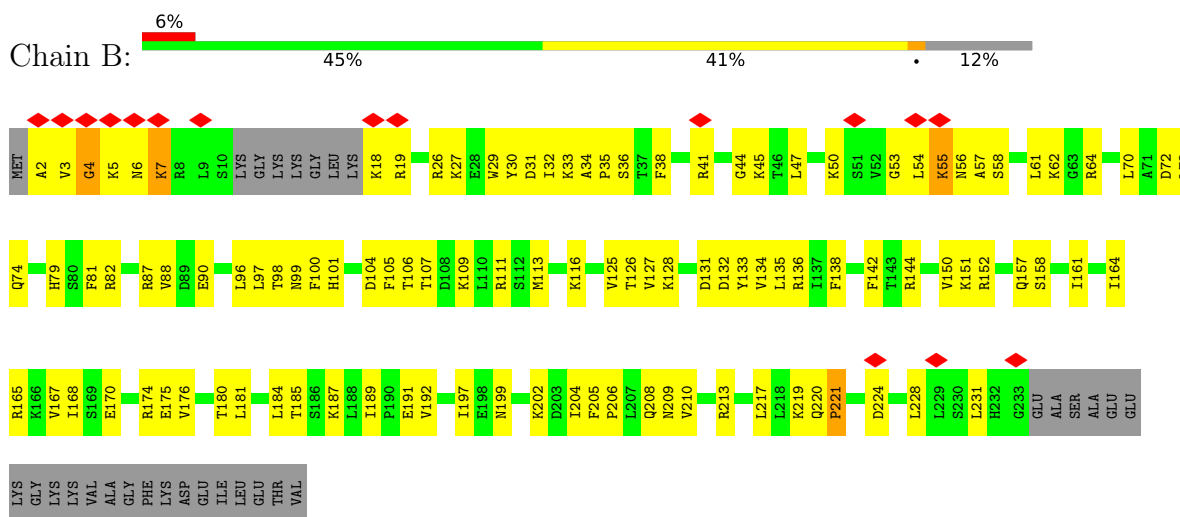
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A1501	U1432	G1363	G1297	A1237	G1168	U1103	G1040	A976	C909	G845	A780	U719	C657
A1503	G1433	C1364	G1298	U1238	G1169	C1104	G1041	A977	U910	A846	A781	G720	C658
	A1434	C1365	A1299	U1239	A1170	U1105	A1042	A978	G912		A782	U721	G659
U1506	G1437	G1366	U1300	G1240	G1171	G1106	U1043	A979	G913	G852	C783	G722	A660
C1507	C1438	U1367	U1301	G1241	G1172	G1107	C1044	G979	A914	A854	C784	G723	C661
		U1368	U1302	G1242	G1173	G1108	G1045		U915	A855	C785	G724	U862
G1510	U1441	C1370	C1305	A1243	G1177	G1109	G1046	A982	U916	U856	A787	G725	U863
U1511	A1442	U1371		C1244	G1178	G1110	U1047	G983	U917	G857	A788	U726	U663
G1512	G1443	C1372	U1309	C1245	C1179	G1111	U1048	G984	A918	U858	A789	G727	U664
A1513	A1444	U1373	U1310	U1246	G1180	A1112	G1049	G985	U919	U859	A790	C728	U665
A1514				C1247	U1181	G1113	G1050	G986	U920	U860	A791	G729	U666
U1515	U1447	U1376	U1313	U1248	U1182	G1114	U1051	A987	U921	A861	A792	A728	G670
C1516	U1448	C1377	G1314	U1249	A1183	A1115	G1052	U988	G922	U862	A793	G730	G671
U1517	C1449	U1378	G1315	C1250	U1184	U1119	U1053	G989	A922	A863	U794	G731	C669
U1518	U1450	U1379	U1316	U1251	A1185	C1120	U1054	G990	A923	U864	A795	G732	G672
G1519	A1380	G1317	G1317	U1252	G1187	G1121	U1055	A991	G924	G865	C796	G733	
U1520				U1253	G1188	G1122	U1056	A992	A925	G866	C797	G734	
G1521	C1454	G1381	A1320	G1254	A1189	U1123	U1057	U995	U927	G867	A798	G735	
A1522	G1455		A1321	U1255	C1189	A1124	C1058	G996	A928	A868	U799	A733	
A1523	C1457		G1322	U1256	B8N1190	G1125	U1059	A997	A929	C869	U799	A734	
	A1458		G1323	U1257		G1126	U1060	U998	C930	C870	G801	G736	
U1526	C1459	U1388	A1324	U1258	A1193		U1061	U999	U931	G871	A802	C737	
C1527		U1390	A1325	U1259	C1194	A1131	U1062	A1000	A932	U872	A803	C738	
C1528		C1391	C1326	U1260	A1195	A1132	G1063		C933	C873	U804	C739	
G1529	G1464	G1392	G1327	G1261	G1196	C1133		U1003	G935	G874	A811	G740	
U1530	C1465		A1328	G1262	G1197	G1134	G1066	A1004	U944	G875	U812	C741	
G1531	A1467	U1396	G1329	U1263	G1198	U1135	C1067	C1005	A938	G876	U813	G742	
G1532	C1468	C1397	A1330	G1264	G1199	U1136	A1068	C1006	U945	G877	G814	U743	
U1533	A1469	A1398	G1331	G1265	G1200	A1137	C1069	G1007	U946	G878	G815	U744	
C1534	C1470	A1399	C1332	G1266	A1201	A1138	U1070	U1008	A947	C879	A816	C745	
G1535	U1471	G1400	U1333	U1267	A1202	A1139	C1071	C1009	U950	A880	C817	C746	
U1536	A1472	C1401	U1334	G1268	C1204	G1140	G1072	G1010	U944	U881	G818	C747	
G1537	A1473	G1402	A1335	G1270	C1205	A1141	A1075	A1012	U945	A883	U819	C748	
G1538	C1474	G1403	U1336	U1271	C1206	U1142	A1076	G1013	U946	G884	U821	U749	
G1539	G1475	A1404	C1337	G1272	A1207	U1143	C1076	U1014	U947	U885	G822	G751	
U1540	C1476	U1405	C1338	G1273	G1208	U1144	C1077	C1015	A950	U888	G823	U752	
A1541	A1477	U1406	U1339	A1274	C1209	G1145	U1078	U1016	A951	C889	U824	A753	
U1542	G1478	G1407	A1340	U1275	A1210	U1146	A1080	C1020	G952	A890	C826	A754	
A1543	C1479	A1408	C1341	G1276	G1211	A1147	C1081	C1021	G953	A891	U827	A755	
G1544	A1480	U1409	U1342	G1277	U1212	G1148	A1082	A1022	G954	U892	A828	A756	
A1545	G1481	G1410	A1343	C1278	G1215	G1149	G1083	C1023	U958	U893	U829	A757	
C1546	C1482	U1411	A1344	C1279	A1216	A1150	A1084	U1024	U959	G894	U830	U758	
G1547	C1483	U1412	A1345	G1280	G1217	A1151	G1085	A1025	U960	C896	U831	U759	
A1548	G1484	U1413	U1346	U1281	A1218	G1152	A1086	A1026	U961	A897	U832	A760	
U1549	A1485	G1414	A1347	U1282	G1219	G1153	A1087	U1027	C962	G898	U833	A761	
U1550	G1486	A1415		C1283	A1220	G1154	A1087	C1028	A962	G900	U834	A762	
G1551	U1487	G1416	G1350	U1284		C1155		U1028	U963	U899	U835	G763	
U1552	A1488	G1417	U1351	U1285	U1224	A1156	A1090	A1029	U964	A966	G836	U764	
A1553	C1489	C1418	U1352	A1286	G1227	C1157	A1091	U1030	U965	U902	G837	G765	
U1554	A1490	A1491	G1353	G1287	U1228	C1158	A1092	C1032	A967	U903	U838	U766	
U1555	C1495		C1354	U1288	G1229	A1159		G1031	U968	A804	U839	C767	
U1556	A1496	U1425	U1355	U1289	A1229	C1161	U1096	U1034	A969	A905	U840	A771	
A1557	U1497	G1426	G1356	G1290	U1230	A1162	U1097	G1033	C968	A906	U842	C772	
U1558	G1498	G1427	C1357	G1291		G1163	U1098	G1034	U969		U843	C773	
U1559	C1499	U1428	C1358	U1292	A1233	G1164	U1099	A1035				C774	
G1560		C1497	A1359	G1293	G1234	A1165	G1100	C1036				C775	
U1561		C1498	C1360	U1294	A1235	G1166	G1101	U1037				C776	
U1562			U1361	A1295				A1038				C777	
												C778	



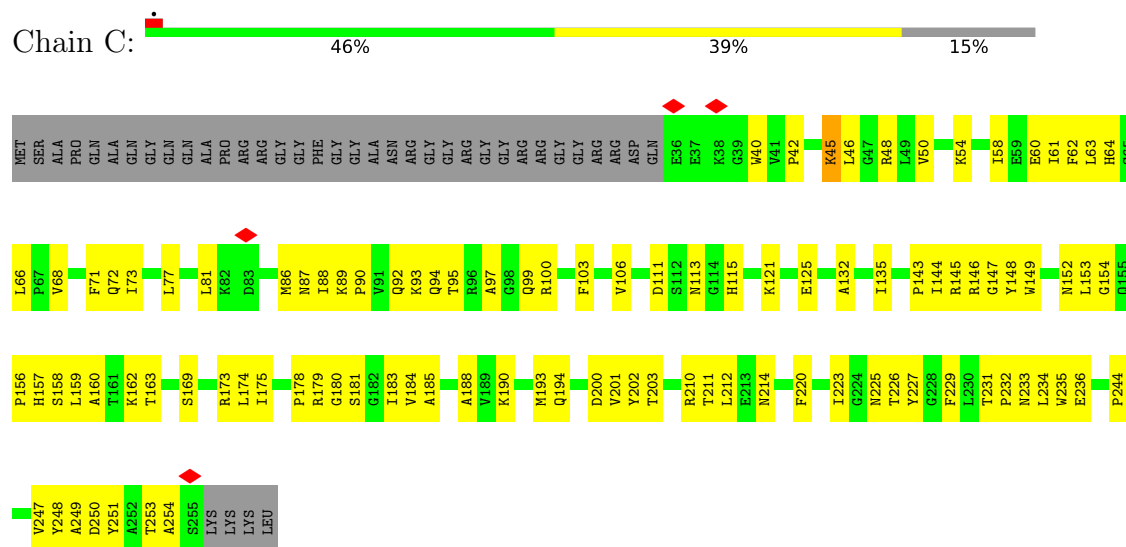
• Molecule 2: Small ribosomal subunit protein uS2



• Molecule 3: Small ribosomal subunit protein eS1



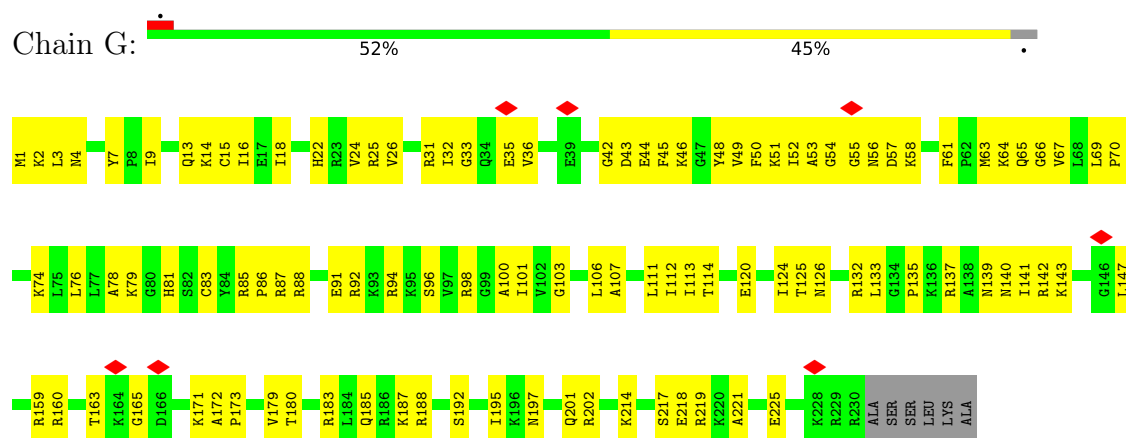
• Molecule 4: Small ribosomal subunit protein uS5



• Molecule 5: 40S ribosomal protein S4

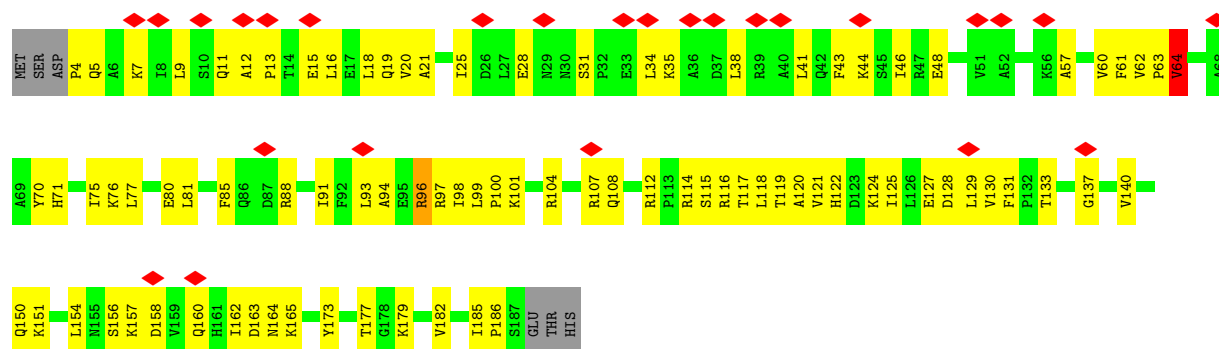


• Molecule 6: Small ribosomal subunit protein eS6

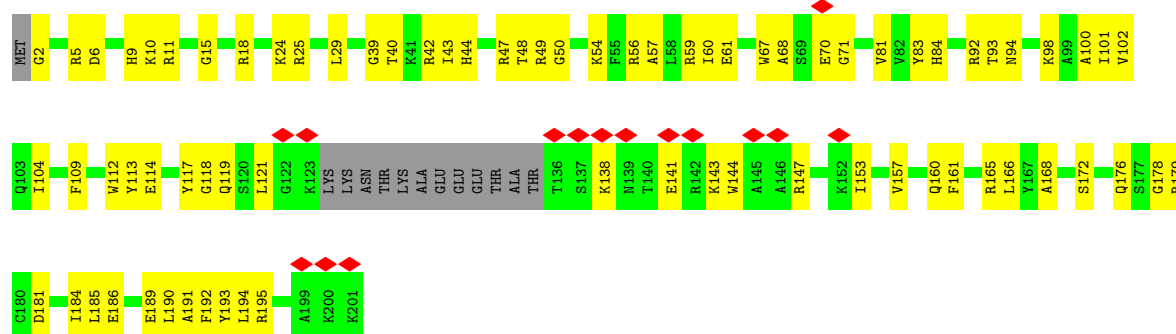


• Molecule 7: 40S ribosomal protein S7

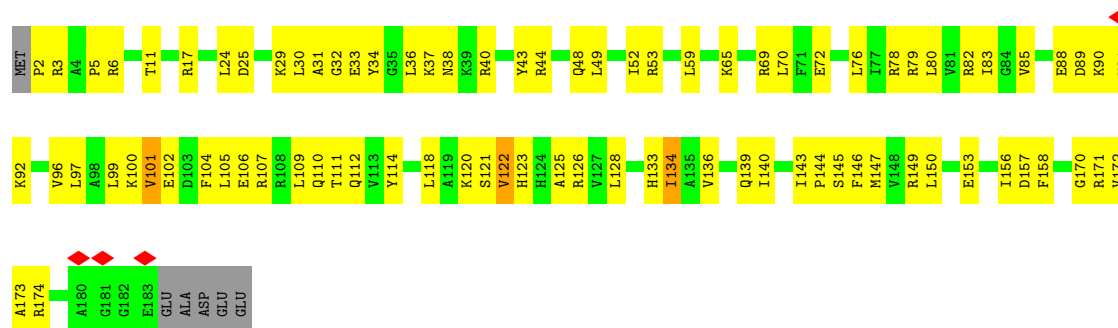




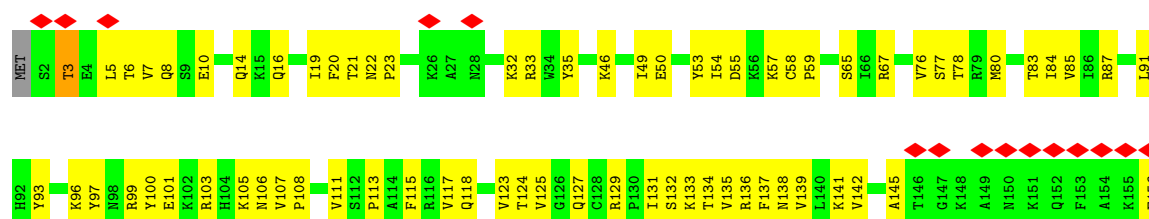
• Molecule 8: 40S ribosomal protein S8



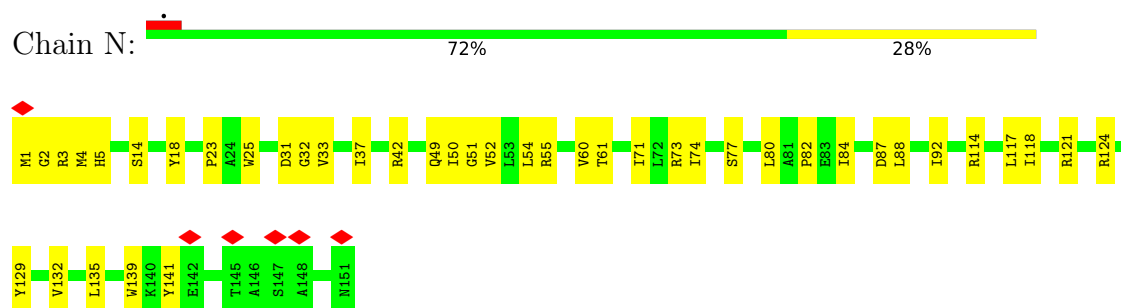
• Molecule 9: KLLA0E23673p



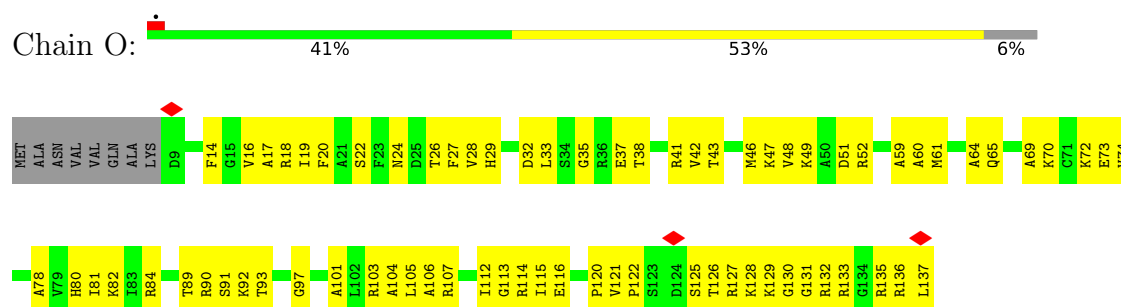
• Molecule 10: KLLA0A10483p



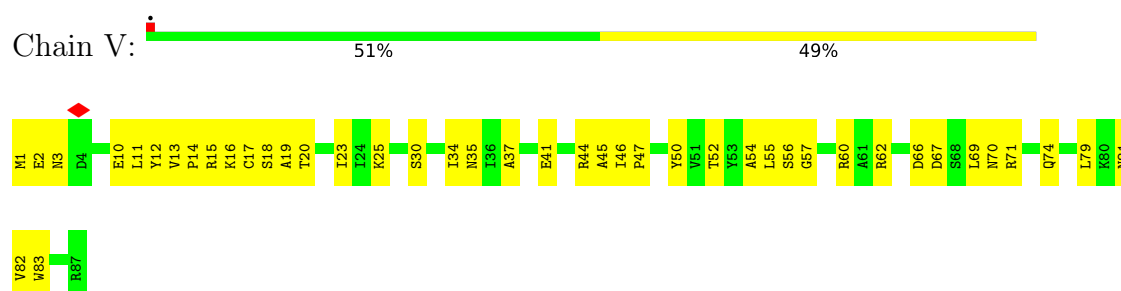
- Molecule 11: KLLA0F18040p



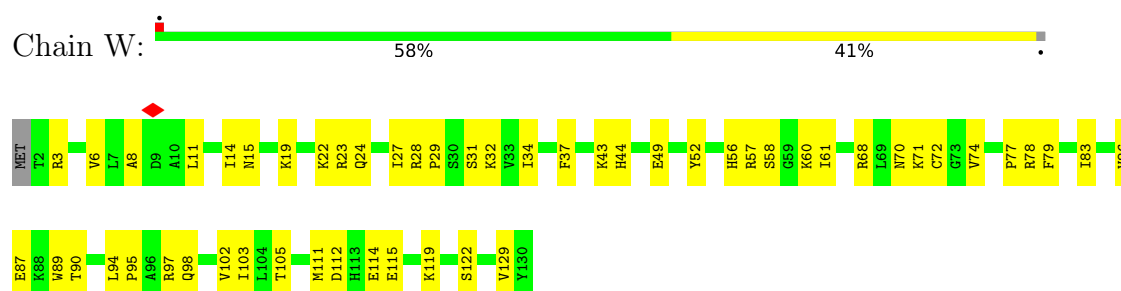
- Molecule 12: Small ribosomal subunit protein uS11



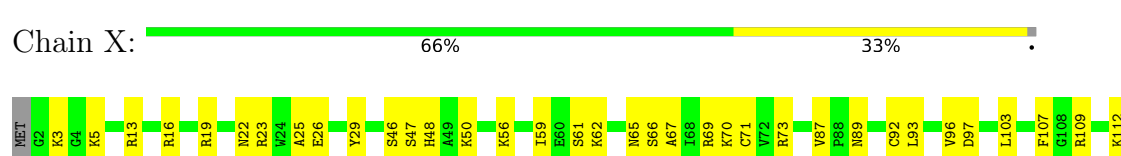
- Molecule 13: 40S ribosomal protein S21



- Molecule 14: Small ribosomal subunit protein uS8



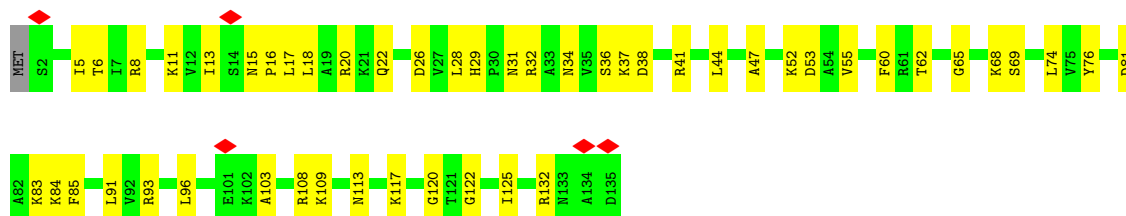
- Molecule 15: KLLA0B11231p





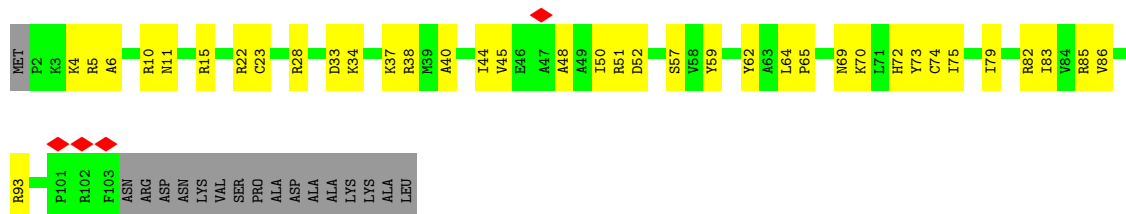
- Molecule 16: 40S ribosomal protein S24

Chain Y: 63% 36%



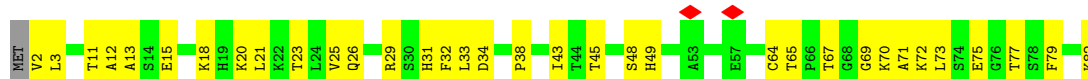
- Molecule 17: 40S ribosomal protein S26

Chain a: 55% 31% 14%



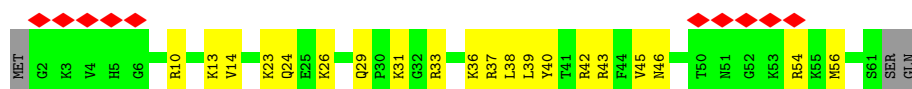
- Molecule 18: 40S ribosomal protein S27

Chain b: 57% 41%



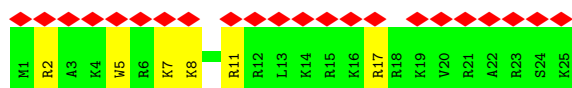
- Molecule 19: 40S ribosomal protein S30

Chain e: 16% 63% 32% 5%



- Molecule 20: 40S ribosomal protein L41-A

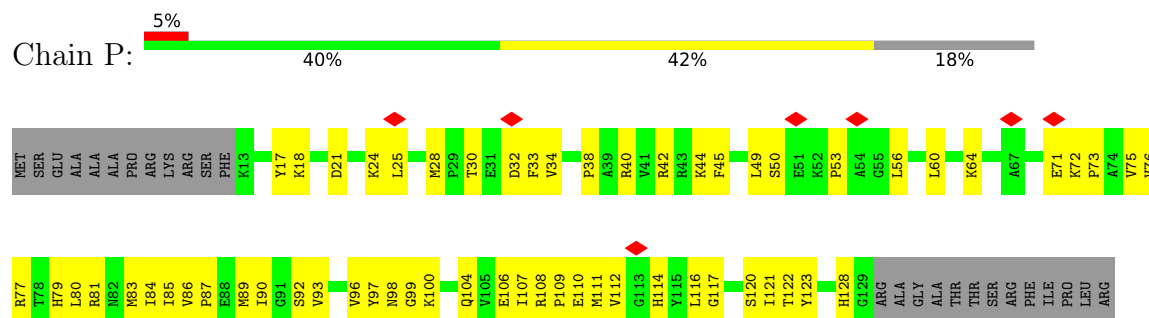
Chain h: 88% 76% 24%



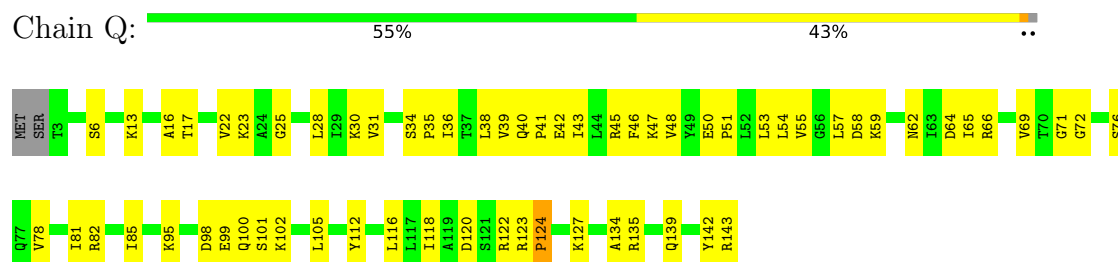
- Molecule 21: 40S ribosomal protein S3



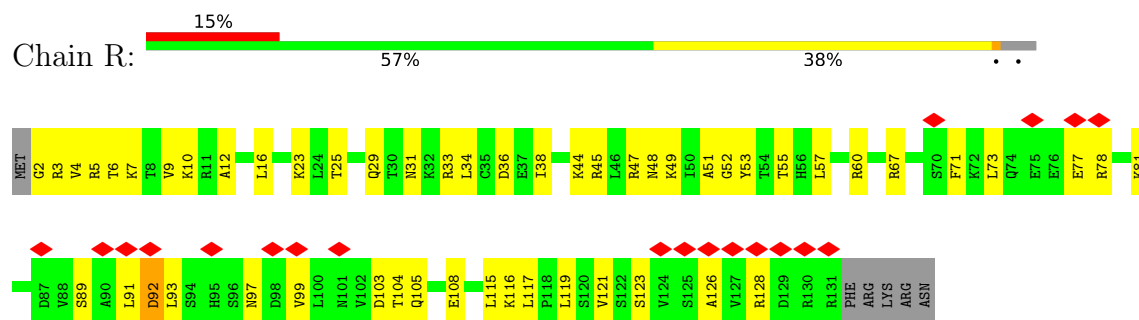
• Molecule 25: KLLA0F07843p



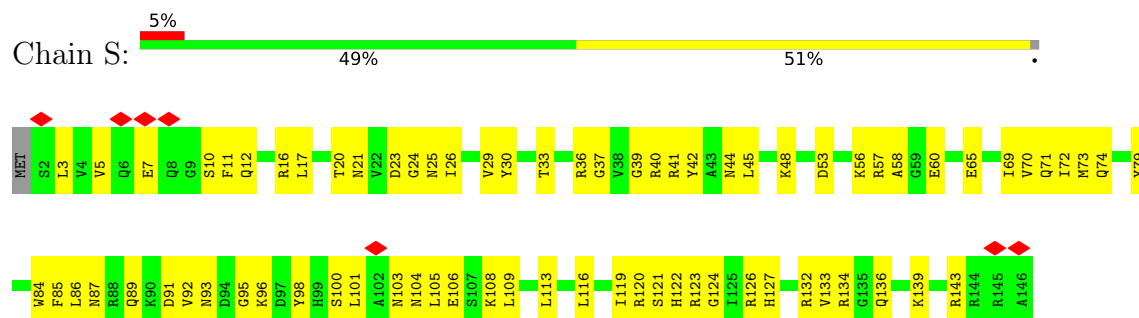
• Molecule 26: Small ribosomal subunit protein uS9



• Molecule 27: KLLA0B01474p

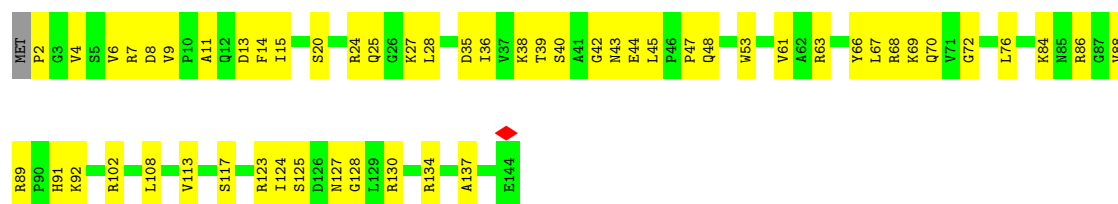


• Molecule 28: KLLA0B01562p

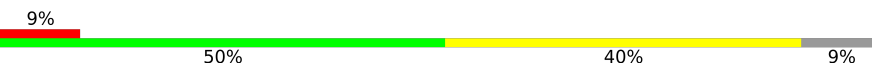


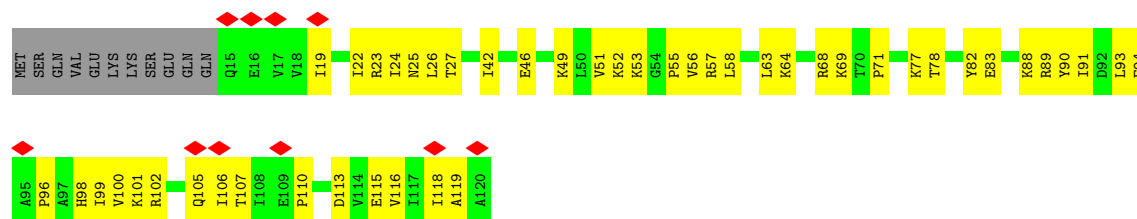
• Molecule 29: KLLA0A07194p

Chain T: 



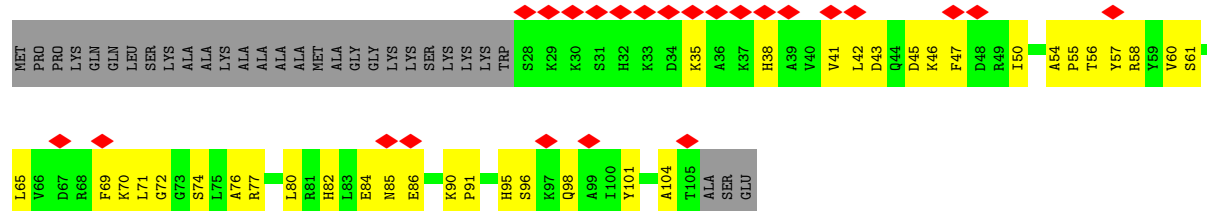
- Molecule 30: Small ribosomal subunit protein uS10

Chain U: 



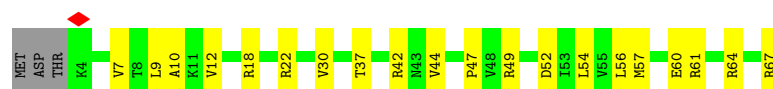
- Molecule 31: 40S ribosomal protein S25

Chain Z: 



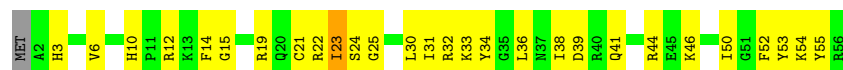
- Molecule 32: Small ribosomal subunit protein eS28

Chain c: 



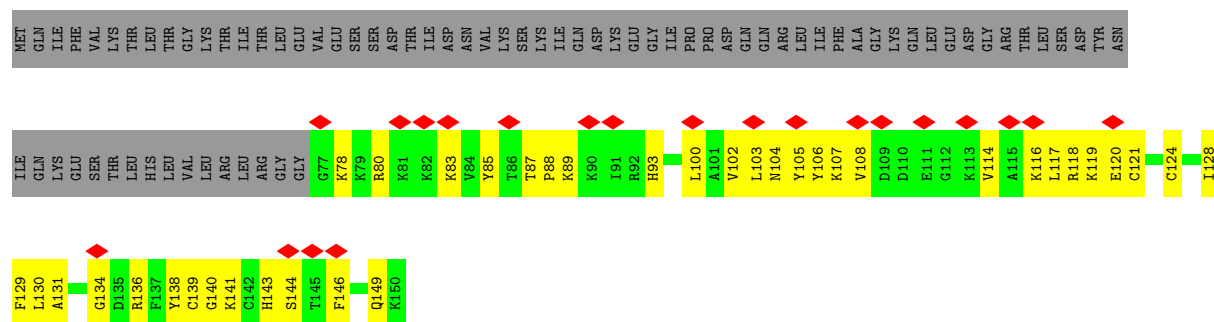
- Molecule 33: Small ribosomal subunit protein uS14

Chain d: 

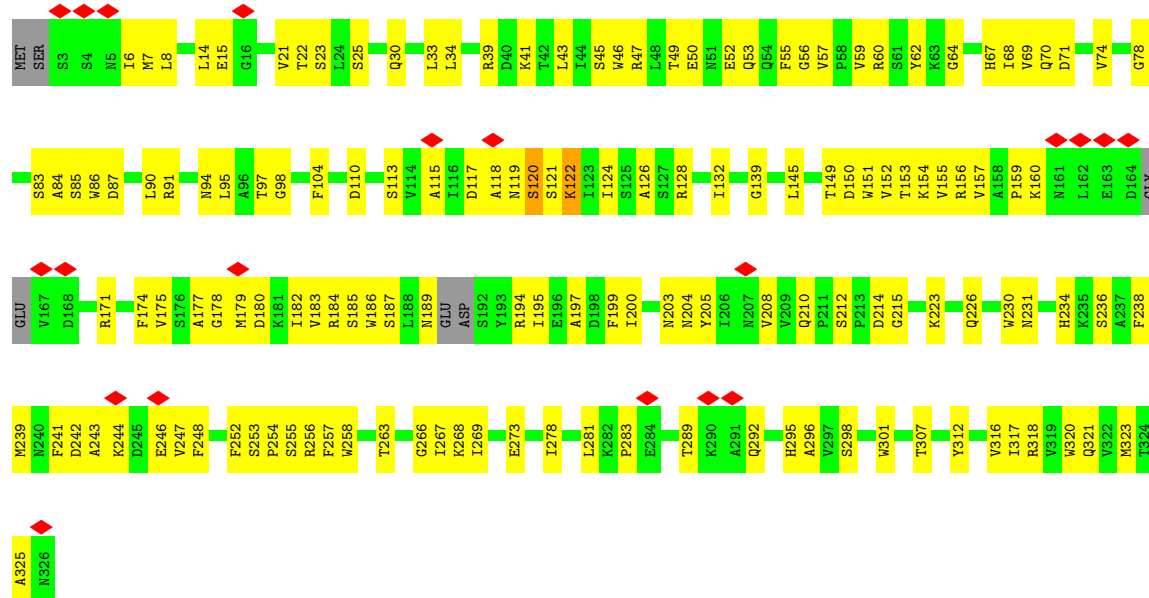


- Molecule 34: Small ribosomal subunit protein eS31

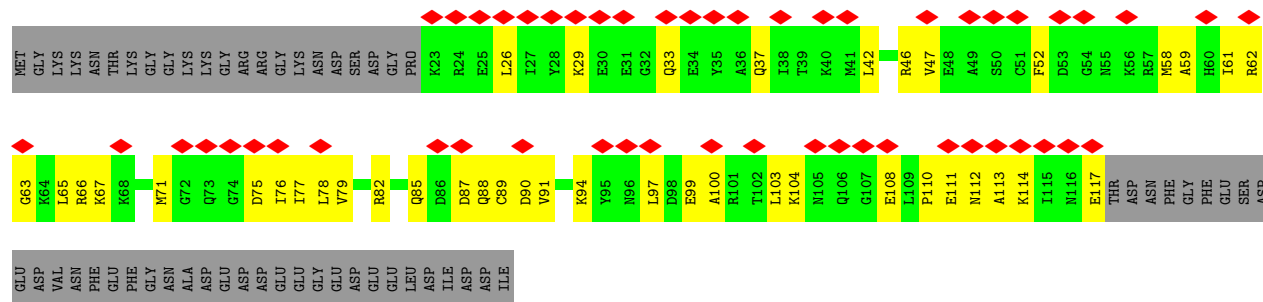
Chain f: 



• Molecule 35: KLLA0E12277p



• Molecule 36: Eukaryotic translation initiation factor 1A



• Molecule 37: mRNA (5'-R(P*AP*AP*U)-3')





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24107	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	0.481	Depositor
Minimum map value	-0.273	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.07	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: 5MC, T6A, B8N, ZN, MA6, M2G, 2MG, 1MA, H2U, RIA, 1MG, MG, GCP, 7MG, PSU

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	0.22	0/42410	0.35	0/66079
2	A	0.21	0/1742	0.47	2/2383 (0.1%)
3	B	0.24	0/1820	0.52	0/2448
4	C	0.27	0/1678	0.50	0/2277
5	E	0.24	0/2122	0.48	0/2861
6	G	0.16	0/1855	0.39	0/2479
7	H	0.25	0/1507	0.52	0/2028
8	I	0.22	0/1515	0.41	0/2029
9	J	0.26	0/1495	0.48	0/2001
10	L	0.28	0/1276	0.51	0/1718
11	N	0.21	0/1218	0.40	0/1638
12	O	0.24	0/966	0.53	0/1297
13	V	0.23	0/696	0.50	1/938 (0.1%)
14	W	0.27	0/1039	0.46	0/1399
15	X	0.25	0/1137	0.49	0/1516
16	Y	0.21	0/1075	0.41	0/1433
17	a	0.23	0/810	0.47	0/1087
18	b	0.23	0/619	0.48	0/837
19	e	0.22	0/480	0.47	0/640
20	h	0.20	0/234	0.47	0/300
21	D	0.22	0/1800	0.44	0/2421
22	F	0.24	0/1628	0.45	0/2198
23	K	0.21	0/831	0.48	0/1123
24	M	0.33	0/891	0.62	0/1201
25	P	0.23	0/942	0.55	0/1269
26	Q	0.26	0/1125	0.80	2/1510 (0.1%)
27	R	0.28	0/1044	0.53	0/1402
28	S	0.19	0/1208	0.50	0/1624
29	T	0.22	0/1129	0.40	0/1520
30	U	0.21	0/857	0.42	0/1158
31	Z	0.31	0/603	0.46	0/814
32	c	0.21	0/501	0.42	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.23	0/473	0.46	1/629 (0.2%)
34	f	0.18	0/597	0.59	0/795
35	g	0.22	0/2523	0.47	0/3434
36	i	0.18	0/773	0.48	0/1031
37	3	0.15	0/595	0.28	0/920
38	1	0.25	1/1529 (0.1%)	0.51	4/2376 (0.2%)
39	j	0.21	0/2177	0.52	0/2931
40	k	0.17	0/3657	0.45	0/4946
41	l	0.14	0/1099	0.38	0/1469
All	All	0.22	1/91676 (0.0%)	0.42	10/132832 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	37	T6A	O3'-P	5.11	1.61	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q	124	PRO	CA-C-N	15.92	143.49	121.20
26	Q	124	PRO	C-N-CA	15.92	143.49	121.20
38	1	45	U	C4'-C3'-O3'	8.08	125.12	113.00
38	1	45	U	N1-C1'-C2'	-7.12	101.32	112.00
2	A	197	ILE	CA-C-N	6.27	130.21	120.68
2	A	197	ILE	C-N-CA	6.27	130.21	120.68
38	1	45	U	C2'-C3'-O3'	-6.20	104.40	113.70
33	d	23	ILE	N-CA-C	-5.92	105.92	111.48
38	1	45	U	C3'-C2'-O2'	5.89	119.53	110.70
13	V	12	TYR	CA-CB-CG	5.53	123.85	113.90

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	38190	0	19213	1408	0
2	A	1702	0	1695	78	0
3	B	1796	0	1874	130	0
4	C	1648	0	1727	105	0
5	E	2078	0	2157	108	0
6	G	1832	0	1919	89	0
7	H	1483	0	1579	94	0
8	I	1489	0	1504	84	0
9	J	1471	0	1554	82	0
10	L	1248	0	1311	62	0
11	N	1195	0	1263	41	0
12	O	955	0	987	77	0
13	V	687	0	682	38	0
14	W	1021	0	1056	51	0
15	X	1119	0	1198	45	0
16	Y	1061	0	1111	46	0
17	a	797	0	835	42	0
18	b	609	0	630	27	0
19	e	472	0	508	28	0
20	h	233	0	284	11	0
21	D	1774	0	1855	57	0
22	F	1609	0	1679	92	0
23	K	809	0	810	48	0
24	M	885	0	917	62	0
25	P	923	0	960	56	0
26	Q	1105	0	1170	70	0
27	R	1033	0	1082	50	0
28	S	1189	0	1211	79	0
29	T	1110	0	1124	52	0
30	U	845	0	913	44	0
31	Z	594	0	590	35	0
32	c	499	0	536	18	0
33	d	461	0	448	34	0
34	f	584	0	600	37	0
35	g	2469	0	2403	118	0
36	i	764	0	763	38	0
37	3	536	0	277	11	0
38	1	1639	0	852	61	0
39	j	2145	0	2216	109	0
40	k	3596	0	3713	146	0
41	l	1083	0	1123	22	0
42	2	111	0	0	0	0
42	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	N	1	0	0	0	0
42	Q	1	0	0	0	0
42	i	1	0	0	0	0
42	k	1	0	0	0	0
43	a	1	0	0	0	0
43	b	1	0	0	0	0
43	f	1	0	0	0	0
44	k	32	0	13	4	0
45	k	8	0	8	4	0
46	2	3	0	0	0	0
All	All	86900	0	68350	3295	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 22.

All (3295) 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)
3:B:5:LYS:NZ	3:B:7:LYS:HA	1.36	1.40
7:H:94:ALA:O	7:H:96:ARG:HD2	1.27	1.29
3:B:5:LYS:NZ	3:B:7:LYS:CA	2.13	1.11
7:H:94:ALA:O	7:H:96:ARG:CD	2.00	1.09
24:M:95:GLY:HA3	24:M:104:ARG:HH11	1.19	1.08
26:Q:34:SER:HB2	26:Q:38:LEU:HD12	1.30	1.06
3:B:5:LYS:NZ	3:B:7:LYS:HD2	1.71	1.05
1:2:910:U:H3	3:B:5:LYS:HG3	1.16	1.04
3:B:144:ARG:HB2	3:B:208:GLN:HB2	1.41	1.02
7:H:96:ARG:HH22	7:H:124:LYS:HB3	1.20	1.01
1:2:691:U:C4	1:2:692:C:N4	2.29	0.98
24:M:102:ASN:OD1	24:M:103:ALA:N	1.97	0.97
3:B:5:LYS:HZ1	3:B:7:LYS:HA	1.18	0.96
7:H:96:ARG:NH2	7:H:124:LYS:HB3	1.79	0.95
1:2:910:U:H3	3:B:5:LYS:CG	1.78	0.95
7:H:96:ARG:HH12	7:H:124:LYS:CB	1.80	0.94
39:j:71:ALA:HB1	39:j:85:LEU:HD21	1.50	0.93
26:Q:34:SER:HB2	26:Q:38:LEU:CD1	1.97	0.93
1:2:143:G:H1	1:2:170:A:N6	1.65	0.93
3:B:5:LYS:HZ3	3:B:7:LYS:HA	1.22	0.93
1:2:143:G:H1	1:2:170:A:H61	0.95	0.92
1:2:159:C:N4	1:2:160:U:C4	2.38	0.92
1:2:1661:G:H1	1:2:1736:U:H3	1.15	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Q:35:PRO:HD2	26:Q:38:LEU:HD11	1.51	0.90
1:2:521:U:H5''	16:Y:37:LYS:HG3	1.52	0.89
7:H:96:ARG:NH2	7:H:124:LYS:HD3	1.88	0.88
1:2:7:G:N7	4:C:210:ARG:NH2	2.22	0.88
40:k:314:ARG:HD2	40:k:344:ASN:HD21	1.40	0.87
1:2:1152:G:OP1	17:a:82:ARG:NH1	2.07	0.86
1:2:485:G:H1	1:2:500:U:H3	1.20	0.86
7:H:96:ARG:HG3	7:H:121:VAL:HG13	1.57	0.86
27:R:31:ASN:HD22	27:R:55:THR:HG22	1.41	0.85
1:2:299:A:H2'	1:2:300:A:C8	2.12	0.84
24:M:95:GLY:CA	24:M:104:ARG:HH11	1.90	0.84
3:B:5:LYS:HZ1	3:B:7:LYS:HD2	1.37	0.84
7:H:96:ARG:HH12	7:H:124:LYS:HB3	1.43	0.84
18:b:20:LYS:HG3	18:b:21:LEU:HD12	1.58	0.83
18:b:34:ASP:OD1	18:b:82:LYS:NZ	2.12	0.83
39:j:205:LEU:HD13	40:k:330:ILE:HB	1.59	0.83
1:2:910:U:N3	3:B:5:LYS:HG3	1.92	0.83
22:F:126:LEU:HG	31:Z:58:ARG:HH21	1.41	0.83
1:2:38:C:O3'	9:J:6:ARG:NH2	2.12	0.83
35:g:70:GLN:HB2	35:g:86:TRP:HE1	1.43	0.83
1:2:28:A:N1	1:2:597:U:C4	2.47	0.82
1:2:1290:G:H1	1:2:1323:G:H22	1.22	0.82
1:2:1386:A:H5''	27:R:48:ASN:HD21	1.44	0.82
7:H:44:LYS:HD2	7:H:63:PRO:HA	1.60	0.82
1:2:143:G:OP1	6:G:143:LYS:NZ	2.11	0.82
4:C:87:ASN:HB2	4:C:212:LEU:HD23	1.61	0.82
24:M:96:LYS:H	24:M:104:ARG:HD3	1.45	0.82
21:D:105:MET:HG3	21:D:184:ILE:HD13	1.62	0.82
24:M:127:LEU:O	24:M:131:PHE:HB2	1.80	0.81
1:2:1486:G:H3'	1:2:1513:A:H61	1.45	0.81
16:Y:13:ILE:HG22	16:Y:22:GLN:HE21	1.43	0.81
41:l:186:ARG:HH22	41:l:244:THR:HG23	1.44	0.81
40:k:390:ALA:HB1	40:k:396:ILE:HD13	1.63	0.81
28:S:44:ASN:OD1	28:S:48:LYS:NZ	2.14	0.81
7:H:96:ARG:NH1	7:H:124:LYS:HB3	1.96	0.80
12:O:49:LYS:O	39:j:89:ARG:NH1	2.14	0.80
20:h:2:ARG:HD3	20:h:5:TRP:HE1	1.47	0.80
1:2:1586:G:H1	1:2:1606:U:H3	1.29	0.80
27:R:115:LEU:HB3	27:R:117:LEU:HD23	1.64	0.80
15:X:56:LYS:O	36:i:85:GLN:NE2	2.13	0.80
1:2:901:G:OP1	12:O:90:ARG:NH2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1531:C:OP2	31:Z:77:ARG:NH2	2.14	0.79
29:T:27:LYS:HG3	29:T:28:LEU:H	1.46	0.79
40:k:307:ARG:HD3	40:k:392:PRO:HG2	1.62	0.79
18:b:34:ASP:HB3	18:b:43:ILE:HD11	1.65	0.79
24:M:101:GLY:O	24:M:102:ASN:OD1	2.00	0.79
22:F:65:GLN:HE22	22:F:68:LYS:HB2	1.46	0.79
1:2:905:A:OP1	12:O:52:ARG:NH1	2.16	0.79
16:Y:41:ARG:NH1	16:Y:55:VAL:O	2.16	0.79
1:2:916:U:O2	12:O:41:ARG:NH1	2.15	0.78
1:2:396:A:H4'	8:I:50:GLY:HA2	1.62	0.78
35:g:90:LEU:HB2	35:g:104:PHE:HB2	1.65	0.78
40:k:127:ARG:NH1	44:k:601:GCP:O2A	2.15	0.78
1:2:28:A:N1	1:2:597:U:O4	2.17	0.78
12:O:81:ILE:HB	12:O:115:ILE:HG12	1.65	0.78
26:Q:39:VAL:HG22	26:Q:45:ARG:HE	1.48	0.78
1:2:59:C:N4	1:2:63:G:O6	2.15	0.78
4:C:233:ASN:ND2	13:V:1:MET:SD	2.55	0.78
22:F:28:ALA:HB3	26:Q:28:LEU:HB3	1.66	0.78
1:2:114:C:N4	1:2:244:U:O2	2.17	0.78
35:g:14:LEU:HB2	35:g:317:ILE:HB	1.66	0.78
1:2:899:A:H3'	1:2:900:G:H21	1.49	0.78
1:2:1388:U:H5'	27:R:3:ARG:HH11	1.49	0.78
21:D:126:VAL:HG11	21:D:188:ILE:HD12	1.66	0.78
1:2:1434:A:OP2	21:D:27:ARG:NH2	2.17	0.77
1:2:1656:G:O6	1:2:1741:U:O2	2.03	0.77
2:A:189:PRO:O	13:V:44:ARG:NH2	2.16	0.77
1:2:910:U:C2	3:B:5:LYS:HD2	2.20	0.77
1:2:1338:C:O2'	1:2:1340:A:N7	2.16	0.77
1:2:787:A:OP2	5:E:108:ARG:NH2	2.18	0.77
8:I:39:GLY:HA2	8:I:61:GLU:HB3	1.67	0.77
1:2:283:G:N7	6:G:188:ARG:NH1	2.33	0.77
1:2:328:G:H2'	1:2:329:G:H8	1.50	0.77
3:B:30:TYR:HD2	3:B:61:LEU:HD21	1.50	0.77
21:D:64:ARG:O	21:D:67:ASN:HB2	1.85	0.77
1:2:1239:U:O2'	1:2:1240:G:N2	2.18	0.76
7:H:96:ARG:CZ	7:H:124:LYS:HB3	2.14	0.76
2:A:188:LEU:HD12	2:A:189:PRO:HD2	1.67	0.76
19:e:39:LEU:HD23	19:e:43:ARG:HH12	1.49	0.76
6:G:32:ILE:HD12	6:G:54:GLY:H	1.49	0.76
25:P:75:VAL:HG22	25:P:104:GLN:HE22	1.49	0.76
5:E:155:LYS:HE3	5:E:156:VAL:H	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1355:U:H3	1:2:1366:G:H1	1.32	0.76
5:E:160:VAL:HG11	5:E:169:ILE:HG12	1.68	0.76
29:T:86:ARG:HH21	29:T:92:LYS:HG3	1.50	0.76
1:2:1609:A:O3'	22:F:97:ASN:ND2	2.16	0.76
5:E:26:CYS:SG	9:J:2:PRO:O	2.42	0.76
35:g:6:ILE:HA	35:g:325:ALA:H	1.51	0.76
1:2:752:A:H2	1:2:796:G:H1	1.31	0.76
10:L:3:THR:HG21	10:L:7:VAL:HG23	1.68	0.76
1:2:789:U:H5	1:2:790:A:C5	2.04	0.75
4:C:235:TRP:HB3	14:W:68:ARG:HE	1.51	0.75
26:Q:34:SER:CB	26:Q:38:LEU:HD12	2.13	0.75
1:2:518:C:N4	1:2:532:U:O2	2.20	0.75
7:H:96:ARG:HH22	7:H:124:LYS:HD3	1.51	0.75
31:Z:85:ASN:ND2	31:Z:86:GLU:OE1	2.20	0.75
4:C:190:LYS:HG2	4:C:194:GLN:HE22	1.52	0.75
1:2:999:C:OP1	39:j:55:ARG:NH1	2.19	0.75
34:f:118:ARG:O	34:f:119:LYS:HG3	1.87	0.75
2:A:42:PRO:O	27:R:128:ARG:NH2	2.20	0.74
10:L:77:SER:HB3	10:L:85:VAL:HB	1.68	0.74
1:2:512:U:H2'	1:2:513:G:C8	2.22	0.74
1:2:654:G:O6	1:2:676:U:O2	2.05	0.74
5:E:15:PRO:HG2	5:E:18:TRP:HZ3	1.51	0.74
7:H:96:ARG:NH1	7:H:124:LYS:CB	2.48	0.74
39:j:152:GLU:OE2	39:j:170:LYS:NZ	2.20	0.74
1:2:1170:A:H2'	1:2:1171:G:C8	2.23	0.74
3:B:199:ASN:OD1	3:B:202:LYS:NZ	2.19	0.74
34:f:116:LYS:HZ2	34:f:129:PHE:HE1	1.33	0.74
39:j:216:MET:HE2	39:j:234:ALA:HA	1.69	0.74
1:2:960:U:H5''	11:N:71:ILE:HD13	1.69	0.74
1:2:1315:G:O2'	27:R:10:LYS:NZ	2.21	0.74
20:h:7:LYS:O	20:h:11:ARG:HG2	1.86	0.74
28:S:41:ARG:NH2	29:T:36:ILE:O	2.19	0.74
1:2:236:C:H5''	1:2:237:U:H5'	1.68	0.74
1:2:1134:U:OP2	15:X:121:ARG:NH2	2.18	0.74
1:2:910:U:H3	3:B:5:LYS:CD	1.99	0.74
1:2:917:U:H2'	1:2:918:A:H8	1.53	0.74
8:I:67:TRP:O	8:I:71:GLY:HA2	1.88	0.74
24:M:36:ARG:HG2	24:M:112:VAL:HG23	1.68	0.74
38:1:74:C:H4'	38:1:75:C:H5'	1.70	0.74
40:k:355:ILE:HB	40:k:373:ILE:HB	1.70	0.74
30:U:51:VAL:HG23	30:U:94:GLU:HB3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:99:C:OP2	1:2:377:A:O2'	2.06	0.74
38:1:11:C:H2'	38:1:12:G:H8	1.52	0.74
1:2:691:U:N3	1:2:692:C:N4	2.35	0.73
1:2:867:G:H2'	1:2:868:A:H8	1.51	0.73
28:S:7:GLU:HB3	28:S:10:SER:HB3	1.69	0.73
1:2:1046:G:H1	1:2:1070:U:H3	1.36	0.73
40:k:95:ILE:HD11	40:k:187:ARG:HA	1.70	0.73
1:2:206:U:O2	8:I:179:ARG:NH2	2.21	0.73
1:2:1293:G:H1	1:2:1302:U:H3	1.37	0.73
1:2:68:A:OP1	6:G:160:ARG:NH2	2.21	0.73
1:2:910:U:N3	3:B:5:LYS:HD2	2.04	0.73
1:2:1521:G:N7	29:T:68:ARG:NH1	2.37	0.73
1:2:563:G:N2	1:2:576:G:OP1	2.22	0.73
1:2:521:U:O4'	16:Y:34:ASN:ND2	2.22	0.73
1:2:1500:G:N7	29:T:102:ARG:NH2	2.36	0.73
6:G:58:LYS:HA	6:G:107:ALA:HB2	1.69	0.73
25:P:50:SER:HB2	25:P:53:PRO:HD2	1.71	0.73
1:2:1561:C:OP1	29:T:84:LYS:NZ	2.19	0.73
4:C:148:TYR:O	14:W:98:GLN:NE2	2.21	0.73
26:Q:22:VAL:HG12	26:Q:65:ILE:HG12	1.71	0.73
1:2:589:C:H2'	1:2:590:A:H8	1.52	0.73
2:A:70:PRO:HB2	2:A:94:GLY:HA3	1.70	0.73
25:P:18:LYS:HD3	28:S:92:VAL:HG23	1.70	0.73
40:k:119:ALA:O	40:k:288:LYS:NZ	2.20	0.73
1:2:472:A:OP1	9:J:44:ARG:NE	2.22	0.73
1:2:1443:G:N2	34:f:87:THR:O	2.22	0.73
6:G:1:MET:N	6:G:18:ILE:O	2.22	0.72
21:D:28:GLU:HB2	23:K:58:GLN:HE22	1.54	0.72
1:2:437:A:H1'	1:2:464:G:H22	1.54	0.72
3:B:113:MET:HE3	3:B:209:ASN:HB3	1.71	0.72
12:O:131:GLY:O	17:a:22:ARG:NH2	2.22	0.72
1:2:870:G:H2'	1:2:871:G:C8	2.23	0.72
30:U:63:LEU:HD11	33:d:34:TYR:CE2	2.25	0.72
40:k:403:ASP:OD2	40:k:405:THR:OG1	2.08	0.72
1:2:317:U:O3'	8:I:11:ARG:NH1	2.22	0.72
1:2:860:U:O2'	14:W:56:HIS:O	2.08	0.72
35:g:312:TYR:HE2	35:g:318:ARG:HD2	1.53	0.72
1:2:159:C:N4	1:2:160:U:N3	2.38	0.72
1:2:761:G:N2	1:2:762:A:N7	2.36	0.72
1:2:1592:G:OP2	1:2:1594:C:N4	2.23	0.72
1:2:162:G:N2	1:2:162:G:OP2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:14:PRO:HG2	13:V:23:ILE:HD11	1.72	0.71
22:F:119:THR:HG21	22:F:196:LEU:HD22	1.72	0.71
1:2:444:A:OP2	5:E:59:ARG:NH2	2.22	0.71
1:2:671:C:H41	1:2:672:G:H21	1.38	0.71
1:2:1496:G:H5''	29:T:72:GLY:HA3	1.72	0.71
1:2:1544:G:OP1	28:S:127:HIS:NE2	2.23	0.71
18:b:2:VAL:HG22	18:b:3:LEU:H	1.54	0.71
40:k:383:GLU:H	45:k:603:MET:HE1	1.53	0.71
1:2:207:U:H2'	1:2:208:U:C6	2.25	0.71
3:B:70:LEU:HD23	3:B:82:ARG:HH11	1.53	0.71
1:2:13:C:O2'	1:2:1298:G:N2	2.22	0.71
1:2:1038:A:O2'	1:2:1039:G:O5'	2.08	0.71
10:L:132:SER:O	10:L:136:ARG:NH1	2.23	0.71
13:V:66:ASP:OD1	13:V:67:ASP:N	2.23	0.71
29:T:42:GLY:HA2	29:T:84:LYS:HG3	1.72	0.71
40:k:342:ILE:O	40:k:393:GLY:N	2.22	0.71
1:2:10:G:N2	4:C:92:GLN:O	2.22	0.71
1:2:126:A:OP2	6:G:201:GLN:NE2	2.24	0.71
1:2:1589:C:H2'	1:2:1590:A:H8	1.55	0.71
1:2:1793:U:H3'	17:a:5:ARG:HH22	1.54	0.71
6:G:69:LEU:HD12	6:G:70:PRO:HD2	1.73	0.71
39:j:174:SER:O	39:j:178:THR:OG1	2.09	0.71
3:B:199:ASN:O	3:B:202:LYS:NZ	2.23	0.71
5:E:47:PHE:HZ	5:E:99:PHE:HD2	1.38	0.71
35:g:223:LYS:HA	35:g:246:GLU:HG2	1.73	0.71
24:M:117:TRP:HE1	24:M:124:ARG:HB3	1.56	0.70
1:2:142:G:H2'	1:2:143:G:C8	2.26	0.70
1:2:905:A:H2'	1:2:906:A:C8	2.26	0.70
1:2:1653:A:N6	1:2:1743:G:O2'	2.19	0.70
3:B:5:LYS:NZ	3:B:7:LYS:N	2.39	0.70
16:Y:38:ASP:HA	16:Y:41:ARG:HG3	1.72	0.70
22:F:43:LYS:HD2	22:F:49:SER:HA	1.73	0.70
1:2:1794:C:O5'	17:a:5:ARG:NH1	2.20	0.70
12:O:133:ARG:HH21	12:O:136:ARG:HH12	1.39	0.70
35:g:86:TRP:HA	35:g:110:ASP:HB2	1.73	0.70
1:2:638:U:OP1	7:H:112:ARG:NH2	2.21	0.70
1:2:1401:C:OP1	27:R:2:GLY:N	2.25	0.70
18:b:49:HIS:HA	18:b:70:LYS:HA	1.74	0.70
40:k:377:ILE:HA	40:k:400:THR:HG22	1.73	0.70
1:2:12:U:OP1	4:C:89:LYS:NZ	2.24	0.70
12:O:107:ARG:NH1	32:c:60:GLU:OE2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:67:GLN:NE2	16:Y:17:LEU:O	2.24	0.70
1:2:866:G:OP2	11:N:3:ARG:NH2	2.25	0.70
40:k:115:THR:HG21	44:k:601:GCP:H2'	1.74	0.70
1:2:29:U:H2'	1:2:30:G:H8	1.55	0.70
1:2:1554:A:H8	25:P:40:ARG:HH22	1.40	0.70
1:2:1670:G:H2'	1:2:1671:G:H8	1.55	0.70
3:B:6:ASN:O	3:B:7:LYS:CB	2.39	0.70
3:B:6:ASN:O	3:B:7:LYS:HB2	1.92	0.70
21:D:29:LEU:HB3	21:D:34:TYR:HB2	1.71	0.70
32:c:7:VAL:HA	32:c:56:LEU:O	1.90	0.70
40:k:235:ALA:HA	40:k:238:ILE:HD12	1.73	0.70
41:l:161:PRO:HG2	41:l:180:ILE:HG13	1.73	0.70
1:2:1754:A:OP2	36:i:67:LYS:NZ	2.25	0.70
16:Y:103:ALA:O	16:Y:108:ARG:NH1	2.25	0.70
39:j:216:MET:HE1	39:j:239:LYS:HB3	1.74	0.70
2:A:74:VAL:HG22	2:A:96:THR:HB	1.74	0.70
6:G:76:LEU:HB2	6:G:94:ARG:HE	1.56	0.70
1:2:216:A:H2'	1:2:217:A:C8	2.27	0.69
1:2:824:U:H2'	1:2:825:U:H6	1.57	0.69
1:2:898:G:N7	3:B:5:LYS:HB2	2.07	0.69
1:2:1115:A:OP1	20:h:17:ARG:NH2	2.26	0.69
1:2:1364:C:H5'	26:Q:66:ARG:HH21	1.57	0.69
2:A:206:ASN:HB2	2:A:209:GLU:HG2	1.74	0.69
7:H:156:SER:HA	7:H:185:ILE:HD11	1.73	0.69
1:2:874:G:OP1	3:B:158:SER:N	2.26	0.69
1:2:925:A:OP1	1:2:1015:C:O2'	2.11	0.69
1:2:1335:A:O2'	26:Q:123:ARG:NH1	2.25	0.69
1:2:58:U:O2'	1:2:450:A:N3	2.24	0.69
1:2:1346:U:OP1	30:U:23:ARG:NH2	2.26	0.69
12:O:20:PHE:HB3	12:O:27:PHE:HB2	1.74	0.69
39:j:196:GLU:HG3	40:k:401:LYS:HE2	1.75	0.69
1:2:685:A:H2'	1:2:686:C:C6	2.27	0.69
1:2:1194:C:N4	26:Q:143:ARG:O	2.25	0.69
10:L:123:VAL:HG22	10:L:142:VAL:HG22	1.75	0.69
1:2:327:A:H2'	1:2:328:G:H8	1.57	0.69
1:2:650:G:N1	1:2:684:A:N6	2.40	0.69
1:2:855:A:N6	7:H:115:SER:O	2.26	0.69
1:2:1162:A:N3	1:2:1611:U:O2'	2.26	0.69
1:2:1500:G:N2	1:2:1503:A:OP2	2.25	0.69
1:2:1752:A:O2'	36:i:46:ARG:NH2	2.26	0.69
10:L:80:MET:SD	10:L:83:THR:OG1	2.48	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:103:ARG:NH2	17:a:48:ALA:O	2.26	0.69
38:1:20:A:H62	38:1:57:G:H1'	1.58	0.69
40:k:359:ILE:HB	40:k:371:LYS:HB2	1.75	0.69
4:C:225:ASN:OD1	13:V:25:LYS:NZ	2.24	0.69
6:G:120:GLU:OE2	6:G:125:THR:OG1	2.11	0.69
40:k:205:LEU:HB2	40:k:465:ASN:HD22	1.57	0.69
1:2:1172:C:OP1	28:S:132:ARG:NH2	2.25	0.69
3:B:104:ASP:OD1	3:B:105:PHE:N	2.25	0.69
6:G:85:ARG:O	6:G:87:ARG:NH1	2.26	0.69
40:k:236:ILE:HG23	40:k:241:LEU:HB2	1.75	0.69
1:2:1252:U:H5''	34:f:128:ILE:HD11	1.75	0.68
1:2:141:U:OP1	6:G:139:ASN:ND2	2.26	0.68
1:2:357:U:H2'	1:2:359:A:C8	2.28	0.68
1:2:1595:A:OP2	33:d:32:ARG:NH1	2.26	0.68
4:C:145:ARG:HB2	4:C:227:TYR:CE1	2.28	0.68
8:I:67:TRP:O	8:I:71:GLY:CA	2.42	0.68
39:j:222:LEU:HD11	40:k:324:ASN:HB3	1.76	0.68
1:2:910:U:N3	3:B:5:LYS:CD	2.56	0.68
1:2:1798:A:N6	37:3:19:A:O2'	2.26	0.68
8:I:47:ARG:NH1	8:I:48:THR:O	2.27	0.68
26:Q:143:ARG:NH2	38:1:35:A:OP2	2.26	0.68
38:1:19:G:OP1	38:1:57:G:N2	2.20	0.68
1:2:485:G:O6	1:2:500:U:O4	2.11	0.68
1:2:930:C:OP1	17:a:70:LYS:NZ	2.19	0.68
2:A:13:ASP:OD1	2:A:179:ARG:NH2	2.26	0.68
15:X:65:ASN:ND2	15:X:116:ASP:OD2	2.23	0.68
19:e:38:LEU:HD21	19:e:42:ARG:HH21	1.59	0.68
27:R:78:ARG:HH21	27:R:81:LYS:HG3	1.59	0.68
40:k:98:GLN:NE2	40:k:389:PHE:O	2.26	0.68
1:2:590:A:H2'	1:2:591:G:C8	2.29	0.68
8:I:57:ALA:HB2	8:I:178:GLY:HA2	1.76	0.68
24:M:102:ASN:CG	24:M:103:ALA:H	2.01	0.68
40:k:76:PRO:O	40:k:97:ARG:NH1	2.26	0.68
1:2:708:C:O2'	1:2:710:U:OP2	2.11	0.68
1:2:1659:U:H2'	1:2:1660:G:C8	2.29	0.68
5:E:11:ARG:NH1	5:E:21:ASP:OD1	2.27	0.68
21:D:6:SER:OG	21:D:9:ARG:NH1	2.26	0.68
6:G:4:ASN:OD1	6:G:13:GLN:NE2	2.26	0.68
18:b:34:ASP:CG	18:b:82:LYS:HZ3	2.01	0.68
1:2:110:U:OP1	1:2:753:A:O2'	2.12	0.68
1:2:1661:G:N2	1:2:1736:U:O2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:114:TYR:HE2	9:J:121:SER:H	1.42	0.68
41:l:161:PRO:HG3	41:l:183:LYS:HD2	1.76	0.68
1:2:367:U:O2'	1:2:602:U:O2'	2.10	0.68
1:2:585:G:OP1	19:e:23:LYS:NZ	2.27	0.68
1:2:1513:A:O2'	1:2:1515:U:OP2	2.10	0.68
1:2:522:G:N1	1:2:527:U:OP2	2.27	0.67
7:H:96:ARG:HH22	7:H:124:LYS:CB	2.02	0.67
1:2:780:A:C8	16:Y:8:ARG:HG2	2.29	0.67
1:2:925:A:H2'	1:2:926:C:C6	2.29	0.67
26:Q:35:PRO:HD2	26:Q:38:LEU:CD1	2.22	0.67
1:2:758:U:OP1	5:E:22:LYS:NZ	2.27	0.67
1:2:1544:G:P	28:S:123:ARG:HH21	2.16	0.67
1:2:1682:U:O2	1:2:1715:G:O6	2.11	0.67
1:2:1143:U:H2'	1:2:1144:U:C6	2.27	0.67
4:C:211:THR:HG23	4:C:214:ASN:HB2	1.75	0.67
1:2:917:U:H2'	1:2:918:A:C8	2.29	0.67
1:2:1300:U:OP1	4:C:93:LYS:NZ	2.26	0.67
18:b:73:LEU:HD12	18:b:75:GLU:H	1.59	0.67
3:B:5:LYS:HZ3	3:B:7:LYS:CA	1.89	0.67
29:T:61:VAL:HG22	29:T:76:LEU:HD21	1.76	0.67
30:U:55:PRO:HA	30:U:91:ILE:HG22	1.76	0.67
1:2:1207:A:O2'	34:f:78:LYS:NZ	2.28	0.67
7:H:15:GLU:O	7:H:19:GLN:NE2	2.27	0.67
1:2:303:U:H2'	1:2:304:C:H6	1.60	0.67
1:2:297:C:O3'	5:E:30:ARG:NH2	2.27	0.67
1:2:533:A:H3'	1:2:534:A:H8	1.60	0.67
1:2:1540:G:N2	1:2:1567:A:OP2	2.28	0.66
2:A:18:LEU:HD13	2:A:23:HIS:CD2	2.29	0.66
1:2:121:U:H2'	1:2:122:U:C6	2.30	0.66
1:2:1490:A:O2'	1:2:1491:A:O4'	2.13	0.66
1:2:1746:G:H2'	1:2:1747:A:C8	2.30	0.66
5:E:72:VAL:HB	5:E:77:ARG:HG3	1.77	0.66
26:Q:30:LYS:NZ	29:T:8:ASP:OD1	2.28	0.66
1:2:923:A:H2'	1:2:924:G:C8	2.29	0.66
1:2:1219:C:H2'	1:2:1220:A:H8	1.61	0.66
1:2:1580:U:OP1	26:Q:135:ARG:NH1	2.27	0.66
1:2:1784:G:OP2	12:O:133:ARG:NH2	2.27	0.66
2:A:16:LEU:HG	2:A:172:LEU:HD11	1.77	0.66
5:E:86:PHE:CD1	5:E:87:MET:HG2	2.31	0.66
11:N:54:LEU:HD12	11:N:60:VAL:HG21	1.78	0.66
24:M:129:GLU:OE2	24:M:130:HIS:ND1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:T:4:VAL:HG11	29:T:137:ALA:HB2	1.77	0.66
1:2:562:U:O2'	19:e:13:LYS:NZ	2.28	0.66
1:2:1300:U:O5'	4:C:93:LYS:HD2	1.96	0.66
5:E:94:ALA:HB1	16:Y:16:PRO:HB2	1.77	0.66
5:E:79:ASP:HB3	5:E:82:PHE:HB2	1.76	0.66
15:X:130:VAL:HG23	15:X:140:LYS:HE3	1.76	0.66
40:k:357:PRO:HG2	40:k:415:GLN:HE21	1.60	0.66
1:2:1770:C:H3'	20:h:2:ARG:HH21	1.60	0.66
2:A:44:GLY:HA3	27:R:128:ARG:HE	1.61	0.66
1:2:1403:G:H2'	1:2:1404:A:H8	1.60	0.66
3:B:26:ARG:HG3	3:B:50:LYS:HE3	1.77	0.66
26:Q:42:GLU:O	26:Q:43:ILE:HD13	1.96	0.66
1:2:916:U:H1'	12:O:41:ARG:HH22	1.60	0.66
1:2:1240:G:O2'	1:2:1241:A:O4'	2.13	0.66
1:2:175:C:N4	1:2:265:A:OP2	2.28	0.66
22:F:103:GLY:C	22:F:105:ASN:H	2.04	0.66
40:k:104:GLY:HA3	40:k:211:MET:HE3	1.78	0.66
40:k:238:ILE:HG23	40:k:514:TRP:HB3	1.77	0.66
1:2:640:G:N2	7:H:177:THR:O	2.28	0.65
1:2:1367:G:H5''	29:T:69:LYS:HG2	1.77	0.65
21:D:76:ARG:O	21:D:78:LYS:NZ	2.27	0.65
1:2:95:G:OP1	5:E:6:LYS:NZ	2.28	0.65
4:C:180:GLY:N	4:C:200:ASP:OD2	2.29	0.65
1:2:630:G:N2	1:2:1103:U:OP1	2.28	0.65
1:2:990:G:N2	1:2:1012:A:H62	1.94	0.65
28:S:45:LEU:HD23	28:S:85:PHE:CE2	2.31	0.65
31:Z:43:ASP:HB2	31:Z:46:LYS:HG2	1.78	0.65
41:l:184:LEU:HD22	41:l:234:VAL:HG11	1.78	0.65
1:2:635:A:H5''	14:W:31:SER:HB2	1.79	0.65
1:2:637:U:O2	7:H:114:ARG:NE	2.24	0.65
1:2:1771:C:H2'	1:2:1772:G:H8	1.60	0.65
6:G:64:LYS:HZ2	6:G:81:HIS:HB3	1.62	0.65
20:h:2:ARG:HD3	20:h:5:TRP:NE1	2.11	0.65
1:2:563:G:N1	1:2:579:A:OP2	2.23	0.65
1:2:739:G:H2'	1:2:740:A:C8	2.32	0.65
1:2:1481:A:H2'	1:2:1482:G:C8	2.31	0.65
2:A:60:ALA:HA	2:A:63:ILE:HD12	1.77	0.65
9:J:49:LEU:HD13	9:J:101:VAL:HG12	1.78	0.65
35:g:14:LEU:N	35:g:317:ILE:O	2.29	0.65
35:g:243:ALA:O	35:g:268:LYS:NZ	2.30	0.65
1:2:1269:G:H1'	34:f:80:ARG:HH22	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:90:GLU:HB2	3:B:97:LEU:HB2	1.78	0.65
5:E:87:MET:HE1	5:E:236:ILE:HD13	1.77	0.65
6:G:32:ILE:HG23	6:G:53:ALA:HA	1.79	0.65
23:K:11:ILE:HD11	23:K:42:VAL:HG22	1.79	0.65
25:P:81:ARG:NH2	25:P:117:GLY:O	2.30	0.65
35:g:69:VAL:HG22	35:g:85:SER:HB3	1.78	0.65
1:2:299:A:H2'	1:2:300:A:H8	1.57	0.65
1:2:1794:C:N3	17:a:5:ARG:HA	2.12	0.65
1:2:204:U:H2'	1:2:205:A:H8	1.62	0.65
1:2:707:A:H61	1:2:730:G:H1	1.45	0.65
12:O:107:ARG:NH2	17:a:52:ASP:OD1	2.29	0.65
14:W:49:GLU:OE1	14:W:49:GLU:N	2.30	0.65
1:2:68:A:OP2	6:G:171:LYS:NZ	2.30	0.65
1:2:367:U:O4	1:2:368:A:N6	2.30	0.65
1:2:842:U:H2'	1:2:843:A:H8	1.59	0.65
4:C:149:TRP:O	14:W:97:ARG:NH2	2.29	0.65
1:2:342:C:H2'	1:2:343:A:H8	1.63	0.64
1:2:938:A:H2'	1:2:939:A:C8	2.32	0.64
6:G:124:ILE:HG23	6:G:125:THR:HG23	1.78	0.64
21:D:143:ARG:NH2	37:3:38:C:O2	2.29	0.64
32:c:42:ARG:NH1	32:c:61:ARG:O	2.30	0.64
34:f:108:VAL:HG12	34:f:114:VAL:HG22	1.79	0.64
1:2:321:G:O2'	8:I:10:LYS:NZ	2.30	0.64
1:2:488:C:N3	1:2:489:C:N4	2.45	0.64
1:2:1794:C:C4	17:a:5:ARG:HA	2.33	0.64
2:A:83:GLN:HB3	2:A:99:ALA:HB1	1.78	0.64
3:B:5:LYS:HZ2	3:B:7:LYS:HD2	1.57	0.64
22:F:60:LEU:HD22	22:F:140:ILE:HA	1.79	0.64
35:g:52:GLU:CD	35:g:53:GLN:H	2.05	0.64
1:2:550:G:H2'	1:2:551:G:H8	1.62	0.64
1:2:1791:G:H3'	17:a:4:LYS:HE3	1.79	0.64
22:F:31:ILE:O	22:F:36:GLN:NE2	2.30	0.64
22:F:83:ARG:HH22	32:c:18:ARG:HH22	1.45	0.64
39:j:173:ILE:HG23	39:j:177:LEU:HD12	1.79	0.64
40:k:214:ALA:HB3	40:k:244:VAL:HG22	1.79	0.64
41:l:163:PRO:HG2	41:l:223:GLU:HG2	1.79	0.64
5:E:95:THR:HG22	16:Y:16:PRO:HD2	1.79	0.64
38:1:29:G:H2'	38:1:30:G:C8	2.32	0.64
39:j:13:TYR:CE2	39:j:78:LYS:HA	2.33	0.64
1:2:702:G:H2'	1:2:703:G:C8	2.32	0.64
1:2:1228:G:N2	1:2:1254:G:O2'	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1556:U:OP1	28:S:122:HIS:ND1	2.30	0.64
9:J:37:LYS:HG3	19:e:33:ARG:HB2	1.80	0.64
21:D:75:LYS:NZ	23:K:20:VAL:O	2.31	0.64
5:E:125:LYS:HB2	5:E:226:PHE:CE1	2.32	0.64
12:O:106:ALA:HA	12:O:112:ILE:HD11	1.78	0.64
23:K:9:LYS:HD2	23:K:80:LEU:HD13	1.79	0.64
30:U:68:ARG:HH12	30:U:77:LYS:HA	1.60	0.64
29:T:127:ASN:OD1	29:T:130:ARG:NH2	2.31	0.64
31:Z:60:VAL:HG13	31:Z:65:LEU:HD11	1.80	0.64
1:2:565:C:OP2	36:i:62:ARG:NH1	2.31	0.64
1:2:792:A:H5'	1:2:793:U:H4'	1.79	0.64
1:2:990:G:H21	1:2:1012:A:H62	1.43	0.64
1:2:142:G:P	6:G:139:ASN:HD22	2.20	0.64
21:D:40:ARG:HH11	30:U:110:PRO:HG3	1.63	0.64
1:2:1314:U:OP1	1:2:1327:G:N2	2.31	0.63
5:E:85:GLY:N	5:E:88:ASP:OD2	2.29	0.63
5:E:112:HIS:NE2	5:E:237:SER:O	2.30	0.63
38:1:62:C:H2'	38:1:63:G:H8	1.62	0.63
1:2:1044:C:H2'	1:2:1045:G:H8	1.64	0.63
1:2:1315:G:OP1	27:R:7:LYS:N	2.30	0.63
1:2:1381:G:O4'	30:U:89:ARG:NH2	2.32	0.63
12:O:80:HIS:ND1	12:O:113:GLY:O	2.31	0.63
21:D:28:GLU:OE2	21:D:29:LEU:HD22	1.98	0.63
27:R:91:LEU:O	27:R:93:LEU:N	2.31	0.63
39:j:205:LEU:HD12	39:j:220:VAL:HB	1.80	0.63
40:k:283:ILE:HD12	40:k:294:VAL:HG21	1.80	0.63
1:2:590:A:H5''	9:J:24:LEU:HD11	1.80	0.63
1:2:598:A:N3	15:X:47:SER:OG	2.31	0.63
39:j:19:ILE:HG21	39:j:98:CYS:SG	2.38	0.63
1:2:328:G:H5''	8:I:98:LYS:HB3	1.79	0.63
1:2:1352:U:O2	1:2:1370:G:O6	2.17	0.63
1:2:1488:A:OP1	21:D:9:ARG:NH2	2.31	0.63
4:C:61:ILE:HA	4:C:66:LEU:HD12	1.80	0.63
5:E:147:ILE:HG21	5:E:169:ILE:HG13	1.80	0.63
1:2:1182:A:N3	1:2:1209:C:O2'	2.29	0.63
1:2:1771:C:H2'	1:2:1772:G:C8	2.33	0.63
7:H:96:ARG:NH2	7:H:124:LYS:CD	2.62	0.63
38:1:62:C:H2'	38:1:63:G:C8	2.33	0.63
40:k:315:LEU:HD11	40:k:398:VAL:HG21	1.81	0.63
1:2:1080:A:O2'	1:2:1081:C:H2'	1.99	0.63
1:2:1279:C:OP1	33:d:44:ARG:NH2	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:5:LYS:HZ2	3:B:7:LYS:CA	2.09	0.63
40:k:373:ILE:HD13	40:k:406:LEU:HD11	1.79	0.63
1:2:1244:G:OP1	33:d:3:HIS:NE2	2.31	0.63
5:E:175:PHE:HE1	5:E:195:ILE:HD13	1.62	0.63
14:W:71:LYS:HG2	14:W:72:CYS:O	1.99	0.63
22:F:176:LEU:HD21	22:F:215:LYS:HB2	1.81	0.63
1:2:72:A:H4'	1:2:73:U:H5'	1.79	0.63
1:2:1645:U:H2'	1:2:1646:A:C8	2.34	0.63
2:A:56:LYS:HE2	13:V:70:ASN:HD21	1.63	0.63
2:A:214:THR:OG1	27:R:81:LYS:NZ	2.29	0.63
10:L:131:ILE:HB	10:L:135:VAL:HG23	1.79	0.63
35:g:210:GLN:NE2	35:g:252:PHE:H	1.97	0.63
38:1:66:C:H2'	38:1:67:G:C8	2.33	0.63
40:k:322:ASP:OD2	40:k:408:ARG:NH1	2.31	0.63
1:2:383:G:H2'	1:2:384:A:C8	2.34	0.63
1:2:1408:A:H5''	26:Q:118:ILE:HD11	1.79	0.63
28:S:30:TYR:O	28:S:33:THR:OG1	2.17	0.63
35:g:160:LYS:NZ	35:g:171:ARG:O	2.32	0.63
35:g:267:ILE:HB	35:g:281:LEU:HB2	1.80	0.63
1:2:736:C:HO2'	1:2:737:A:H8	1.45	0.62
28:S:29:VAL:HG11	28:S:44:ASN:HA	1.81	0.62
36:i:76:ILE:HD12	36:i:100:ALA:HB1	1.80	0.62
1:2:198:G:H2'	1:2:199:A:H8	1.64	0.62
1:2:687:C:H5'	14:W:119:LYS:HZ3	1.64	0.62
1:2:752:A:C2	1:2:796:G:N1	2.63	0.62
1:2:917:U:O3'	12:O:18:ARG:NH2	2.32	0.62
24:M:34:LEU:HD23	24:M:36:ARG:HD3	1.81	0.62
34:f:107:LYS:HB2	34:f:117:LEU:HD11	1.80	0.62
1:2:207:U:O4'	8:I:179:ARG:NH2	2.32	0.62
1:2:1198:G:O2'	1:2:1199:G:OP2	2.13	0.62
2:A:53:THR:HG22	2:A:161:PRO:HG2	1.81	0.62
3:B:133:TYR:HE2	3:B:181:LEU:HD22	1.64	0.62
38:1:23:C:O5'	39:j:64:ARG:NH1	2.31	0.62
1:2:1645:U:H4'	36:i:58:MET:HE1	1.82	0.62
1:2:1778:G:H2'	1:2:1779:A:C8	2.34	0.62
12:O:26:THR:HG21	12:O:97:GLY:HA3	1.82	0.62
15:X:69:ARG:HG3	15:X:117:ILE:HG12	1.81	0.62
24:M:95:GLY:HA3	24:M:104:ARG:NH1	2.04	0.62
24:M:120:ASP:HA	24:M:124:ARG:HG3	1.80	0.62
25:P:92:SER:HB2	25:P:107:ILE:HD13	1.81	0.62
39:j:47:LEU:HD12	39:j:49:SER:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:152:G:H2'	1:2:153:G:H8	1.64	0.62
1:2:1797:U:H4'	1:2:1798:A:OP2	1.99	0.62
6:G:79:LYS:HB2	6:G:86:PRO:HG3	1.80	0.62
7:H:140:VAL:HB	14:W:52:TYR:HB3	1.82	0.62
29:T:113:VAL:HG12	29:T:128:GLY:HA2	1.82	0.62
38:1:23:C:H2'	38:1:24:G:C8	2.34	0.62
9:J:134:ILE:H	9:J:134:ILE:HD12	1.63	0.62
35:g:269:ILE:HG23	35:g:278:ILE:HB	1.80	0.62
1:2:886:A:H2'	1:2:887:U:H6	1.64	0.62
1:2:1219:C:H5''	23:K:52:LYS:HE3	1.82	0.62
35:g:34:LEU:HB3	35:g:46:TRP:HB2	1.80	0.62
1:2:327:A:H2'	1:2:328:G:C8	2.35	0.62
6:G:1:MET:HE1	6:G:24:VAL:HG21	1.82	0.62
16:Y:15:ASN:HD22	16:Y:20:ARG:HH12	1.46	0.62
22:F:146:GLU:HB2	32:c:57:MET:HE1	1.80	0.62
35:g:64:GLY:O	35:g:91:ARG:NH1	2.31	0.62
1:2:1784:G:OP2	12:O:136:ARG:NH2	2.32	0.62
5:E:21:ASP:OD2	5:E:24:SER:OG	2.17	0.62
35:g:60:ARG:HH11	35:g:98:GLY:HA3	1.64	0.62
38:1:11:C:H2'	38:1:12:G:C8	2.34	0.62
1:2:493:U:H2'	1:2:494:C:H4'	1.81	0.62
1:2:811:A:H62	1:2:857:G:H2'	1.65	0.62
1:2:885:U:H2'	1:2:886:A:C8	2.35	0.62
1:2:893:U:H2'	1:2:894:G:H8	1.65	0.62
1:2:1336:A:O5'	26:Q:123:ARG:NH1	2.33	0.62
2:A:84:ARG:HH12	2:A:205:ARG:HG2	1.63	0.62
12:O:65:GLN:NE2	12:O:104:ALA:HB1	2.15	0.62
1:2:165:C:O2'	6:G:133:LEU:O	2.17	0.61
1:2:824:U:H2'	1:2:825:U:C6	2.33	0.61
1:2:883:A:H2'	1:2:884:G:C8	2.35	0.61
1:2:1574:A:O2'	38:1:40:C:O2'	2.17	0.61
1:2:1589:C:H2'	1:2:1590:A:C8	2.34	0.61
16:Y:53:ASP:HB3	16:Y:96:LEU:HD21	1.82	0.61
23:K:20:VAL:HG12	23:K:67:THR:HA	1.82	0.61
23:K:62:GLN:HE22	33:d:24:SER:HA	1.65	0.61
27:R:33:ARG:NH1	35:g:110:ASP:OD2	2.33	0.61
28:S:25:ASN:O	28:S:57:ARG:NH1	2.30	0.61
30:U:69:LYS:HB2	30:U:78:THR:HG23	1.82	0.61
39:j:94:ASP:HA	39:j:97:LYS:HE3	1.82	0.61
1:2:853:U:O4	1:2:854:A:N6	2.32	0.61
1:2:984:G:H1	1:2:1015:C:H5	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:328:G:H2'	1:2:329:G:C8	2.32	0.61
1:2:1126:G:P	20:h:11:ARG:HH22	2.24	0.61
39:j:154:VAL:HG23	39:j:155:TRP:HD1	1.64	0.61
1:2:198:G:H2'	1:2:199:A:C8	2.35	0.61
1:2:1256:U:H4'	23:K:8:ARG:HH12	1.66	0.61
3:B:58:SER:OG	3:B:62:LYS:NZ	2.33	0.61
3:B:131:ASP:OD1	3:B:132:ASP:N	2.32	0.61
25:P:83:MET:HB3	25:P:116:LEU:HD13	1.80	0.61
28:S:57:ARG:NH2	31:Z:74:SER:OG	2.33	0.61
30:U:64:LYS:O	33:d:33:LYS:NZ	2.33	0.61
1:2:1617:C:H2'	1:2:1618:C:H6	1.64	0.61
1:2:1754:A:OP1	36:i:66:ARG:NH1	2.33	0.61
14:W:28:ARG:HB3	14:W:29:PRO:HD3	1.82	0.61
30:U:118:ILE:HG13	30:U:119:ALA:H	1.64	0.61
35:g:49:THR:N	35:g:55:PHE:O	2.22	0.61
1:2:334:U:O2'	10:L:129:ARG:NH1	2.34	0.61
1:2:609:G:O2'	1:2:612:G:O2'	2.17	0.61
1:2:842:U:H2'	1:2:843:A:C8	2.35	0.61
1:2:1229:A:N6	1:2:1230:U:O2	2.34	0.61
4:C:232:PRO:HA	4:C:235:TRP:CD2	2.34	0.61
16:Y:28:LEU:HG	16:Y:68:LYS:HG2	1.83	0.61
1:2:63:G:O2'	1:2:169:U:OP1	2.18	0.61
1:2:610:U:OP2	15:X:19:ARG:NH2	2.34	0.61
1:2:702:G:H2'	1:2:703:G:H8	1.63	0.61
22:F:78:ARG:O	22:F:85:ARG:NH2	2.34	0.61
30:U:24:ILE:HD12	30:U:91:ILE:HD11	1.82	0.61
40:k:89:PRO:HB3	40:k:307:ARG:HH22	1.65	0.61
1:2:893:U:H2'	1:2:894:G:C8	2.36	0.61
30:U:98:HIS:CE1	30:U:99:ILE:HG23	2.35	0.61
38:l:18:G:O6	39:j:176:ARG:NE	2.33	0.61
1:2:292:U:H2'	1:2:293:C:C6	2.36	0.61
1:2:383:G:H2'	1:2:384:A:H8	1.65	0.61
1:2:399:A:OP1	8:I:25:ARG:NH1	2.34	0.61
1:2:658:C:H2'	1:2:659:G:H8	1.66	0.61
1:2:983:G:H2'	1:2:984:G:H8	1.66	0.61
1:2:1670:G:H2'	1:2:1671:G:C8	2.36	0.61
2:A:41:ARG:HG2	2:A:43:ASP:H	1.66	0.61
6:G:76:LEU:HD11	6:G:92:ARG:HB3	1.83	0.61
21:D:150:MET:HE3	21:D:152:PHE:CZ	2.36	0.61
26:Q:41:PRO:HG2	26:Q:78:VAL:HG21	1.83	0.61
40:k:254:MET:HA	40:k:254:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:12:U:H2'	1:2:13:C:H6	1.64	0.60
1:2:28:A:C6	1:2:597:U:O4	2.54	0.60
1:2:460:G:H2'	1:2:461:G:C8	2.36	0.60
1:2:510:A:H5'	9:J:173:ALA:HB2	1.83	0.60
1:2:855:A:OP1	7:H:97:ARG:NH1	2.34	0.60
1:2:911:U:O2	1:2:913:G:N1	2.33	0.60
1:2:1652:G:H22	1:2:1743:G:H2'	1.66	0.60
3:B:167:VAL:HA	3:B:170:GLU:OE2	2.01	0.60
5:E:80:THR:HG23	5:E:81:THR:HG23	1.83	0.60
1:2:803:A:N3	14:W:105:THR:OG1	2.30	0.60
1:2:871:G:H2'	1:2:872:U:O4'	2.01	0.60
1:2:990:G:H21	1:2:1012:A:N6	1.99	0.60
4:C:92:GLN:C	4:C:93:LYS:HD3	2.26	0.60
10:L:78:THR:HG22	10:L:84:ILE:HD11	1.83	0.60
14:W:70:ASN:OD1	14:W:71:LYS:N	2.34	0.60
34:f:131:ALA:N	34:f:138:TYR:O	2.33	0.60
40:k:94:ILE:HG23	40:k:391:VAL:HG21	1.82	0.60
40:k:247:LEU:HD23	40:k:281:VAL:HB	1.82	0.60
40:k:346:VAL:HG22	40:k:392:PRO:HD3	1.82	0.60
3:B:5:LYS:HZ2	3:B:7:LYS:N	1.99	0.60
7:H:157:LYS:HD2	7:H:158:ASP:HB2	1.83	0.60
1:2:420:A:H2'	1:2:421:G:H5''	1.84	0.60
1:2:1407:G:N2	1:2:1410:G:OP2	2.34	0.60
1:2:1541:A:N6	1:2:1566:C:O2'	2.35	0.60
3:B:132:ASP:HB3	3:B:221:PRO:HD3	1.84	0.60
7:H:91:ILE:HG21	7:H:129:LEU:HD12	1.83	0.60
1:2:700:C:O2'	1:2:701:U:OP1	2.19	0.60
1:2:843:A:H2'	1:2:844:G:C8	2.37	0.60
1:2:855:A:H62	7:H:116:ARG:HD3	1.67	0.60
1:2:1485:A:OP1	33:d:34:TYR:OH	2.19	0.60
2:A:84:ARG:NH1	2:A:205:ARG:HG2	2.17	0.60
1:2:1679:A:N6	1:2:1718:G:O2'	2.34	0.60
1:2:1786:G:H5''	12:O:132:ARG:HH12	1.65	0.60
3:B:87:ARG:NH1	3:B:220:GLN:OE1	2.35	0.60
22:F:114:ARG:HE	31:Z:95:HIS:CE1	2.19	0.60
27:R:44:LYS:HA	27:R:47:ARG:HG2	1.84	0.60
31:Z:71:LEU:HD13	31:Z:76:ALA:HA	1.84	0.60
31:Z:90:LYS:HD2	31:Z:104:ALA:HA	1.84	0.60
40:k:313:PRO:HA	40:k:345:GLY:HA3	1.83	0.60
1:2:104:A:N6	1:2:307:C:O4'	2.35	0.60
1:2:223:C:H2'	1:2:224:A:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:624:C:H2'	1:2:625:U:C6	2.36	0.60
8:I:68:ALA:N	8:I:186:GLU:OE1	2.34	0.60
8:I:81:VAL:HG12	8:I:94:ASN:HA	1.84	0.60
9:J:123:HIS:ND1	19:e:37:ARG:HD2	2.17	0.60
1:2:407:C:O2'	1:2:1730:A:O2'	2.18	0.60
1:2:1740:U:H2'	1:2:1741:U:O4'	2.02	0.60
4:C:42:PRO:HB2	4:C:48:ARG:HG2	1.84	0.60
4:C:154:GLY:HA2	13:V:3:ASN:HD21	1.66	0.60
10:L:91:LEU:HD12	10:L:100:TYR:HB3	1.82	0.60
10:L:117:VAL:HG22	10:L:142:VAL:HG21	1.83	0.60
22:F:78:ARG:NH2	22:F:81:ASN:OD1	2.35	0.60
26:Q:42:GLU:C	26:Q:43:ILE:HD13	2.26	0.60
32:c:64:ARG:NH1	37:3:23:A:O2'	2.35	0.60
40:k:495:ILE:HG23	40:k:496:ASN:H	1.65	0.60
1:2:29:U:H2'	1:2:30:G:C8	2.35	0.60
1:2:122:U:O3'	5:E:77:ARG:NH2	2.35	0.60
1:2:935:G:O6	17:a:15:ARG:NH2	2.35	0.60
5:E:136:ILE:HG21	5:E:148:ARG:HH11	1.67	0.60
25:P:96:VAL:HG13	25:P:120:SER:HB3	1.82	0.60
1:2:444:A:H5'	5:E:59:ARG:HH12	1.66	0.60
1:2:760:A:N1	1:2:789:U:C4	2.69	0.60
1:2:895:U:H2'	1:2:896:C:C2	2.36	0.60
10:L:14:GLN:HB2	10:L:54:ILE:HD13	1.82	0.60
21:D:106:LYS:HG3	21:D:175:VAL:HG22	1.83	0.60
22:F:124:ASN:O	22:F:128:ASP:HA	2.02	0.60
35:g:94:ASN:ND2	35:g:97:THR:OG1	2.35	0.60
40:k:416:VAL:HG21	40:k:492:CYS:HB2	1.82	0.60
1:2:1571:A:H4'	1:2:1572:G:O5'	2.01	0.59
39:j:13:TYR:HE2	39:j:78:LYS:HA	1.64	0.59
39:j:189:GLU:HB2	39:j:265:THR:HG23	1.84	0.59
40:k:109:VAL:HG21	40:k:197:HIS:HD2	1.67	0.59
40:k:453:VAL:HG13	40:k:503:ARG:HH12	1.67	0.59
1:2:10:G:O6	1:2:1143:U:O2	2.20	0.59
1:2:255:A:H2'	1:2:256:A:C8	2.37	0.59
1:2:1157:C:N3	1:2:1161:C:N4	2.49	0.59
6:G:197:ASN:OD1	6:G:201:GLN:NE2	2.34	0.59
11:N:31:ASP:OD1	11:N:32:GLY:N	2.35	0.59
35:g:182:ILE:HD12	35:g:184:ARG:HD3	1.83	0.59
39:j:54:ARG:HD3	39:j:57:ARG:HH22	1.67	0.59
1:2:910:U:N3	3:B:5:LYS:CG	2.55	0.59
1:2:1559:U:H2'	1:2:1560:G:H8	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:64:HIS:HD2	13:V:15:ARG:HH21	1.50	0.59
17:a:51:ARG:NH2	32:c:37:THR:O	2.32	0.59
28:S:69:ILE:O	28:S:73:MET:HG2	2.00	0.59
35:g:119:ASN:OD1	35:g:120:SER:N	2.32	0.59
1:2:1240:G:O2'	1:2:1241:A:O5'	2.20	0.59
16:Y:122:GLY:HA2	16:Y:125:ILE:HD13	1.85	0.59
22:F:190:LYS:NZ	22:F:198:GLU:OE1	2.30	0.59
38:1:66:C:H2'	38:1:67:G:H8	1.66	0.59
7:H:137:GLY:HA2	11:N:18:TYR:HE2	1.68	0.59
11:N:1:MET:SD	11:N:1:MET:N	2.76	0.59
14:W:27:ILE:HB	14:W:61:ILE:HB	1.85	0.59
39:j:244:LEU:HD13	39:j:268:PRO:HB3	1.84	0.59
1:2:1203:A:H61	33:d:15:GLY:HA3	1.66	0.59
1:2:1537:G:H4'	28:S:40:ARG:HH22	1.68	0.59
9:J:88:GLU:OE1	9:J:88:GLU:N	2.36	0.59
12:O:22:SER:OG	12:O:24:ASN:O	2.21	0.59
12:O:92:LYS:HZ1	12:O:122:PRO:HD2	1.68	0.59
22:F:96:THR:HG22	22:F:116:VAL:HG11	1.85	0.59
40:k:148:TYR:HB3	40:k:183:TYR:HB3	1.85	0.59
1:2:78:A:O2'	6:G:173:PRO:O	2.20	0.59
1:2:683:C:N4	1:2:684:A:H62	2.00	0.59
1:2:1464:G:O2'	1:2:1600:C:OP1	2.20	0.59
3:B:36:SER:OG	3:B:41:ARG:NH2	2.35	0.59
9:J:118:LEU:HD22	9:J:158:PHE:HE2	1.67	0.59
22:F:178:THR:OG1	22:F:182:ARG:NH2	2.36	0.59
25:P:81:ARG:NH1	25:P:97:TYR:O	2.35	0.59
29:T:38:LYS:O	29:T:39:THR:OG1	2.19	0.59
1:2:332:A:H62	8:I:49:ARG:HH22	1.49	0.59
1:2:1343:A:H2'	1:2:1344:A:C8	2.37	0.59
4:C:236:GLU:OE1	4:C:236:GLU:N	2.36	0.59
26:Q:55:VAL:HG12	26:Q:59:LYS:HB3	1.84	0.59
35:g:117:ASP:HB2	35:g:122:LYS:H	1.66	0.59
1:2:625:U:H2'	1:2:626:C:H6	1.67	0.59
1:2:776:G:N7	16:Y:11:LYS:NZ	2.47	0.59
1:2:1475:G:H1'	29:T:48:GLN:HG3	1.83	0.59
3:B:142:PHE:O	3:B:208:GLN:N	2.36	0.59
28:S:86:LEU:O	28:S:89:GLN:NE2	2.36	0.59
1:2:332:A:OP1	8:I:48:THR:OG1	2.21	0.58
1:2:929:A:O2'	3:B:111:ARG:NH2	2.35	0.58
6:G:180:THR:HG23	6:G:183:ARG:H	1.68	0.58
35:g:312:TYR:CE2	35:g:318:ARG:HD2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:33:TYR:HA	39:j:45:MET:HA	1.85	0.58
40:k:453:VAL:HG13	40:k:503:ARG:NH1	2.17	0.58
1:2:694:U:H2'	7:H:98:ILE:HG22	1.85	0.58
1:2:872:U:O2'	1:2:1046:G:OP1	2.22	0.58
4:C:145:ARG:HB2	4:C:227:TYR:HE1	1.66	0.58
14:W:11:LEU:HA	14:W:14:ILE:HG22	1.84	0.58
16:Y:13:ILE:HG22	16:Y:22:GLN:NE2	2.17	0.58
17:a:85:ARG:HG2	17:a:85:ARG:HH11	1.68	0.58
29:T:130:ARG:HH11	29:T:134:ARG:HH21	1.50	0.58
36:i:52:PHE:HB3	36:i:110:PRO:HD2	1.85	0.58
1:2:1626:U:H2'	1:2:1627:G:H8	1.68	0.58
1:2:1676:A:OP1	8:I:59:ARG:NH2	2.29	0.58
3:B:164:ILE:O	3:B:168:ILE:HG12	2.04	0.58
1:2:115:G:OP2	10:L:65:SER:OG	2.20	0.58
1:2:906:A:N3	1:2:996:G:O2'	2.29	0.58
2:A:84:ARG:HD2	2:A:204:TYR:HA	1.85	0.58
4:C:50:VAL:HG21	4:C:73:ILE:HG23	1.84	0.58
12:O:92:LYS:HZ3	12:O:121:VAL:HA	1.68	0.58
35:g:152:VAL:HA	35:g:178:GLY:HA3	1.85	0.58
35:g:179:MET:HA	35:g:205:TYR:HB2	1.85	0.58
1:2:12:U:H2'	1:2:13:C:C6	2.39	0.58
1:2:128:U:H4'	1:2:130:C:H5	1.66	0.58
1:2:566:A:OP1	15:X:70:LYS:NZ	2.36	0.58
1:2:955:C:OP1	1:2:1071:C:O2'	2.20	0.58
1:2:1145:G:H2'	1:2:1146:A:C8	2.38	0.58
9:J:114:TYR:HE2	9:J:121:SER:N	2.01	0.58
15:X:143:PRO:C	15:X:144:ARG:HD3	2.29	0.58
27:R:77:GLU:O	27:R:81:LYS:HG2	2.03	0.58
1:2:31:C:O2'	1:2:546:U:OP1	2.21	0.58
1:2:90:C:H2'	1:2:91:G:C8	2.38	0.58
1:2:160:U:OP2	6:G:87:ARG:NH2	2.35	0.58
4:C:132:ALA:HA	4:C:135:ILE:HG22	1.84	0.58
9:J:110:GLN:HE22	9:J:126:ARG:HA	1.67	0.58
21:D:71:LEU:HD22	23:K:90:THR:HG22	1.86	0.58
24:M:96:LYS:N	24:M:104:ARG:HD3	2.17	0.58
34:f:104:ASN:O	34:f:118:ARG:NH2	2.35	0.58
35:g:115:ALA:HB3	35:g:124:ILE:HB	1.84	0.58
1:2:1609:A:O2'	22:F:97:ASN:OD1	2.15	0.58
12:O:60:ALA:HB1	12:O:101:ALA:HB2	1.86	0.58
22:F:29:THR:HG23	26:Q:28:LEU:HB2	1.86	0.58
1:2:326:U:O2'	10:L:10:GLU:OE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:332:A:N7	8:I:49:ARG:NH2	2.51	0.58
7:H:150:GLN:OE1	7:H:179:LYS:NZ	2.29	0.58
22:F:95:LEU:HA	22:F:174:ILE:HD11	1.85	0.58
23:K:22:VAL:HG23	23:K:23:ALA:H	1.68	0.58
1:2:158:U:O5'	16:Y:117:LYS:NZ	2.29	0.58
1:2:1216:A:N6	23:K:28:ASN:OD1	2.34	0.58
1:2:1499:C:OP2	29:T:102:ARG:NH1	2.37	0.58
1:2:1626:U:H2'	1:2:1627:G:C8	2.39	0.58
2:A:184:LEU:HD12	13:V:45:ALA:HB2	1.85	0.58
7:H:9:LEU:HD13	7:H:43:PHE:HB2	1.85	0.58
13:V:1:MET:HG2	13:V:10:GLU:HB2	1.86	0.58
22:F:103:GLY:O	22:F:105:ASN:N	2.36	0.58
33:d:15:GLY:O	33:d:19:ARG:NH1	2.37	0.58
1:2:86:A:H2'	1:2:87:C:H6	1.69	0.57
1:2:589:C:H2'	1:2:590:A:C8	2.37	0.57
1:2:1472:G:H2'	1:2:1473:A:C8	2.39	0.57
9:J:128:LEU:O	9:J:133:HIS:HB2	2.04	0.57
19:e:45:VAL:HG12	19:e:46:ASN:HD22	1.69	0.57
21:D:228:THR:O	35:g:171:ARG:NH2	2.37	0.57
28:S:103:ASN:HA	28:S:106:GLU:OE2	2.04	0.57
1:2:160:U:O2'	1:2:161:A:OP2	2.19	0.57
9:J:107:ARG:HD2	9:J:112:GLN:HE21	1.69	0.57
25:P:17:TYR:CD2	25:P:18:LYS:HG2	2.39	0.57
28:S:12:GLN:OE1	28:S:12:GLN:N	2.37	0.57
28:S:100:SER:HB3	28:S:105:LEU:HA	1.86	0.57
30:U:49:LYS:HE3	30:U:49:LYS:HA	1.86	0.57
39:j:244:LEU:HD22	39:j:268:PRO:HD3	1.85	0.57
1:2:127:G:O3'	1:2:177:U:N3	2.33	0.57
1:2:1198:G:N2	33:d:30:LEU:O	2.37	0.57
5:E:194:THR:N	5:E:211:LYS:O	2.37	0.57
14:W:11:LEU:HD12	14:W:72:CYS:HB2	1.87	0.57
35:g:69:VAL:HA	35:g:85:SER:HA	1.85	0.57
35:g:85:SER:OG	35:g:87:ASP:OD1	2.18	0.57
1:2:107:C:H5''	1:2:382:G:O2'	2.04	0.57
1:2:1427:G:H2'	1:2:1428:U:C6	2.39	0.57
1:2:1590:A:H2'	1:2:1591:A:H8	1.69	0.57
3:B:61:LEU:HA	3:B:64:ARG:HH11	1.70	0.57
24:M:50:GLY:O	24:M:76:ASN:ND2	2.37	0.57
24:M:129:GLU:HA	24:M:133:GLN:HB2	1.85	0.57
25:P:108:ARG:NH2	25:P:110:GLU:OE1	2.37	0.57
38:1:27:C:H2'	38:1:28:A:H8	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:593:A:OP2	9:J:38:ASN:ND2	2.37	0.57
1:2:681:U:O2'	1:2:682:U:O4'	2.19	0.57
1:2:1448:U:H2'	1:2:1449:C:C6	2.40	0.57
1:2:1632:C:H1'	37:3:35:C:H41	1.69	0.57
36:i:62:ARG:HD3	36:i:90:ASP:HB2	1.86	0.57
1:2:2:A:H5''	4:C:202:TYR:HE1	1.68	0.57
1:2:140:A:N6	6:G:187:LYS:HD2	2.19	0.57
1:2:588:C:O2'	19:e:56:MET:HE1	2.05	0.57
1:2:865:G:H2'	1:2:866:G:H8	1.70	0.57
1:2:1415:A:H2'	1:2:1416:G:O4'	2.04	0.57
1:2:1585:A:O2'	22:F:106:ASN:OD1	2.18	0.57
24:M:27:THR:HG21	24:M:119:ALA:HB3	1.87	0.57
28:S:17:LEU:O	28:S:20:THR:OG1	2.18	0.57
36:i:26:LEU:HB3	36:i:99:GLU:HG2	1.86	0.57
40:k:195:PRO:HB2	40:k:200:LEU:HD23	1.85	0.57
40:k:314:ARG:HE	40:k:494:GLU:HG2	1.70	0.57
1:2:396:A:OP2	8:I:47:ARG:NH2	2.37	0.57
1:2:931:U:H3'	3:B:116:LYS:HE3	1.85	0.57
1:2:996:G:O6	1:2:1006:5MC:N4	2.37	0.57
1:2:1056:U:H3	1:2:1059:U:H3'	1.68	0.57
24:M:60:THR:O	24:M:61:GLU:HG3	2.04	0.57
27:R:23:LYS:HD2	35:g:179:MET:SD	2.45	0.57
35:g:128:ARG:HD3	35:g:151:TRP:CZ2	2.40	0.57
1:2:25:C:H5''	1:2:26:A:H5'	1.86	0.57
1:2:332:A:H2'	1:2:333:G:C8	2.40	0.57
1:2:1632:C:H1'	37:3:35:C:N4	2.20	0.57
1:2:1659:U:H2'	1:2:1660:G:H8	1.68	0.57
4:C:193:MET:HA	4:C:193:MET:HE3	1.87	0.57
39:j:47:LEU:N	39:j:50:GLU:OE1	2.37	0.57
1:2:709:C:H41	1:2:731:C:H6	1.52	0.57
1:2:911:U:H1'	1:2:913:G:C6	2.40	0.57
1:2:997:A:N6	1:2:1003:U:OP2	2.38	0.57
1:2:1096:U:O3'	4:C:173:ARG:NH1	2.37	0.57
8:I:113:TYR:HE2	8:I:121:LEU:HD11	1.70	0.57
12:O:19:ILE:HD12	12:O:28:VAL:HG22	1.86	0.57
12:O:112:ILE:O	17:a:57:SER:OG	2.17	0.57
15:X:26:GLU:OE1	15:X:26:GLU:N	2.28	0.57
30:U:63:LEU:HD11	33:d:34:TYR:HE2	1.67	0.57
1:2:903:G:OP1	12:O:135:ARG:NH2	2.38	0.57
1:2:1063:G:O2'	3:B:204:ILE:O	2.23	0.57
1:2:1198:G:H1	33:d:31:ILE:HD11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1788:A:P	17:a:10:ARG:HH12	2.28	0.57
3:B:174:ARG:NE	3:B:175:GLU:OE2	2.25	0.57
5:E:18:TRP:HH2	5:E:38:LEU:O	1.87	0.57
41:l:134:LEU:HA	41:l:137:ARG:HG3	1.87	0.57
9:J:136:VAL:HG22	9:J:156:ILE:HG22	1.87	0.56
22:F:121:GLU:O	22:F:125:VAL:HG22	2.05	0.56
35:g:171:ARG:NH2	35:g:187:SER:OG	2.38	0.56
38:1:20:A:N6	38:1:57:G:H1'	2.20	0.56
39:j:58:SER:HB2	39:j:61:LYS:HB3	1.87	0.56
40:k:92:ALA:HA	40:k:95:ILE:HG22	1.87	0.56
41:l:172:THR:OG1	41:l:215:GLY:O	2.22	0.56
1:2:331:U:O2'	8:I:5:ARG:NH1	2.38	0.56
1:2:603:A:H2'	1:2:604:A:O4'	2.05	0.56
1:2:952:G:H2'	1:2:953:G:H8	1.69	0.56
1:2:1522:A:H2'	1:2:1523:A:C8	2.40	0.56
1:2:1563:C:H2'	1:2:1564:U:C6	2.40	0.56
12:O:32:ASP:OD1	12:O:35:GLY:N	2.38	0.56
22:F:39:GLN:C	22:F:41:GLU:H	2.13	0.56
36:i:114:LYS:HE3	41:l:166:LEU:HD21	1.87	0.56
1:2:326:U:H2'	1:2:327:A:C8	2.41	0.56
1:2:434:C:H2'	1:2:435:A:O4'	2.05	0.56
1:2:1403:G:H2'	1:2:1404:A:C8	2.41	0.56
2:A:119:ARG:HH12	4:C:249:ALA:HB2	1.69	0.56
2:A:163:ASN:O	2:A:169:SER:OG	2.20	0.56
3:B:152:ARG:NH1	3:B:152:ARG:O	2.38	0.56
5:E:11:ARG:NE	5:E:27:TYR:O	2.37	0.56
25:P:28:MET:SD	25:P:32:ASP:HB3	2.44	0.56
30:U:82:TYR:HB3	33:d:52:PHE:HB3	1.87	0.56
38:1:64:RIA:O3A	38:1:65:G:OP2	2.22	0.56
39:j:7:ARG:HG3	39:j:40:ASP:HB3	1.86	0.56
1:2:272:G:H2'	1:2:273:G:H8	1.69	0.56
1:2:471:U:H2'	1:2:472:A:C8	2.40	0.56
1:2:1159:A:H2'	1:2:1160:C:C6	2.40	0.56
1:2:1233:A:H4'	34:f:143:HIS:CD2	2.41	0.56
1:2:1647:G:OP1	15:X:73:ARG:NH2	2.33	0.56
5:E:71:LYS:HB3	5:E:91:THR:HB	1.86	0.56
7:H:96:ARG:HH12	7:H:124:LYS:C	2.13	0.56
10:L:50:GLU:OE1	10:L:50:GLU:N	2.38	0.56
14:W:103:ILE:HD11	14:W:129:VAL:HG22	1.87	0.56
19:e:45:VAL:HG12	19:e:46:ASN:ND2	2.20	0.56
26:Q:95:LYS:NZ	35:g:98:GLY:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:394:U:H3	1:2:398:A:H62	1.54	0.56
1:2:1123:A:H2'	1:2:1124:A:C8	2.41	0.56
1:2:1590:A:H2'	1:2:1591:A:C8	2.40	0.56
8:I:192:PHE:HA	8:I:195:ARG:HH11	1.71	0.56
13:V:74:GLN:OE1	13:V:83:TRP:N	2.31	0.56
23:K:9:LYS:HZ2	23:K:80:LEU:HB2	1.71	0.56
24:M:71:LEU:HD11	34:f:106:TYR:HD2	1.71	0.56
1:2:127:G:O2'	1:2:177:U:O2	2.18	0.56
12:O:116:GLU:N	12:O:116:GLU:OE2	2.39	0.56
21:D:113:LEU:HD22	21:D:118:ALA:HB2	1.88	0.56
1:2:1315:G:OP1	27:R:6:THR:OG1	2.22	0.56
9:J:153:GLU:O	9:J:156:ILE:HG12	2.06	0.56
18:b:18:LYS:HE3	18:b:23:THR:HA	1.88	0.56
21:D:32:GLU:OE2	21:D:57:ASP:HB3	2.06	0.56
26:Q:55:VAL:HG13	26:Q:105:LEU:HD11	1.86	0.56
32:c:57:MET:N	32:c:57:MET:SD	2.79	0.56
36:i:67:LYS:HD3	37:3:32:U:O3'	2.06	0.56
1:2:598:A:H2'	1:2:599:U:C6	2.41	0.56
1:2:946:U:H2'	1:2:947:G:C8	2.41	0.56
1:2:1785:C:OP2	12:O:132:ARG:N	2.39	0.56
13:V:30:SER:O	13:V:60:ARG:NH1	2.37	0.56
23:K:55:VAL:HG22	23:K:68:LEU:HD23	1.88	0.56
27:R:5:ARG:HD2	27:R:53:TYR:HB2	1.88	0.56
28:S:65:GLU:O	28:S:69:ILE:HG12	2.05	0.56
30:U:52:LYS:HB3	30:U:93:LEU:HD12	1.87	0.56
35:g:258:TRP:HB3	35:g:269:ILE:HD11	1.86	0.56
36:i:61:ILE:HA	36:i:91:VAL:HG12	1.86	0.56
40:k:71:GLU:HB3	40:k:182:ARG:HH22	1.71	0.56
40:k:349:LEU:HD23	40:k:388:LYS:HA	1.85	0.56
1:2:715:U:H3	1:2:723:G:H22	1.52	0.56
1:2:1230:U:OP1	1:2:1258:U:O2'	2.17	0.56
1:2:1736:U:H2'	1:2:1737:C:H6	1.71	0.56
1:2:1768:U:H2'	1:2:1769:U:H6	1.71	0.56
5:E:122:LYS:NZ	5:E:145:ARG:HH22	2.04	0.56
6:G:221:ALA:O	6:G:225:GLU:HG2	2.06	0.56
7:H:63:PRO:O	7:H:64:VAL:HB	2.06	0.56
33:d:30:LEU:HA	33:d:39:ASP:HA	1.88	0.56
1:2:140:A:N6	6:G:183:ARG:HG2	2.20	0.56
1:2:885:U:H2'	1:2:886:A:H8	1.70	0.56
1:2:1355:U:O4	1:2:1366:G:O6	2.22	0.56
39:j:198:ILE:HG22	39:j:202:LYS:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:115:G:H5'	10:L:129:ARG:HD3	1.87	0.55
7:H:133:THR:HG21	7:H:154:LEU:HD23	1.88	0.55
27:R:25:THR:O	27:R:31:ASN:ND2	2.39	0.55
1:2:65:A:N7	1:2:83:G:N1	2.55	0.55
1:2:216:A:H2'	1:2:217:A:H8	1.71	0.55
1:2:1791:G:C2	17:a:75:ILE:HD11	2.41	0.55
5:E:41:SER:OG	5:E:42:LEU:N	2.39	0.55
13:V:19:ALA:O	14:W:23:ARG:NH1	2.23	0.55
34:f:102:VAL:HA	34:f:105:TYR:HB2	1.86	0.55
36:i:42:LEU:H	36:i:47:VAL:HA	1.70	0.55
1:2:1086:A:OP2	1:2:1086:A:H8	1.89	0.55
1:2:1652:G:N2	1:2:1743:G:H2'	2.20	0.55
8:I:114:GLU:HA	8:I:118:GLY:HA2	1.88	0.55
9:J:100:LYS:O	9:J:102:GLU:N	2.38	0.55
26:Q:143:ARG:NH1	38:1:35:A:OP1	2.39	0.55
28:S:136:GLN:N	28:S:136:GLN:OE1	2.39	0.55
35:g:39:ARG:HA	35:g:68:ILE:HG23	1.88	0.55
38:1:16:H2U:O3'	38:1:18:G:OP1	2.25	0.55
1:2:473:A:H5'	9:J:144:PRO:HD2	1.89	0.55
1:2:910:U:C2	3:B:5:LYS:CD	2.90	0.55
1:2:1060:U:H5''	1:2:1061:A:H2	1.72	0.55
1:2:1739:U:H2'	1:2:1740:U:C6	2.42	0.55
4:C:162:LYS:HE3	14:W:95:PRO:HA	1.88	0.55
9:J:59:LEU:HD12	9:J:69:ARG:HA	1.88	0.55
34:f:121:CYS:HB3	34:f:128:ILE:HG23	1.88	0.55
39:j:23:ASN:O	39:j:34:VAL:HB	2.06	0.55
40:k:320:SER:HB2	40:k:412:LEU:HB2	1.88	0.55
1:2:495:G:H2'	1:2:496:G:C8	2.42	0.55
2:A:8:ASP:OD1	2:A:9:LEU:N	2.38	0.55
6:G:3:LEU:HD23	6:G:111:LEU:HD21	1.89	0.55
7:H:117:THR:HG22	7:H:119:THR:H	1.71	0.55
14:W:31:SER:H	14:W:34:ILE:HD13	1.69	0.55
40:k:118:ARG:HD3	40:k:124:GLN:HG3	1.88	0.55
1:2:348:U:OP2	10:L:106:ASN:ND2	2.39	0.55
1:2:658:C:H2'	1:2:659:G:C8	2.42	0.55
1:2:1523:A:N3	1:2:1587:C:O2'	2.36	0.55
1:2:1570:2MG:O2'	22:F:187:ARG:NH2	2.39	0.55
2:A:207:PRO:HA	2:A:210:ILE:HG22	1.89	0.55
6:G:48:TYR:HB3	6:G:50:PHE:HE1	1.72	0.55
24:M:101:GLY:O	24:M:102:ASN:CG	2.49	0.55
39:j:25:GLN:HE22	39:j:35:LYS:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:204:MET:HE3	40:k:232:HIS:CE1	2.41	0.55
1:2:224:A:H3'	1:2:225:A:H8	1.71	0.55
1:2:606:G:H5'	1:2:612:G:N2	2.21	0.55
1:2:1359:A:N6	1:2:1363:G:O6	2.39	0.55
1:2:1610:U:P	22:F:97:ASN:HD21	2.28	0.55
1:2:1794:C:N4	17:a:6:ALA:H	2.04	0.55
2:A:18:LEU:HA	2:A:23:HIS:CD2	2.42	0.55
6:G:69:LEU:HG	6:G:71:THR:H	1.71	0.55
22:F:36:GLN:HG3	26:Q:57:LEU:HD22	1.89	0.55
35:g:70:GLN:HB2	35:g:86:TRP:NE1	2.19	0.55
35:g:283:PRO:HG3	35:g:320:TRP:HH2	1.71	0.55
40:k:466:ILE:HA	40:k:499:ILE:HG12	1.87	0.55
1:2:167:A:H5'	6:G:137:ARG:HD3	1.88	0.55
1:2:799:U:H2'	1:2:800:G:C8	2.41	0.55
1:2:933:C:N4	1:2:1076:C:O3'	2.39	0.55
24:M:78:PRO:HB2	24:M:128:LEU:HD22	1.88	0.55
31:Z:91:PRO:HA	31:Z:101:TYR:CD1	2.42	0.55
39:j:25:GLN:HG2	39:j:26:GLN:HG2	1.89	0.55
1:2:761:G:O2'	9:J:72:GLU:OE2	2.20	0.55
1:2:1480:C:O2'	26:Q:72:GLY:O	2.24	0.55
1:2:1544:G:OP2	28:S:123:ARG:NH2	2.33	0.55
16:Y:52:LYS:O	16:Y:55:VAL:HG12	2.06	0.55
21:D:216:PRO:O	35:g:203:ASN:ND2	2.38	0.55
31:Z:91:PRO:HA	31:Z:101:TYR:HD1	1.71	0.55
1:2:152:G:H2'	1:2:153:G:C8	2.42	0.55
1:2:245:G:H2'	1:2:246:A:C8	2.42	0.55
1:2:1788:A:O5'	17:a:10:ARG:NH1	2.40	0.55
3:B:38:PHE:CD2	3:B:73:LEU:HD23	2.42	0.55
9:J:32:GLY:HA3	19:e:40:TYR:CG	2.42	0.55
23:K:9:LYS:HE2	23:K:9:LYS:HA	1.88	0.55
24:M:94:LEU:O	24:M:104:ARG:NH1	2.39	0.55
29:T:13:ASP:OD1	29:T:14:PHE:N	2.40	0.55
1:2:565:C:H5'	36:i:62:ARG:NH1	2.21	0.54
1:2:586:C:H5'	19:e:24:GLN:HE22	1.72	0.54
1:2:620:A:HO2'	1:2:1105:U:HO2'	1.52	0.54
1:2:866:G:H21	11:N:87:ASP:CG	2.15	0.54
1:2:1044:C:H2'	1:2:1045:G:C8	2.42	0.54
1:2:1276:G:H2'	1:2:1277:G:C8	2.42	0.54
1:2:1378:U:H2'	1:2:1379:U:O4'	2.06	0.54
21:D:28:GLU:HB2	23:K:58:GLN:NE2	2.22	0.54
22:F:49:SER:OG	22:F:130:ASN:ND2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:96:LYS:HB2	28:S:98:TYR:CE1	2.41	0.54
35:g:33:LEU:HD21	35:g:95:LEU:HD21	1.87	0.54
40:k:93:GLU:HA	40:k:97:ARG:HH21	1.72	0.54
40:k:317:VAL:HG11	40:k:412:LEU:HB3	1.89	0.54
1:2:738:G:H2'	1:2:739:G:C8	2.42	0.54
5:E:130:GLN:HB2	5:E:138:TYR:CZ	2.42	0.54
24:M:95:GLY:CA	24:M:104:ARG:NH1	2.66	0.54
35:g:145:LEU:HD12	35:g:186:TRP:HZ3	1.72	0.54
41:l:195:LEU:HD21	41:l:222:MET:HE1	1.88	0.54
1:2:649:U:H2'	1:2:650:G:C8	2.43	0.54
1:2:886:A:H2'	1:2:887:U:C6	2.43	0.54
1:2:1458:A:H5''	25:P:128:HIS:HD2	1.72	0.54
1:2:1481:A:H4'	26:Q:71:GLY:HA2	1.89	0.54
1:2:1622:C:H2'	1:2:1623:C:C6	2.43	0.54
5:E:18:TRP:HB3	5:E:20:LEU:HG	1.89	0.54
5:E:63:ALA:HA	5:E:66:MET:HE2	1.89	0.54
12:O:16:VAL:HG21	12:O:82:LYS:HE3	1.90	0.54
17:a:44:ILE:HG23	17:a:45:VAL:HG13	1.88	0.54
19:e:39:LEU:HD23	19:e:43:ARG:NH1	2.21	0.54
21:D:25:PHE:O	21:D:29:LEU:HB2	2.07	0.54
28:S:23:ASP:OD1	28:S:24:GLY:N	2.41	0.54
30:U:118:ILE:HG13	30:U:119:ALA:N	2.23	0.54
40:k:71:GLU:C	40:k:182:ARG:HH12	2.15	0.54
1:2:7:G:O6	4:C:210:ARG:NH1	2.27	0.54
1:2:14:C:OP1	4:C:169:SER:OG	2.23	0.54
1:2:968:C:H4'	1:2:1103:U:O2'	2.07	0.54
1:2:1182:A:H61	25:P:99:GLY:HA3	1.73	0.54
5:E:15:PRO:HG3	5:E:39:ARG:NE	2.22	0.54
7:H:46:ILE:HG12	7:H:60:VAL:HG12	1.89	0.54
8:I:113:TYR:CE1	8:I:117:TYR:HB2	2.43	0.54
9:J:85:VAL:HG11	9:J:104:PHE:HD1	1.73	0.54
10:L:97:TYR:O	10:L:99:ARG:HG2	2.07	0.54
13:V:17:CYS:HB2	13:V:56:SER:HB3	1.89	0.54
22:F:103:GLY:C	22:F:105:ASN:N	2.64	0.54
26:Q:112:TYR:HD1	26:Q:116:LEU:HD11	1.73	0.54
39:j:104:LYS:HB3	39:j:140:HIS:CE1	2.43	0.54
1:2:373:U:H2'	1:2:374:U:C6	2.43	0.54
1:2:601:U:H2'	1:2:602:U:C6	2.42	0.54
1:2:1683:G:H2'	1:2:1684:C:C6	2.42	0.54
9:J:40:ARG:HA	9:J:43:TYR:HD2	1.72	0.54
28:S:71:GLN:OE1	28:S:74:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:154:LYS:HG2	35:g:208:VAL:HG23	1.89	0.54
36:i:59:ALA:HA	36:i:89:CYS:O	2.08	0.54
1:2:26:A:H2'	1:2:27:U:C6	2.42	0.54
1:2:67:A:O2'	1:2:69:G:OP1	2.25	0.54
1:2:266:U:OP1	6:G:183:ARG:NE	2.37	0.54
1:2:357:U:O2'	1:2:359:A:OP1	2.26	0.54
1:2:898:G:C5	3:B:5:LYS:HB2	2.42	0.54
1:2:921:G:H2'	1:2:922:A:H8	1.73	0.54
1:2:946:U:H2'	1:2:947:G:H8	1.71	0.54
1:2:1513:A:O2'	1:2:1514:A:OP1	2.25	0.54
3:B:133:TYR:CD2	3:B:181:LEU:HB3	2.43	0.54
7:H:160:GLN:HA	7:H:163:ASP:HB2	1.89	0.54
10:L:49:ILE:H	10:L:49:ILE:HD12	1.71	0.54
22:F:42:ILE:HG23	22:F:71:TYR:CE1	2.42	0.54
22:F:194:GLU:OE2	31:Z:61:SER:OG	2.22	0.54
35:g:159:PRO:HD2	35:g:215:GLY:HA2	1.88	0.54
38:1:6:C:H2'	38:1:7:G:C8	2.42	0.54
39:j:27:ILE:HG13	39:j:32:ALA:HB2	1.88	0.54
40:k:106:ILE:HD13	40:k:236:ILE:HD12	1.89	0.54
1:2:1170:A:H2'	1:2:1171:G:H8	1.69	0.54
3:B:107:THR:O	3:B:111:ARG:HG2	2.08	0.54
6:G:7:TYR:HD1	6:G:113:ILE:HG13	1.72	0.54
12:O:65:GLN:HE22	12:O:104:ALA:HB1	1.71	0.54
16:Y:29:HIS:HB2	16:Y:32:ARG:HB3	1.89	0.54
22:F:42:ILE:HG22	22:F:69:PRO:HB2	1.89	0.54
22:F:114:ARG:HD3	26:Q:43:ILE:HD12	1.90	0.54
25:P:123:TYR:OH	28:S:122:HIS:NE2	2.32	0.54
38:1:36:U:H2'	38:1:37:T6A:H8	1.72	0.54
39:j:132:TRP:O	39:j:136:ARG:HG2	2.07	0.54
1:2:71:A:H3'	1:2:72:A:H5''	1.90	0.54
1:2:463:A:C2	1:2:464:G:C8	2.95	0.54
1:2:531:U:H2'	1:2:532:U:O4'	2.07	0.54
1:2:650:G:H1	1:2:684:A:N6	2.06	0.54
1:2:1145:G:H2'	1:2:1146:A:H8	1.72	0.54
1:2:1543:A:H3'	28:S:134:ARG:HH21	1.72	0.54
2:A:24:LEU:HD12	2:A:41:ARG:HH22	1.73	0.54
3:B:35:PRO:HB3	3:B:231:LEU:HD13	1.89	0.54
23:K:9:LYS:NZ	23:K:80:LEU:HB2	2.22	0.54
1:2:2:A:H2'	4:C:202:TYR:HD1	1.72	0.54
1:2:305:U:OP2	10:L:105:LYS:NZ	2.41	0.54
1:2:928:A:H2	3:B:111:ARG:HH12	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1617:C:H2'	1:2:1618:C:C6	2.43	0.54
1:2:1749:C:H2'	1:2:1750:U:H6	1.73	0.54
22:F:39:GLN:C	22:F:41:GLU:N	2.66	0.54
29:T:86:ARG:NE	29:T:92:LYS:HE2	2.22	0.54
40:k:315:LEU:HD12	40:k:347:PHE:HE2	1.73	0.54
1:2:428:G:H2'	1:2:429:G:H8	1.73	0.54
1:2:880:A:H2'	1:2:881:U:O4'	2.08	0.54
1:2:1219:C:H2'	1:2:1220:A:C8	2.43	0.54
1:2:1768:U:H2'	1:2:1769:U:C6	2.42	0.54
3:B:133:TYR:CE2	3:B:181:LEU:HD22	2.43	0.54
6:G:120:GLU:OE1	6:G:126:ASN:ND2	2.41	0.54
7:H:185:ILE:HD12	7:H:186:PRO:HD2	1.89	0.54
10:L:76:VAL:HG21	10:L:87:ARG:HD2	1.90	0.54
12:O:128:LYS:HB3	17:a:22:ARG:HD3	1.90	0.54
13:V:55:LEU:HD11	13:V:69:LEU:HD22	1.89	0.54
22:F:147:ASP:OD1	22:F:148:THR:N	2.34	0.54
33:d:21:CYS:C	33:d:23:ILE:H	2.15	0.54
39:j:130:ILE:HG13	39:j:158:ILE:HD13	1.89	0.54
1:2:40:A:H3'	1:2:41:A:H8	1.73	0.53
1:2:399:A:H5''	8:I:25:ARG:HA	1.90	0.53
1:2:915:U:O2	12:O:41:ARG:NH2	2.33	0.53
1:2:1379:U:O4	1:2:1380:A:N6	2.41	0.53
3:B:133:TYR:HD2	3:B:181:LEU:HB3	1.71	0.53
4:C:125:GLU:N	4:C:125:GLU:OE2	2.41	0.53
5:E:86:PHE:HE1	5:E:87:MET:HE2	1.72	0.53
8:I:92:ARG:HH21	8:I:93:THR:HG22	1.73	0.53
24:M:53:ALA:HB3	24:M:79:LEU:HD23	1.89	0.53
28:S:109:LEU:O	28:S:113:LEU:HG	2.08	0.53
35:g:194:ARG:HG3	35:g:195:ILE:H	1.73	0.53
35:g:212:SER:OG	35:g:214:ASP:OD1	2.24	0.53
36:i:37:GLN:OE1	36:i:75:ASP:N	2.41	0.53
38:1:44:A:O2'	38:1:45:U:O4'	2.20	0.53
1:2:566:A:N3	19:e:14:VAL:HG11	2.24	0.53
22:F:167:LEU:HD23	32:c:47:PRO:HG2	1.90	0.53
35:g:34:LEU:HD22	35:g:46:TRP:CD1	2.44	0.53
41:l:230:ILE:HA	41:l:234:VAL:HB	1.90	0.53
1:2:230:U:O2'	1:2:232:C:OP2	2.24	0.53
2:A:77:SER:O	2:A:100:GLY:N	2.41	0.53
3:B:74:GLN:HG2	3:B:79:HIS:CE1	2.43	0.53
3:B:128:LYS:NZ	3:B:132:ASP:O	2.31	0.53
5:E:246:LEU:HD21	5:E:254:ARG:HH21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:96:ARG:HH22	7:H:124:LYS:CD	2.19	0.53
35:g:231:ASN:HB3	35:g:234:HIS:HB2	1.89	0.53
35:g:283:PRO:HG2	35:g:318:ARG:HH11	1.74	0.53
39:j:240:GLY:HA2	39:j:243:GLN:NE2	2.22	0.53
1:2:122:U:N3	1:2:123:G:N7	2.57	0.53
1:2:650:G:N1	1:2:684:A:C6	2.76	0.53
1:2:815:G:H2'	1:2:816:A:H8	1.72	0.53
1:2:1159:A:H2'	1:2:1160:C:H6	1.74	0.53
1:2:1187:G:O2'	1:2:1428:U:OP1	2.22	0.53
1:2:1497:G:H2'	1:2:1498:C:H6	1.73	0.53
3:B:79:HIS:CG	3:B:82:ARG:HH12	2.26	0.53
4:C:93:LYS:HB2	4:C:100:ARG:HE	1.73	0.53
4:C:147:GLY:N	4:C:158:SER:O	2.25	0.53
25:P:108:ARG:HB2	25:P:111:MET:HG2	1.90	0.53
40:k:234:ALA:O	40:k:238:ILE:HG13	2.08	0.53
40:k:473:ALA:HB1	40:k:485:LEU:HB3	1.91	0.53
1:2:213:G:N2	1:2:251:U:O4	2.42	0.53
1:2:405:U:H2'	1:2:406:A:C8	2.44	0.53
1:2:408:C:H2'	1:2:409:A:H8	1.73	0.53
1:2:574:C:N4	15:X:65:ASN:HD21	2.07	0.53
1:2:1749:C:H2'	1:2:1750:U:C6	2.44	0.53
2:A:14:ALA:O	2:A:18:LEU:HD23	2.09	0.53
11:N:23:PRO:HB2	11:N:25:TRP:CD1	2.44	0.53
21:D:47:GLU:OE2	21:D:87:TYR:N	2.42	0.53
27:R:71:PHE:HE2	27:R:73:LEU:HB3	1.73	0.53
28:S:121:SER:O	28:S:124:GLY:N	2.42	0.53
29:T:130:ARG:O	29:T:134:ARG:HG3	2.09	0.53
1:2:691:U:O4	1:2:692:C:N4	2.41	0.53
1:2:1101:G:H2'	1:2:1102:U:O4'	2.09	0.53
1:2:1203:A:N6	33:d:15:GLY:HA3	2.24	0.53
1:2:1297:U:O2'	1:2:1298:G:O5'	2.19	0.53
24:M:55:LEU:HD12	24:M:65:SER:HA	1.89	0.53
40:k:71:GLU:O	40:k:182:ARG:NH1	2.39	0.53
1:2:716:C:H42	1:2:722:G:H1	1.56	0.53
1:2:1353:G:O6	1:2:1368:U:O2	2.27	0.53
1:2:1518:U:H4'	1:2:1521:G:N2	2.24	0.53
3:B:30:TYR:CD2	3:B:61:LEU:HD21	2.38	0.53
3:B:135:LEU:HD23	3:B:217:LEU:HA	1.90	0.53
8:I:157:VAL:HG12	8:I:161:PHE:CZ	2.43	0.53
21:D:23:GLU:HG3	21:D:24:PHE:N	2.24	0.53
28:S:104:ASN:HB3	28:S:108:LYS:HZ1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:T:70:GLN:OE1	29:T:70:GLN:N	2.42	0.53
35:g:307:THR:HG22	35:g:321:GLN:HG3	1.91	0.53
38:1:21:A:N6	38:1:48:5MC:OP1	2.42	0.53
1:2:945:U:H5'	3:B:165:ARG:NH1	2.24	0.53
1:2:1228:G:O6	24:M:39:ARG:HB3	2.09	0.53
1:2:1562:U:H2'	1:2:1563:C:C6	2.44	0.53
3:B:57:ALA:O	3:B:61:LEU:HD12	2.09	0.53
11:N:33:VAL:O	11:N:37:ILE:HG12	2.09	0.53
27:R:45:ARG:O	27:R:49:LYS:HG2	2.08	0.53
40:k:353:ILE:HG13	40:k:419:ALA:HA	1.89	0.53
1:2:318:U:O2'	1:2:322:A:N7	2.38	0.53
1:2:650:G:C6	1:2:684:A:N6	2.76	0.53
1:2:841:C:H2'	1:2:842:U:C6	2.43	0.53
1:2:1144:U:N3	1:2:1145:G:N7	2.57	0.53
1:2:1177:G:H5'	1:2:1189:C:H42	1.73	0.53
1:2:1465:C:H2'	1:2:1466:U:C6	2.44	0.53
1:2:1479:C:OP1	29:T:63:ARG:NH1	2.34	0.53
3:B:33:LYS:O	3:B:98:THR:HG22	2.09	0.53
3:B:106:THR:HG23	3:B:109:LYS:H	1.74	0.53
4:C:232:PRO:HA	4:C:235:TRP:CE2	2.44	0.53
6:G:22:HIS:HA	6:G:25:ARG:HG2	1.91	0.53
13:V:74:GLN:NE2	13:V:83:TRP:O	2.42	0.53
17:a:62:TYR:HD1	17:a:64:LEU:H	1.57	0.53
25:P:108:ARG:HB2	25:P:111:MET:HE3	1.90	0.53
35:g:145:LEU:HD12	35:g:186:TRP:CZ3	2.43	0.53
39:j:183:LYS:HB2	39:j:185:ARG:HH11	1.74	0.53
1:2:473:A:N6	1:2:593:A:OP1	2.42	0.53
1:2:653:C:HO2'	1:2:654:G:H8	1.56	0.53
1:2:778:G:H3'	1:2:780:A:H2	1.74	0.53
1:2:855:A:H1'	7:H:64:VAL:HG11	1.90	0.53
1:2:902:U:O4	12:O:52:ARG:NH2	2.31	0.53
2:A:163:ASN:OD1	2:A:165:ARG:HG2	2.09	0.53
14:W:44:HIS:NE2	14:W:112:ASP:OD2	2.42	0.53
14:W:98:GLN:OE1	14:W:98:GLN:N	2.34	0.53
25:P:24:LYS:O	25:P:28:MET:HB2	2.09	0.53
26:Q:99:GLU:O	26:Q:102:LYS:HG3	2.09	0.53
27:R:126:ALA:O	27:R:128:ARG:NH1	2.42	0.53
1:2:513:G:N7	1:2:536:G:N2	2.56	0.52
1:2:976:A:N7	1:2:1023:U:O4	2.41	0.52
3:B:6:ASN:O	3:B:7:LYS:CG	2.57	0.52
10:L:107:VAL:HG11	10:L:137:PHE:HD2	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:92:LYS:NZ	12:O:122:PRO:HD2	2.24	0.52
38:1:10:2MG:H2'	38:1:11:C:C6	2.44	0.52
40:k:207:GLY:O	40:k:211:MET:HG3	2.09	0.52
40:k:356:ARG:HE	40:k:424:PRO:HD2	1.74	0.52
1:2:804:U:O2'	14:W:78:ARG:NH1	2.43	0.52
1:2:885:U:O2'	12:O:121:VAL:O	2.27	0.52
1:2:1201:A:H2'	1:2:1454:C:H41	1.73	0.52
1:2:1437:C:H2'	1:2:1438:C:H6	1.75	0.52
1:2:1679:A:C8	6:G:66:GLY:HA3	2.43	0.52
1:2:1786:G:OP2	12:O:132:ARG:NH1	2.42	0.52
7:H:21:ALA:O	7:H:25:ILE:HG12	2.09	0.52
12:O:64:ALA:HB1	12:O:105:LEU:HD22	1.91	0.52
15:X:107:PHE:CE2	15:X:114:LYS:HG3	2.45	0.52
26:Q:39:VAL:HG22	26:Q:45:ARG:NE	2.22	0.52
39:j:25:GLN:N	39:j:25:GLN:OE1	2.43	0.52
40:k:463:MET:HB3	40:k:502:SER:OG	2.09	0.52
1:2:367:U:O2	1:2:372:G:O6	2.27	0.52
1:2:905:A:P	12:O:52:ARG:HD2	2.49	0.52
1:2:1485:A:H2'	1:2:1486:G:C8	2.44	0.52
1:2:1577:U:H2'	1:2:1578:C:C6	2.44	0.52
2:A:127:ARG:HH21	2:A:152:PRO:HD3	1.75	0.52
6:G:159:ARG:HD2	6:G:172:ALA:HB2	1.92	0.52
6:G:163:THR:HG22	6:G:165:GLY:H	1.74	0.52
9:J:34:TYR:CD2	9:J:105:LEU:HB3	2.45	0.52
18:b:65:THR:O	18:b:72:LYS:N	2.36	0.52
23:K:25:LYS:HB3	23:K:62:GLN:HB3	1.92	0.52
1:2:194:G:O2'	1:2:195:G:H5'	2.09	0.52
1:2:979:G:H4'	1:2:1774:A:H4'	1.91	0.52
1:2:1239:U:H2'	1:2:1241:A:OP2	2.10	0.52
1:2:1553:A:H5''	25:P:44:LYS:HZ3	1.75	0.52
3:B:3:VAL:HG11	39:j:72:VAL:HG21	1.90	0.52
4:C:58:ILE:HD12	4:C:62:PHE:HE2	1.75	0.52
8:I:67:TRP:O	8:I:71:GLY:N	2.42	0.52
19:e:46:ASN:HD22	19:e:46:ASN:N	2.08	0.52
22:F:93:GLU:O	22:F:96:THR:OG1	2.26	0.52
22:F:119:THR:O	22:F:123:ILE:HG12	2.10	0.52
25:P:90:ILE:HD13	25:P:109:PRO:HA	1.91	0.52
29:T:38:LYS:HZ2	29:T:38:LYS:HB3	1.75	0.52
36:i:71:MET:HE1	36:i:94:LYS:HB2	1.92	0.52
1:2:116:U:O2'	1:2:332:A:N3	2.30	0.52
1:2:131:C:H4'	1:2:132:U:H4'	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:751:G:H2'	1:2:752:A:H8	1.75	0.52
1:2:1050:G:H3'	1:2:1051:U:H4'	1.92	0.52
1:2:1315:G:P	27:R:6:THR:HG1	2.32	0.52
1:2:1316:C:H5'	27:R:10:LYS:NZ	2.25	0.52
1:2:1426:2MG:HM22	1:2:1427:G:C2	2.45	0.52
3:B:82:ARG:NE	3:B:191:GLU:OE1	2.43	0.52
22:F:211:TYR:OH	22:F:215:LYS:NZ	2.42	0.52
36:i:82:ARG:HH21	36:i:88:GLN:HG3	1.75	0.52
39:j:100:GLU:O	39:j:104:LYS:HG2	2.09	0.52
1:2:220:A:H2'	1:2:221:A:C8	2.45	0.52
1:2:415:A:H5'	1:2:416:A:C8	2.44	0.52
1:2:689:G:H2'	1:2:690:A:C8	2.45	0.52
1:2:975:G:H1	1:2:1022:A:HO2'	1.57	0.52
1:2:1107:G:H2'	15:X:25:ALA:HB1	1.92	0.52
1:2:1209:C:H2'	1:2:1210:A:H8	1.75	0.52
4:C:152:ASN:ND2	13:V:2:GLU:O	2.43	0.52
5:E:15:PRO:HG2	5:E:18:TRP:CZ3	2.39	0.52
6:G:51:LYS:HB3	6:G:112:ILE:HB	1.91	0.52
10:L:5:LEU:O	10:L:6:THR:OG1	2.23	0.52
22:F:102:ASN:O	22:F:104:ARG:N	2.43	0.52
22:F:152:GLY:HA3	22:F:157:ALA:HA	1.92	0.52
26:Q:36:ILE:HD11	26:Q:48:VAL:HG22	1.91	0.52
30:U:46:GLU:O	30:U:49:LYS:HD2	2.09	0.52
39:j:240:GLY:HA2	39:j:243:GLN:HG2	1.92	0.52
1:2:511:A:H2'	1:2:512:U:O4'	2.10	0.52
1:2:513:G:N7	9:J:171:ARG:NH1	2.58	0.52
1:2:550:G:H2'	1:2:551:G:C8	2.43	0.52
1:2:749:U:H2'	1:2:750:U:C6	2.45	0.52
1:2:1259:U:O2'	1:2:1260:G:H8	1.93	0.52
2:A:154:GLU:OE1	2:A:154:GLU:N	2.42	0.52
5:E:124:ALA:HA	5:E:142:HIS:HE1	1.75	0.52
8:I:48:THR:OG1	8:I:49:ARG:N	2.42	0.52
30:U:22:ILE:HG21	30:U:100:VAL:HG11	1.91	0.52
35:g:283:PRO:HG3	35:g:320:TRP:CH2	2.44	0.52
1:2:125:U:O2	1:2:292:U:N3	2.43	0.52
1:2:262:C:H2'	1:2:263:G:C8	2.44	0.52
1:2:1316:C:H5'	27:R:10:LYS:HZ1	1.75	0.52
2:A:122:ILE:HA	2:A:144:ILE:O	2.09	0.52
3:B:6:ASN:O	3:B:7:LYS:HG2	2.09	0.52
13:V:46:ILE:HD12	13:V:47:PRO:HD2	1.91	0.52
15:X:103:LEU:HD23	15:X:126:LYS:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:40:ALA:HB3	17:a:69:ASN:HB2	1.92	0.52
18:b:23:THR:OG1	18:b:25:VAL:O	2.24	0.52
35:g:132:ILE:HB	35:g:145:LEU:HB2	1.90	0.52
39:j:7:ARG:HG2	39:j:12:LYS:HA	1.91	0.52
1:2:863:U:O4	14:W:60:LYS:NZ	2.32	0.52
1:2:991:A:N7	1:2:1011:U:O4	2.43	0.52
1:2:1240:G:C8	25:P:79:HIS:CG	2.98	0.52
1:2:1413:U:OP1	27:R:45:ARG:NH2	2.36	0.52
1:2:1469:A:OP1	22:F:187:ARG:NH2	2.42	0.52
1:2:1594:C:OP1	33:d:19:ARG:NH2	2.42	0.52
2:A:37:VAL:HG23	2:A:46:ASN:HB3	1.92	0.52
7:H:96:ARG:NH1	7:H:124:LYS:HB2	2.25	0.52
8:I:179:ARG:NH1	8:I:181:ASP:OD2	2.43	0.52
22:F:167:LEU:HG	22:F:171:ASN:HD21	1.75	0.52
24:M:56:VAL:HG13	24:M:83:ALA:HA	1.92	0.52
1:2:298:A:P	5:E:30:ARG:HH22	2.33	0.52
1:2:1791:G:C4	17:a:75:ILE:HD11	2.45	0.52
5:E:15:PRO:HG3	5:E:39:ARG:HE	1.75	0.52
5:E:23:LEU:HD12	9:J:3:ARG:HH21	1.74	0.52
9:J:31:ALA:HA	9:J:36:LEU:HD12	1.92	0.52
10:L:21:THR:OG1	10:L:32:LYS:N	2.43	0.52
11:N:129:TYR:HA	11:N:132:VAL:HG12	1.92	0.52
15:X:3:LYS:O	15:X:5:LYS:N	2.37	0.52
22:F:42:ILE:HD12	22:F:42:ILE:H	1.75	0.52
22:F:99:LEU:O	22:F:182:ARG:NH2	2.42	0.52
23:K:14:HIS:ND1	23:K:35:ILE:HD13	2.25	0.52
35:g:115:ALA:HB1	35:g:157:VAL:HG13	1.92	0.52
36:i:67:LYS:NZ	37:3:33:C:OP1	2.39	0.52
38:1:2:G:H2'	38:1:3:C:C6	2.45	0.52
40:k:112:GLY:HA3	44:k:601:GCP:H8	1.91	0.52
40:k:297:PHE:HD1	40:k:300:LYS:HD3	1.74	0.52
1:2:239:C:H4'	1:2:240:U:OP2	2.09	0.51
1:2:295:U:H2'	1:2:296:U:C6	2.44	0.51
1:2:589:C:H5''	19:e:43:ARG:NH2	2.25	0.51
1:2:1059:U:H2'	1:2:1060:U:O2	2.10	0.51
1:2:1350:G:H2'	1:2:1351:U:C6	2.46	0.51
1:2:1455:C:O2'	1:2:1456:G:H5'	2.11	0.51
3:B:87:ARG:HB2	3:B:101:HIS:HB2	1.92	0.51
4:C:46:LEU:HD21	4:C:68:VAL:HG12	1.92	0.51
7:H:117:THR:HG22	7:H:119:THR:N	2.25	0.51
22:F:101:MET:HA	22:F:101:MET:HE3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:82:LEU:HD23	23:K:86:ILE:HD13	1.93	0.51
24:M:71:LEU:HD21	34:f:106:TYR:CE2	2.45	0.51
39:j:109:HIS:HD1	39:j:127:TYR:HH	1.58	0.51
1:2:339:U:H2'	1:2:340:A:C8	2.44	0.51
1:2:611:U:OP2	15:X:5:LYS:NZ	2.42	0.51
1:2:855:A:N7	7:H:116:ARG:NE	2.58	0.51
6:G:67:VAL:H	6:G:100:ALA:HB2	1.75	0.51
8:I:160:GLN:HB3	8:I:166:LEU:HD13	1.91	0.51
9:J:89:ASP:HB3	9:J:90:LYS:HD3	1.92	0.51
12:O:16:VAL:HG22	12:O:18:ARG:HG3	1.91	0.51
12:O:46:MET:HE3	12:O:46:MET:HA	1.92	0.51
13:V:30:SER:OG	13:V:57:GLY:HA3	2.10	0.51
14:W:87:GLU:O	14:W:90:THR:OG1	2.19	0.51
23:K:77:ARG:O	23:K:81:ASN:N	2.43	0.51
27:R:57:LEU:HD23	27:R:60:ARG:HH21	1.76	0.51
28:S:42:TYR:HA	28:S:85:PHE:CZ	2.45	0.51
35:g:117:ASP:OD1	35:g:118:ALA:N	2.43	0.51
1:2:339:U:H2'	1:2:340:A:H8	1.76	0.51
1:2:983:G:H2'	1:2:984:G:C8	2.45	0.51
1:2:1418:C:OP1	33:d:54:LYS:NZ	2.44	0.51
1:2:1485:A:H2'	1:2:1486:G:H8	1.75	0.51
1:2:1532:G:OP2	31:Z:74:SER:HB3	2.10	0.51
2:A:139:VAL:HG13	2:A:141:ILE:HG13	1.92	0.51
6:G:57:ASP:HB3	6:G:61:PHE:H	1.75	0.51
7:H:162:ILE:HG23	7:H:165:LYS:HB2	1.91	0.51
40:k:166:SER:HB2	40:k:383:GLU:HG2	1.93	0.51
1:2:743:U:H2'	1:2:744:U:C6	2.46	0.51
1:2:977:A:C4	1:2:978:A:C8	2.98	0.51
3:B:88:VAL:HA	3:B:98:THR:HA	1.91	0.51
7:H:99:LEU:HD22	7:H:112:ARG:HB2	1.92	0.51
10:L:33:ARG:NH2	10:L:53:TYR:O	2.40	0.51
24:M:34:LEU:HB3	24:M:36:ARG:HG3	1.93	0.51
32:c:67:ARG:HD2	37:3:24:U:C6	2.45	0.51
35:g:68:ILE:O	35:g:86:TRP:N	2.32	0.51
38:l:27:C:H4'	41:l:214:LYS:HE3	1.93	0.51
39:j:127:TYR:HA	39:j:131:ALA:HB3	1.92	0.51
1:2:318:U:H5'	8:I:11:ARG:HH12	1.76	0.51
1:2:471:U:H2'	1:2:472:A:H8	1.76	0.51
1:2:478:C:O3'	9:J:120:LYS:NZ	2.44	0.51
1:2:1591:A:H2'	1:2:1592:G:H8	1.75	0.51
1:2:1710:A:C6	1:2:1711:G:H1'	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:ILE:HG13	5:E:61:VAL:HG21	1.91	0.51
9:J:83:ILE:O	9:J:107:ARG:NH2	2.42	0.51
10:L:108:PRO:HB2	10:L:135:VAL:HG12	1.93	0.51
21:D:164:VAL:HG23	21:D:168:ILE:HD12	1.93	0.51
25:P:72:LYS:CD	25:P:106:GLU:HG3	2.41	0.51
1:2:387:G:O3'	1:2:424:A:N6	2.44	0.51
1:2:780:A:N7	16:Y:8:ARG:NH1	2.57	0.51
1:2:1056:U:C4	1:2:1059:U:H5''	2.45	0.51
3:B:133:TYR:HE1	3:B:221:PRO:HD2	1.75	0.51
4:C:94:GLN:HG2	4:C:99:GLN:OE1	2.09	0.51
10:L:35:TYR:CE2	10:L:49:ILE:HG23	2.45	0.51
18:b:11:THR:HG22	18:b:13:ALA:H	1.76	0.51
22:F:144:PRO:O	22:F:169:ARG:HG2	2.11	0.51
22:F:202:ASN:HB2	22:F:210:SER:HB2	1.92	0.51
25:P:50:SER:HB2	25:P:53:PRO:CD	2.40	0.51
30:U:19:ILE:HG21	30:U:94:GLU:HG3	1.91	0.51
33:d:21:CYS:O	33:d:22:ARG:HG2	2.10	0.51
36:i:33:GLN:HB3	36:i:78:LEU:HD21	1.92	0.51
39:j:154:VAL:HG23	39:j:155:TRP:CD1	2.46	0.51
1:2:799:U:H2'	1:2:800:G:H8	1.76	0.51
3:B:197:ILE:HG21	3:B:210:VAL:HG11	1.92	0.51
21:D:167:PHE:O	21:D:190:LYS:NZ	2.28	0.51
26:Q:142:TYR:O	26:Q:143:ARG:HG3	2.11	0.51
35:g:21:VAL:HG11	35:g:317:ILE:HG12	1.93	0.51
36:i:87:ASP:OD1	36:i:88:GLN:N	2.43	0.51
1:2:391:G:H5''	1:2:1727:C:O2'	2.10	0.51
1:2:1582:G:H22	1:2:1609:A:P	2.34	0.51
2:A:38:TYR:CE2	2:A:39:LYS:HE2	2.45	0.51
5:E:86:PHE:CE1	5:E:87:MET:HE2	2.46	0.51
14:W:11:LEU:HD11	14:W:37:PHE:HE2	1.75	0.51
16:Y:13:ILE:CG2	16:Y:22:GLN:HE21	2.19	0.51
21:D:169:GLU:HG3	21:D:190:LYS:HZ2	1.76	0.51
1:2:105:A:OP1	8:I:18:ARG:NH2	2.39	0.51
1:2:157:U:O2'	1:2:159:C:OP2	2.16	0.51
1:2:253:A:H2'	1:2:254:U:C6	2.45	0.51
1:2:384:A:H2'	1:2:385:G:C8	2.46	0.51
1:2:627:G:OP1	11:N:124:ARG:NE	2.43	0.51
1:2:860:U:H2'	1:2:861:A:O4'	2.11	0.51
1:2:1038:A:H4'	13:V:62:ARG:NH2	2.25	0.51
1:2:1161:C:H4'	32:c:22:ARG:HG3	1.92	0.51
1:2:1247:C:OP2	34:f:93:HIS:ND1	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1389:A:H2'	1:2:1390:U:C6	2.46	0.51
1:2:1631:A:H1'	4:C:94:GLN:HE22	1.76	0.51
1:2:1750:U:H2'	1:2:1751:A:C8	2.46	0.51
9:J:32:GLY:HA3	19:e:40:TYR:CD1	2.46	0.51
18:b:45:THR:HG23	18:b:82:LYS:NZ	2.25	0.51
29:T:108:LEU:HD22	29:T:113:VAL:HG21	1.92	0.51
30:U:63:LEU:O	30:U:83:GLU:HA	2.10	0.51
1:2:1165:A:H5''	22:F:103:GLY:H	1.76	0.51
1:2:1350:G:H2'	1:2:1351:U:H6	1.76	0.51
1:2:1622:C:H2'	1:2:1623:C:H6	1.76	0.51
4:C:247:VAL:HG13	4:C:248:TYR:CD1	2.45	0.51
17:a:33:ASP:OD1	17:a:34:LYS:N	2.44	0.51
17:a:50:ILE:HG13	17:a:51:ARG:N	2.26	0.51
24:M:71:LEU:HD21	34:f:106:TYR:HE2	1.76	0.51
25:P:111:MET:HE1	28:S:119:ILE:HA	1.93	0.51
34:f:116:LYS:HE2	34:f:120:GLU:HB3	1.93	0.51
35:g:150:ASP:N	35:g:180:ASP:OD2	2.44	0.51
1:2:1448:U:H2'	1:2:1449:C:H6	1.76	0.50
2:A:126:PRO:HG2	2:A:147:THR:HG22	1.93	0.50
5:E:67:GLN:OE1	5:E:69:HIS:ND1	2.44	0.50
15:X:89:ASN:HB2	15:X:92:CYS:HB3	1.93	0.50
24:M:120:ASP:HA	24:M:124:ARG:CG	2.40	0.50
35:g:171:ARG:NH1	35:g:189:ASN:OD1	2.43	0.50
39:j:70:VAL:O	39:j:87:LYS:HG3	2.11	0.50
1:2:303:U:H2'	1:2:304:C:C6	2.45	0.50
1:2:1070:U:H2'	1:2:1071:C:C6	2.46	0.50
1:2:1107:G:H1	15:X:22:ASN:ND2	2.08	0.50
4:C:71:PHE:CG	4:C:135:ILE:HG13	2.47	0.50
4:C:174:LEU:HD13	4:C:203:THR:HG22	1.93	0.50
25:P:71:GLU:OE2	25:P:72:LYS:N	2.44	0.50
30:U:24:ILE:HG12	30:U:116:VAL:HG22	1.91	0.50
40:k:314:ARG:HD2	40:k:344:ASN:ND2	2.19	0.50
1:2:961:C:H2'	1:2:962:A:O4'	2.12	0.50
1:2:1086:A:H2'	1:2:1087:A:C8	2.47	0.50
1:2:1351:U:H2'	1:2:1352:U:O4'	2.11	0.50
1:2:1433:G:O6	23:K:64:TYR:OH	2.23	0.50
1:2:1736:U:H2'	1:2:1737:C:C6	2.46	0.50
9:J:65:LYS:HA	9:J:70:LEU:HD11	1.93	0.50
14:W:29:PRO:O	14:W:58:SER:OG	2.25	0.50
18:b:65:THR:N	18:b:72:LYS:O	2.33	0.50
26:Q:13:LYS:HG2	26:Q:76:SER:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:124:CYS:HB2	34:f:128:ILE:HG21	1.93	0.50
40:k:121:SER:HB3	40:k:145:ALA:HB2	1.93	0.50
1:2:392:C:OP2	8:I:2:GLY:N	2.44	0.50
1:2:683:C:H3'	1:2:684:A:H8	1.77	0.50
1:2:1104:C:H2'	1:2:1105:U:H6	1.76	0.50
1:2:1235:A:N6	1:2:1236:G:O6	2.44	0.50
1:2:1472:G:H2'	1:2:1473:A:H8	1.76	0.50
1:2:1544:G:N2	28:S:87:ASN:O	2.43	0.50
3:B:180:THR:HG22	3:B:181:LEU:H	1.75	0.50
7:H:118:LEU:O	7:H:122:HIS:ND1	2.41	0.50
10:L:135:VAL:HG23	10:L:135:VAL:O	2.12	0.50
39:j:217:GLN:O	39:j:232:THR:HG23	2.12	0.50
40:k:330:ILE:HD12	40:k:333:LEU:HD11	1.94	0.50
1:2:14:C:H5'	4:C:169:SER:OG	2.12	0.50
1:2:234:G:H2'	1:2:235:A:C8	2.46	0.50
1:2:521:U:H2'	1:2:522:G:O4'	2.12	0.50
1:2:1066:C:OP1	3:B:151:LYS:N	2.32	0.50
1:2:1588:G:OP1	29:T:91:HIS:HB2	2.12	0.50
1:2:1742:A:H3'	1:2:1743:G:H8	1.77	0.50
15:X:56:LYS:NZ	15:X:96:VAL:HB	2.27	0.50
34:f:139:CYS:SG	34:f:140:GLY:N	2.83	0.50
35:g:289:THR:OG1	35:g:292:GLN:NE2	2.37	0.50
1:2:3:U:O2	9:J:17:ARG:NH2	2.43	0.50
1:2:371:G:H1'	1:2:611:U:H3	1.76	0.50
1:2:1131:A:H2'	1:2:1132:A:H8	1.76	0.50
1:2:1573:7MG:HN22	38:1:42:U:H4'	1.76	0.50
4:C:58:ILE:HD11	4:C:115:HIS:CE1	2.47	0.50
5:E:36:HIS:HB2	5:E:41:SER:HB2	1.92	0.50
12:O:80:HIS:HD1	12:O:114:ARG:HB2	1.76	0.50
22:F:55:VAL:HG21	22:F:61:VAL:HB	1.94	0.50
25:P:72:LYS:HD3	25:P:106:GLU:HG3	1.92	0.50
38:1:23:C:H2'	38:1:24:G:H8	1.75	0.50
39:j:113:ARG:HA	39:j:123:LEU:HD21	1.93	0.50
1:2:373:U:H2'	1:2:374:U:H6	1.77	0.50
1:2:768:C:C2	9:J:143:ILE:HD13	2.47	0.50
1:2:898:G:C8	3:B:5:LYS:HB2	2.46	0.50
1:2:1207:A:H4'	1:2:1269:G:OP2	2.12	0.50
11:N:4:MET:HE3	11:N:5:HIS:ND1	2.26	0.50
23:K:23:ALA:HB3	23:K:66:TYR:HE2	1.77	0.50
40:k:127:ARG:HG2	40:k:133:GLU:HA	1.94	0.50
40:k:292:ASP:OD1	40:k:293:ALA:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:643:U:H2'	1:2:644:C:C6	2.47	0.50
1:2:866:G:N2	11:N:87:ASP:OD1	2.41	0.50
1:2:1067:C:H2'	1:2:1068:A:C8	2.46	0.50
1:2:1546:G:H2'	1:2:1547:C:C6	2.47	0.50
5:E:121:TYR:OH	5:E:235:TRP:O	2.25	0.50
10:L:133:LYS:HG3	10:L:134:THR:HG23	1.93	0.50
13:V:18:SER:N	13:V:54:ALA:O	2.42	0.50
15:X:56:LYS:HD3	15:X:93:LEU:HD21	1.94	0.50
15:X:70:LYS:HB3	15:X:93:LEU:HD12	1.93	0.50
15:X:87:VAL:HG12	15:X:92:CYS:SG	2.51	0.50
17:a:79:ILE:HD11	17:a:86:VAL:HG23	1.93	0.50
22:F:130:ASN:OD1	22:F:131:PRO:HD2	2.12	0.50
35:g:126:ALA:HB1	35:g:152:VAL:HG23	1.93	0.50
40:k:134:ARG:HH22	41:l:266:ARG:HA	1.76	0.50
41:l:211:LEU:HD21	41:l:213:ILE:HD11	1.94	0.50
1:2:752:A:H2	1:2:796:G:N1	2.06	0.50
1:2:966:A:OP2	11:N:124:ARG:NH2	2.28	0.50
1:2:1357:G:H2'	1:2:1358:C:C6	2.47	0.50
1:2:1405:U:H2'	1:2:1406:G:H8	1.75	0.50
4:C:148:TYR:OH	4:C:153:LEU:O	2.18	0.50
24:M:117:TRP:NE1	24:M:124:ARG:HB3	2.25	0.50
25:P:18:LYS:HE3	28:S:95:GLY:HA2	1.94	0.50
35:g:171:ARG:HH11	35:g:189:ASN:CG	2.20	0.50
39:j:198:ILE:HG13	40:k:404:PRO:HD3	1.93	0.50
40:k:216:LEU:HD23	40:k:246:ILE:HD12	1.93	0.50
1:2:616:U:H2'	1:2:617:U:O2	2.12	0.49
1:2:1121:G:N2	1:2:1124:A:OP2	2.44	0.49
1:2:1386:A:H5'	1:2:1387:C:C6	2.46	0.49
1:2:1543:A:H5''	28:S:134:ARG:HE	1.77	0.49
1:2:1577:U:H2'	1:2:1578:C:H6	1.77	0.49
1:2:1793:U:H3'	17:a:5:ARG:NH2	2.23	0.49
2:A:49:ASN:O	2:A:53:THR:HG23	2.11	0.49
24:M:94:LEU:C	24:M:104:ARG:NH1	2.70	0.49
40:k:130:ASP:N	40:k:133:GLU:OE1	2.44	0.49
40:k:426:ILE:HG12	40:k:492:CYS:SG	2.52	0.49
1:2:95:G:H5'	5:E:8:HIS:HB2	1.94	0.49
1:2:789:U:C5	1:2:790:A:C5	2.95	0.49
1:2:865:G:H2'	1:2:866:G:C8	2.47	0.49
1:2:932:A:C6	1:2:934:U:N3	2.80	0.49
1:2:958:U:O5'	11:N:14:SER:HB2	2.12	0.49
1:2:1554:A:H8	25:P:40:ARG:NH2	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:142:PRO:HB3	13:V:34:ILE:HD11	1.95	0.49
5:E:141:THR:OG1	5:E:142:HIS:N	2.45	0.49
8:I:191:ALA:O	8:I:194:LEU:HG	2.11	0.49
11:N:5:HIS:HD2	11:N:117:LEU:HD22	1.77	0.49
12:O:19:ILE:N	12:O:82:LYS:O	2.45	0.49
29:T:6:VAL:O	29:T:9:VAL:HG12	2.12	0.49
30:U:25:ASN:OD1	30:U:115:GLU:HB3	2.12	0.49
40:k:353:ILE:HG12	40:k:417:VAL:HG12	1.93	0.49
1:2:296:U:H2'	1:2:297:C:C6	2.47	0.49
1:2:1506:U:H2'	1:2:1507:C:C6	2.47	0.49
6:G:214:LYS:O	6:G:218:GLU:HG2	2.12	0.49
7:H:61:PHE:HE1	7:H:93:LEU:HD12	1.77	0.49
14:W:22:LYS:HA	18:b:3:LEU:HD12	1.93	0.49
16:Y:18:LEU:HD12	16:Y:20:ARG:NH1	2.27	0.49
22:F:63:TYR:CD2	22:F:166:PRO:HB2	2.47	0.49
28:S:100:SER:OG	28:S:108:LYS:HD2	2.13	0.49
1:2:52:U:H2'	1:2:53:G:C8	2.47	0.49
1:2:331:U:N3	1:2:334:U:OP2	2.33	0.49
1:2:904:A:H5'	12:O:52:ARG:HD3	1.93	0.49
5:E:86:PHE:HD1	5:E:87:MET:HG2	1.76	0.49
6:G:78:ALA:HB2	6:G:92:ARG:HG3	1.95	0.49
11:N:4:MET:SD	11:N:124:ARG:NH1	2.85	0.49
14:W:6:VAL:HG23	14:W:34:ILE:HD11	1.95	0.49
15:X:97:ASP:HB2	15:X:142:LYS:HE3	1.94	0.49
16:Y:8:ARG:HB3	16:Y:26:ASP:OD1	2.13	0.49
22:F:127:THR:O	22:F:129:GLN:HB2	2.12	0.49
26:Q:39:VAL:HG11	26:Q:48:VAL:HG11	1.93	0.49
39:j:172:TYR:CE2	39:j:176:ARG:HD2	2.48	0.49
1:2:103:A:H4'	1:2:105:A:C8	2.47	0.49
1:2:403:G:H2'	1:2:404:C:C6	2.47	0.49
1:2:763:G:OP2	9:J:79:ARG:HD3	2.13	0.49
1:2:1757:C:H2'	1:2:1758:G:H8	1.78	0.49
4:C:185:ALA:HB2	4:C:203:THR:HG21	1.94	0.49
10:L:124:THR:OG1	10:L:141:LYS:HB3	2.12	0.49
14:W:94:LEU:H	14:W:94:LEU:HD12	1.78	0.49
22:F:65:GLN:NE2	22:F:68:LYS:HB2	2.23	0.49
39:j:104:LYS:O	39:j:108:VAL:HG23	2.12	0.49
39:j:188:VAL:HG11	39:j:251:ILE:HD13	1.93	0.49
1:2:141:U:H2'	1:2:142:G:H8	1.78	0.49
1:2:430:C:H2'	1:2:431:G:C8	2.47	0.49
1:2:624:C:H2'	1:2:625:U:H6	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:748:U:O2'	14:W:122:SER:O	2.23	0.49
1:2:1210:A:H2'	1:2:1211:G:O4'	2.13	0.49
7:H:48:GLU:OE2	7:H:57:ALA:N	2.43	0.49
7:H:75:ILE:HG13	7:H:76:LYS:N	2.27	0.49
9:J:126:ARG:HG2	19:e:33:ARG:HD3	1.94	0.49
18:b:67:THR:OG1	18:b:70:LYS:O	2.30	0.49
22:F:72:VAL:HB	26:Q:47:LYS:HD3	1.94	0.49
23:K:12:TYR:HB3	23:K:76:LEU:HD11	1.95	0.49
40:k:215:LEU:HD13	40:k:245:ILE:HB	1.95	0.49
1:2:78:A:H2'	1:2:79:C:C6	2.48	0.49
1:2:129:U:H5'	1:2:263:G:H1	1.77	0.49
1:2:688:G:OP2	14:W:119:LYS:NZ	2.29	0.49
1:2:901:G:H2'	1:2:902:U:C6	2.48	0.49
1:2:1358:C:H2'	1:2:1359:A:C8	2.48	0.49
3:B:5:LYS:CE	3:B:7:LYS:HD2	2.42	0.49
13:V:71:ARG:HG3	13:V:83:TRP:CH2	2.48	0.49
14:W:43:LYS:NZ	14:W:115:GLU:OE2	2.39	0.49
23:K:11:ILE:CD1	23:K:42:VAL:HG22	2.42	0.49
25:P:49:LEU:O	25:P:50:SER:OG	2.26	0.49
25:P:84:ILE:HD12	25:P:114:HIS:O	2.12	0.49
25:P:85:ILE:HG22	25:P:112:VAL:HG12	1.95	0.49
35:g:257:PHE:HD2	35:g:273:GLU:HG3	1.77	0.49
40:k:90:LEU:HD22	40:k:187:ARG:HG2	1.94	0.49
40:k:108:HIS:HB3	40:k:111:HIS:CD2	2.48	0.49
1:2:452:U:H2'	1:2:453:U:H5''	1.95	0.49
1:2:555:A:N3	1:2:589:C:H1'	2.27	0.49
1:2:625:U:H2'	1:2:626:C:C6	2.46	0.49
1:2:1405:U:C2	1:2:1406:G:C8	3.01	0.49
1:2:1564:U:H5''	28:S:39:GLY:N	2.27	0.49
2:A:109:ASN:O	2:A:112:THR:HG22	2.13	0.49
3:B:187:LYS:HZ2	3:B:192:VAL:HG11	1.77	0.49
8:I:43:ILE:HA	8:I:56:ARG:O	2.13	0.49
12:O:14:PHE:HD1	12:O:78:ALA:HB3	1.77	0.49
12:O:70:LYS:O	12:O:73:GLU:HG3	2.12	0.49
18:b:64:CYS:SG	18:b:71:ALA:HB3	2.53	0.49
22:F:92:VAL:O	22:F:96:THR:HG23	2.12	0.49
26:Q:120:ASP:OD1	26:Q:122:ARG:HG2	2.12	0.49
27:R:71:PHE:CE2	27:R:73:LEU:HB3	2.47	0.49
29:T:6:VAL:HB	29:T:66:TYR:CE1	2.48	0.49
1:2:566:A:H1'	19:e:14:VAL:HG13	1.94	0.49
1:2:855:A:N7	7:H:116:ARG:CZ	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:867:G:H2'	1:2:868:A:C8	2.41	0.49
1:2:1254:G:N7	24:M:39:ARG:NH1	2.60	0.49
1:2:1450:U:OP1	33:d:10:HIS:ND1	2.46	0.49
1:2:1687:A:H2	1:2:1709:C:N4	2.11	0.49
3:B:127:VAL:HG21	3:B:176:VAL:HG11	1.94	0.49
5:E:181:VAL:HG21	5:E:225:VAL:HG13	1.95	0.49
8:I:40:THR:N	8:I:61:GLU:OE1	2.44	0.49
8:I:117:TYR:CE1	8:I:147:ARG:HD3	2.48	0.49
21:D:215:GLU:HG2	21:D:217:VAL:HG12	1.94	0.49
22:F:202:ASN:HA	22:F:205:LYS:HE2	1.93	0.49
23:K:46:LEU:HG	23:K:66:TYR:CE2	2.47	0.49
26:Q:23:LYS:HB2	26:Q:64:ASP:OD2	2.12	0.49
27:R:103:ASP:OD2	27:R:105:GLN:HG2	2.12	0.49
30:U:71:PRO:HB3	33:d:41:GLN:OE1	2.11	0.49
35:g:239:MET:HE3	35:g:241:PHE:HZ	1.77	0.49
39:j:134:LEU:HD22	39:j:144:ALA:HB1	1.94	0.49
1:2:296:U:H2'	1:2:297:C:H6	1.78	0.49
1:2:477:A:H5'	19:e:33:ARG:HH22	1.78	0.49
1:2:891:A:H2'	1:2:892:U:O4'	2.12	0.49
1:2:952:G:H2'	1:2:953:G:C8	2.48	0.49
1:2:1336:A:P	26:Q:123:ARG:HH12	2.36	0.49
1:2:1527:C:H2'	1:2:1528:C:C6	2.48	0.49
1:2:1563:C:H2'	1:2:1564:U:H6	1.77	0.49
2:A:79:ARG:NH2	2:A:164:ASN:O	2.46	0.49
4:C:81:LEU:HD23	4:C:111:ASP:HB3	1.95	0.49
6:G:57:ASP:OD1	6:G:58:LYS:N	2.46	0.49
7:H:46:ILE:H	7:H:46:ILE:HD12	1.77	0.49
8:I:42:ARG:HD3	8:I:44:HIS:HE1	1.78	0.49
9:J:170:GLY:HA2	9:J:174:ARG:HD3	1.94	0.49
12:O:14:PHE:HB2	12:O:33:LEU:HD12	1.94	0.49
12:O:51:ASP:HB2	12:O:52:ARG:HH12	1.78	0.49
28:S:139:LYS:O	28:S:143:ARG:NH2	2.46	0.49
35:g:296:ALA:HA	35:g:312:TYR:HA	1.94	0.49
38:l:76:A:C4	40:k:337:VAL:HG21	2.47	0.49
39:j:21:MET:HE2	39:j:68:ASN:HB3	1.94	0.49
39:j:212:SER:HB2	39:j:217:GLN:HA	1.94	0.49
40:k:300:LYS:HG3	40:k:301:THR:HG23	1.95	0.49
40:k:436:LEU:HD22	40:k:453:VAL:HG11	1.95	0.49
1:2:365:A:OP1	1:2:758:U:O2'	2.28	0.48
1:2:756:A:C4	1:2:757:A:C8	3.01	0.48
1:2:802:A:O2'	7:H:104:ARG:NH2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1285:U:H2'	1:2:1286:A:H8	1.78	0.48
1:2:1301:U:H2'	1:2:1302:U:H6	1.78	0.48
1:2:1558:U:H3'	1:2:1559:U:H6	1.79	0.48
2:A:55:GLU:O	2:A:58:VAL:HG12	2.12	0.48
2:A:175:TYR:CD2	2:A:199:PRO:HB3	2.48	0.48
3:B:6:ASN:HD21	39:j:91:SER:CB	2.26	0.48
3:B:18:LYS:O	3:B:19:ARG:HD3	2.13	0.48
4:C:60:GLU:O	4:C:64:HIS:ND1	2.46	0.48
12:O:114:ARG:HA	17:a:62:TYR:OH	2.13	0.48
16:Y:62:THR:HA	16:Y:69:SER:HA	1.95	0.48
29:T:27:LYS:HG3	29:T:28:LEU:N	2.24	0.48
29:T:63:ARG:CZ	29:T:67:LEU:HD11	2.43	0.48
29:T:117:SER:HA	29:T:123:ARG:HE	1.78	0.48
31:Z:74:SER:O	31:Z:77:ARG:NH2	2.45	0.48
1:2:97:C:H2'	1:2:98:U:C6	2.48	0.48
1:2:295:U:H2'	1:2:296:U:H6	1.77	0.48
1:2:326:U:OP2	10:L:57:LYS:NZ	2.46	0.48
1:2:1066:C:H5''	3:B:150:VAL:HG12	1.95	0.48
1:2:1650:C:H2'	1:2:1651:C:H6	1.78	0.48
3:B:185:THR:O	3:B:189:ILE:HG12	2.13	0.48
5:E:26:CYS:HG	9:J:2:PRO:C	2.18	0.48
5:E:104:ASP:N	5:E:108:ARG:O	2.44	0.48
9:J:30:LEU:O	9:J:33:GLU:HG2	2.13	0.48
20:h:2:ARG:HB2	20:h:5:TRP:CD1	2.48	0.48
22:F:97:ASN:O	22:F:100:MET:HG2	2.14	0.48
24:M:89:GLY:HA2	24:M:94:LEU:HD13	1.95	0.48
28:S:3:LEU:HD22	31:Z:82:HIS:CG	2.48	0.48
35:g:45:SER:OG	35:g:60:ARG:N	2.45	0.48
36:i:29:LYS:HB2	36:i:33:GLN:O	2.13	0.48
40:k:297:PHE:HA	40:k:300:LYS:HG2	1.95	0.48
1:2:250:A:H2'	1:2:251:U:O4'	2.12	0.48
1:2:1134:U:H2'	1:2:1135:U:C6	2.48	0.48
1:2:1201:A:H61	1:2:1455:C:H5'	1.78	0.48
1:2:1405:U:H2'	1:2:1406:G:C8	2.49	0.48
1:2:1555:U:O2'	1:2:1556:U:H2'	2.12	0.48
1:2:1565:U:H2'	1:2:1566:C:H1'	1.95	0.48
1:2:1588:G:H2'	1:2:1589:C:C6	2.48	0.48
1:2:1591:A:H2'	1:2:1592:G:C8	2.48	0.48
1:2:1673:C:N3	1:2:1725:G:N1	2.61	0.48
1:2:1688:G:N2	1:2:1689:A:N1	2.60	0.48
3:B:131:ASP:CG	3:B:132:ASP:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:149:TRP:CG	14:W:97:ARG:HH22	2.32	0.48
10:L:20:PHE:CZ	10:L:23:PRO:HD3	2.48	0.48
16:Y:20:ARG:HE	16:Y:74:LEU:HD21	1.78	0.48
20:h:8:LYS:HA	20:h:11:ARG:HG2	1.95	0.48
22:F:84:PHE:CE2	32:c:49:ARG:HG3	2.48	0.48
23:K:14:HIS:HA	23:K:17:GLN:HG2	1.95	0.48
23:K:81:ASN:HD21	24:M:30:VAL:HG22	1.78	0.48
25:P:38:PRO:HA	25:P:42:ARG:HH12	1.77	0.48
30:U:106:ILE:HG13	30:U:107:THR:HG23	1.94	0.48
1:2:220:A:C6	1:2:840:U:C4	3.01	0.48
1:2:272:G:H2'	1:2:273:G:C8	2.47	0.48
1:2:460:G:H2'	1:2:461:G:H8	1.78	0.48
1:2:877:G:H2'	1:2:878:G:H8	1.78	0.48
1:2:1031:G:H2'	1:2:1032:C:H6	1.78	0.48
1:2:1187:G:H2'	1:2:1188:A:O4'	2.13	0.48
1:2:1227:G:O2'	34:f:100:LEU:HG	2.12	0.48
1:2:1467:A:H4'	1:2:1539:G:H4'	1.95	0.48
5:E:181:VAL:HB	5:E:195:ILE:HD11	1.95	0.48
10:L:93:TYR:HD2	10:L:100:TYR:HE1	1.61	0.48
21:D:28:GLU:OE1	21:D:65:ARG:NH2	2.46	0.48
31:Z:38:HIS:HB3	31:Z:72:GLY:HA2	1.95	0.48
31:Z:54:ALA:HB3	31:Z:55:PRO:HD3	1.94	0.48
31:Z:76:ALA:O	31:Z:80:LEU:CB	2.62	0.48
35:g:226:GLN:HA	35:g:242:ASP:HA	1.95	0.48
38:1:53:G:H2'	38:1:54:A:C8	2.49	0.48
1:2:82:U:H2'	1:2:83:G:O4'	2.14	0.48
1:2:92:A:H5''	1:2:93:A:H5''	1.95	0.48
1:2:223:C:H2'	1:2:224:A:H8	1.75	0.48
1:2:752:A:N1	1:2:796:G:O6	2.47	0.48
1:2:1248:U:H2'	1:2:1249:U:C6	2.47	0.48
1:2:1667:U:H3'	1:2:1668:G:H8	1.79	0.48
2:A:68:PRO:HD2	2:A:119:ARG:NH2	2.28	0.48
5:E:125:LYS:HB2	5:E:226:PHE:CD1	2.49	0.48
5:E:208:VAL:HG21	5:E:225:VAL:HG21	1.96	0.48
7:H:96:ARG:HH11	7:H:125:ILE:HG13	1.78	0.48
8:I:101:ILE:HD11	8:I:193:TYR:CD1	2.48	0.48
29:T:86:ARG:CZ	29:T:92:LYS:HE2	2.42	0.48
38:1:63:G:N2	38:1:64:RIA:O5'	2.32	0.48
1:2:812:U:O2'	1:2:813:A:H4'	2.13	0.48
1:2:1169:G:H21	1:2:1569:C:H4'	1.79	0.48
1:2:1230:U:H3	1:2:1253:U:H3	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1645:U:H2'	1:2:1646:A:H8	1.77	0.48
2:A:76:ILE:HD13	2:A:121:VAL:HG13	1.96	0.48
25:P:56:LEU:HD12	25:P:60:LEU:HD13	1.96	0.48
35:g:45:SER:O	35:g:59:VAL:N	2.35	0.48
39:j:198:ILE:HG12	40:k:335:GLY:HA2	1.96	0.48
1:2:129:U:P	1:2:131:C:H41	2.36	0.48
1:2:218:A:N6	1:2:842:U:O2	2.46	0.48
1:2:446:U:H2'	1:2:447:C:O4'	2.13	0.48
1:2:760:A:H1'	1:2:790:A:H2	1.79	0.48
1:2:900:G:C6	1:2:901:G:C6	3.01	0.48
1:2:1107:G:H4'	1:2:1108:G:H5''	1.96	0.48
1:2:1217:G:H22	1:2:1442:A:P	2.36	0.48
1:2:1487:U:H2'	1:2:1512:U:O4	2.14	0.48
1:2:1502:G:H2'	1:2:1503:A:C8	2.48	0.48
2:A:52:LYS:NZ	13:V:81:ASN:O	2.46	0.48
4:C:40:TRP:CG	4:C:72:GLN:HE21	2.31	0.48
10:L:16:GLN:HB3	10:L:19:ILE:HD12	1.95	0.48
12:O:84:ARG:HH21	12:O:120:PRO:HG2	1.78	0.48
21:D:42:THR:OG1	21:D:45:LYS:O	2.23	0.48
24:M:77:VAL:N	24:M:78:PRO:HD2	2.29	0.48
25:P:34:VAL:HG22	25:P:45:PHE:CD2	2.49	0.48
35:g:94:ASN:HB3	35:g:97:THR:HB	1.94	0.48
38:1:18:G:H1	39:j:176:ARG:HE	1.61	0.48
1:2:10:G:O6	1:2:1143:U:C2	2.67	0.48
1:2:652:C:H2'	1:2:653:C:O4'	2.14	0.48
1:2:1040:G:H2'	1:2:1041:G:C8	2.48	0.48
1:2:1210:A:O2'	25:P:100:LYS:O	2.31	0.48
1:2:1573:7MG:N2	38:1:42:U:O2'	2.46	0.48
1:2:1738:A:H2'	1:2:1739:U:C6	2.48	0.48
2:A:59:LEU:HD22	13:V:79:LEU:HD21	1.96	0.48
6:G:192:SER:HA	6:G:195:ILE:HG22	1.95	0.48
7:H:71:HIS:HB3	7:H:131:PHE:CZ	2.49	0.48
8:I:39:GLY:N	8:I:60:ILE:O	2.46	0.48
19:e:29:GLN:O	19:e:31:LYS:HG3	2.13	0.48
21:D:31:GLU:N	21:D:31:GLU:OE1	2.45	0.48
25:P:60:LEU:O	25:P:64:LYS:HG2	2.14	0.48
26:Q:69:VAL:HG11	26:Q:81:ILE:HD11	1.95	0.48
28:S:70:VAL:O	28:S:74:GLN:HG3	2.13	0.48
40:k:460:GLU:O	40:k:474:ARG:HA	2.14	0.48
1:2:88:U:H2'	1:2:89:G:H8	1.78	0.48
1:2:332:A:N6	8:I:49:ARG:HH22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:751:G:H2'	1:2:752:A:C8	2.49	0.48
1:2:788:A:C2	1:2:789:U:H1'	2.49	0.48
1:2:1067:C:H2'	1:2:1068:A:H8	1.78	0.48
1:2:1501:A:H8	1:2:1501:A:OP1	1.96	0.48
1:2:1537:G:C4'	28:S:40:ARG:HH12	2.26	0.48
4:C:178:PRO:HG2	4:C:181:SER:HB2	1.94	0.48
11:N:49:GLN:HA	11:N:52:VAL:HG12	1.96	0.48
12:O:17:ALA:HB3	12:O:81:ILE:HA	1.96	0.48
22:F:118:HIS:CG	31:Z:98:GLN:HE22	2.32	0.48
27:R:116:LYS:HD2	27:R:117:LEU:N	2.29	0.48
28:S:100:SER:C	28:S:101:LEU:HD12	2.39	0.48
39:j:230:LEU:HD12	39:j:244:LEU:HD21	1.95	0.48
1:2:187:A:C6	1:2:197:A:C4	3.02	0.48
1:2:379:U:C4	9:J:5:PRO:HB3	2.49	0.48
1:2:381:C:P	5:E:10:LYS:HD2	2.54	0.48
1:2:496:G:OP2	1:2:496:G:H8	1.97	0.48
1:2:1015:C:H2'	1:2:1016:U:O4'	2.13	0.48
1:2:1038:A:O2'	1:2:1039:G:H8	1.96	0.48
1:2:1322:C:H2'	1:2:1323:G:C8	2.49	0.48
1:2:1430:U:H4'	1:2:1431:G:O5'	2.14	0.48
1:2:1598:A:H2'	1:2:1599:G:H5''	1.94	0.48
1:2:1676:A:P	8:I:59:ARG:HH12	2.36	0.48
1:2:1679:A:H8	6:G:66:GLY:HA3	1.79	0.48
2:A:18:LEU:HD13	2:A:23:HIS:NE2	2.29	0.48
9:J:25:ASP:OD2	19:e:54:ARG:NH2	2.47	0.48
31:Z:55:PRO:O	31:Z:56:THR:OG1	2.23	0.48
35:g:104:PHE:CE1	35:g:139:GLY:HA2	2.49	0.48
36:i:77:ILE:HD12	36:i:91:VAL:HG23	1.94	0.48
1:2:90:C:H2'	1:2:91:G:H8	1.79	0.47
1:2:775:G:C6	1:2:785:C:N4	2.82	0.47
1:2:910:U:C4	3:B:5:LYS:HG3	2.49	0.47
1:2:1171:G:H21	29:T:88:VAL:HG21	1.78	0.47
1:2:1326:C:H2'	1:2:1327:G:H8	1.79	0.47
1:2:1714:C:H2'	1:2:1715:G:O4'	2.14	0.47
2:A:84:ARG:CD	2:A:204:TYR:HA	2.43	0.47
3:B:3:VAL:O	3:B:3:VAL:HG22	2.14	0.47
4:C:54:LYS:HB3	4:C:248:TYR:CD2	2.49	0.47
4:C:58:ILE:HG22	4:C:61:ILE:HD12	1.96	0.47
7:H:11:GLN:HG3	7:H:13:PRO:HD3	1.96	0.47
9:J:110:GLN:NE2	9:J:126:ARG:HD3	2.29	0.47
22:F:101:MET:HB2	22:F:182:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:13:GLN:NE2	23:K:17:GLN:OE1	2.37	0.47
26:Q:31:VAL:N	26:Q:34:SER:O	2.44	0.47
34:f:130:LEU:HD11	34:f:146:PHE:CD2	2.49	0.47
39:j:147:LEU:O	39:j:151:ASP:N	2.27	0.47
1:2:212:A:H2'	1:2:213:G:O4'	2.13	0.47
1:2:680:U:O2'	1:2:682:U:H5'	2.14	0.47
1:2:693:U:H2'	1:2:695:U:C5	2.49	0.47
1:2:741:C:O2	7:H:107:ARG:NH1	2.38	0.47
1:2:754:A:H5''	1:2:755:A:H5''	1.95	0.47
1:2:1021:C:O2'	1:2:1124:A:N1	2.47	0.47
1:2:1314:U:O2	27:R:4:VAL:HG11	2.15	0.47
1:2:1657:A:H2'	1:2:1658:A:C8	2.49	0.47
1:2:1794:C:N4	17:a:93:ARG:HH22	2.11	0.47
4:C:40:TRP:CD1	4:C:72:GLN:HE21	2.32	0.47
5:E:131:LEU:HA	5:E:137:PRO:HA	1.96	0.47
8:I:143:LYS:HB3	8:I:147:ARG:NH1	2.29	0.47
10:L:67:ARG:O	10:L:127:GLN:HB3	2.14	0.47
11:N:92:ILE:HD12	11:N:141:TYR:CE1	2.50	0.47
17:a:62:TYR:HE1	17:a:65:PRO:HD3	1.80	0.47
27:R:47:ARG:HG3	27:R:48:ASN:N	2.27	0.47
39:j:50:GLU:N	39:j:50:GLU:OE2	2.47	0.47
40:k:199:ILE:HG12	40:k:508:HIS:CD2	2.49	0.47
1:2:369:A:H2'	1:2:370:G:H8	1.78	0.47
1:2:406:A:H1'	1:2:1669:A:H2	1.80	0.47
1:2:789:U:O4	1:2:790:A:N6	2.47	0.47
1:2:1169:G:C2	1:2:1170:A:C8	3.02	0.47
1:2:1576:U:H2'	1:2:1577:U:H6	1.78	0.47
1:2:1632:C:H5'	1:2:1633:A:C8	2.50	0.47
5:E:141:THR:HG23	5:E:143:ASP:H	1.78	0.47
6:G:132:ARG:NH1	6:G:133:LEU:HB3	2.29	0.47
8:I:117:TYR:O	8:I:144:TRP:NE1	2.46	0.47
12:O:29:HIS:CE1	12:O:41:ARG:HH11	2.32	0.47
22:F:71:TYR:HE2	26:Q:53:LEU:HD21	1.79	0.47
25:P:81:ARG:HB3	25:P:117:GLY:HA3	1.97	0.47
28:S:56:LYS:HG2	28:S:60:GLU:HB3	1.96	0.47
30:U:58:LEU:HD11	30:U:90:TYR:HD2	1.80	0.47
38:l:55:U:N3	38:l:58:1MA:OP2	2.37	0.47
39:j:73:VAL:HG22	39:j:85:LEU:HD12	1.96	0.47
39:j:109:HIS:ND1	39:j:127:TYR:OH	2.42	0.47
40:k:356:ARG:NH2	40:k:422:HIS:O	2.47	0.47
1:2:108:A:H2'	1:2:109:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:180:A:H2'	1:2:181:A:C8	2.49	0.47
1:2:773:C:OP1	5:E:22:LYS:N	2.43	0.47
1:2:865:G:P	11:N:1:MET:H2	2.36	0.47
1:2:1264:G:H2'	1:2:1265:U:C6	2.49	0.47
1:2:1477:A:C2	1:2:1478:G:C8	3.03	0.47
1:2:1772:G:H2'	1:2:1773:U:C6	2.49	0.47
21:D:13:ALA:HA	21:D:16:VAL:HG22	1.96	0.47
21:D:105:MET:HE2	21:D:122:VAL:HG21	1.96	0.47
23:K:7:ASP:HA	23:K:10:LYS:HG2	1.97	0.47
29:T:25:GLN:CD	29:T:27:LYS:H	2.22	0.47
30:U:96:PRO:HG2	30:U:99:ILE:HG12	1.96	0.47
31:Z:45:ASP:OD1	31:Z:46:LYS:N	2.48	0.47
31:Z:95:HIS:HD2	31:Z:96:SER:N	2.13	0.47
33:d:53:TYR:HB2	33:d:55:TYR:HE1	1.79	0.47
1:2:161:A:OP1	6:G:83:CYS:N	2.43	0.47
1:2:1197:G:C6	1:2:1199:G:C6	3.02	0.47
1:2:1457:C:OP1	28:S:126:ARG:NH1	2.32	0.47
1:2:1595:A:C8	33:d:14:PHE:HB2	2.49	0.47
1:2:1683:G:C6	1:2:1715:G:C6	3.03	0.47
3:B:101:HIS:C	3:B:217:LEU:HD13	2.39	0.47
6:G:57:ASP:HA	6:G:106:LEU:HD13	1.96	0.47
38:1:20:A:N3	38:1:20:A:H2'	2.29	0.47
40:k:198:ASP:O	40:k:201:MET:HE3	2.14	0.47
1:2:28:A:C6	1:2:29:U:C4	3.02	0.47
1:2:54:C:O3'	16:Y:109:LYS:HD3	2.15	0.47
1:2:416:A:H1'	1:2:417:G:N2	2.30	0.47
1:2:671:C:H41	1:2:672:G:N2	2.09	0.47
1:2:1166:G:H2'	1:2:1167:U:H6	1.78	0.47
1:2:1290:G:H22	1:2:1323:G:N2	2.13	0.47
3:B:6:ASN:C	3:B:7:LYS:HG2	2.39	0.47
6:G:35:GLU:OE2	6:G:51:LYS:HD3	2.14	0.47
9:J:85:VAL:HG11	9:J:104:PHE:CD1	2.48	0.47
17:a:85:ARG:HG2	17:a:85:ARG:NH1	2.29	0.47
39:j:185:ARG:HA	39:j:230:LEU:O	2.15	0.47
1:2:44:U:OP2	1:2:436:A:N6	2.46	0.47
1:2:179:A:H3'	1:2:180:A:H8	1.79	0.47
1:2:219:A:C8	1:2:831:U:H1'	2.49	0.47
1:2:384:A:H5''	8:I:25:ARG:HH21	1.80	0.47
1:2:517:A:H1'	1:2:533:A:H62	1.80	0.47
1:2:782:G:HO2'	1:2:783:C:H6	1.62	0.47
1:2:865:G:OP1	11:N:2:GLY:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:918:A:H2'	1:2:919:U:C6	2.49	0.47
1:2:998:PSU:OP1	39:j:53:ARG:NH1	2.48	0.47
1:2:1359:A:C6	1:2:1363:G:C6	3.03	0.47
1:2:1437:C:H2'	1:2:1438:C:C6	2.48	0.47
1:2:1651:C:H2'	1:2:1652:G:O4'	2.14	0.47
1:2:1710:A:H3'	1:2:1711:G:H4'	1.96	0.47
2:A:21:ARG:HB3	2:A:24:LEU:HB3	1.96	0.47
3:B:5:LYS:HZ3	3:B:7:LYS:N	2.09	0.47
3:B:205:PHE:CD2	3:B:206:PRO:HD2	2.50	0.47
4:C:231:THR:O	4:C:234:LEU:N	2.42	0.47
5:E:3:ARG:HD3	5:E:3:ARG:H	1.79	0.47
6:G:7:TYR:CE2	6:G:9:ILE:HB	2.50	0.47
6:G:43:ASP:O	6:G:46:LYS:HG3	2.14	0.47
10:L:97:TYR:HE2	15:X:16:ARG:HG3	1.80	0.47
12:O:42:VAL:HG23	12:O:46:MET:HG3	1.97	0.47
21:D:222:VAL:HG11	35:g:236:SER:HA	1.97	0.47
24:M:55:LEU:HD23	24:M:55:LEU:H	1.80	0.47
25:P:30:THR:HG22	25:P:86:VAL:HG21	1.96	0.47
28:S:122:HIS:O	28:S:126:ARG:HG2	2.15	0.47
33:d:3:HIS:HB3	33:d:6:VAL:HG22	1.97	0.47
35:g:154:LYS:HE3	35:g:156:ARG:HD2	1.96	0.47
40:k:284:SER:HB2	40:k:287:LEU:HB2	1.96	0.47
1:2:623:G:H2'	1:2:624:C:C6	2.49	0.47
1:2:895:U:O4'	12:O:38:THR:OG1	2.32	0.47
1:2:1076:C:H2'	1:2:1077:C:C6	2.50	0.47
1:2:1096:U:H1'	4:C:173:ARG:HH11	1.79	0.47
1:2:1119:U:H2'	1:2:1120:C:C6	2.49	0.47
1:2:1386:A:C6	1:2:1409:A:N7	2.83	0.47
1:2:1600:C:H2'	1:2:1601:U:C6	2.50	0.47
3:B:224:ASP:O	3:B:228:LEU:HD23	2.15	0.47
8:I:119:GLN:OE1	8:I:121:LEU:HD23	2.14	0.47
9:J:88:GLU:O	9:J:91:LYS:NZ	2.25	0.47
17:a:10:ARG:HA	17:a:34:LYS:HB2	1.96	0.47
25:P:98:ASN:OD1	25:P:122:THR:HA	2.14	0.47
35:g:153:THR:H	35:g:178:GLY:HA2	1.80	0.47
39:j:22:VAL:HG12	39:j:36:LEU:HG	1.97	0.47
1:2:34:G:N1	1:2:474:A:N7	2.63	0.47
1:2:54:C:OP1	16:Y:113:ASN:ND2	2.48	0.47
1:2:357:U:H2'	1:2:359:A:H8	1.77	0.47
1:2:655:G:H2'	1:2:656:U:O4'	2.15	0.47
1:2:786:G:C6	1:2:787:A:C6	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:904:A:H5'	12:O:52:ARG:CD	2.45	0.47
1:2:984:G:N1	1:2:1015:C:H5	2.12	0.47
1:2:1343:A:H4'	1:2:1344:A:OP1	2.14	0.47
6:G:61:PHE:CE1	6:G:96:SER:HB2	2.50	0.47
8:I:104:ILE:HD11	8:I:168:ALA:HB3	1.96	0.47
15:X:46:SER:OG	15:X:48:HIS:O	2.28	0.47
16:Y:44:LEU:HA	16:Y:47:ALA:HB3	1.97	0.47
35:g:43:LEU:HB2	35:g:62:TYR:CD1	2.50	0.47
35:g:84:ALA:HA	35:g:90:LEU:HD23	1.97	0.47
38:1:1:A:H2'	38:1:2:G:C8	2.49	0.47
38:1:18:G:H4'	38:1:60:A:N3	2.29	0.47
39:j:241:ILE:O	39:j:245:GLU:HG2	2.15	0.47
40:k:89:PRO:HB3	40:k:307:ARG:NH2	2.30	0.47
1:2:93:A:H61	1:2:395:G:H1'	1.80	0.47
1:2:204:U:H2'	1:2:205:A:C8	2.47	0.47
1:2:391:G:OP1	8:I:24:LYS:HD2	2.15	0.47
1:2:512:U:H2'	1:2:513:G:H8	1.74	0.47
1:2:762:A:OP1	9:J:79:ARG:NH2	2.47	0.47
1:2:1163:G:H2'	1:2:1164:G:H8	1.79	0.47
1:2:1548:A:H2'	1:2:1549:U:C6	2.50	0.47
9:J:125:ALA:HA	9:J:128:LEU:HB2	1.97	0.47
14:W:57:ARG:HD2	18:b:26:GLN:OE1	2.14	0.47
22:F:50:PHE:CD2	22:F:69:PRO:HA	2.50	0.47
24:M:35:ALA:HB2	24:M:115:LYS:HD3	1.97	0.47
25:P:98:ASN:HB2	25:P:120:SER:HB2	1.97	0.47
27:R:52:GLY:O	27:R:55:THR:OG1	2.30	0.47
29:T:20:SER:O	29:T:24:ARG:HG3	2.15	0.47
30:U:101:LYS:HD2	30:U:101:LYS:HA	1.63	0.47
31:Z:84:GLU:OE2	31:Z:91:PRO:HD3	2.15	0.47
34:f:102:VAL:HA	34:f:105:TYR:CD2	2.50	0.47
39:j:248:ILE:HD12	39:j:264:ILE:HG12	1.97	0.47
1:2:219:A:N7	1:2:831:U:H1'	2.30	0.46
1:2:369:A:C4	1:2:370:G:C8	3.03	0.46
1:2:929:A:H1'	3:B:111:ARG:HH22	1.80	0.46
1:2:1210:A:N3	25:P:97:TYR:OH	2.45	0.46
1:2:1539:G:N1	1:2:1567:A:OP2	2.47	0.46
1:2:1676:A:H2'	1:2:1677:G:O4'	2.15	0.46
5:E:155:LYS:HE3	5:E:156:VAL:HG23	1.97	0.46
5:E:199:GLU:HA	5:E:199:GLU:OE2	2.15	0.46
5:E:255:ARG:O	5:E:259:HIS:ND1	2.48	0.46
9:J:85:VAL:HG12	9:J:107:ARG:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:79:LEU:HD22	13:V:82:VAL:HG21	1.97	0.46
14:W:114:GLU:HG2	14:W:115:GLU:N	2.30	0.46
21:D:34:TYR:OH	21:D:37:VAL:HG23	2.15	0.46
35:g:175:VAL:HG12	35:g:185:SER:HA	1.97	0.46
1:2:29:U:O3'	15:X:126:LYS:NZ	2.40	0.46
1:2:34:G:O2'	1:2:514:A:O2'	2.33	0.46
1:2:273:G:C6	1:2:274:C:C4	3.03	0.46
1:2:520:A:H2'	1:2:521:U:C6	2.50	0.46
1:2:523:U:H1'	1:2:526:A:N7	2.30	0.46
1:2:1198:G:H3'	1:2:1198:G:N3	2.31	0.46
3:B:27:LYS:HB3	3:B:47:LEU:HG	1.97	0.46
3:B:158:SER:HA	3:B:161:ILE:HD13	1.97	0.46
8:I:42:ARG:HE	8:I:59:ARG:HD2	1.79	0.46
22:F:126:LEU:HG	31:Z:58:ARG:NH2	2.21	0.46
35:g:15:GLU:HA	35:g:316:VAL:HG12	1.96	0.46
1:2:168:A:OP1	6:G:137:ARG:HD2	2.15	0.46
1:2:318:U:OP1	8:I:11:ARG:NH2	2.42	0.46
1:2:418:G:H2'	1:2:419:A:H8	1.80	0.46
1:2:559:U:H2'	1:2:560:G:C8	2.50	0.46
1:2:959:U:O2'	11:N:51:GLY:HA3	2.15	0.46
1:2:997:A:N1	1:2:1005:C:N4	2.60	0.46
1:2:1243:A:H2'	1:2:1243:A:N3	2.30	0.46
1:2:1538:G:H2'	1:2:1539:G:O4'	2.15	0.46
1:2:1624:U:H2'	1:2:1625:U:C6	2.51	0.46
4:C:87:ASN:OD1	4:C:88:ILE:N	2.48	0.46
7:H:62:VAL:HG12	7:H:64:VAL:H	1.79	0.46
12:O:137:LEU:HD11	37:3:25:A:C6	2.50	0.46
14:W:43:LYS:NZ	14:W:112:ASP:OD2	2.48	0.46
22:F:60:LEU:HB3	22:F:64:ILE:HD12	1.98	0.46
30:U:42:ILE:HG23	30:U:52:LYS:HZ1	1.80	0.46
38:1:60:A:H3'	38:1:61:C:C5	2.51	0.46
39:j:60:GLN:HA	39:j:63:ILE:HG22	1.96	0.46
39:j:240:GLY:HA2	39:j:243:GLN:HE21	1.81	0.46
40:k:315:LEU:HD12	40:k:347:PHE:CE2	2.51	0.46
1:2:159:C:N3	1:2:160:U:C2	2.83	0.46
1:2:322:A:OP2	8:I:10:LYS:HD3	2.15	0.46
1:2:525:A:OP2	16:Y:93:ARG:NH2	2.48	0.46
1:2:991:A:H5'	1:2:992:A:OP2	2.15	0.46
1:2:1389:A:H2'	1:2:1390:U:H6	1.79	0.46
1:2:1627:G:H2'	1:2:1628:U:C6	2.50	0.46
7:H:16:LEU:O	7:H:20:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:6:ASP:OD1	8:I:9:HIS:ND1	2.46	0.46
9:J:78:ARG:HH22	9:J:82:ARG:HD3	1.80	0.46
9:J:109:LEU:HB2	9:J:146:PHE:HB3	1.98	0.46
13:V:37:ALA:HA	13:V:50:TYR:HB3	1.97	0.46
24:M:86:LYS:HD2	24:M:107:VAL:O	2.16	0.46
28:S:116:LEU:HA	28:S:119:ILE:HG12	1.96	0.46
35:g:238:PHE:CD2	35:g:239:MET:HG2	2.51	0.46
35:g:247:VAL:HA	35:g:263:THR:HA	1.97	0.46
38:1:27:C:H2'	38:1:28:A:C8	2.50	0.46
1:2:838:U:H2'	1:2:839:U:C6	2.51	0.46
1:2:922:A:H2'	1:2:923:A:C8	2.51	0.46
1:2:978:A:C4	1:2:979:G:C8	3.04	0.46
1:2:1317:G:H5'	27:R:67:ARG:NH1	2.31	0.46
1:2:1573:7MG:H82	1:2:1573:7MG:O5'	2.16	0.46
1:2:1671:G:H2'	1:2:1672:C:H6	1.80	0.46
3:B:3:VAL:O	3:B:4:GLY:C	2.58	0.46
4:C:234:LEU:O	4:C:234:LEU:HD23	2.16	0.46
5:E:247:THR:HB	5:E:250:GLU:HG2	1.97	0.46
6:G:113:ILE:HG13	6:G:113:ILE:O	2.15	0.46
7:H:41:LEU:HD22	7:H:70:TYR:HE1	1.80	0.46
9:J:100:LYS:O	9:J:100:LYS:HG2	2.16	0.46
12:O:89:THR:O	12:O:128:LYS:HE3	2.15	0.46
16:Y:6:THR:CG2	16:Y:28:LEU:HB2	2.45	0.46
38:1:9:1MG:O5'	38:1:46:7MG:H1'	2.15	0.46
38:1:47:H2U:H5''	38:1:47:H2U:H61	1.96	0.46
39:j:21:MET:HG3	39:j:69:ASP:C	2.40	0.46
1:2:388:G:P	1:2:424:A:H61	2.39	0.46
1:2:477:A:OP1	19:e:37:ARG:NH1	2.48	0.46
1:2:751:G:C6	1:2:798:A:C6	3.04	0.46
1:2:1146:A:H2'	1:2:1147:C:C6	2.50	0.46
1:2:1537:G:H4'	28:S:40:ARG:HH12	1.79	0.46
11:N:117:LEU:O	11:N:121:ARG:HG3	2.15	0.46
21:D:158:ILE:O	21:D:168:ILE:HD11	2.15	0.46
28:S:48:LYS:HE2	29:T:35:ASP:OD1	2.15	0.46
33:d:36:LEU:O	33:d:38:ILE:HG23	2.16	0.46
33:d:53:TYR:HB2	33:d:55:TYR:CE1	2.51	0.46
35:g:177:ALA:HB2	35:g:183:VAL:HG22	1.97	0.46
40:k:129:LYS:O	40:k:131:GLU:N	2.49	0.46
1:2:11:A:N1	1:2:1142:A:H2	2.13	0.46
1:2:448:C:H2'	1:2:449:U:C6	2.51	0.46
1:2:783:C:H2'	1:2:784:U:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:818:G:C4	1:2:852:G:N2	2.84	0.46
1:2:1209:C:H2'	1:2:1210:A:C8	2.51	0.46
1:2:1568:A:H2'	1:2:1569:C:O4'	2.15	0.46
1:2:1582:G:O5'	26:Q:122:ARG:HB2	2.15	0.46
2:A:207:PRO:O	2:A:210:ILE:HG22	2.15	0.46
4:C:233:ASN:HD22	13:V:1:MET:N	2.14	0.46
5:E:86:PHE:CE1	5:E:87:MET:HG2	2.50	0.46
7:H:12:ALA:HB1	7:H:18:LEU:HD21	1.97	0.46
7:H:117:THR:HB	7:H:120:ALA:HB3	1.97	0.46
10:L:115:PHE:HE2	10:L:142:VAL:H	1.63	0.46
30:U:27:THR:OG1	30:U:113:ASP:HB3	2.15	0.46
35:g:14:LEU:HB3	35:g:46:TRP:CZ3	2.51	0.46
40:k:248:GLN:HE21	40:k:262:HIS:HD2	1.63	0.46
1:2:57:G:C4	1:2:91:G:N2	2.84	0.46
1:2:85:A:H2'	1:2:86:A:C8	2.51	0.46
1:2:86:A:H2'	1:2:87:C:C6	2.48	0.46
1:2:325:G:H2'	1:2:326:U:C6	2.50	0.46
1:2:387:G:C6	1:2:409:A:C6	3.04	0.46
1:2:497:G:H1'	1:2:499:C:N4	2.30	0.46
1:2:597:U:O4	1:2:598:A:C6	2.68	0.46
1:2:954:A:H2'	1:2:955:C:C6	2.50	0.46
1:2:979:G:OP2	1:2:1013:G:O2'	2.33	0.46
1:2:1279:C:H5'	33:d:44:ARG:NH2	2.31	0.46
7:H:130:VAL:HG13	7:H:130:VAL:O	2.16	0.46
16:Y:76:TYR:HE2	16:Y:85:PHE:HB2	1.81	0.46
16:Y:81:ASP:HA	16:Y:84:LYS:HG2	1.97	0.46
17:a:73:TYR:HE2	17:a:83:ILE:HG12	1.81	0.46
18:b:33:LEU:HD13	18:b:79:PHE:HB2	1.98	0.46
24:M:120:ASP:HA	24:M:124:ARG:HD2	1.98	0.46
28:S:5:VAL:HA	31:Z:42:LEU:HD22	1.98	0.46
28:S:71:GLN:HA	28:S:74:GLN:HE21	1.81	0.46
34:f:130:LEU:HD11	34:f:146:PHE:HD2	1.81	0.46
39:j:24:VAL:HG13	39:j:65:VAL:HA	1.97	0.46
39:j:94:ASP:O	39:j:97:LYS:HG2	2.16	0.46
1:2:142:G:O2'	1:2:143:G:H5'	2.16	0.46
1:2:271:U:O2'	1:2:283:G:N2	2.48	0.46
1:2:506:U:H3'	1:2:507:U:H5''	1.97	0.46
1:2:682:U:C4	1:2:683:C:H1'	2.51	0.46
1:2:958:U:H6	11:N:61:THR:HG23	1.81	0.46
1:2:1036:C:H2'	1:2:1037:U:C6	2.51	0.46
1:2:1277:G:H2'	1:2:1278:C:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1365:C:O3'	29:T:7:ARG:NE	2.48	0.46
1:2:1694:G:H2'	1:2:1706:U:O2'	2.16	0.46
3:B:53:GLY:HA2	3:B:56:ASN:OD1	2.16	0.46
3:B:197:ILE:CG2	3:B:210:VAL:HG11	2.45	0.46
4:C:113:ASN:C	4:C:146:ARG:HH12	2.24	0.46
5:E:125:LYS:HB2	5:E:226:PHE:HE1	1.78	0.46
7:H:34:LEU:HG	7:H:38:LEU:HD22	1.97	0.46
7:H:34:LEU:HD22	7:H:76:LYS:HZ2	1.80	0.46
8:I:70:GLU:HG3	8:I:112:TRP:CH2	2.50	0.46
10:L:76:VAL:HG21	10:L:87:ARG:HB2	1.97	0.46
10:L:101:GLU:HG2	10:L:103:ARG:HD3	1.97	0.46
23:K:54:PHE:O	23:K:69:THR:HG22	2.16	0.46
27:R:36:ASP:OD1	27:R:47:ARG:HD3	2.15	0.46
28:S:16:ARG:NH1	28:S:21:ASN:OD1	2.44	0.46
39:j:252:THR:O	39:j:256:THR:HG23	2.16	0.46
1:2:79:C:H3'	1:2:80:A:C8	2.51	0.46
1:2:123:G:H21	5:E:146:THR:HG21	1.80	0.46
1:2:405:U:H2'	1:2:406:A:H8	1.80	0.46
1:2:441:C:H2'	1:2:442:C:C6	2.50	0.46
1:2:858:A:N3	11:N:73:ARG:NH2	2.64	0.46
1:2:983:G:H1	1:2:1016:U:H5	1.64	0.46
1:2:1007:G:H2'	1:2:1008:U:H6	1.80	0.46
1:2:1097:U:O3'	14:W:71:LYS:NZ	2.46	0.46
1:2:1141:A:H2'	1:2:1142:A:O4'	2.16	0.46
1:2:1386:A:C2	1:2:1410:G:C4	3.04	0.46
1:2:1683:G:H2'	1:2:1684:C:H6	1.80	0.46
1:2:1787:G:OP2	12:O:132:ARG:NH2	2.25	0.46
5:E:36:HIS:CE1	5:E:85:GLY:HA3	2.51	0.46
5:E:136:ILE:HG23	5:E:149:TYR:CE1	2.51	0.46
7:H:96:ARG:NH2	7:H:124:LYS:CB	2.64	0.46
14:W:34:ILE:HD12	14:W:34:ILE:H	1.81	0.46
27:R:6:THR:O	27:R:9:VAL:HG12	2.16	0.46
35:g:255:SER:OG	35:g:256:ARG:HD2	2.16	0.46
40:k:148:TYR:OH	40:k:169:GLU:O	2.18	0.46
1:2:477:A:H2	1:2:509:G:H22	1.64	0.45
1:2:559:U:H2'	1:2:560:G:H8	1.80	0.45
1:2:1290:G:O5'	1:2:1290:G:H8	1.98	0.45
1:2:1431:G:H2'	1:2:1432:U:C6	2.51	0.45
4:C:40:TRP:CH2	4:C:72:GLN:HG2	2.51	0.45
4:C:45:LYS:HE2	4:C:253:THR:HG22	1.98	0.45
5:E:94:ALA:C	5:E:96:ASN:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:17:CYS:SG	13:V:20:THR:N	2.72	0.45
15:X:59:ILE:HD12	15:X:71:CYS:SG	2.56	0.45
26:Q:53:LEU:HD12	26:Q:54:LEU:N	2.30	0.45
35:g:149:THR:OG1	35:g:180:ASP:OD1	2.26	0.45
39:j:25:GLN:HE22	39:j:35:LYS:N	2.13	0.45
40:k:142:TYR:CE1	40:k:190:SER:HB2	2.52	0.45
40:k:456:LEU:HD22	40:k:462:LEU:HD11	1.97	0.45
41:l:134:LEU:HD12	41:l:134:LEU:H	1.81	0.45
1:2:107:C:H2'	1:2:108:A:C8	2.51	0.45
1:2:107:C:H2'	1:2:108:A:H8	1.81	0.45
1:2:446:U:O2'	5:E:27:TYR:O	2.35	0.45
1:2:1240:G:OP1	25:P:77:ARG:NH1	2.49	0.45
1:2:1526:U:OP1	22:F:111:LYS:HG3	2.17	0.45
1:2:1788:A:H2'	1:2:1789:A:C8	2.51	0.45
11:N:4:MET:HG2	11:N:5:HIS:ND1	2.31	0.45
15:X:69:ARG:NH1	15:X:116:ASP:OD1	2.48	0.45
17:a:83:ILE:H	17:a:83:ILE:HD12	1.81	0.45
21:D:225:TYR:HB2	35:g:197:ALA:HA	1.98	0.45
23:K:77:ARG:NH2	23:K:86:ILE:O	2.30	0.45
35:g:152:VAL:HG23	35:g:152:VAL:O	2.16	0.45
36:i:97:LEU:HA	36:i:100:ALA:HB3	1.97	0.45
1:2:143:G:H2'	1:2:144:A:H8	1.81	0.45
1:2:241:U:OP1	6:G:219:ARG:NH1	2.46	0.45
1:2:610:U:P	15:X:19:ARG:HH12	2.39	0.45
1:2:1035:A:H2'	1:2:1036:C:H6	1.82	0.45
1:2:1309:U:H2'	1:2:1310:U:C6	2.51	0.45
1:2:1466:U:O2'	1:2:1540:G:OP1	2.33	0.45
1:2:1533:U:H5	22:F:189:ILE:HA	1.82	0.45
3:B:34:ALA:N	3:B:41:ARG:O	2.36	0.45
3:B:54:LEU:O	3:B:55:LYS:HG2	2.16	0.45
6:G:135:PRO:HG2	6:G:141:ILE:HG12	1.98	0.45
7:H:15:GLU:HG2	7:H:19:GLN:HE22	1.81	0.45
11:N:23:PRO:HB2	11:N:25:TRP:HD1	1.81	0.45
21:D:221:SER:HB3	35:g:200:ILE:O	2.17	0.45
24:M:88:LEU:O	24:M:92:ALA:HB2	2.17	0.45
26:Q:81:ILE:O	26:Q:85:ILE:HG12	2.17	0.45
30:U:102:ARG:O	30:U:105:GLN:HG2	2.16	0.45
34:f:104:ASN:O	34:f:117:LEU:HD22	2.17	0.45
35:g:199:PHE:HB3	35:g:230:TRP:CE3	2.51	0.45
39:j:149:ILE:HD11	39:j:177:LEU:HB2	1.99	0.45
40:k:109:VAL:HG23	44:k:601:GCP:O2G	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:l:206:ASP:O	41:l:210:ARG:HG2	2.17	0.45
1:2:6:G:C5	4:C:210:ARG:NH2	2.85	0.45
1:2:284:G:H2'	1:2:285:C:C6	2.52	0.45
1:2:689:G:H2'	1:2:690:A:H8	1.81	0.45
1:2:736:C:O2'	1:2:737:A:H8	1.97	0.45
1:2:811:A:N6	1:2:857:G:H2'	2.30	0.45
1:2:822:G:C5	1:2:823:G:C8	3.05	0.45
1:2:827:U:O4	1:2:828:A:N6	2.50	0.45
1:2:1180:U:H2'	1:2:1181:U:O4'	2.16	0.45
1:2:1754:A:N6	36:i:66:ARG:O	2.29	0.45
3:B:144:ARG:HB3	3:B:206:PRO:HB2	1.99	0.45
8:I:185:LEU:CD1	8:I:189:GLU:HB3	2.46	0.45
8:I:185:LEU:HD12	8:I:189:GLU:HB3	1.97	0.45
23:K:46:LEU:O	23:K:50:THR:HG23	2.17	0.45
25:P:89:MET:HE3	25:P:107:ILE:HG12	1.97	0.45
26:Q:58:ASP:N	26:Q:58:ASP:OD1	2.50	0.45
31:Z:76:ALA:O	31:Z:80:LEU:HB2	2.16	0.45
1:2:154:U:OP2	16:Y:132:ARG:NH1	2.50	0.45
1:2:324:G:O6	1:2:343:A:N6	2.49	0.45
1:2:654:G:N7	1:2:677:G:N1	2.64	0.45
1:2:657:C:H2'	1:2:658:C:C5	2.52	0.45
1:2:813:A:O2'	1:2:814:G:O5'	2.28	0.45
1:2:1582:G:H3'	26:Q:124:PRO:HA	1.97	0.45
1:2:1649:A:H2'	1:2:1650:C:C6	2.52	0.45
1:2:1781:C:H5	20:h:5:TRP:HB3	1.79	0.45
5:E:54:TYR:HB3	16:Y:15:ASN:HD21	1.81	0.45
5:E:64:ILE:HA	5:E:67:GLN:HE21	1.82	0.45
5:E:103:TYR:HE1	5:E:109:PHE:CE1	2.35	0.45
6:G:52:ILE:HG13	6:G:52:ILE:O	2.16	0.45
7:H:96:ARG:CZ	7:H:124:LYS:CB	2.92	0.45
17:a:10:ARG:O	17:a:11:ASN:HB2	2.14	0.45
21:D:41:VAL:HG13	21:D:46:THR:HG22	1.98	0.45
24:M:26:ARG:O	24:M:30:VAL:HG23	2.17	0.45
35:g:253:SER:HB2	35:g:256:ARG:O	2.16	0.45
36:i:79:VAL:HG23	36:i:90:ASP:C	2.42	0.45
36:i:103:LEU:HD22	36:i:108:GLU:HG3	1.98	0.45
39:j:53:ARG:HA	39:j:88:ARG:HE	1.82	0.45
39:j:220:VAL:HG22	39:j:230:LEU:HD22	1.98	0.45
40:k:148:TYR:O	40:k:162:ARG:N	2.48	0.45
40:k:313:PRO:HB2	40:k:347:PHE:HE1	1.82	0.45
1:2:189:C:O2'	1:2:190:C:O5'	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:734:A:H2'	1:2:735:C:C6	2.52	0.45
1:2:977:A:H2'	1:2:978:A:H8	1.82	0.45
1:2:1137:A:H2'	1:2:1138:A:H8	1.81	0.45
2:A:53:THR:O	2:A:57:ILE:HG13	2.16	0.45
3:B:99:ASN:OD1	3:B:100:PHE:N	2.50	0.45
3:B:126:THR:HG22	3:B:136:ARG:HE	1.82	0.45
5:E:155:LYS:HB2	5:E:174:LYS:NZ	2.31	0.45
10:L:127:GLN:HA	10:L:137:PHE:HD1	1.82	0.45
23:K:35:ILE:HG13	23:K:37:THR:HG22	1.99	0.45
24:M:60:THR:C	24:M:61:GLU:HG3	2.41	0.45
27:R:34:LEU:O	27:R:38:ILE:HG12	2.17	0.45
30:U:69:LYS:HB2	30:U:78:THR:CG2	2.47	0.45
35:g:248:PHE:CE2	35:g:295:HIS:CE1	3.04	0.45
1:2:48:G:C6	1:2:431:G:C2	3.04	0.45
1:2:143:G:N2	1:2:170:A:N1	2.49	0.45
1:2:277:U:O5'	1:2:278:G:N2	2.50	0.45
1:2:431:G:H2'	1:2:432:C:C6	2.52	0.45
1:2:520:A:C2'	16:Y:34:ASN:HD21	2.29	0.45
1:2:692:C:H2'	1:2:693:U:C6	2.51	0.45
1:2:897:A:N6	1:2:911:U:O4'	2.50	0.45
1:2:984:G:H2'	1:2:985:G:H8	1.82	0.45
1:2:1577:U:O2'	26:Q:139:GLN:HG3	2.17	0.45
2:A:75:ALA:HB3	2:A:86:VAL:HG13	1.99	0.45
4:C:86:MET:HB2	4:C:106:VAL:HG13	1.99	0.45
4:C:144:ILE:HG21	4:C:223:ILE:HG13	1.98	0.45
19:e:10:ARG:HA	19:e:10:ARG:HD2	1.78	0.45
21:D:67:ASN:O	21:D:70:THR:OG1	2.30	0.45
28:S:36:ARG:HB3	28:S:105:LEU:HD23	1.98	0.45
41:l:245:GLU:O	41:l:257:MET:HG3	2.16	0.45
1:2:332:A:P	8:I:48:THR:HG1	2.40	0.45
1:2:588:C:H2'	1:2:589:C:C6	2.51	0.45
1:2:635:A:N1	1:2:860:U:C4	2.85	0.45
1:2:700:C:HO2'	1:2:701:U:P	2.39	0.45
1:2:859:U:O2	7:H:114:ARG:NH1	2.50	0.45
1:2:989:C:H2'	1:2:990:G:O4'	2.16	0.45
1:2:1038:A:H4'	13:V:62:ARG:HH22	1.82	0.45
1:2:1212:G:O2'	1:2:1243:A:N6	2.50	0.45
1:2:1238:U:O2	1:2:1245:C:N4	2.50	0.45
1:2:1467:A:H2'	1:2:1468:C:C6	2.52	0.45
1:2:1713:G:H2'	1:2:1714:C:C6	2.52	0.45
1:2:1776:G:N2	1:2:1782:C:C2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1794:C:C4	17:a:93:ARG:NH2	2.79	0.45
3:B:152:ARG:HB3	3:B:152:ARG:CZ	2.45	0.45
3:B:167:VAL:O	3:B:170:GLU:HG2	2.17	0.45
7:H:25:ILE:HA	7:H:28:GLU:CD	2.42	0.45
9:J:76:LEU:O	9:J:80:LEU:HD23	2.16	0.45
10:L:55:ASP:OD2	10:L:113:PRO:HD3	2.17	0.45
28:S:123:ARG:HD2	28:S:133:VAL:CG1	2.47	0.45
40:k:245:ILE:HG12	40:k:279:PRO:HG2	1.97	0.45
40:k:473:ALA:HB2	40:k:487:LEU:HD23	1.98	0.45
1:2:35:U:H2'	1:2:36:C:C6	2.52	0.45
1:2:471:U:H5''	9:J:11:THR:HG22	1.98	0.45
1:2:552:G:H3'	1:2:553:C:H2'	1.99	0.45
1:2:779:A:H1'	1:2:781:A:N6	2.32	0.45
1:2:908:U:H2'	1:2:909:C:C6	2.51	0.45
1:2:1000:A:OP1	38:l:38:A:O2'	2.32	0.45
1:2:1198:G:H1	33:d:31:ILE:CD1	2.30	0.45
1:2:1200:G:N2	1:2:1598:A:O4'	2.48	0.45
1:2:1275:U:OP1	21:D:147:ALA:N	2.40	0.45
1:2:1424:C:H3'	1:2:1425:A:H4'	1.97	0.45
2:A:153:SER:O	2:A:156:VAL:HG12	2.17	0.45
4:C:95:THR:HG23	4:C:97:ALA:H	1.82	0.45
4:C:159:LEU:HD21	4:C:223:ILE:HD12	1.99	0.45
5:E:230:GLU:N	5:E:230:GLU:OE1	2.50	0.45
26:Q:99:GLU:N	26:Q:99:GLU:OE1	2.50	0.45
35:g:23:SER:OG	35:g:71:ASP:HA	2.17	0.45
1:2:85:A:N3	1:2:147:U:O2'	2.43	0.45
1:2:300:A:C6	1:2:301:U:C4	3.05	0.45
1:2:523:U:H1'	1:2:526:A:C8	2.52	0.45
1:2:609:G:C6	1:2:613:C:C2	3.05	0.45
1:2:857:G:OP1	7:H:116:ARG:NH2	2.33	0.45
1:2:875:G:C6	1:2:935:G:C6	3.05	0.45
1:2:897:A:C2	1:2:914:A:C5	3.04	0.45
1:2:908:U:H2'	1:2:909:C:H6	1.82	0.45
1:2:1760:A:C2	1:2:1761:A:C8	3.05	0.45
2:A:105:GLY:H	2:A:135:GLU:CD	2.22	0.45
6:G:31:ARG:HB3	6:G:101:ILE:HD13	1.99	0.45
7:H:5:GLN:O	7:H:9:LEU:HD23	2.16	0.45
7:H:85:PHE:HB3	7:H:88:ARG:HE	1.82	0.45
7:H:101:LYS:HA	7:H:112:ARG:CZ	2.47	0.45
8:I:81:VAL:HA	8:I:102:VAL:HG12	1.99	0.45
10:L:125:VAL:HA	10:L:139:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:42:ARG:HH21	11:N:80:LEU:HD11	1.81	0.45
16:Y:15:ASN:OD1	16:Y:17:LEU:HB2	2.16	0.45
22:F:71:TYR:CE2	26:Q:53:LEU:HD21	2.52	0.45
22:F:221:ARG:HH12	39:j:45:MET:HE3	1.81	0.45
31:Z:80:LEU:HD21	31:Z:101:TYR:HE2	1.82	0.45
35:g:67:HIS:CE1	35:g:68:ILE:HG12	2.51	0.45
40:k:113:LYS:HG2	40:k:217:LEU:HD12	1.99	0.45
40:k:431:GLU:OE1	40:k:482:MET:HE3	2.17	0.45
1:2:27:U:H2'	1:2:28:A:H8	1.82	0.44
1:2:38:C:H2'	1:2:39:A:C8	2.53	0.44
1:2:139:C:N4	1:2:280:G:OP1	2.34	0.44
1:2:410:C:H2'	1:2:411:A:O4'	2.17	0.44
1:2:904:A:O3'	12:O:52:ARG:HD2	2.16	0.44
1:2:1077:C:H2'	1:2:1078:U:C6	2.52	0.44
1:2:1166:G:C4	1:2:1167:U:C5	3.05	0.44
1:2:1203:A:N3	1:2:1203:A:H2'	2.32	0.44
1:2:1217:G:N2	1:2:1441:U:O3'	2.50	0.44
1:2:1337:C:H2'	1:2:1338:C:O4'	2.17	0.44
1:2:1478:G:H3'	1:2:1479:C:H6	1.82	0.44
1:2:1624:U:H2'	1:2:1625:U:H6	1.82	0.44
1:2:1711:G:C6	1:2:1712:A:C2	3.05	0.44
2:A:55:GLU:OE2	13:V:79:LEU:HA	2.17	0.44
3:B:31:ASP:O	3:B:96:LEU:HG	2.16	0.44
5:E:124:ALA:HB1	5:E:141:THR:OG1	2.17	0.44
6:G:7:TYR:CZ	6:G:9:ILE:HB	2.51	0.44
15:X:107:PHE:CD1	15:X:123:LYS:HG3	2.52	0.44
16:Y:62:THR:HG22	16:Y:69:SER:HB2	1.99	0.44
21:D:154:ASP:OD1	21:D:155:GLY:N	2.50	0.44
22:F:55:VAL:HG12	22:F:136:VAL:HG21	1.99	0.44
22:F:72:VAL:HG12	22:F:74:HIS:HB3	2.00	0.44
30:U:102:ARG:HA	30:U:105:GLN:CD	2.43	0.44
31:Z:74:SER:HA	31:Z:77:ARG:HH22	1.81	0.44
32:c:12:VAL:HG12	32:c:52:ASP:O	2.18	0.44
35:g:122:LYS:HA	35:g:122:LYS:HD3	1.81	0.44
35:g:157:VAL:HG12	35:g:174:PHE:HB3	1.99	0.44
38:1:40:C:P	39:j:57:ARG:HD2	2.57	0.44
41:l:174:PHE:HD2	41:l:177:ILE:HB	1.81	0.44
1:2:240:U:H2'	1:2:241:U:C6	2.52	0.44
1:2:393:C:C4	1:2:403:G:N2	2.86	0.44
1:2:508:G:H2'	1:2:509:G:C8	2.52	0.44
1:2:1334:U:N3	1:2:1335:A:N7	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1335:A:O3'	26:Q:123:ARG:NH2	2.47	0.44
1:2:1459:C:OP2	28:S:143:ARG:HA	2.17	0.44
1:2:1501:A:C6	28:S:84:TRP:CG	3.05	0.44
1:2:1563:C:C2	1:2:1564:U:C5	3.04	0.44
1:2:1661:G:H2'	1:2:1662:C:C6	2.53	0.44
3:B:180:THR:HG22	3:B:181:LEU:HD23	2.00	0.44
4:C:64:HIS:CE1	4:C:244:PRO:HD3	2.52	0.44
5:E:122:LYS:HG2	5:E:123:LEU:N	2.32	0.44
6:G:140:ASN:O	6:G:143:LYS:HG2	2.17	0.44
8:I:121:LEU:HD11	8:I:153:ILE:HD11	1.98	0.44
14:W:77:PRO:O	14:W:79:PHE:N	2.50	0.44
22:F:210:SER:HB3	22:F:213:ILE:HG22	2.00	0.44
26:Q:98:ASP:HB3	26:Q:101:SER:HB2	1.99	0.44
26:Q:99:GLU:OE2	35:g:60:ARG:HA	2.18	0.44
27:R:12:ALA:O	27:R:16:LEU:HD23	2.17	0.44
34:f:134:GLY:O	34:f:136:ARG:HG2	2.16	0.44
35:g:113:SER:OG	35:g:155:VAL:HG12	2.17	0.44
1:2:278:G:C6	1:2:280:G:C6	3.06	0.44
1:2:281:C:H2'	1:2:282:U:O4'	2.17	0.44
1:2:783:C:H2'	1:2:784:U:C6	2.52	0.44
1:2:867:G:N3	1:2:868:A:C8	2.85	0.44
1:2:1043:U:H2'	1:2:1044:C:C6	2.52	0.44
1:2:1601:U:H2'	1:2:1602:U:C6	2.52	0.44
1:2:1779:A:N6	1:2:1780:MA6:H102	2.32	0.44
3:B:138:PHE:HB2	3:B:213:ARG:O	2.17	0.44
7:H:93:LEU:HD22	7:H:125:ILE:HG23	2.00	0.44
7:H:107:ARG:HG3	7:H:108:GLN:OE1	2.18	0.44
17:a:23:CYS:HB2	17:a:74:CYS:HB3	1.99	0.44
18:b:15:GLU:O	18:b:29:ARG:NH2	2.50	0.44
27:R:29:GLN:O	27:R:33:ARG:HG2	2.18	0.44
28:S:29:VAL:O	28:S:33:THR:HG23	2.16	0.44
29:T:38:LYS:NZ	29:T:43:ASN:O	2.43	0.44
36:i:117:GLU:HA	41:l:167:ARG:O	2.17	0.44
39:j:20:VAL:HG23	39:j:71:ALA:HB3	1.98	0.44
1:2:31:C:H1'	1:2:546:U:H5''	1.99	0.44
1:2:161:A:OP2	1:2:161:A:H8	2.01	0.44
1:2:221:A:H2'	1:2:222:U:C6	2.52	0.44
1:2:224:A:H3'	1:2:225:A:C8	2.52	0.44
1:2:365:A:H2'	1:2:366:A:H8	1.82	0.44
1:2:780:A:O5'	1:2:781:A:N6	2.49	0.44
1:2:887:U:H2'	1:2:888:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1289:PSU:H2'	1:2:1290:G:C8	2.53	0.44
1:2:1518:U:H4'	1:2:1521:G:H22	1.82	0.44
10:L:93:TYR:CD2	10:L:100:TYR:HE1	2.35	0.44
12:O:48:VAL:HG11	12:O:59:ALA:HB2	1.99	0.44
15:X:143:PRO:O	15:X:144:ARG:HD3	2.18	0.44
18:b:38:PRO:HD3	18:b:77:THR:HA	1.99	0.44
21:D:142:LEU:O	21:D:143:ARG:HG2	2.17	0.44
23:K:33:GLU:O	23:K:34:GLU:HG3	2.18	0.44
24:M:54:VAL:HG22	24:M:80:ILE:HG23	1.99	0.44
34:f:88:PRO:O	34:f:89:LYS:HG2	2.17	0.44
34:f:124:CYS:SG	34:f:141:LYS:HB3	2.58	0.44
40:k:104:GLY:CA	40:k:211:MET:HE3	2.45	0.44
1:2:89:G:C6	1:2:90:C:C4	3.06	0.44
1:2:222:U:H2'	1:2:223:C:C6	2.53	0.44
1:2:249:C:H2'	1:2:250:A:C8	2.53	0.44
1:2:565:C:H5'	36:i:62:ARG:CZ	2.47	0.44
1:2:597:U:C5	1:2:598:A:C5	3.06	0.44
1:2:880:A:N1	1:2:947:G:C6	2.85	0.44
1:2:967:U:H2'	1:2:968:C:O4'	2.18	0.44
1:2:1036:C:H2'	1:2:1037:U:H6	1.82	0.44
1:2:1426:2MG:HM22	1:2:1427:G:N3	2.33	0.44
1:2:1486:G:H3'	1:2:1513:A:N6	2.25	0.44
1:2:1559:U:H2'	1:2:1560:G:C8	2.50	0.44
1:2:1680:U:H2'	1:2:1681:U:C6	2.53	0.44
1:2:1712:A:H2'	1:2:1713:G:C8	2.52	0.44
5:E:103:TYR:O	5:E:182:TYR:OH	2.34	0.44
14:W:19:LYS:HE3	14:W:19:LYS:HB3	1.89	0.44
22:F:43:LYS:HD3	22:F:43:LYS:HA	1.73	0.44
40:k:134:ARG:NH2	41:l:266:ARG:HA	2.32	0.44
40:k:199:ILE:HG23	40:k:508:HIS:HD2	1.81	0.44
1:2:1060:U:H5''	1:2:1061:A:C2	2.50	0.44
1:2:1171:G:N2	29:T:88:VAL:HG21	2.33	0.44
1:2:1607:U:H2'	1:2:1608:G:O4'	2.17	0.44
2:A:43:ASP:O	27:R:128:ARG:NE	2.50	0.44
2:A:72:ASP:HB3	2:A:119:ARG:HB2	2.00	0.44
10:L:127:GLN:HA	10:L:137:PHE:CD1	2.53	0.44
11:N:88:LEU:O	11:N:92:ILE:HG12	2.17	0.44
15:X:107:PHE:HE2	15:X:114:LYS:HG3	1.80	0.44
18:b:21:LEU:HA	18:b:26:GLN:HG3	1.99	0.44
23:K:78:GLU:C	23:K:81:ASN:H	2.26	0.44
25:P:121:ILE:HD12	25:P:121:ILE:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:106:GLU:OE1	28:S:106:GLU:N	2.35	0.44
39:j:155:TRP:CE3	39:j:166:LEU:HD22	2.53	0.44
40:k:94:ILE:HG12	40:k:389:PHE:HE2	1.83	0.44
1:2:163:A:H2'	1:2:164:G:C8	2.53	0.44
1:2:176:U:H3'	1:2:177:U:H2'	2.00	0.44
1:2:875:G:O6	17:a:15:ARG:NH2	2.48	0.44
1:2:1576:U:H2'	1:2:1577:U:C6	2.52	0.44
1:2:1658:A:H2'	1:2:1659:U:C6	2.52	0.44
7:H:9:LEU:HD21	7:H:21:ALA:HB2	2.00	0.44
7:H:77:LEU:O	7:H:81:LEU:HD23	2.17	0.44
10:L:118:GLN:NE2	10:L:145:ALA:O	2.45	0.44
15:X:130:VAL:HG13	15:X:135:LEU:HD11	1.99	0.44
21:D:28:GLU:CB	23:K:58:GLN:HE22	2.27	0.44
36:i:62:ARG:HB2	36:i:91:VAL:O	2.17	0.44
36:i:67:LYS:HD3	37:3:33:C:P	2.58	0.44
39:j:160:PRO:HG3	39:j:166:LEU:HD11	2.00	0.44
40:k:216:LEU:HD11	40:k:229:THR:HB	1.99	0.44
40:k:381:PHE:O	45:k:603:MET:N	2.51	0.44
1:2:894:G:H4'	12:O:37:GLU:OE1	2.18	0.44
1:2:1169:G:N3	1:2:1169:G:H2'	2.32	0.44
1:2:1391:C:H2'	1:2:1392:G:H8	1.81	0.44
1:2:1398:A:H2'	1:2:1399:A:C8	2.53	0.44
1:2:1606:U:H2'	1:2:1607:U:C6	2.53	0.44
5:E:179:LYS:HB3	5:E:195:ILE:HD12	2.00	0.44
22:F:43:LYS:HE3	22:F:49:SER:HB2	1.99	0.44
27:R:104:THR:O	27:R:108:GLU:HG3	2.17	0.44
29:T:40:SER:OG	29:T:43:ASN:N	2.43	0.44
30:U:56:VAL:HG22	30:U:90:TYR:O	2.18	0.44
34:f:136:ARG:HA	34:f:149:GLN:HA	1.99	0.44
35:g:263:THR:N	35:g:266:GLY:O	2.51	0.44
36:i:63:GLY:C	36:i:65:LEU:H	2.26	0.44
1:2:142:G:H2'	1:2:143:G:H8	1.80	0.44
1:2:156:A:H2	1:2:418:G:H21	1.65	0.44
1:2:208:U:N3	1:2:209:A:N7	2.66	0.44
1:2:323:U:OP1	10:L:133:LYS:NZ	2.46	0.44
1:2:564:C:H5''	1:2:565:C:C5	2.53	0.44
1:2:812:U:O3'	10:L:156:PHE:HA	2.17	0.44
1:2:1177:G:H5'	1:2:1189:C:N4	2.33	0.44
1:2:1584:A:H2'	1:2:1585:A:O4'	2.17	0.44
1:2:1716:A:H2'	1:2:1717:A:C8	2.53	0.44
1:2:1774:A:H2'	1:2:1775:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:109:LYS:O	3:B:113:MET:HB2	2.18	0.44
7:H:162:ILE:O	7:H:164:ASN:N	2.50	0.44
8:I:113:TYR:HE1	8:I:117:TYR:CD2	2.35	0.44
13:V:79:LEU:HD13	13:V:82:VAL:HB	1.99	0.44
27:R:57:LEU:CD2	27:R:60:ARG:HH21	2.31	0.44
31:Z:38:HIS:CD2	31:Z:69:PHE:HA	2.53	0.44
35:g:8:LEU:HD23	35:g:8:LEU:H	1.83	0.44
36:i:104:LYS:HE3	36:i:114:LYS:HA	1.99	0.44
39:j:187:ASP:OD2	39:j:227:LEU:HD22	2.18	0.44
40:k:412:LEU:HD23	40:k:415:GLN:OE1	2.18	0.44
1:2:340:A:H2'	1:2:341:C:C6	2.53	0.43
1:2:760:A:H3'	1:2:761:G:H8	1.83	0.43
1:2:798:A:O3'	5:E:201:HIS:CE1	2.71	0.43
1:2:1398:A:O3'	27:R:60:ARG:NH1	2.50	0.43
1:2:1417:G:H2'	1:2:1418:C:C6	2.53	0.43
1:2:1660:G:C2	1:2:1661:G:C8	3.06	0.43
1:2:1783:U:H2'	1:2:1784:G:H8	1.83	0.43
7:H:76:LYS:O	7:H:80:GLU:HG3	2.18	0.43
15:X:93:LEU:C	15:X:93:LEU:HD23	2.42	0.43
21:D:113:LEU:HD23	21:D:114:ALA:N	2.33	0.43
22:F:132:LEU:HA	22:F:135:VAL:HG12	2.00	0.43
25:P:28:MET:HE1	25:P:33:PHE:HB2	1.99	0.43
25:P:53:PRO:HB3	25:P:83:MET:SD	2.58	0.43
26:Q:25:GLY:N	26:Q:62:ASN:O	2.52	0.43
28:S:84:TRP:O	28:S:85:PHE:HB3	2.17	0.43
40:k:431:GLU:OE2	40:k:519:LYS:N	2.51	0.43
1:2:69:G:H2'	1:2:70:C:H6	1.84	0.43
1:2:236:C:H4'	1:2:237:U:C6	2.52	0.43
1:2:418:G:H2'	1:2:419:A:C8	2.52	0.43
1:2:616:U:C4	1:2:1092:A:C5	3.06	0.43
1:2:813:A:HO2'	1:2:814:G:P	2.41	0.43
1:2:1163:G:H2'	1:2:1164:G:C8	2.53	0.43
1:2:1341:C:H2'	1:2:1342:U:C6	2.54	0.43
3:B:6:ASN:HD21	39:j:91:SER:HB3	1.83	0.43
6:G:50:PHE:CD2	6:G:111:LEU:HD23	2.52	0.43
7:H:28:GLU:HB3	7:H:38:LEU:HD23	2.00	0.43
10:L:8:GLN:NE2	10:L:14:GLN:O	2.51	0.43
10:L:132:SER:OG	10:L:135:VAL:HG22	2.18	0.43
12:O:81:ILE:O	12:O:115:ILE:HA	2.18	0.43
26:Q:98:ASP:OD1	26:Q:99:GLU:N	2.51	0.43
29:T:35:ASP:OD1	29:T:35:ASP:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:33:LYS:HD3	33:d:34:TYR:CE2	2.53	0.43
38:1:63:G:C6	38:1:64:RIA:C6	3.07	0.43
41:l:133:GLU:O	41:l:137:ARG:HG3	2.18	0.43
1:2:71:A:H2'	1:2:72:A:C4	2.53	0.43
1:2:140:A:H8	6:G:179:VAL:HG22	1.84	0.43
1:2:153:G:N3	6:G:56:ASN:ND2	2.66	0.43
1:2:208:U:H2'	1:2:209:A:C8	2.53	0.43
1:2:363:G:N2	1:2:380:C:C2	2.87	0.43
1:2:365:A:H2'	1:2:366:A:C8	2.53	0.43
1:2:670:G:O2'	1:2:671:C:OP1	2.27	0.43
1:2:747:C:H2'	1:2:748:U:O4'	2.18	0.43
1:2:1201:A:N6	1:2:1455:C:OP1	2.52	0.43
1:2:1202:A:C5	1:2:1553:A:C6	3.07	0.43
1:2:1292:U:H1'	2:A:111:ILE:HD12	2.00	0.43
1:2:1377:C:O2'	26:Q:17:THR:HG21	2.18	0.43
1:2:1379:U:H1'	1:2:1514:A:N6	2.33	0.43
1:2:1449:C:P	33:d:12:ARG:HH22	2.41	0.43
1:2:1514:A:O2'	1:2:1515:U:H5'	2.18	0.43
4:C:145:ARG:HE	4:C:160:ALA:HB2	1.84	0.43
5:E:8:HIS:O	5:E:30:ARG:HD2	2.18	0.43
5:E:108:ARG:H	5:E:108:ARG:HG2	1.70	0.43
6:G:63:MET:HG3	6:G:98:ARG:CG	2.48	0.43
6:G:142:ARG:HG2	6:G:147:LEU:HD23	2.01	0.43
10:L:59:PRO:HD3	10:L:138:ASN:OD1	2.18	0.43
15:X:109:ARG:HG3	15:X:112:LYS:HB2	2.00	0.43
30:U:58:LEU:HD12	30:U:88:LYS:HB2	2.00	0.43
35:g:50:GLU:OE1	35:g:50:GLU:N	2.49	0.43
38:1:74:C:H4'	38:1:75:C:C5'	2.42	0.43
39:j:192:CYS:HB2	40:k:403:ASP:CG	2.43	0.43
1:2:93:A:C4'	5:E:3:ARG:HH12	2.32	0.43
1:2:178:A:N1	6:G:202:ARG:NH1	2.67	0.43
1:2:414:C:O2'	1:2:415:A:H5''	2.18	0.43
1:2:638:U:C5	7:H:100:PRO:HA	2.54	0.43
1:2:707:A:N1	1:2:730:G:N2	2.60	0.43
1:2:772:G:N2	1:2:774:A:H1'	2.34	0.43
1:2:921:G:H2'	1:2:922:A:C8	2.52	0.43
1:2:1372:C:H2'	1:2:1373:U:C6	2.54	0.43
1:2:1470:C:H4'	1:2:1471:U:O5'	2.18	0.43
1:2:1606:U:H2'	1:2:1607:U:H6	1.83	0.43
2:A:114:SER:OG	2:A:116:LYS:NZ	2.52	0.43
5:E:155:LYS:HD2	5:E:155:LYS:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:LYS:HA	5:E:231:PRO:HD3	2.01	0.43
6:G:14:LYS:HE2	6:G:16:ILE:HD11	2.00	0.43
7:H:124:LYS:HA	7:H:127:GLU:HG2	2.01	0.43
22:F:89:CYS:SG	22:F:94:ARG:HD2	2.58	0.43
22:F:119:THR:HG21	22:F:196:LEU:CD2	2.46	0.43
24:M:60:THR:C	24:M:62:GLU:H	2.26	0.43
25:P:60:LEU:HD12	25:P:76:VAL:HG11	2.00	0.43
25:P:87:PRO:C	25:P:89:MET:H	2.25	0.43
29:T:86:ARG:HH11	29:T:89:ARG:HE	1.65	0.43
30:U:22:ILE:HD13	30:U:100:VAL:CG1	2.48	0.43
34:f:143:HIS:CG	34:f:144:SER:N	2.86	0.43
38:1:2:G:H2'	38:1:3:C:H6	1.82	0.43
40:k:466:ILE:HB	40:k:469:THR:OG1	2.18	0.43
1:2:208:U:H2'	1:2:209:A:H8	1.83	0.43
1:2:939:A:H2'	1:2:940:A:O4'	2.19	0.43
1:2:1194:C:OP1	30:U:77:LYS:NZ	2.40	0.43
1:2:1387:C:H5'	27:R:49:LYS:NZ	2.33	0.43
1:2:1447:U:H2'	1:2:1448:U:C6	2.54	0.43
1:2:1768:U:O4'	1:2:1792:A:N6	2.51	0.43
2:A:122:ILE:HG21	2:A:174:TRP:CH2	2.54	0.43
2:A:188:LEU:HD13	2:A:195:TRP:HE3	1.83	0.43
4:C:149:TRP:CD1	14:W:97:ARG:HH22	2.35	0.43
5:E:124:ALA:HA	5:E:142:HIS:CE1	2.54	0.43
6:G:49:VAL:HG13	6:G:114:THR:HB	2.00	0.43
7:H:15:GLU:HA	7:H:18:LEU:HG	2.00	0.43
8:I:11:ARG:HD3	8:I:15:GLY:O	2.17	0.43
9:J:145:SER:C	9:J:147:MET:H	2.25	0.43
10:L:111:VAL:HA	10:L:139:VAL:HG22	2.00	0.43
25:P:30:THR:O	25:P:34:VAL:HG23	2.18	0.43
25:P:123:TYR:OH	28:S:126:ARG:HD3	2.19	0.43
26:Q:35:PRO:O	26:Q:38:LEU:HG	2.18	0.43
26:Q:50:GLU:N	26:Q:51:PRO:HD2	2.34	0.43
27:R:119:LEU:HD21	27:R:121:VAL:HG13	2.00	0.43
28:S:92:VAL:HG13	28:S:92:VAL:O	2.19	0.43
35:g:289:THR:N	35:g:292:GLN:OE1	2.48	0.43
36:i:104:LYS:HE2	36:i:111:GLU:HA	1.99	0.43
1:2:10:G:C5	1:2:11:A:C8	3.06	0.43
1:2:106:U:H2'	1:2:107:C:O4'	2.19	0.43
1:2:722:G:C5	1:2:723:G:H1'	2.54	0.43
1:2:737:A:O2'	1:2:738:G:O5'	2.33	0.43
1:2:910:U:O2	3:B:5:LYS:CD	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1356:G:H2'	1:2:1357:G:C8	2.53	0.43
1:2:1522:A:N3	1:2:1588:G:O2'	2.42	0.43
2:A:88:LYS:O	2:A:92:HIS:ND1	2.51	0.43
7:H:164:ASN:OD1	7:H:165:LYS:HD2	2.18	0.43
8:I:172:SER:OG	8:I:179:ARG:O	2.35	0.43
9:J:49:LEU:HD12	9:J:104:PHE:HE2	1.82	0.43
12:O:17:ALA:N	12:O:80:HIS:O	2.35	0.43
12:O:42:VAL:HG21	12:O:47:LYS:NZ	2.33	0.43
12:O:61:MET:O	12:O:65:GLN:HG2	2.18	0.43
12:O:129:LYS:HD3	12:O:130:GLY:N	2.33	0.43
18:b:32:PHE:O	18:b:33:LEU:HD23	2.19	0.43
23:K:45:ALA:O	23:K:49:LEU:HD23	2.19	0.43
24:M:23:VAL:O	24:M:27:THR:HG23	2.18	0.43
34:f:100:LEU:HB3	34:f:103:LEU:HD23	2.00	0.43
38:1:36:U:H2'	38:1:37:T6A:C8	2.54	0.43
1:2:278:G:H2'	1:2:279:U:O4'	2.18	0.43
1:2:346:G:H5'	10:L:80:MET:HE2	2.01	0.43
1:2:698:U:H2'	1:2:699:U:C6	2.53	0.43
1:2:899:A:OP1	12:O:43:THR:OG1	2.28	0.43
1:2:1297:U:C4	1:2:1298:G:N2	2.87	0.43
1:2:1356:G:H2'	1:2:1357:G:H8	1.83	0.43
1:2:1359:A:O2'	29:T:2:PRO:HB2	2.18	0.43
1:2:1552:U:H2'	1:2:1553:A:O4'	2.18	0.43
1:2:1687:A:H2'	1:2:1688:G:N7	2.33	0.43
3:B:79:HIS:CD2	3:B:82:ARG:HH12	2.37	0.43
4:C:178:PRO:HB2	9:J:97:LEU:HD23	2.00	0.43
4:C:212:LEU:HD12	4:C:212:LEU:HA	1.74	0.43
4:C:235:TRP:O	13:V:16:LYS:NZ	2.51	0.43
6:G:9:ILE:H	6:G:9:ILE:HD12	1.83	0.43
6:G:42:GLY:HA3	6:G:45:PHE:HD2	1.83	0.43
12:O:103:ARG:NH1	32:c:60:GLU:OE1	2.51	0.43
14:W:3:ARG:HH22	14:W:28:ARG:HD3	1.84	0.43
14:W:15:ASN:HD21	14:W:71:LYS:HG3	1.84	0.43
14:W:83:ILE:O	14:W:86:VAL:HB	2.18	0.43
18:b:45:THR:HG23	18:b:82:LYS:HZ2	1.82	0.43
22:F:145:ARG:NH1	22:F:220:GLU:OE2	2.51	0.43
26:Q:6:SER:OG	26:Q:23:LYS:HG2	2.17	0.43
29:T:124:ILE:HG22	29:T:125:SER:O	2.18	0.43
38:1:64:RIA:H2A	38:1:65:G:H8	1.83	0.43
40:k:219:ALA:O	40:k:262:HIS:NE2	2.51	0.43
1:2:46:A:H4'	1:2:47:A:H5'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:88:U:C2	1:2:89:G:C8	3.07	0.43
1:2:330:A:OP1	8:I:56:ARG:NH1	2.51	0.43
1:2:430:C:H2'	1:2:431:G:H8	1.83	0.43
1:2:564:C:H1'	15:X:66:SER:OG	2.19	0.43
1:2:620:A:O2'	1:2:1105:U:O2'	2.25	0.43
1:2:887:U:O2	1:2:987:A:O2'	2.37	0.43
1:2:1071:C:H2'	1:2:1072:G:C8	2.53	0.43
1:2:1079:U:H2'	1:2:1080:A:C8	2.53	0.43
1:2:1300:U:P	4:C:93:LYS:HD2	2.59	0.43
1:2:1344:A:H5'	30:U:53:LYS:NZ	2.34	0.43
1:2:1481:A:C6	1:2:1522:A:C5	3.07	0.43
1:2:1563:C:H4'	28:S:85:PHE:CD1	2.54	0.43
1:2:1680:U:O4	1:2:1718:G:N2	2.52	0.43
4:C:54:LYS:HB3	4:C:248:TYR:CE2	2.54	0.43
4:C:162:LYS:HD3	4:C:175:ILE:HD12	2.01	0.43
9:J:134:ILE:HG23	9:J:157:ASP:C	2.44	0.43
29:T:47:PRO:HG2	29:T:53:TRP:CE2	2.54	0.43
35:g:50:GLU:H	35:g:50:GLU:CD	2.26	0.43
36:i:62:ARG:HD2	36:i:62:ARG:HA	1.89	0.43
40:k:315:LEU:HD23	40:k:316:ILE:N	2.34	0.43
1:2:255:A:C6	1:2:256:A:C6	3.07	0.43
1:2:511:A:OP2	9:J:172:VAL:HB	2.19	0.43
1:2:586:C:H5'	19:e:26:LYS:HE2	2.00	0.43
1:2:897:A:C8	1:2:911:U:C4	3.07	0.43
1:2:1052:G:C2	1:2:1066:C:C2	3.07	0.43
1:2:1139:G:C2	1:2:1140:G:C8	3.06	0.43
1:2:1561:C:H2'	1:2:1562:U:C6	2.53	0.43
1:2:1681:U:H2'	1:2:1682:U:O4'	2.18	0.43
6:G:74:LYS:HG2	6:G:94:ARG:HG3	2.00	0.43
7:H:31:SER:HA	7:H:35:LYS:HG3	2.00	0.43
8:I:70:GLU:HG3	8:I:112:TRP:HH2	1.84	0.43
15:X:23:ARG:HG2	15:X:29:TYR:CD2	2.54	0.43
15:X:62:LYS:HE3	15:X:118:PRO:HB3	2.01	0.43
24:M:36:ARG:HD2	24:M:94:LEU:HD11	2.01	0.43
24:M:123:GLU:O	24:M:124:ARG:C	2.62	0.43
39:j:181:ALA:HA	39:j:235:LEU:HA	2.00	0.43
40:k:382:ALA:HB2	40:k:396:ILE:HG12	2.00	0.43
1:2:93:A:N7	1:2:398:A:C4	2.87	0.43
1:2:168:A:P	6:G:137:ARG:HD2	2.59	0.43
1:2:520:A:H2'	16:Y:34:ASN:HD21	1.84	0.43
1:2:772:G:H21	1:2:774:A:H1'	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:789:U:H5	1:2:790:A:C6	2.36	0.43
1:2:1004:A:H2'	1:2:1005:C:C6	2.54	0.43
1:2:1649:A:H2'	1:2:1650:C:H6	1.84	0.43
1:2:1712:A:H2'	1:2:1713:G:H8	1.84	0.43
3:B:18:LYS:C	3:B:19:ARG:HD3	2.43	0.43
4:C:58:ILE:HG23	4:C:77:LEU:HB3	2.01	0.43
5:E:31:PRO:HG2	5:E:38:LEU:HB2	2.01	0.43
8:I:161:PHE:CD1	8:I:166:LEU:HD21	2.54	0.43
10:L:111:VAL:HG23	10:L:139:VAL:HG21	2.00	0.43
22:F:119:THR:HG23	22:F:197:ALA:HB2	2.00	0.43
25:P:75:VAL:HG22	25:P:104:GLN:NE2	2.25	0.43
28:S:24:GLY:HA2	28:S:58:ALA:HB3	2.00	0.43
35:g:67:HIS:CG	35:g:68:ILE:H	2.36	0.43
35:g:199:PHE:HB3	35:g:230:TRP:CZ3	2.54	0.43
40:k:388:LYS:HD2	40:k:389:PHE:N	2.34	0.43
1:2:199:A:H2'	1:2:200:G:C8	2.54	0.42
1:2:1073:G:H2'	1:2:1074:C:C6	2.54	0.42
1:2:1404:A:H2'	1:2:1405:U:C6	2.54	0.42
1:2:1437:C:C2	1:2:1438:C:C5	3.07	0.42
3:B:125:VAL:HG22	3:B:127:VAL:HG13	2.01	0.42
5:E:136:ILE:HG21	5:E:148:ARG:NH1	2.32	0.42
7:H:34:LEU:HD22	7:H:76:LYS:NZ	2.34	0.42
9:J:85:VAL:HG21	9:J:104:PHE:HE1	1.84	0.42
9:J:107:ARG:HH11	9:J:112:GLN:NE2	2.17	0.42
10:L:96:LYS:HD3	10:L:97:TYR:CZ	2.54	0.42
10:L:107:VAL:HG11	10:L:137:PHE:CD2	2.54	0.42
21:D:177:LEU:HD23	21:D:177:LEU:HA	1.88	0.42
21:D:218:LEU:HG	21:D:221:SER:HB2	2.01	0.42
22:F:117:LYS:O	22:F:121:GLU:HG2	2.19	0.42
34:f:138:TYR:OH	34:f:143:HIS:HB2	2.19	0.42
35:g:281:LEU:HD23	35:g:320:TRP:CE2	2.54	0.42
40:k:356:ARG:NH2	40:k:423:LEU:HA	2.33	0.42
1:2:216:A:O2'	1:2:217:A:OP1	2.22	0.42
1:2:243:A:O3'	5:E:155:LYS:NZ	2.53	0.42
1:2:409:A:H2'	1:2:410:C:O4'	2.19	0.42
1:2:453:U:C2	5:E:66:MET:SD	3.12	0.42
1:2:802:A:N7	7:H:104:ARG:HD2	2.34	0.42
1:2:826:C:H2'	1:2:827:U:C5	2.54	0.42
1:2:976:A:N6	1:2:1023:U:C2	2.87	0.42
1:2:1689:A:N6	1:2:1708:U:O2'	2.51	0.42
1:2:1751:A:H2'	1:2:1752:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4:PRO:HG3	13:V:41:GLU:O	2.19	0.42
2:A:84:ARG:O	2:A:88:LYS:HG2	2.19	0.42
3:B:5:LYS:HZ1	3:B:7:LYS:CD	2.21	0.42
3:B:157:GLN:O	3:B:161:ILE:HD12	2.19	0.42
4:C:121:LYS:HG2	4:C:132:ALA:CB	2.49	0.42
7:H:122:HIS:O	7:H:173:TYR:OH	2.28	0.42
8:I:104:ILE:O	8:I:165:ARG:HA	2.18	0.42
9:J:82:ARG:O	9:J:149:ARG:HB2	2.19	0.42
12:O:70:LYS:O	12:O:74:VAL:HG22	2.20	0.42
19:e:36:LYS:HA	19:e:36:LYS:HD3	1.69	0.42
24:M:41:SER:O	24:M:45:LEU:HD23	2.19	0.42
28:S:30:TYR:C	28:S:33:THR:HG1	2.26	0.42
35:g:210:GLN:HE22	35:g:252:PHE:H	1.66	0.42
39:j:15:GLU:OE1	39:j:39:TYR:OH	2.28	0.42
40:k:142:TYR:CE2	45:k:603:MET:HE2	2.55	0.42
40:k:463:MET:HB2	40:k:509:TRP:CE3	2.54	0.42
1:2:296:U:O3'	5:E:37:LYS:HA	2.19	0.42
1:2:388:G:C2	1:2:408:C:C2	3.07	0.42
1:2:396:A:H2'	1:2:397:G:O4'	2.19	0.42
1:2:751:G:C6	1:2:798:A:N1	2.87	0.42
1:2:790:A:H2'	1:2:791:U:C6	2.54	0.42
1:2:906:A:H2'	1:2:907:U:C6	2.54	0.42
1:2:910:U:O2	3:B:5:LYS:HD2	2.19	0.42
1:2:1031:G:H2'	1:2:1032:C:C6	2.54	0.42
1:2:1096:U:H1'	4:C:173:ARG:NH1	2.34	0.42
1:2:1294:G:H2'	1:2:1295:A:H8	1.84	0.42
1:2:1298:G:O2'	1:2:1299:A:H5'	2.19	0.42
1:2:1339:U:H1'	1:2:1376:U:H5'	2.01	0.42
1:2:1476:G:OP1	29:T:39:THR:OG1	2.34	0.42
4:C:58:ILE:HA	4:C:61:ILE:HD12	2.01	0.42
4:C:63:LEU:O	4:C:63:LEU:HD23	2.19	0.42
7:H:5:GLN:HE21	7:H:21:ALA:HB3	1.84	0.42
11:N:25:TRP:HH2	18:b:45:THR:HG21	1.84	0.42
12:O:91:SER:O	12:O:93:THR:HG23	2.20	0.42
16:Y:31:ASN:O	16:Y:31:ASN:ND2	2.52	0.42
23:K:35:ILE:HG23	23:K:37:THR:H	1.84	0.42
25:P:80:LEU:HB3	25:P:83:MET:HB2	2.01	0.42
35:g:33:LEU:HD11	35:g:95:LEU:HD23	2.02	0.42
35:g:204:ASN:CG	35:g:223:LYS:HB3	2.44	0.42
39:j:46:ILE:HG23	39:j:50:GLU:HG2	2.00	0.42
1:2:11:A:O2'	1:2:12:U:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:60:U:H3	1:2:63:G:P	2.42	0.42
1:2:72:A:H1'	1:2:73:U:C6	2.54	0.42
1:2:474:A:OP1	9:J:126:ARG:NE	2.49	0.42
1:2:990:G:O2'	1:2:1013:G:N2	2.53	0.42
1:2:1179:C:H2'	1:2:1180:U:C6	2.55	0.42
1:2:1200:G:N2	1:2:1598:A:N3	2.67	0.42
1:2:1396:U:H3'	1:2:1397:C:H5'	2.00	0.42
1:2:1481:A:C2	1:2:1605:G:H1'	2.54	0.42
1:2:1599:G:OP1	29:T:86:ARG:NH2	2.46	0.42
1:2:1778:G:C6	1:2:1779:A:C6	3.08	0.42
1:2:1786:G:OP1	12:O:127:ARG:NH1	2.53	0.42
2:A:22:VAL:HG22	2:A:169:SER:HB2	2.00	0.42
2:A:179:ARG:HD3	2:A:183:ARG:NE	2.35	0.42
3:B:176:VAL:HG13	3:B:184:LEU:HD22	2.01	0.42
4:C:54:LYS:HE3	4:C:251:TYR:CE2	2.55	0.42
4:C:90:PRO:HB3	4:C:103:PHE:HE1	1.84	0.42
5:E:126:VAL:HG12	5:E:158:ASP:O	2.18	0.42
6:G:43:ASP:OD1	6:G:44:GLU:N	2.52	0.42
10:L:33:ARG:HD3	10:L:49:ILE:O	2.20	0.42
10:L:101:GLU:OE2	15:X:13:ARG:NH1	2.53	0.42
24:M:97:ILE:HG23	24:M:101:GLY:HA2	2.02	0.42
30:U:42:ILE:HG23	30:U:52:LYS:NZ	2.34	0.42
35:g:22:THR:O	35:g:298:SER:HB3	2.20	0.42
36:i:112:ASN:OD1	36:i:113:ALA:N	2.52	0.42
38:1:63:G:H2'	38:1:64:RIA:H1A	2.00	0.42
40:k:464:VAL:HG23	40:k:471:THR:OG1	2.19	0.42
1:2:270:A:C2	1:2:271:U:H1'	2.55	0.42
1:2:369:A:C6	1:2:370:G:C5	3.07	0.42
1:2:1647:G:H5''	15:X:73:ARG:NH2	2.33	0.42
2:A:188:LEU:HD13	2:A:195:TRP:CE3	2.55	0.42
5:E:115:THR:HG23	5:E:118:GLU:H	1.85	0.42
8:I:168:ALA:HA	8:I:185:LEU:HD23	2.01	0.42
12:O:51:ASP:HB2	12:O:52:ARG:NH1	2.34	0.42
13:V:11:LEU:O	13:V:11:LEU:HD12	2.19	0.42
13:V:35:ASN:OD1	13:V:52:THR:HG22	2.19	0.42
35:g:43:LEU:HD11	35:g:83:SER:HB3	2.01	0.42
40:k:198:ASP:CG	40:k:228:GLN:HE21	2.28	0.42
40:k:388:LYS:HE3	40:k:389:PHE:HD1	1.85	0.42
1:2:97:C:H2'	1:2:98:U:H6	1.84	0.42
1:2:179:A:H2'	1:2:180:A:O4'	2.20	0.42
1:2:277:U:P	1:2:278:G:H21	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:388:G:N2	1:2:408:C:C2	2.87	0.42
1:2:683:C:N4	1:2:684:A:N6	2.66	0.42
1:2:1035:A:H2'	1:2:1036:C:C6	2.55	0.42
2:A:90:ALA:HA	2:A:95:ALA:HB3	2.00	0.42
4:C:132:ALA:O	4:C:135:ILE:HG22	2.20	0.42
5:E:104:ASP:HB2	5:E:110:ALA:HB2	2.02	0.42
5:E:222:LEU:HD12	5:E:222:LEU:O	2.20	0.42
7:H:157:LYS:HE3	7:H:157:LYS:HB3	1.93	0.42
12:O:133:ARG:HA	17:a:28:ARG:HD2	2.02	0.42
22:F:71:TYR:HB3	26:Q:46:PHE:HB3	2.01	0.42
26:Q:50:GLU:HG3	26:Q:112:TYR:CE1	2.54	0.42
27:R:10:LYS:HG2	27:R:53:TYR:CE2	2.55	0.42
28:S:96:LYS:HB2	28:S:98:TYR:CZ	2.55	0.42
32:c:10:ALA:HB1	32:c:30:VAL:HB	2.00	0.42
38:1:76:A:O2'	45:k:603:MET:O	2.36	0.42
39:j:232:THR:HG21	39:j:243:GLN:NE2	2.35	0.42
40:k:108:HIS:ND1	40:k:228:GLN:OE1	2.48	0.42
1:2:95:G:H4'	5:E:8:HIS:CD2	2.55	0.42
1:2:141:U:H3'	1:2:141:U:OP2	2.20	0.42
1:2:221:A:OP2	1:2:832:U:H1'	2.20	0.42
1:2:912:G:H5'	1:2:913:G:C8	2.55	0.42
1:2:984:G:N3	1:2:985:G:C8	2.87	0.42
1:2:1238:U:H2'	1:2:1239:U:C6	2.54	0.42
1:2:1472:G:C2	1:2:1473:A:C5	3.08	0.42
1:2:1513:A:H1'	1:2:1516:C:N4	2.35	0.42
1:2:1550:U:H2'	1:2:1551:G:O4'	2.19	0.42
1:2:1656:G:O6	1:2:1741:U:C2	2.72	0.42
2:A:122:ILE:HG12	2:A:144:ILE:HB	2.02	0.42
2:A:200:ASP:HB2	27:R:89:SER:HB2	2.01	0.42
3:B:113:MET:CE	3:B:209:ASN:HB3	2.45	0.42
14:W:94:LEU:HD11	14:W:102:VAL:HG23	2.02	0.42
21:D:59:VAL:HG12	21:D:63:GLY:HA2	2.02	0.42
23:K:81:ASN:ND2	24:M:30:VAL:HG22	2.34	0.42
33:d:21:CYS:HB3	33:d:25:GLY:H	1.84	0.42
39:j:35:LYS:NZ	39:j:41:ASN:HB3	2.35	0.42
1:2:10:G:C6	1:2:11:A:C5	3.08	0.42
1:2:1125:G:H2'	1:2:1126:G:H8	1.85	0.42
1:2:1156:A:C2	1:2:1159:A:C8	3.07	0.42
1:2:1259:U:HO2'	1:2:1260:G:H8	1.67	0.42
1:2:1664:U:H2'	1:2:1665:A:O4'	2.20	0.42
1:2:1741:U:H2'	1:2:1742:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1758:G:C6	1:2:1759:U:C4	3.07	0.42
1:2:1798:A:N6	37:3:19:A:HO2'	2.17	0.42
3:B:32:ILE:HB	3:B:44:GLY:H	1.84	0.42
3:B:72:ASP:OD1	17:a:59:TYR:OH	2.35	0.42
4:C:148:TYR:CE2	4:C:156:PRO:HB3	2.55	0.42
5:E:75:LYS:HB2	5:E:75:LYS:HE2	1.89	0.42
6:G:50:PHE:CE1	6:G:113:ILE:HG22	2.55	0.42
8:I:138:LYS:HD2	8:I:141:GLU:HB2	2.02	0.42
10:L:125:VAL:HG23	10:L:138:ASN:C	2.44	0.42
17:a:37:LYS:HG2	17:a:72:HIS:ND1	2.34	0.42
21:D:24:PHE:CZ	23:K:65:TYR:HD2	2.37	0.42
26:Q:82:ARG:NH2	26:Q:116:LEU:HD23	2.34	0.42
26:Q:127:LYS:HA	26:Q:134:ALA:HA	2.02	0.42
35:g:242:ASP:OD1	35:g:243:ALA:N	2.53	0.42
35:g:254:PRO:HD3	35:g:301:TRP:HB3	2.01	0.42
38:1:55:U:H5'	39:j:175:LYS:NZ	2.35	0.42
39:j:42:ILE:HG22	39:j:43:GLU:H	1.84	0.42
1:2:43:A:C6	1:2:377:A:C6	3.08	0.42
1:2:426:C:H1'	1:2:458:G:H1'	2.01	0.42
1:2:461:G:C6	1:2:462:U:C4	3.08	0.42
1:2:843:A:H2'	1:2:844:G:H8	1.83	0.42
1:2:863:U:H3'	14:W:28:ARG:HH21	1.85	0.42
1:2:1052:G:H2'	1:2:1053:U:H6	1.83	0.42
1:2:1473:A:H2'	1:2:1474:C:C6	2.54	0.42
1:2:1474:C:H2'	1:2:1475:G:H8	1.85	0.42
1:2:1519:G:N2	1:2:1521:G:O4'	2.52	0.42
1:2:1557:A:C8	28:S:134:ARG:HB3	2.54	0.42
1:2:1770:C:O5'	20:h:2:ARG:NE	2.53	0.42
2:A:121:VAL:HG23	2:A:141:ILE:HG21	2.02	0.42
3:B:181:LEU:O	3:B:185:THR:HG23	2.19	0.42
8:I:84:HIS:HD2	8:I:100:ALA:HB2	1.85	0.42
9:J:123:HIS:CE1	19:e:37:ARG:HD2	2.55	0.42
23:K:50:THR:HG22	23:K:55:VAL:O	2.19	0.42
30:U:52:LYS:O	30:U:53:LYS:HD2	2.19	0.42
39:j:190:VAL:HB	40:k:405:THR:HG21	2.01	0.42
40:k:398:VAL:HG12	40:k:400:THR:HG23	2.01	0.42
40:k:402:VAL:HG11	40:k:406:LEU:HD22	2.01	0.42
1:2:249:C:H2'	1:2:250:A:H8	1.85	0.42
1:2:521:U:O3'	16:Y:60:PHE:HB2	2.20	0.42
1:2:732:G:H1'	1:2:734:A:H61	1.85	0.42
1:2:732:G:H1'	1:2:734:A:N6	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:760:A:C6	1:2:761:G:C4	3.08	0.42
1:2:983:G:N3	1:2:984:G:C8	2.88	0.42
1:2:1014:U:H3'	1:2:1015:C:O2	2.20	0.42
1:2:1148:G:H1	1:2:1626:U:H3	1.68	0.42
1:2:1162:A:H2'	1:2:1163:G:O4'	2.20	0.42
1:2:1253:U:H2'	1:2:1254:G:C8	2.55	0.42
1:2:1316:C:H2'	1:2:1317:G:O4'	2.20	0.42
1:2:1643:G:C6	1:2:1755:G:O6	2.73	0.42
1:2:1757:C:H2'	1:2:1758:G:C8	2.54	0.42
4:C:180:GLY:O	9:J:53:ARG:NH2	2.51	0.42
8:I:161:PHE:HD1	8:I:166:LEU:HD21	1.85	0.42
28:S:91:ASP:O	28:S:93:ASN:N	2.39	0.42
38:1:24:G:H2'	38:1:25:C:C6	2.55	0.42
40:k:93:GLU:HA	40:k:97:ARG:NH2	2.35	0.42
1:2:86:A:H5'	16:Y:120:GLY:HA2	2.02	0.41
1:2:536:G:C6	9:J:171:ARG:HD2	2.55	0.41
1:2:593:A:OP2	9:J:37:LYS:NZ	2.51	0.41
1:2:678:G:H2'	1:2:679:U:H4'	2.00	0.41
1:2:959:U:H5'	11:N:55:ARG:HH11	1.85	0.41
1:2:1280:G:H2'	1:2:1281:U:C6	2.54	0.41
1:2:1296:G:H5'	1:2:1297:U:OP2	2.19	0.41
2:A:26:ALA:HB1	2:A:149:LEU:HB2	2.01	0.41
3:B:144:ARG:CZ	3:B:206:PRO:HB3	2.50	0.41
4:C:48:ARG:NH1	4:C:254:ALA:H	2.18	0.41
5:E:122:LYS:HZ2	5:E:145:ARG:HH22	1.68	0.41
7:H:71:HIS:NE2	7:H:128:ASP:OD1	2.48	0.41
8:I:109:PHE:CZ	8:I:184:ILE:HD11	2.55	0.41
9:J:139:GLN:NE2	9:J:140:ILE:O	2.49	0.41
10:L:76:VAL:CG2	10:L:87:ARG:HB2	2.49	0.41
12:O:80:HIS:ND1	12:O:114:ARG:HB2	2.35	0.41
14:W:111:MET:HE1	14:W:115:GLU:C	2.44	0.41
16:Y:5:ILE:H	16:Y:5:ILE:HD12	1.85	0.41
16:Y:83:LYS:HE3	16:Y:96:LEU:HD23	2.02	0.41
18:b:31:HIS:O	18:b:48:SER:OG	2.25	0.41
24:M:95:GLY:HA3	24:M:104:ARG:CD	2.50	0.41
28:S:26:ILE:H	28:S:26:ILE:HD12	1.85	0.41
28:S:45:LEU:HD11	29:T:36:ILE:HD13	2.01	0.41
31:Z:65:LEU:HB3	31:Z:71:LEU:HD12	2.01	0.41
34:f:131:ALA:HB3	34:f:138:TYR:HB3	2.02	0.41
35:g:7:MET:HE2	35:g:323:MET:CE	2.50	0.41
38:1:35:A:H2'	38:1:36:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:76:A:N6	40:k:379:SER:OG	2.48	0.41
39:j:15:GLU:HG2	39:j:18:ASP:HB3	2.02	0.41
40:k:330:ILE:HG23	40:k:333:LEU:HD11	2.01	0.41
1:2:35:U:H2'	1:2:36:C:H6	1.85	0.41
1:2:97:C:O2	1:2:424:A:O2'	2.37	0.41
1:2:105:A:P	8:l:18:ARG:HH12	2.42	0.41
1:2:151:U:O2'	6:G:15:CYS:HB2	2.20	0.41
1:2:366:A:H2'	1:2:367:U:O4'	2.19	0.41
1:2:369:A:H2'	1:2:370:G:C8	2.55	0.41
1:2:760:A:C4	1:2:790:A:C2	3.08	0.41
1:2:835:U:H2'	1:2:836:G:H8	1.85	0.41
1:2:862:A:C4	1:2:864:A:C8	3.08	0.41
1:2:899:A:C8	1:2:900:G:N2	2.88	0.41
1:2:959:U:OP2	11:N:55:ARG:NH1	2.51	0.41
1:2:1029:A:C5	1:2:1790:G:C6	3.09	0.41
1:2:1252:U:C2	1:2:1253:U:C5	3.08	0.41
1:2:1281:U:H2'	1:2:1282:U:H6	1.85	0.41
1:2:1431:G:C2	33:d:41:GLN:HG3	2.55	0.41
1:2:1613:C:OP2	32:c:47:PRO:HB3	2.20	0.41
1:2:1622:C:C2	1:2:1623:C:C5	3.08	0.41
1:2:1715:G:C6	1:2:1716:A:C5	3.08	0.41
8:l:29:LEU:HD23	8:l:29:LEU:H	1.85	0.41
9:J:145:SER:O	9:J:147:MET:N	2.53	0.41
10:L:20:PHE:CE2	10:L:22:ASN:HA	2.55	0.41
11:N:50:ILE:O	11:N:54:LEU:HD23	2.20	0.41
23:K:32:HIS:O	23:K:35:ILE:HG22	2.20	0.41
28:S:45:LEU:HD21	29:T:36:ILE:HD12	2.02	0.41
31:Z:50:ILE:HD11	31:Z:70:LYS:HD2	2.03	0.41
39:j:201:ILE:HG22	40:k:330:ILE:HG21	2.02	0.41
40:k:210:VAL:HG11	40:k:395:LEU:HD21	2.02	0.41
1:2:425:G:C2	1:2:426:C:C5	3.07	0.41
1:2:487:G:H2'	1:2:488:C:O4'	2.20	0.41
1:2:649:U:O2'	1:2:650:G:OP1	2.38	0.41
1:2:749:U:C4	1:2:800:G:O6	2.73	0.41
1:2:883:A:H2'	1:2:884:G:H8	1.84	0.41
1:2:1228:G:N1	24:M:40:GLU:OE2	2.43	0.41
1:2:1481:A:C6	1:2:1522:A:C6	3.08	0.41
1:2:1660:G:C2	1:2:1738:A:C2	3.09	0.41
2:A:188:LEU:HD22	2:A:195:TRP:CE3	2.56	0.41
6:G:185:GLN:HA	6:G:188:ARG:HE	1.86	0.41
8:l:192:PHE:HD1	8:l:195:ARG:HH12	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:71:ILE:H	11:N:71:ILE:HD12	1.84	0.41
22:F:86:LYS:HD2	22:F:94:ARG:NH2	2.34	0.41
24:M:56:VAL:HG21	24:M:85:ALA:HA	2.02	0.41
31:Z:46:LYS:O	31:Z:50:ILE:HG12	2.20	0.41
40:k:238:ILE:CG2	40:k:514:TRP:HB3	2.48	0.41
1:2:15:U:H2'	1:2:16:G:O4'	2.21	0.41
1:2:55:A:H2'	1:2:402:G:H1	1.86	0.41
1:2:1408:A:O2'	1:2:1409:A:O5'	2.37	0.41
1:2:1513:A:OP1	21:D:7:LYS:NZ	2.47	0.41
1:2:1515:U:OP2	1:2:1516:C:N4	2.40	0.41
1:2:1628:U:HO2'	1:2:1762:C:HO2'	1.62	0.41
1:2:1691:A:N6	1:2:1695:G:OP1	2.53	0.41
1:2:1735:G:H2'	1:2:1736:U:O4'	2.20	0.41
6:G:88:ARG:HB3	6:G:91:GLU:CD	2.46	0.41
8:I:185:LEU:HB3	8:I:190:LEU:HG	2.01	0.41
9:J:48:GLN:O	9:J:52:ILE:HG12	2.20	0.41
9:J:49:LEU:HD12	9:J:104:PHE:CE2	2.55	0.41
14:W:8:ALA:HA	14:W:74:VAL:HG21	2.02	0.41
25:P:21:ASP:O	25:P:25:LEU:HG	2.20	0.41
26:Q:30:LYS:O	26:Q:66:ARG:HA	2.20	0.41
28:S:116:LEU:O	28:S:124:GLY:HA3	2.19	0.41
30:U:64:LYS:HE3	30:U:64:LYS:HB2	1.65	0.41
38:1:41:C:H2'	38:1:42:U:C6	2.56	0.41
40:k:230:SER:HB3	40:k:269:PHE:CZ	2.55	0.41
1:2:57:G:C6	1:2:91:G:N1	2.88	0.41
1:2:65:A:O2'	1:2:66:U:H5''	2.21	0.41
1:2:434:C:OP2	15:X:50:LYS:HB2	2.20	0.41
1:2:637:U:OP2	14:W:32:LYS:HD2	2.20	0.41
1:2:898:G:C6	1:2:899:A:C5	3.08	0.41
1:2:1047:G:O3'	18:b:69:GLY:HA3	2.20	0.41
1:2:1173:C:OP1	28:S:136:GLN:HB3	2.20	0.41
1:2:1475:G:C4	1:2:1476:G:C8	3.09	0.41
1:2:1623:C:H2'	1:2:1624:U:H6	1.86	0.41
2:A:88:LYS:NZ	2:A:201:LEU:HG	2.35	0.41
2:A:200:ASP:HA	2:A:203:PHE:CD1	2.56	0.41
7:H:4:PRO:HA	7:H:7:LYS:HE3	2.02	0.41
9:J:170:GLY:HA2	9:J:174:ARG:NH1	2.34	0.41
24:M:35:ALA:HB3	24:M:113:VAL:HG13	2.01	0.41
24:M:105:LYS:HD2	24:M:106:VAL:HG12	2.03	0.41
26:Q:16:ALA:HB2	26:Q:72:GLY:HA3	2.02	0.41
29:T:11:ALA:O	29:T:15:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1:61:C:H2'	38:1:62:C:C6	2.56	0.41
39:j:18:ASP:OD1	39:j:73:VAL:HB	2.20	0.41
39:j:35:LYS:HZ3	39:j:41:ASN:HB3	1.86	0.41
39:j:195:TYR:HE1	40:k:374:PHE:H	1.69	0.41
40:k:155:CYS:HA	40:k:156:PRO:HD2	1.92	0.41
1:2:5:U:O2'	1:2:552:G:H4'	2.21	0.41
1:2:332:A:H5''	8:I:54:LYS:HE3	2.03	0.41
1:2:646:G:C6	1:2:688:G:C6	3.09	0.41
1:2:820:U:C4	1:2:821:U:C4	3.08	0.41
1:2:985:G:O2'	1:2:986:G:H5'	2.21	0.41
1:2:1270:G:H2'	1:2:1271:U:C6	2.55	0.41
1:2:1279:C:H4'	30:U:69:LYS:HB3	2.02	0.41
1:2:1621:C:H2'	1:2:1622:C:H6	1.86	0.41
1:2:1742:A:H2'	1:2:1743:G:H5'	2.03	0.41
3:B:134:VAL:HB	3:B:219:LYS:HB3	2.02	0.41
4:C:62:PHE:CD2	4:C:143:PRO:HG3	2.56	0.41
4:C:153:LEU:HG	4:C:154:GLY:H	1.85	0.41
4:C:183:ILE:HD12	4:C:201:VAL:HG12	2.01	0.41
4:C:184:VAL:HG21	4:C:202:TYR:CD1	2.55	0.41
5:E:131:LEU:HD12	5:E:131:LEU:O	2.19	0.41
12:O:69:ALA:O	12:O:72:LYS:HG2	2.20	0.41
14:W:24:GLN:N	14:W:24:GLN:OE1	2.53	0.41
21:D:196:THR:HA	21:D:200:LYS:NZ	2.36	0.41
22:F:211:TYR:O	22:F:215:LYS:HG2	2.20	0.41
24:M:38:LEU:HD13	34:f:102:VAL:HG21	2.01	0.41
26:Q:39:VAL:HB	26:Q:41:PRO:HD2	2.03	0.41
26:Q:112:TYR:CD1	26:Q:116:LEU:HD11	2.54	0.41
27:R:51:ALA:O	27:R:55:THR:HG23	2.20	0.41
28:S:72:ILE:HA	28:S:79:TYR:CD2	2.55	0.41
36:i:26:LEU:H	36:i:26:LEU:HD23	1.85	0.41
39:j:160:PRO:HG3	39:j:166:LEU:HD21	2.03	0.41
1:2:277:U:H4'	1:2:278:G:O5'	2.21	0.41
1:2:360:C:H2'	1:2:361:G:H8	1.86	0.41
1:2:519:A:C6	1:2:520:A:C6	3.09	0.41
1:2:594:G:H2'	1:2:595:C:C6	2.56	0.41
1:2:681:U:H2'	1:2:682:U:C6	2.55	0.41
1:2:953:G:H2'	1:2:954:A:C8	2.54	0.41
1:2:1052:G:H2'	1:2:1053:U:C6	2.56	0.41
1:2:1198:G:HO2'	1:2:1199:G:P	2.40	0.41
1:2:1246:U:H5''	34:f:93:HIS:HB2	2.02	0.41
1:2:1671:G:H2'	1:2:1672:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1677:G:O2'	1:2:1678:G:H5'	2.20	0.41
3:B:81:PHE:O	3:B:106:THR:N	2.53	0.41
4:C:157:HIS:NE2	4:C:179:ARG:HG2	2.36	0.41
6:G:33:GLY:HA2	6:G:51:LYS:HE2	2.02	0.41
6:G:55:GLY:HA3	6:G:63:MET:HE1	2.03	0.41
6:G:103:GLY:H	6:G:106:LEU:HD23	1.85	0.41
15:X:61:SER:OG	15:X:67:ALA:N	2.49	0.41
16:Y:91:LEU:HD23	16:Y:91:LEU:HA	1.82	0.41
23:K:33:GLU:C	23:K:34:GLU:HG3	2.45	0.41
31:Z:42:LEU:HD21	31:Z:47:PHE:HB2	2.03	0.41
32:c:9:LEU:HA	32:c:54:LEU:O	2.20	0.41
39:j:14:PRO:HG3	39:j:39:TYR:HD2	1.86	0.41
40:k:140:LEU:O	40:k:319:ARG:NH1	2.54	0.41
1:2:8:U:O2	1:2:1137:A:H3'	2.21	0.41
1:2:218:A:C6	1:2:842:U:H1'	2.56	0.41
1:2:479:G:C6	1:2:508:G:C6	3.09	0.41
1:2:484:A:H2'	1:2:485:G:C8	2.56	0.41
1:2:1096:U:H6	4:C:173:ARG:HD2	1.86	0.41
1:2:1125:G:H5'	20:h:11:ARG:NH2	2.36	0.41
1:2:1276:G:C5	1:2:1277:G:C5	3.09	0.41
1:2:1477:A:N3	1:2:1478:G:C8	2.89	0.41
1:2:1537:G:H4'	28:S:40:ARG:NH2	2.35	0.41
1:2:1604:C:H2'	1:2:1605:G:C8	2.56	0.41
4:C:227:TYR:O	4:C:229:PHE:N	2.52	0.41
5:E:6:LYS:HB3	5:E:6:LYS:HE3	1.92	0.41
6:G:214:LYS:O	6:G:217:SER:OG	2.28	0.41
8:I:83:TYR:HB3	8:I:101:ILE:HB	2.03	0.41
9:J:29:LYS:HE2	9:J:29:LYS:HB2	1.90	0.41
9:J:114:TYR:CG	9:J:122:VAL:HG12	2.56	0.41
11:N:74:ILE:O	11:N:77:SER:OG	2.25	0.41
21:D:179:GLN:O	21:D:179:GLN:HG3	2.21	0.41
25:P:40:ARG:HD2	25:P:40:ARG:HA	1.90	0.41
28:S:53:ASP:HB3	28:S:56:LYS:HB2	2.03	0.41
30:U:26:LEU:O	30:U:88:LYS:HA	2.21	0.41
31:Z:55:PRO:C	31:Z:57:TYR:H	2.28	0.41
32:c:44:VAL:CG2	32:c:54:LEU:HD21	2.50	0.41
39:j:182:VAL:HG11	39:j:270:ALA:HB1	2.02	0.41
39:j:247:ALA:HA	39:j:250:LYS:HE3	2.03	0.41
40:k:166:SER:HB2	40:k:383:GLU:OE2	2.20	0.41
40:k:227:PRO:HB2	40:k:442:GLY:HA2	2.02	0.41
1:2:13:C:OP1	4:C:211:THR:OG1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:208:U:C2	1:2:209:A:C8	3.08	0.41
1:2:242:G:H2'	1:2:243:A:C8	2.56	0.41
1:2:324:G:C6	1:2:343:A:C6	3.09	0.41
1:2:357:U:H4'	1:2:358:A:C2	2.56	0.41
1:2:548:G:H1	1:2:588:C:H5	1.68	0.41
1:2:586:C:C5'	19:e:24:GLN:HE22	2.32	0.41
1:2:644:C:H2'	1:2:645:U:O4'	2.20	0.41
1:2:654:G:H3'	1:2:655:G:H8	1.85	0.41
1:2:665:A:H2'	1:2:666:U:C6	2.56	0.41
1:2:691:U:H5'	1:2:692:C:OP2	2.20	0.41
1:2:833:G:H8	1:2:833:G:OP2	2.03	0.41
1:2:846:A:O5'	1:2:846:A:H8	2.04	0.41
1:2:877:G:H2'	1:2:878:G:C8	2.56	0.41
1:2:888:U:H2'	1:2:889:C:C6	2.56	0.41
1:2:1166:G:H2'	1:2:1167:U:C6	2.55	0.41
1:2:1274:A:N3	21:D:141:LYS:NZ	2.46	0.41
1:2:1322:C:H2'	1:2:1323:G:O4'	2.21	0.41
1:2:1331:C:O2'	21:D:162:GLN:HB3	2.21	0.41
1:2:1357:G:H4'	29:T:130:ARG:HG2	2.03	0.41
1:2:1389:A:C4	1:2:1390:U:C5	3.09	0.41
1:2:1456:G:HO2'	1:2:1457:C:C5'	2.32	0.41
1:2:1475:G:C6	1:2:1529:G:C6	3.09	0.41
1:2:1653:A:H62	1:2:1743:G:HO2'	1.55	0.41
1:2:1678:G:OP2	1:2:1678:G:H8	2.03	0.41
1:2:1680:U:H4'	6:G:65:GLN:HE22	1.85	0.41
1:2:1789:A:C4	1:2:1791:G:C8	3.09	0.41
2:A:4:PRO:HG2	2:A:6:THR:OG1	2.21	0.41
2:A:25:GLY:HA2	2:A:45:VAL:CG1	2.50	0.41
3:B:2:ALA:HA	39:j:89:ARG:HH22	1.86	0.41
3:B:152:ARG:O	3:B:152:ARG:HG2	2.21	0.41
4:C:54:LYS:HD2	4:C:248:TYR:CE2	2.56	0.41
4:C:163:THR:HG21	4:C:226:THR:HA	2.02	0.41
4:C:220:PHE:O	4:C:223:ILE:HG22	2.21	0.41
6:G:2:LYS:C	6:G:3:LEU:HD12	2.46	0.41
6:G:76:LEU:HB2	6:G:94:ARG:NE	2.32	0.41
7:H:5:GLN:NE2	7:H:18:LEU:HA	2.35	0.41
7:H:151:LYS:HG3	7:H:182:VAL:HG13	2.03	0.41
9:J:92:LYS:HA	9:J:92:LYS:HD2	1.89	0.41
9:J:150:LEU:O	9:J:153:GLU:HG3	2.21	0.41
11:N:135:LEU:HD13	11:N:139:TRP:CD2	2.55	0.41
13:V:17:CYS:HG	13:V:20:THR:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:12:ALA:HA	18:b:15:GLU:HG2	2.02	0.41
21:D:66:ILE:HG13	21:D:67:ASN:N	2.35	0.41
22:F:65:GLN:HG3	22:F:88:GLN:C	2.45	0.41
22:F:114:ARG:HD3	26:Q:43:ILE:CD1	2.50	0.41
26:Q:40:GLN:HA	26:Q:40:GLN:OE1	2.21	0.41
26:Q:100:GLN:HB3	35:g:57:VAL:HG13	2.01	0.41
28:S:11:PHE:CE2	31:Z:41:VAL:HG11	2.55	0.41
34:f:83:LYS:HD2	34:f:85:TYR:HE1	1.86	0.41
35:g:39:ARG:C	35:g:41:LYS:H	2.29	0.41
35:g:113:SER:OG	35:g:126:ALA:HB3	2.21	0.41
35:g:243:ALA:O	35:g:244:LYS:HG2	2.20	0.41
39:j:15:GLU:H	39:j:15:GLU:CD	2.29	0.41
39:j:30:MET:O	39:j:48:LEU:HG	2.21	0.41
41:l:157:LYS:HD2	41:l:242:ILE:HG21	2.02	0.41
1:2:71:A:H1'	1:2:81:G:N1	2.36	0.41
1:2:278:G:N1	1:2:280:G:C6	2.89	0.41
1:2:643:U:H2'	1:2:644:C:H6	1.86	0.41
1:2:823:G:N3	1:2:823:G:H2'	2.35	0.41
1:2:826:C:O2'	1:2:827:U:O5'	2.32	0.41
1:2:1120:C:N4	1:2:1126:G:O6	2.54	0.41
1:2:1137:A:H2'	1:2:1138:A:C8	2.55	0.41
1:2:1144:U:C2	1:2:1145:G:C8	3.09	0.41
1:2:1387:C:H3'	1:2:1387:C:O2	2.21	0.41
1:2:1414:G:C6	1:2:1415:A:C5	3.09	0.41
1:2:1573:7MG:HN22	38:1:42:U:C4'	2.34	0.41
2:A:147:THR:O	2:A:161:PRO:HA	2.21	0.41
3:B:29:TRP:HB3	3:B:45:LYS:CE	2.50	0.41
3:B:29:TRP:HB3	3:B:45:LYS:HE2	2.03	0.41
8:I:117:TYR:HE1	8:I:147:ARG:HD3	1.85	0.41
9:J:140:ILE:HG21	16:Y:65:GLY:HA3	2.02	0.41
16:Y:36:SER:O	16:Y:38:ASP:N	2.54	0.41
22:F:195:THR:HA	22:F:198:GLU:HG2	2.03	0.41
24:M:31:HIS:O	24:M:116:ASN:ND2	2.45	0.41
24:M:71:LEU:HD11	34:f:106:TYR:CD2	2.52	0.41
29:T:44:GLU:CD	29:T:45:LEU:HG	2.46	0.41
33:d:21:CYS:C	33:d:23:ILE:N	2.79	0.41
40:k:174:CYS:HA	40:k:183:TYR:CE2	2.56	0.41
40:k:200:LEU:O	40:k:201:MET:HE2	2.21	0.41
1:2:19:A:H2'	1:2:20:G:H8	1.87	0.40
1:2:323:U:N3	1:2:324:G:N7	2.68	0.40
1:2:519:A:H3'	1:2:520:A:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:544:A:H2'	19:e:31:LYS:HD2	2.03	0.40
1:2:703:G:H3'	1:2:704:C:H3'	2.03	0.40
1:2:752:A:N1	1:2:796:G:C6	2.89	0.40
1:2:903:G:C6	1:2:904:A:C5	3.09	0.40
1:2:1034:G:OP1	11:N:1:MET:HG2	2.21	0.40
1:2:1085:A:OP1	1:2:1085:A:H8	2.04	0.40
1:2:1157:C:N4	1:2:1162:A:H61	2.20	0.40
1:2:1201:A:H61	1:2:1455:C:C5'	2.35	0.40
1:2:1252:U:C2	1:2:1253:U:H5	2.39	0.40
1:2:1359:A:N1	1:2:1363:G:C6	2.88	0.40
1:2:1370:G:H2'	1:2:1370:G:N3	2.36	0.40
1:2:1679:A:H2	1:2:1718:G:H21	1.68	0.40
4:C:121:LYS:HG2	4:C:132:ALA:HB3	2.04	0.40
6:G:57:ASP:HB2	6:G:61:PHE:O	2.21	0.40
13:V:13:VAL:HA	13:V:14:PRO:HD3	1.96	0.40
21:D:69:LEU:HD23	21:D:69:LEU:HA	1.93	0.40
21:D:105:MET:HE1	21:D:118:ALA:C	2.45	0.40
22:F:136:VAL:HA	22:F:139:ILE:HG12	2.02	0.40
24:M:52:LEU:HD11	24:M:127:LEU:HD11	2.04	0.40
25:P:73:PRO:HD2	25:P:93:VAL:HG23	2.03	0.40
35:g:30:GLN:OE1	35:g:78:GLY:HA3	2.22	0.40
40:k:134:ARG:HH11	41:l:256:PHE:HE1	1.68	0.40
1:2:413:C:C4	1:2:414:C:C4	3.09	0.40
1:2:788:A:H2'	1:2:788:A:N3	2.36	0.40
1:2:958:U:C6	11:N:61:THR:HG23	2.56	0.40
1:2:1165:A:H2'	1:2:1166:G:O4'	2.21	0.40
1:2:1215:C:O2'	1:2:1442:A:N1	2.47	0.40
1:2:1238:U:H2'	1:2:1239:U:N1	2.36	0.40
1:2:1473:A:C6	1:2:1474:C:C4	3.09	0.40
1:2:1656:G:C5	1:2:1742:A:C6	3.09	0.40
3:B:180:THR:HG22	3:B:181:LEU:N	2.36	0.40
5:E:195:ILE:H	5:E:195:ILE:HG13	1.61	0.40
9:J:96:VAL:O	9:J:99:LEU:HD23	2.21	0.40
9:J:121:SER:O	9:J:123:HIS:N	2.53	0.40
10:L:46:LYS:HA	10:L:49:ILE:HD13	2.04	0.40
14:W:79:PHE:HD2	14:W:89:TRP:HZ2	1.68	0.40
17:a:37:LYS:O	17:a:38:ARG:HD3	2.19	0.40
22:F:129:GLN:O	22:F:130:ASN:C	2.64	0.40
23:K:9:LYS:HD3	23:K:9:LYS:O	2.21	0.40
24:M:88:LEU:O	24:M:92:ALA:CB	2.68	0.40
28:S:37:GLY:O	28:S:87:ASN:ND2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:119:ILE:O	28:S:120:ARG:HG2	2.21	0.40
38:1:25:C:C4	38:1:26:M2G:C8	3.09	0.40
40:k:78:GLN:N	40:k:97:ARG:HH12	2.19	0.40
40:k:78:GLN:HE22	40:k:98:GLN:NE2	2.20	0.40
1:2:30:G:C6	1:2:596:G:C6	3.09	0.40
1:2:47:A:H4'	1:2:48:G:H5''	2.03	0.40
1:2:210:U:OP1	10:L:20:PHE:HB2	2.22	0.40
1:2:331:U:H1'	8:I:5:ARG:HH11	1.84	0.40
1:2:778:G:C6	1:2:782:G:C6	3.10	0.40
1:2:836:G:C2	1:2:837:G:C5	3.10	0.40
1:2:1172:C:H5'	1:2:1541:A:O2'	2.21	0.40
1:2:1178:G:H2'	1:2:1179:C:C6	2.56	0.40
1:2:1333:U:H2'	1:2:1334:U:O4'	2.20	0.40
1:2:1521:G:N2	1:2:1521:G:OP2	2.54	0.40
3:B:152:ARG:HG2	3:B:152:ARG:HH11	1.87	0.40
4:C:93:LYS:HE2	4:C:100:ARG:NE	2.36	0.40
5:E:197:HIS:HB3	5:E:209:HIS:HB2	2.04	0.40
6:G:26:VAL:HG22	6:G:36:VAL:HG21	2.03	0.40
8:I:104:ILE:HD11	8:I:168:ALA:CB	2.51	0.40
8:I:117:TYR:C	8:I:144:TRP:HE1	2.29	0.40
8:I:157:VAL:HA	8:I:160:GLN:OE1	2.21	0.40
9:J:106:GLU:O	9:J:111:THR:OG1	2.37	0.40
11:N:82:PRO:HB2	11:N:84:ILE:O	2.22	0.40
22:F:221:ARG:NH1	39:j:45:MET:HE3	2.37	0.40
23:K:21:LEU:HD23	23:K:21:LEU:HA	1.89	0.40
23:K:46:LEU:HG	23:K:66:TYR:CD2	2.55	0.40
25:P:81:ARG:NH1	25:P:120:SER:OG	2.51	0.40
27:R:78:ARG:NH2	27:R:81:LYS:HG3	2.32	0.40
27:R:103:ASP:OD1	27:R:123:SER:HA	2.22	0.40
30:U:57:ARG:HG3	30:U:89:ARG:HG2	2.04	0.40
33:d:46:LYS:O	33:d:50:ILE:HG12	2.21	0.40
35:g:47:ARG:O	35:g:56:GLY:HA2	2.22	0.40
1:2:31:C:C4	1:2:32:U:C4	3.09	0.40
1:2:67:A:C4	1:2:84:A:C6	3.09	0.40
1:2:330:A:C6	1:2:331:U:C4	3.09	0.40
1:2:566:A:H5''	15:X:70:LYS:NZ	2.37	0.40
1:2:867:G:OP2	11:N:121:ARG:NH2	2.55	0.40
1:2:885:U:C2	1:2:886:A:C8	3.10	0.40
1:2:895:U:H2'	1:2:896:C:N1	2.36	0.40
1:2:1236:G:C2	1:2:1237:A:N7	2.90	0.40
1:2:1328:A:C4	1:2:1329:G:C8	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1444:A:OP2	1:2:1444:A:H8	2.04	0.40
1:2:1474:C:C2	1:2:1475:G:C8	3.09	0.40
1:2:1564:U:H5''	28:S:39:GLY:H	1.86	0.40
4:C:250:ASP:N	4:C:250:ASP:OD1	2.54	0.40
5:E:175:PHE:CE1	5:E:195:ILE:HD13	2.50	0.40
8:I:190:LEU:O	8:I:191:ALA:C	2.64	0.40
10:L:55:ASP:HB3	10:L:58:CYS:HB2	2.03	0.40
12:O:125:SER:O	12:O:126:THR:OG1	2.38	0.40
39:j:12:LYS:HE2	39:j:13:TYR:CE1	2.57	0.40
1:2:10:G:N7	1:2:1631:A:C2	2.90	0.40
1:2:152:G:C6	1:2:161:A:C6	3.10	0.40
1:2:167:A:H2'	1:2:168:A:C8	2.55	0.40
1:2:179:A:C2	1:2:180:A:H1'	2.55	0.40
1:2:888:U:H2'	1:2:889:C:H6	1.86	0.40
1:2:965:A:N1	1:2:966:A:N6	2.69	0.40
1:2:1023:U:H5	1:2:1026:A:N1	2.19	0.40
1:2:1038:A:P	1:2:1038:A:H3'	2.62	0.40
1:2:1104:C:H2'	1:2:1105:U:C6	2.55	0.40
1:2:1282:U:OP2	1:2:1283:C:O2'	2.26	0.40
1:2:1480:C:H2'	1:2:1481:A:H5''	2.03	0.40
4:C:188:ALA:CB	4:C:212:LEU:HD11	2.51	0.40
8:I:83:TYR:CD2	8:I:101:ILE:HD12	2.57	0.40
9:J:120:LYS:O	9:J:121:SER:HB3	2.21	0.40
11:N:114:ARG:O	11:N:118:ILE:HG12	2.21	0.40
15:X:109:ARG:HG3	15:X:109:ARG:O	2.22	0.40
22:F:38:ALA:O	22:F:40:GLN:N	2.55	0.40
23:K:40:LEU:O	23:K:44:LYS:HG2	2.22	0.40
23:K:41:PHE:HA	23:K:44:LYS:HB2	2.04	0.40
35:g:25:SER:OG	35:g:74:VAL:HG12	2.22	0.40
38:1:58:1MA:H1'	38:1:60:A:N7	2.36	0.40
38:1:69:C:H2'	38:1:70:G:C8	2.57	0.40
40:k:157:GLU:N	40:k:158:PRO:HD2	2.36	0.40
40:k:207:GLY:O	40:k:211:MET:N	2.51	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%)	192 (88%)	25 (12%)	0	100	100
3	B	221/255 (87%)	192 (87%)	25 (11%)	4 (2%)	6	34
4	C	218/259 (84%)	195 (89%)	22 (10%)	1 (0%)	24	60
5	E	258/261 (99%)	234 (91%)	24 (9%)	0	100	100
6	G	228/236 (97%)	215 (94%)	13 (6%)	0	100	100
7	H	182/190 (96%)	159 (87%)	22 (12%)	1 (0%)	24	60
8	I	184/201 (92%)	166 (90%)	18 (10%)	0	100	100
9	J	180/188 (96%)	155 (86%)	22 (12%)	3 (2%)	7	36
10	L	153/156 (98%)	132 (86%)	21 (14%)	0	100	100
11	N	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
12	O	127/137 (93%)	106 (84%)	21 (16%)	0	100	100
13	V	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
14	W	127/130 (98%)	114 (90%)	13 (10%)	0	100	100
15	X	142/145 (98%)	120 (84%)	22 (16%)	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%)	72 (91%)	7 (9%)	0	100	100
19	e	58/63 (92%)	51 (88%)	7 (12%)	0	100	100
20	h	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
21	D	225/237 (95%)	209 (93%)	15 (7%)	1 (0%)	30	65
22	F	204/227 (90%)	173 (85%)	28 (14%)	3 (2%)	8	38
23	K	94/106 (89%)	80 (85%)	14 (15%)	0	100	100
24	M	113/134 (84%)	92 (81%)	19 (17%)	2 (2%)	6	34
25	P	115/142 (81%)	92 (80%)	23 (20%)	0	100	100
26	Q	139/143 (97%)	130 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	R	128/136 (94%)	109 (85%)	16 (12%)	3 (2%)	5	31
28	S	143/146 (98%)	125 (87%)	18 (13%)	0	100	100
29	T	141/144 (98%)	125 (89%)	16 (11%)	0	100	100
30	U	104/117 (89%)	91 (88%)	13 (12%)	0	100	100
31	Z	76/108 (70%)	69 (91%)	6 (8%)	1 (1%)	9	41
32	c	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
33	d	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
34	f	72/150 (48%)	53 (74%)	19 (26%)	0	100	100
35	g	314/326 (96%)	287 (91%)	25 (8%)	2 (1%)	21	57
36	i	93/153 (61%)	80 (86%)	13 (14%)	0	100	100
39	j	263/304 (86%)	245 (93%)	17 (6%)	1 (0%)	30	65
40	k	468/527 (89%)	433 (92%)	32 (7%)	3 (1%)	21	57
41	l	126/285 (44%)	122 (97%)	4 (3%)	0	100	100
All	All	5796/6582 (88%)	5167 (89%)	604 (10%)	25 (0%)	31	65

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	7	LYS
7	H	64	VAL
22	F	103	GLY
27	R	92	ASP
35	g	120	SER
3	B	4	GLY
3	B	55	LYS
22	F	39	GLN
22	F	104	ARG
24	M	123	GLU
40	k	130	ASP
40	k	497	GLU
3	B	221	PRO
24	M	124	ARG
31	Z	35	LYS
35	g	121	SER
4	C	45	LYS
9	J	101	VAL
27	R	97	ASN

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Mol	Chain	Res	Type
27	R	99	VAL
39	j	40	ASP
40	k	507	LYS
9	J	122	VAL
9	J	134	ILE
21	D	220	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/211 (85%)	180 (100%)	0	100	100
3	B	202/228 (89%)	202 (100%)	0	100	100
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%)	192 (100%)	0	100	100
7	H	164/170 (96%)	162 (99%)	2 (1%)	63	73
8	I	147/159 (92%)	146 (99%)	1 (1%)	76	79
9	J	153/158 (97%)	153 (100%)	0	100	100
10	L	136/137 (99%)	135 (99%)	1 (1%)	76	79
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%)	110 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	D	188/196 (96%)	188 (100%)	0	100	100
22	F	174/194 (90%)	172 (99%)	2 (1%)	65	74
23	K	88/96 (92%)	88 (100%)	0	100	100
24	M	93/109 (85%)	92 (99%)	1 (1%)	65	74
25	P	99/119 (83%)	99 (100%)	0	100	100
26	Q	117/119 (98%)	117 (100%)	0	100	100
27	R	116/124 (94%)	115 (99%)	1 (1%)	70	76
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%)	60 (100%)	0	100	100
35	g	264/272 (97%)	263 (100%)	1 (0%)	84	84
36	i	80/130 (62%)	80 (100%)	0	100	100
39	j	240/274 (88%)	240 (100%)	0	100	100
40	k	393/449 (88%)	393 (100%)	0	100	100
41	l	125/246 (51%)	125 (100%)	0	100	100
All	All	4975/5595 (89%)	4966 (100%)	9 (0%)	85	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	64	VAL
7	H	96	ARG
8	I	176	GLN
10	L	3	THR
22	F	40	GLN
22	F	104	ARG
24	M	121	THR
27	R	92	ASP
35	g	122	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	15	GLN
3	B	6	ASN
3	B	79	HIS
3	B	157	GLN
4	C	92	GLN
4	C	94	GLN
4	C	233	ASN
5	E	17	HIS
6	G	139	ASN
6	G	201	GLN
7	H	5	GLN
7	H	19	GLN
7	H	89	HIS
8	I	44	HIS
9	J	112	GLN
10	L	152	GLN
11	N	78	ASN
11	N	151	ASN
12	O	65	GLN
13	V	81	ASN
14	W	15	ASN
14	W	117	HIS
15	X	99	ASN
16	Y	22	GLN
16	Y	31	ASN
18	b	31	HIS
19	e	46	ASN
22	F	36	GLN
22	F	171	ASN
23	K	29	GLN
23	K	39	ASN
23	K	62	GLN
24	M	134	GLN
25	P	104	GLN
27	R	48	ASN
28	S	74	GLN
29	T	17	ASN
29	T	43	ASN
30	U	40	ASN
31	Z	38	HIS
33	d	20	GLN
33	d	48	ASN
34	f	104	ASN

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Mol	Chain	Res	Type
35	g	94	ASN
35	g	210	GLN
36	i	93	HIS
39	j	68	ASN
39	j	243	GLN
40	k	78	GLN
40	k	197	HIS
40	k	232	HIS
40	k	249	ASN
40	k	262	HIS
40	k	344	ASN
40	k	384	GLN
40	k	415	GLN
40	k	433	ASN
40	k	465	ASN
41	l	146	ASN
41	l	218	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	581 (32%)	24 (1%)
37	3	25/49 (51%)	14 (56%)	0
38	1	72/75 (96%)	31 (43%)	6 (8%)
All	All	1894/1922 (98%)	626 (33%)	30 (1%)

All (626) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	5	U
1	2	16	G
1	2	17	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	42	G
1	2	43	A
1	2	45	U
1	2	46	A

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Mol	Chain	Res	Type
1	2	47	A
1	2	50	C
1	2	57	G
1	2	59	C
1	2	63	G
1	2	67	A
1	2	68	A
1	2	72	A
1	2	74	U
1	2	75	U
1	2	77	U
1	2	78	A
1	2	79	C
1	2	100	A
1	2	104	A
1	2	114	C
1	2	115	G
1	2	124	A
1	2	126	A
1	2	127	G
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	134	U
1	2	136	C
1	2	137	U
1	2	139	C
1	2	140	A
1	2	141	U
1	2	143	G
1	2	146	A
1	2	152	G
1	2	158	U
1	2	159	C
1	2	160	U
1	2	161	A
1	2	167	A
1	2	173	U
1	2	176	U
1	2	177	U
1	2	178	A

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Mol	Chain	Res	Type
1	2	184	U
1	2	185	C
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	197	A
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	231	U
1	2	232	C
1	2	235	A
1	2	237	U
1	2	239	C
1	2	240	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	271	U
1	2	275	C
1	2	276	U
1	2	278	G
1	2	280	G
1	2	283	G
1	2	289	G
1	2	298	A
1	2	301	U
1	2	307	C
1	2	308	C

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Mol	Chain	Res	Type
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	349	U
1	2	359	A
1	2	360	C
1	2	390	A
1	2	399	A
1	2	400	A
1	2	401	C
1	2	411	A
1	2	415	A
1	2	416	A
1	2	421	G
1	2	423	C
1	2	424	A
1	2	425	G
1	2	427	A
1	2	433	G
1	2	436	A
1	2	438	U
1	2	439	U
1	2	440	A
1	2	443	C
1	2	459	A
1	2	460	G
1	2	467	A
1	2	474	A
1	2	475	U
1	2	476	A
1	2	479	G
1	2	482	A
1	2	483	C
1	2	488	C
1	2	489	C
1	2	490	C
1	2	491	A
1	2	492	U
1	2	493	U

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Mol	Chain	Res	Type
1	2	494	C
1	2	495	G
1	2	496	G
1	2	499	C
1	2	501	U
1	2	502	G
1	2	505	A
1	2	506	U
1	2	507	U
1	2	509	G
1	2	512	U
1	2	515	G
1	2	516	U
1	2	519	A
1	2	523	U
1	2	526	A
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	547	G
1	2	553	C
1	2	558	C
1	2	560	G
1	2	564	C
1	2	565	C
1	2	567	G
1	2	576	G
1	2	578	A
1	2	584	A
1	2	587	U
1	2	592	U
1	2	593	A
1	2	594	G
1	2	605	A
1	2	608	U
1	2	610	U
1	2	618	A

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Mol	Chain	Res	Type
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	641	G
1	2	642	G
1	2	647	G
1	2	650	G
1	2	651	U
1	2	652	C
1	2	657	C
1	2	659	G
1	2	660	A
1	2	661	C
1	2	663	U
1	2	664	U
1	2	671	C
1	2	672	G
1	2	675	C
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
1	2	691	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	709	C
1	2	710	U
1	2	711	G
1	2	712	U

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Mol	Chain	Res	Type
1	2	714	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	722	G
1	2	724	G
1	2	727	C
1	2	730	G
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	739	G
1	2	741	C
1	2	745	U
1	2	755	A
1	2	765	G
1	2	766	PSU
1	2	771	A
1	2	774	A
1	2	778	G
1	2	779	A
1	2	780	A
1	2	782	G
1	2	783	C
1	2	786	G
1	2	787	A
1	2	788	A
1	2	789	U
1	2	792	A
1	2	793	U
1	2	794	U
1	2	811	A
1	2	812	U
1	2	813	A
1	2	814	G
1	2	819	U
1	2	820	U
1	2	821	U

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Mol	Chain	Res	Type
1	2	822	G
1	2	823	G
1	2	826	C
1	2	827	U
1	2	828	A
1	2	829	U
1	2	832	U
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	864	A
1	2	876	G
1	2	895	U
1	2	896	C
1	2	897	A
1	2	898	G
1	2	901	G
1	2	903	G
1	2	904	A
1	2	905	A
1	2	911	U
1	2	912	G
1	2	913	G
1	2	915	U
1	2	916	U
1	2	917	U
1	2	918	A
1	2	919	U
1	2	920	U
1	2	930	C
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

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Mol	Chain	Res	Type
1	2	963	U
1	2	965	A
1	2	969	A
1	2	972	A
1	2	982	A
1	2	985	G
1	2	986	G
1	2	987	A
1	2	991	A
1	2	992	A
1	2	995	U
1	2	1003	U
1	2	1009	C
1	2	1011	U
1	2	1015	C
1	2	1016	U
1	2	1020	C
1	2	1023	U
1	2	1024	A
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1028	U
1	2	1030	U
1	2	1031	G
1	2	1038	A
1	2	1039	G
1	2	1041	G
1	2	1042	A
1	2	1048	U
1	2	1050	G
1	2	1051	U
1	2	1052	G
1	2	1054	U
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1062	U
1	2	1075	A
1	2	1081	C
1	2	1082	G
1	2	1084	G

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Mol	Chain	Res	Type
1	2	1086	A
1	2	1090	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	1112	A
1	2	1113	G
1	2	1137	A
1	2	1141	A
1	2	1149	G
1	2	1150	A
1	2	1154	G
1	2	1155	C
1	2	1157	C
1	2	1158	C
1	2	1163	G
1	2	1166	G
1	2	1184	U
1	2	1188	A
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	1205	U
1	2	1207	A
1	2	1211	G
1	2	1216	A
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	1237	A
1	2	1240	G
1	2	1241	A

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Mol	Chain	Res	Type
1	2	1243	A
1	2	1244	G
1	2	1245	C
1	2	1246	U
1	2	1247	C
1	2	1250	U
1	2	1255	A
1	2	1257	U
1	2	1258	U
1	2	1259	U
1	2	1260	G
1	2	1262	G
1	2	1266	G
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1275	U
1	2	1283	C
1	2	1284	U
1	2	1287	G
1	2	1292	U
1	2	1296	G
1	2	1297	U
1	2	1298	G
1	2	1299	A
1	2	1305	C
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	1324	A
1	2	1337	C
1	2	1338	C
1	2	1339	U
1	2	1343	A
1	2	1344	A
1	2	1345	A
1	2	1346	U
1	2	1347	A
1	2	1353	G

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Mol	Chain	Res	Type
1	2	1355	U
1	2	1359	A
1	2	1360	C
1	2	1361	U
1	2	1362	U
1	2	1363	G
1	2	1366	G
1	2	1369	U
1	2	1370	G
1	2	1371	A
1	2	1376	U
1	2	1380	A
1	2	1388	U
1	2	1389	A
1	2	1396	U
1	2	1397	C
1	2	1398	A
1	2	1400	G
1	2	1401	C
1	2	1407	G
1	2	1408	A
1	2	1409	A
1	2	1410	G
1	2	1411	U
1	2	1413	U
1	2	1414	G
1	2	1416	G
1	2	1418	C
1	2	1423	A
1	2	1425	A
1	2	1426	2MG
1	2	1427	G
1	2	1429	C
1	2	1430	U
1	2	1431	G
1	2	1434	A
1	2	1442	A
1	2	1444	A
1	2	1455	C
1	2	1457	C
1	2	1458	A
1	2	1459	C

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Mol	Chain	Res	Type
1	2	1464	G
1	2	1469	A
1	2	1471	U
1	2	1472	G
1	2	1476	G
1	2	1481	A
1	2	1482	G
1	2	1483	C
1	2	1484	G
1	2	1487	U
1	2	1488	A
1	2	1489	C
1	2	1490	A
1	2	1491	A
1	2	1494	U
1	2	1499	C
1	2	1500	G
1	2	1510	G
1	2	1514	A
1	2	1521	G
1	2	1522	A
1	2	1532	G
1	2	1534	G
1	2	1535	C
1	2	1538	G
1	2	1540	G
1	2	1555	U
1	2	1556	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	1574	A
1	2	1580	U
1	2	1588	G
1	2	1594	C
1	2	1597	C
1	2	1598	A
1	2	1599	G
1	2	1614	G

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Mol	Chain	Res	Type
1	2	1617	C
1	2	1620	G
1	2	1632	C
1	2	1640	G
1	2	1646	A
1	2	1650	C
1	2	1654	U
1	2	1655	U
1	2	1656	G
1	2	1662	C
1	2	1667	U
1	2	1678	G
1	2	1679	A
1	2	1680	U
1	2	1683	G
1	2	1686	U
1	2	1687	A
1	2	1688	G
1	2	1691	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	1709	C
1	2	1710	A
1	2	1711	G
1	2	1712	A
1	2	1725	G
1	2	1726	U
1	2	1728	A
1	2	1729	A
1	2	1730	A
1	2	1734	G

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Mol	Chain	Res	Type
1	2	1740	U
1	2	1742	A
1	2	1743	G
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	1786	G
1	2	1787	G
1	2	1789	A
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1794	C
1	2	1796	U
1	2	1798	A
37	3	16	U
37	3	17	C
37	3	18	U
37	3	20	A
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	37	U
37	3	38	C
37	3	40	C
38	1	4	G
38	1	8	U
38	1	9	1MG
38	1	10	2MG
38	1	13	C

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Mol	Chain	Res	Type
38	1	14	A
38	1	15	G
38	1	16	H2U
38	1	18	G
38	1	19	G
38	1	20	A
38	1	21	A
38	1	22	G
38	1	23	C
38	1	26	M2G
38	1	41	C
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	50	U
38	1	58	1MA
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 (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	74	U
1	2	216	A
1	2	217	A
1	2	239	C
1	2	277	U
1	2	279	U
1	2	649	U
1	2	670	G
1	2	700	C
1	2	828	A
1	2	855	A
1	2	1080	A

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Mol	Chain	Res	Type
1	2	1198	G
1	2	1206	C
1	2	1240	G
1	2	1343	A
1	2	1430	U
1	2	1470	C
1	2	1513	A
1	2	1571	A
1	2	1573	7MG
1	2	1613	C
1	2	1655	U
1	2	1797	U
38	1	8	U
38	1	9	1MG
38	1	43	G
38	1	44	A
38	1	49	5MC
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
38	RIA	1	64	38	35,38,39	4.66	14 (40%)	50,57,60	2.10	13 (26%)
1	5MC	2	1637	1	19,22,23	3.75	8 (42%)	26,32,35	1.00	1 (3%)
1	PSU	2	998	1	18,21,22	4.36	7 (38%)	21,30,33	1.94	5 (23%)
1	B8N	2	1190	1	25,29,30	3.31	8 (32%)	28,42,45	2.12	8 (28%)
38	M2G	1	26	38	24,27,28	2.63	7 (29%)	33,40,43	1.70	8 (24%)
1	5MC	2	1006	1	19,22,23	3.70	8 (42%)	26,32,35	1.03	2 (7%)
38	1MG	1	9	38	23,26,27	3.27	7 (30%)	33,39,42	2.26	8 (24%)
38	H2U	1	47	38	18,21,22	3.15	4 (22%)	19,30,33	1.43	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	7MG	1	46	38	23,26,27	3.52	10 (43%)	27,39,42	2.26	9 (33%)
1	2MG	2	1570	1	23,26,27	2.94	9 (39%)	33,38,41	2.20	12 (36%)
1	PSU	2	465	1	18,21,22	4.33	7 (38%)	21,30,33	1.91	5 (23%)
1	PSU	2	120	1	18,21,22	4.32	7 (38%)	21,30,33	2.07	5 (23%)
38	2MG	1	10	38	23,26,27	2.86	9 (39%)	33,38,41	2.16	10 (30%)
38	T6A	1	37	38	31,34,35	1.81	8 (25%)	43,49,52	2.19	12 (27%)
1	PSU	2	766	1	18,21,22	4.38	7 (38%)	21,30,33	2.05	6 (28%)
38	H2U	1	16	38	18,21,22	3.08	4 (22%)	19,30,33	1.46	4 (21%)
38	1MA	1	58	38	21,25,26	3.10	6 (28%)	30,37,40	2.40	8 (26%)
1	PSU	2	1289	1	18,21,22	4.33	7 (38%)	21,30,33	1.89	5 (23%)
38	5MC	1	48	38	19,22,23	3.79	8 (42%)	26,32,35	1.15	1 (3%)
38	5MC	1	49	38	19,22,23	3.91	8 (42%)	26,32,35	1.05	1 (3%)
1	7MG	2	1573	1	23,26,27	3.46	10 (43%)	27,39,42	2.31	9 (33%)
1	2MG	2	1426	42,1	23,26,27	2.85	9 (39%)	33,38,41	2.39	11 (33%)
1	MA6	2	1780	1	23,26,27	1.40	4 (17%)	33,38,41	3.48	13 (39%)

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
38	RIA	1	64	38	-	5/17/51/52	0/4/4/4
1	5MC	2	1637	1	-	1/7/25/26	0/2/2/2
1	PSU	2	998	1	-	0/7/25/26	0/2/2/2
1	B8N	2	1190	1	-	5/16/34/35	0/2/2/2
38	M2G	1	26	38	-	4/11/29/30	0/3/3/3
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
38	1MG	1	9	38	-	2/7/25/26	0/3/3/3
38	H2U	1	47	38	-	4/7/38/39	0/2/2/2
38	7MG	1	46	38	-	2/7/37/38	0/3/3/3
1	2MG	2	1570	1	-	1/9/27/28	0/3/3/3
1	PSU	2	465	1	-	0/7/25/26	0/2/2/2
1	PSU	2	120	1	-	0/7/25/26	0/2/2/2
38	2MG	1	10	38	-	2/9/27/28	0/3/3/3
38	T6A	1	37	38	-	5/23/41/42	0/3/3/3
1	PSU	2	766	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	H2U	1	16	38	-	6/7/38/39	0/2/2/2
38	1MA	1	58	38	-	2/7/25/26	0/3/3/3
1	PSU	2	1289	1	-	1/7/25/26	0/2/2/2
38	5MC	1	48	38	-	3/7/25/26	0/2/2/2
38	5MC	1	49	38	-	3/7/25/26	0/2/2/2
1	7MG	2	1573	1	-	4/7/37/38	0/3/3/3
1	2MG	2	1426	42,1	-	0/9/27/28	0/3/3/3
1	MA6	2	1780	1	-	6/11/29/30	0/3/3/3

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	64	RIA	C1'-C2'	-16.39	1.32	1.52
1	2	766	PSU	C6-C5	11.53	1.48	1.35
1	2	1289	PSU	C6-C5	11.43	1.47	1.35
1	2	465	PSU	C6-C5	11.41	1.47	1.35
1	2	998	PSU	C6-C5	11.41	1.47	1.35
1	2	120	PSU	C6-C5	11.38	1.47	1.35
38	1	64	RIA	O1'-C1'	11.09	1.61	1.41
38	1	47	H2U	C2-N1	9.91	1.49	1.35
1	2	998	PSU	C2-N1	9.78	1.49	1.36
1	2	766	PSU	C2-N1	9.77	1.49	1.36
38	1	16	H2U	C2-N1	9.60	1.48	1.35
1	2	465	PSU	C2-N1	9.60	1.49	1.36
1	2	1289	PSU	C2-N1	9.59	1.49	1.36
38	1	58	1MA	C2-N3	9.58	1.48	1.30
1	2	120	PSU	C2-N1	9.56	1.49	1.36
38	1	48	5MC	C6-C5	9.36	1.49	1.34
38	1	64	RIA	C2A-C1A	-9.35	1.30	1.53
38	1	49	5MC	C6-C5	9.21	1.49	1.34
38	1	64	RIA	O4'-C1A	9.15	1.63	1.42
38	1	9	1MG	C2-N2	9.08	1.50	1.34
1	2	1637	5MC	C6-C5	8.96	1.49	1.34
1	2	1006	5MC	C6-C5	8.72	1.48	1.34
1	2	1190	B8N	C6-N1	8.26	1.56	1.36
38	1	46	7MG	C8-N9	8.04	1.51	1.45
1	2	1573	7MG	C8-N9	7.79	1.50	1.45
1	2	1570	2MG	C2-N3	7.68	1.46	1.32
1	2	1190	B8N	C4-N3	-7.62	1.26	1.40
1	2	766	PSU	C2-N3	7.60	1.50	1.37
1	2	120	PSU	C2-N3	7.58	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	998	PSU	C2-N3	7.58	1.50	1.37
38	1	10	2MG	C2-N3	7.53	1.46	1.32
1	2	465	PSU	C2-N3	7.48	1.49	1.37
1	2	1289	PSU	C2-N3	7.44	1.49	1.37
1	2	1190	B8N	C4-C5	7.35	1.64	1.47
1	2	1426	2MG	C2-N3	7.30	1.45	1.32
38	1	58	1MA	C4-N3	7.07	1.50	1.35
38	1	46	7MG	C5-N7	6.99	1.44	1.35
38	1	9	1MG	C2-N3	6.94	1.44	1.33
38	1	49	5MC	C5-C4	6.94	1.49	1.44
38	1	49	5MC	C4-N3	6.91	1.45	1.34
1	2	1637	5MC	C4-N3	6.83	1.45	1.34
38	1	64	RIA	O1'-C4'	-6.68	1.30	1.45
38	1	26	M2G	C4-N3	6.67	1.49	1.34
1	2	1570	2MG	C4-N3	6.65	1.49	1.34
1	2	1006	5MC	C4-N3	6.58	1.44	1.34
38	1	10	2MG	C4-N3	6.56	1.49	1.34
38	1	48	5MC	C4-N3	6.56	1.44	1.34
38	1	47	H2U	C2-N3	6.49	1.49	1.38
38	1	26	M2G	C2-N2	6.46	1.47	1.35
38	1	16	H2U	C2-N3	6.42	1.49	1.38
38	1	9	1MG	C4-N3	6.39	1.48	1.34
1	2	1426	2MG	C4-N3	6.36	1.48	1.34
1	2	1006	5MC	C5-C4	6.34	1.48	1.44
38	1	49	5MC	C2-N3	6.30	1.48	1.36
38	1	64	RIA	O4'-C4A	-6.28	1.31	1.45
38	1	48	5MC	C5-C4	6.24	1.48	1.44
1	2	1573	7MG	C2-N3	6.20	1.48	1.33
1	2	1573	7MG	C5-N7	6.15	1.43	1.35
1	2	1637	5MC	C2-N3	6.15	1.48	1.36
1	2	1006	5MC	C2-N3	6.11	1.48	1.36
1	2	1570	2MG	C2-N2	5.98	1.45	1.33
1	2	1573	7MG	C4-N3	5.96	1.47	1.34
38	1	26	M2G	C2-N3	5.96	1.46	1.32
1	2	1637	5MC	C5-C4	5.94	1.48	1.44
38	1	64	RIA	C6-N6	5.91	1.49	1.34
38	1	48	5MC	C2-N3	5.85	1.47	1.36
38	1	46	7MG	C4-N3	5.83	1.47	1.34
1	2	1426	2MG	C2-N2	5.79	1.45	1.33
38	1	46	7MG	C2-N3	5.77	1.47	1.33
38	1	10	2MG	C2-N2	5.67	1.45	1.33
1	2	1190	B8N	C2-N1	5.59	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1573	7MG	C4-N9	5.27	1.44	1.37
38	1	37	T6A	C10-N11	5.22	1.49	1.35
38	1	9	1MG	C2-N1	5.21	1.46	1.37
38	1	46	7MG	C4-N9	5.20	1.44	1.37
1	2	1289	PSU	C6-N1	5.17	1.44	1.36
1	2	465	PSU	C6-N1	5.15	1.44	1.36
1	2	120	PSU	C6-N1	5.14	1.44	1.36
1	2	766	PSU	C6-N1	5.12	1.44	1.36
1	2	998	PSU	C6-N1	5.12	1.44	1.36
38	1	37	T6A	C10-N6	5.08	1.48	1.37
38	1	47	H2U	C4-N3	5.06	1.46	1.37
1	2	1570	2MG	C2-N1	5.05	1.44	1.36
1	2	1190	B8N	C6-C5	4.99	1.42	1.35
1	2	1573	7MG	C2-N2	4.97	1.45	1.34
38	1	16	H2U	C4-N3	4.91	1.45	1.37
38	1	46	7MG	C2-N2	4.87	1.45	1.34
1	2	1426	2MG	C2-N1	4.83	1.44	1.36
38	1	58	1MA	C2-N1	4.78	1.45	1.35
38	1	10	2MG	C2-N1	4.71	1.44	1.36
38	1	48	5MC	C6-N1	4.66	1.45	1.38
38	1	49	5MC	C6-N1	4.49	1.45	1.38
1	2	1637	5MC	C6-N1	4.47	1.45	1.38
38	1	49	5MC	C4-N4	4.45	1.45	1.34
38	1	49	5MC	C2-N1	4.42	1.49	1.40
38	1	48	5MC	C4-N4	4.40	1.45	1.34
1	2	1637	5MC	C4-N4	4.36	1.45	1.34
1	2	1006	5MC	C4-N4	4.31	1.45	1.34
1	2	1190	B8N	C1'-C5	-4.31	1.40	1.50
38	1	48	5MC	C2-N1	4.30	1.49	1.40
1	2	1637	5MC	C2-N1	4.27	1.49	1.40
1	2	1006	5MC	C6-N1	4.20	1.45	1.38
1	2	1006	5MC	C2-N1	4.05	1.48	1.40
38	1	58	1MA	C5-C6	3.92	1.54	1.43
1	2	998	PSU	C4-N3	3.77	1.45	1.38
1	2	1573	7MG	C2-N1	3.74	1.46	1.37
1	2	465	PSU	C4-N3	3.73	1.45	1.38
38	1	46	7MG	C2-N1	3.72	1.46	1.37
1	2	766	PSU	C4-N3	3.67	1.45	1.38
38	1	9	1MG	O6-C6	-3.67	1.15	1.23
1	2	1289	PSU	C4-N3	3.63	1.45	1.38
1	2	120	PSU	C4-N3	3.62	1.45	1.38
1	2	1780	MA6	C6-N6	3.60	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	46	7MG	C5-C6	3.56	1.52	1.43
38	1	26	M2G	C2-N1	3.54	1.44	1.36
38	1	9	1MG	C5-N7	-3.41	1.32	1.39
1	2	1573	7MG	C5-C6	3.41	1.52	1.43
38	1	9	1MG	C5-C6	3.34	1.54	1.45
38	1	58	1MA	C5-N7	-3.22	1.32	1.39
38	1	46	7MG	C6-N1	3.21	1.44	1.38
38	1	64	RIA	O3A-C3A	-3.19	1.35	1.43
38	1	64	RIA	O2'-C2'	3.07	1.50	1.43
38	1	10	2MG	C5-N7	-2.98	1.33	1.39
1	2	1426	2MG	C5-N7	-2.98	1.33	1.39
1	2	1780	MA6	C5-C4	-2.95	1.33	1.39
38	1	64	RIA	C5-N7	-2.93	1.33	1.39
1	2	1573	7MG	C6-N1	2.92	1.44	1.38
1	2	1006	5MC	O2-C2	-2.89	1.18	1.23
1	2	1637	5MC	O2-C2	-2.86	1.18	1.23
1	2	1570	2MG	C5-N7	-2.85	1.33	1.39
1	2	1573	7MG	O6-C6	-2.85	1.18	1.23
38	1	48	5MC	O2-C2	-2.83	1.18	1.23
38	1	26	M2G	C5-N7	-2.82	1.33	1.39
38	1	46	7MG	O6-C6	-2.81	1.18	1.23
38	1	64	RIA	O2A-C2A	2.77	1.50	1.43
1	2	120	PSU	O4-C4	-2.75	1.18	1.23
1	2	1289	PSU	O4-C4	-2.74	1.18	1.23
38	1	37	T6A	C5-N7	-2.73	1.34	1.39
38	1	49	5MC	O2-C2	-2.71	1.18	1.23
38	1	26	M2G	C5-C6	2.67	1.54	1.44
1	2	1426	2MG	O6-C6	-2.65	1.18	1.23
38	1	26	M2G	C6-N1	2.62	1.43	1.38
1	2	766	PSU	O4-C4	-2.62	1.18	1.23
1	2	465	PSU	O4-C4	-2.60	1.18	1.23
1	2	998	PSU	O4-C4	-2.56	1.18	1.23
38	1	47	H2U	O2-C2	-2.56	1.18	1.23
38	1	10	2MG	O6-C6	-2.53	1.18	1.23
1	2	1570	2MG	O6-C6	-2.51	1.18	1.23
1	2	1570	2MG	C5-C6	2.51	1.53	1.44
38	1	16	H2U	O2-C2	-2.51	1.18	1.23
1	2	1780	MA6	C5-N7	-2.49	1.34	1.39
1	2	1570	2MG	C6-N1	2.43	1.43	1.38
1	2	1426	2MG	C5-C6	2.42	1.53	1.44
38	1	10	2MG	C5-C6	2.41	1.53	1.44
38	1	64	RIA	O3'-C3'	-2.38	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1426	2MG	C6-N1	2.36	1.43	1.38
38	1	37	T6A	ODA-C13	2.31	1.28	1.22
38	1	37	T6A	C5-C4	-2.27	1.35	1.39
38	1	58	1MA	CM1-N1	-2.26	1.42	1.46
1	2	1289	PSU	O2-C2	-2.26	1.18	1.23
1	2	465	PSU	O2-C2	-2.25	1.18	1.23
1	2	766	PSU	O2-C2	-2.24	1.18	1.23
1	2	120	PSU	O2-C2	-2.22	1.18	1.23
38	1	10	2MG	C6-N1	2.20	1.43	1.38
1	2	1780	MA6	C8-N9	-2.20	1.33	1.37
38	1	64	RIA	C2-N1	2.19	1.37	1.33
1	2	998	PSU	O2-C2	-2.18	1.18	1.23
38	1	64	RIA	P'-O5'	2.15	1.67	1.60
38	1	37	T6A	C2-N1	2.11	1.37	1.33
38	1	10	2MG	C4-N9	-2.11	1.32	1.38
38	1	37	T6A	O10-C10	-2.10	1.18	1.23
1	2	1426	2MG	C4-N9	-2.09	1.32	1.38
38	1	37	T6A	C6-N6	2.06	1.43	1.39
1	2	1190	B8N	O2-C2	-2.05	1.18	1.22
1	2	1190	B8N	O4-C4	-2.03	1.18	1.23
1	2	1570	2MG	C4-N9	-2.03	1.32	1.38

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	N1-C6-N6	-13.37	100.56	116.86
1	2	1780	MA6	C5-C6-N6	8.82	139.29	125.33
1	2	1426	2MG	C2-N3-C4	6.97	120.72	112.00
38	1	58	1MA	C1'-N9-C8	-6.90	107.13	126.73
1	2	1570	2MG	C2-N3-C4	6.45	120.07	112.00
38	1	10	2MG	C2-N3-C4	6.30	119.88	112.00
38	1	9	1MG	C1'-N9-C4	-6.19	108.20	126.49
38	1	58	1MA	C1'-N9-C4	5.99	144.19	126.49
38	1	64	RIA	N3-C2-N1	-5.96	119.56	128.58
38	1	37	T6A	N3-C2-N1	-5.80	119.80	128.58
38	1	9	1MG	C1'-N9-C8	5.68	142.86	126.73
1	2	1426	2MG	C5-C4-N3	-5.53	119.60	128.39
1	2	1780	MA6	N1-C2-N3	-5.48	120.28	128.58
38	1	64	RIA	C5-C4-N3	-5.45	119.21	126.72
38	1	26	M2G	C5-C4-N3	-5.38	119.83	128.39
38	1	46	7MG	C5-C6-N1	5.36	120.37	110.94
38	1	9	1MG	C5-C4-N3	-5.31	119.94	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1190	B8N	C5-C4-N3	5.22	125.64	116.15
38	1	10	2MG	C5-C4-N3	-5.20	120.12	128.39
1	2	1573	7MG	C5-C6-N1	5.16	120.02	110.94
1	2	1570	2MG	C5-C4-N3	-5.02	120.41	128.39
1	2	1426	2MG	N1-C2-N2	5.01	121.67	116.56
1	2	766	PSU	C4-N3-C2	-4.95	119.55	126.37
1	2	120	PSU	C4-N3-C2	-4.93	119.58	126.37
38	1	58	1MA	C5-C4-N3	-4.88	120.08	127.27
38	1	37	T6A	C12-N11-C10	4.88	130.10	121.99
38	1	46	7MG	C2-N3-C4	4.87	120.69	112.30
38	1	64	RIA	N6-C6-N1	-4.86	107.55	118.38
38	1	37	T6A	C5-C4-N3	-4.83	120.07	126.72
1	2	1780	MA6	C5-C4-N3	-4.79	120.12	126.72
1	2	998	PSU	C4-N3-C2	-4.77	119.81	126.37
38	1	58	1MA	N1-C2-N3	-4.76	120.33	126.00
1	2	1190	B8N	C4-N3-C2	-4.75	119.77	125.62
1	2	465	PSU	C4-N3-C2	-4.69	119.91	126.37
1	2	1426	2MG	C2-N1-C6	-4.69	118.89	124.55
1	2	1289	PSU	C4-N3-C2	-4.68	119.93	126.37
1	2	1573	7MG	C5-C4-N3	-4.63	119.44	128.13
1	2	120	PSU	N1-C2-N3	4.55	119.97	115.17
1	2	766	PSU	N1-C2-N3	4.52	119.94	115.17
1	2	1573	7MG	C2-N3-C4	4.48	120.01	112.30
38	1	46	7MG	C5-C4-N3	-4.34	119.98	128.13
1	2	465	PSU	N1-C2-N3	4.33	119.74	115.17
1	2	998	PSU	N1-C2-N3	4.30	119.70	115.17
1	2	1289	PSU	N1-C2-N3	4.26	119.66	115.17
38	1	37	T6A	N6-C10-N11	4.20	119.55	113.77
1	2	1780	MA6	N9-C8-N7	-4.20	107.98	113.94
38	1	10	2MG	C2-N1-C6	-4.17	119.51	124.55
38	1	64	RIA	N9-C8-N7	-4.15	108.06	113.94
1	2	1573	7MG	C4-C5-N7	4.14	110.27	105.38
38	1	26	M2G	C2-N3-C4	4.14	120.17	112.51
38	1	48	5MC	C5-C6-N1	-4.03	118.94	123.31
38	1	37	T6A	N9-C8-N7	-3.99	108.28	113.94
38	1	37	T6A	C4-C5-C6	3.97	120.08	116.78
1	2	1570	2MG	C2-N1-C6	-3.95	119.77	124.55
1	2	1190	B8N	N3-C2-N1	3.81	121.37	116.72
1	2	1780	MA6	C4-C5-C6	3.80	119.84	115.91
38	1	46	7MG	C4-C5-N7	3.79	109.85	105.38
38	1	64	RIA	C2-N3-C4	3.72	120.90	111.83
38	1	64	RIA	N3-C4-N9	3.66	133.39	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	58	1MA	C2-N3-C4	3.63	119.66	112.53
38	1	64	RIA	C1'-O2A-C2A	-3.61	109.42	117.98
1	2	1190	B8N	C31-N3-C4	3.56	122.22	117.18
38	1	9	1MG	N9-C4-N3	3.51	132.97	125.95
38	1	64	RIA	C5-C6-N6	3.50	131.94	123.29
1	2	1190	B8N	C1'-C5-C4	3.48	122.88	117.61
1	2	1573	7MG	N9-C4-N3	3.48	130.56	125.46
38	1	9	1MG	C2-N3-C4	3.47	119.78	111.98
38	1	37	T6A	O10-C10-N6	-3.44	117.53	123.64
1	2	120	PSU	C6-C5-C4	3.41	120.47	118.17
38	1	9	1MG	N9-C8-N7	-3.38	107.13	113.40
1	2	465	PSU	C6-N1-C2	-3.34	119.59	122.69
38	1	37	T6A	C2-N3-C4	3.33	119.95	111.83
38	1	47	H2U	N3-C2-N1	3.32	119.98	116.65
1	2	1780	MA6	C2-N1-C6	3.30	119.89	111.83
1	2	998	PSU	C6-N1-C2	-3.28	119.65	122.69
1	2	1289	PSU	C6-N1-C2	-3.27	119.66	122.69
38	1	10	2MG	N1-C2-N2	3.27	119.89	116.56
1	2	1570	2MG	N1-C2-N2	3.27	119.89	116.56
38	1	16	H2U	N3-C2-N1	3.25	119.91	116.65
1	2	120	PSU	C6-N1-C2	-3.24	119.69	122.69
1	2	1780	MA6	C2-N3-C4	3.23	119.72	111.83
38	1	10	2MG	N9-C4-N3	3.21	132.36	125.95
1	2	766	PSU	C6-C5-C4	3.18	120.32	118.17
38	1	49	5MC	C5-C6-N1	-3.17	119.87	123.31
1	2	766	PSU	C6-N1-C2	-3.16	119.76	122.69
1	2	1426	2MG	N9-C4-N3	3.13	132.22	125.95
38	1	26	M2G	N9-C4-N3	3.11	132.17	125.95
1	2	1573	7MG	C2-N1-C6	-3.11	119.48	125.11
38	1	58	1MA	N9-C8-N7	-3.10	107.65	113.40
1	2	1570	2MG	N9-C8-N7	-3.06	107.73	113.40
38	1	46	7MG	C2-N1-C6	-3.05	119.58	125.11
38	1	46	7MG	O6-C6-C5	-3.04	120.16	127.62
38	1	46	7MG	C5-C4-N9	3.01	110.19	106.33
38	1	46	7MG	N9-C4-N3	2.99	129.84	125.46
1	2	1637	5MC	C5-C6-N1	-2.96	120.10	123.31
1	2	1006	5MC	C5-C6-N1	-2.96	120.10	123.31
38	1	64	RIA	C5-N7-C8	2.91	108.03	103.45
38	1	16	H2U	C5-C6-N1	2.90	120.29	111.52
38	1	47	H2U	C5-C6-N1	2.89	120.27	111.52
1	2	1570	2MG	N9-C4-N3	2.88	131.72	125.95
1	2	1573	7MG	C5-C4-N9	2.87	110.01	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1426	2MG	N9-C8-N7	-2.87	108.08	113.40
38	1	10	2MG	N9-C8-N7	-2.86	108.09	113.40
38	1	47	H2U	C5-C4-N3	2.86	119.73	116.69
1	2	120	PSU	O2-C2-N1	-2.84	119.86	122.79
1	2	1570	2MG	C1'-N9-C4	-2.83	118.14	126.49
1	2	1780	MA6	C5-N7-C8	2.82	107.89	103.45
1	2	1573	7MG	O6-C6-C5	-2.82	120.71	127.62
1	2	1426	2MG	C5-C6-N1	2.81	120.41	113.25
1	2	1289	PSU	O2-C2-N1	-2.80	119.90	122.79
1	2	1190	B8N	C32-C31-N3	2.77	117.00	112.16
1	2	766	PSU	O2-C2-N1	-2.77	119.93	122.79
1	2	1780	MA6	N3-C4-N9	2.77	131.88	127.17
1	2	998	PSU	C6-C5-C4	2.76	120.04	118.17
1	2	465	PSU	O2-C2-N1	-2.76	119.94	122.79
38	1	37	T6A	C5-N7-C8	2.74	107.75	103.45
38	1	37	T6A	N3-C4-N9	2.73	131.80	127.17
38	1	16	H2U	C5-C4-N3	2.68	119.53	116.69
1	2	998	PSU	O2-C2-N1	-2.67	120.03	122.79
38	1	10	2MG	C5-C6-N1	2.65	120.01	113.25
38	1	64	RIA	C1'-C2'-C3'	2.64	105.58	102.29
1	2	1570	2MG	C5-C6-N1	2.64	119.98	113.25
1	2	1426	2MG	O6-C6-C5	-2.62	119.62	126.53
38	1	26	M2G	N9-C8-N7	-2.62	108.55	113.40
1	2	1573	7MG	N9-C8-N7	2.61	107.06	103.37
38	1	64	RIA	O1'-C1'-C2'	2.58	108.26	104.98
1	2	1006	5MC	CM5-C5-C6	-2.57	119.38	122.85
38	1	16	H2U	O2-C2-N1	-2.56	120.02	123.10
38	1	9	1MG	C5-C6-N1	2.55	119.73	115.02
38	1	58	1MA	N9-C4-N3	2.54	132.69	126.90
38	1	9	1MG	C8-N7-C5	2.51	108.73	104.26
1	2	1190	B8N	O4-C4-C5	-2.48	118.30	122.58
38	1	10	2MG	O6-C6-C5	-2.43	120.11	126.53
38	1	26	M2G	C5-C6-N1	2.42	119.42	113.25
1	2	1570	2MG	O6-C6-C5	-2.42	120.16	126.53
1	2	1190	B8N	O4-C4-N3	-2.41	116.07	119.99
1	2	1570	2MG	C1'-N9-C8	2.37	133.46	126.73
38	1	47	H2U	O2-C2-N1	-2.36	120.26	123.10
38	1	64	RIA	C4-N9-C8	2.32	108.18	105.74
1	2	1570	2MG	N1-C2-N3	-2.27	119.85	123.68
1	2	1780	MA6	C4-N9-C8	2.23	108.08	105.74
38	1	58	1MA	C8-N7-C5	2.22	108.22	104.26
1	2	1780	MA6	C4-C5-N7	-2.22	108.05	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	465	PSU	C6-C5-C4	2.19	119.65	118.17
1	2	1570	2MG	C8-N7-C5	2.18	108.14	104.26
1	2	766	PSU	O4'-C1'-C2'	2.16	108.14	105.15
38	1	37	T6A	C5-C4-N9	2.13	108.13	105.81
38	1	37	T6A	C4-C5-N7	-2.12	108.16	110.58
38	1	26	M2G	C1'-N9-C8	-2.09	120.78	126.73
38	1	26	M2G	C8-N7-C5	2.08	107.97	104.26
38	1	10	2MG	C1'-N9-C4	-2.08	120.35	126.49
38	1	10	2MG	CM2-N2-C2	-2.08	119.19	123.65
1	2	1426	2MG	C8-N7-C5	2.08	107.96	104.26
1	2	1426	2MG	C1'-N9-C4	-2.07	120.36	126.49
1	2	1426	2MG	N1-C2-N3	-2.06	120.20	123.68
38	1	46	7MG	N9-C8-N7	2.05	106.28	103.37
38	1	64	RIA	C6-C5-C4	2.04	119.97	117.18
1	2	1780	MA6	C5-C4-N9	2.01	108.00	105.81
38	1	26	M2G	O6-C6-C5	-2.01	121.23	126.53
1	2	1289	PSU	C6-C5-C4	2.01	119.53	118.17

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1573	7MG	O4'-C4'-C5'-O5'
1	2	1780	MA6	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	46	7MG	O4'-C4'-C5'-O5'
38	1	64	RIA	O4'-C4A-C5A-O5A
38	1	64	RIA	C3A-C4A-C5A-O5A
1	2	1190	B8N	O4'-C4'-C5'-O5'
1	2	1573	7MG	C3'-C4'-C5'-O5'
38	1	9	1MG	C3'-C4'-C5'-O5'
38	1	16	H2U	C3'-C4'-C5'-O5'
38	1	26	M2G	O4'-C4'-C5'-O5'
38	1	26	M2G	C3'-C4'-C5'-O5'
38	1	46	7MG	C3'-C4'-C5'-O5'
38	1	47	H2U	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
38	1	49	5MC	O4'-C4'-C5'-O5'
38	1	64	RIA	C3'-C4'-C5'-O5'
38	1	47	H2U	C3'-C4'-C5'-O5'
38	1	48	5MC	O4'-C4'-C5'-O5'
38	1	58	1MA	O4'-C4'-C5'-O5'
38	1	64	RIA	O1'-C4'-C5'-O5'
38	1	48	5MC	C3'-C4'-C5'-O5'
38	1	37	T6A	N11-C12-C14-C15
38	1	16	H2U	O4'-C4'-C5'-O5'
38	1	58	1MA	C3'-C4'-C5'-O5'
1	2	766	PSU	C3'-C4'-C5'-O5'
1	2	1190	B8N	C3'-C4'-C5'-O5'
1	2	1780	MA6	C3'-C4'-C5'-O5'
38	1	49	5MC	C3'-C4'-C5'-O5'
38	1	47	H2U	C4'-C5'-O5'-P
1	2	1637	5MC	O4'-C4'-C5'-O5'
38	1	16	H2U	C2'-C1'-N1-C6
38	1	37	T6A	N11-C12-C14-O14
1	2	1780	MA6	C5-C6-N6-C9
1	2	1573	7MG	C2'-C1'-N9-C8
1	2	766	PSU	O4'-C4'-C5'-O5'
38	1	48	5MC	C4'-C5'-O5'-P
1	2	1190	B8N	O4'-C1'-C5-C4
1	2	1190	B8N	N34-C33-C34-O36
38	1	49	5MC	C4'-C5'-O5'-P
1	2	1289	PSU	O4'-C4'-C5'-O5'
38	1	10	2MG	C3'-C4'-C5'-O5'
1	2	1573	7MG	O4'-C1'-N9-C8
1	2	1780	MA6	C4'-C5'-O5'-P
38	1	16	H2U	C2'-C1'-N1-C2
38	1	16	H2U	O4'-C1'-N1-C2
38	1	26	M2G	C2'-C1'-N9-C4
38	1	10	2MG	O4'-C4'-C5'-O5'
38	1	26	M2G	C4'-C5'-O5'-P
38	1	64	RIA	C3A-C2A-O2A-C1'
38	1	47	H2U	O4'-C1'-N1-C6
1	2	1570	2MG	O4'-C4'-C5'-O5'
1	2	1190	B8N	N34-C33-C34-O35

There are no ring outliers.

17 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	1	64	RIA	5	0
1	2	998	PSU	1	0
38	1	26	M2G	1	0
1	2	1006	5MC	1	0
38	1	9	1MG	1	0
38	1	47	H2U	1	0
38	1	46	7MG	1	0
1	2	1570	2MG	1	0
38	1	10	2MG	1	0
38	1	37	T6A	2	0
38	1	16	H2U	1	0
38	1	58	1MA	2	0
1	2	1289	PSU	1	0
38	1	48	5MC	1	0
1	2	1573	7MG	4	0
1	2	1426	2MG	2	0
1	2	1780	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 121 ligands modelled in this entry, 119 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	$\# Z > 2$
45	MET	k	603	-	6,7,8	0.48	0	2,7,9	0.25	0
44	GCP	k	601	-	32,34,34	3.18	12 (37%)	49,54,54	1.65	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
45	MET	k	603	-	-	0/5/6/8	-
44	GCP	k	601	-	-	7/19/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	k	601	GCP	O4'-C1'	8.85	1.62	1.42
44	k	601	GCP	C2'-C1'	-7.35	1.30	1.53
44	k	601	GCP	O4'-C4'	-6.15	1.31	1.45
44	k	601	GCP	PB-O3A	5.92	1.65	1.58
44	k	601	GCP	PA-O3A	5.14	1.65	1.59
44	k	601	GCP	C2-N2	4.91	1.45	1.34
44	k	601	GCP	C6-N1	-3.30	1.32	1.38
44	k	601	GCP	O2'-C2'	2.80	1.49	1.43
44	k	601	GCP	O3'-C3'	-2.79	1.36	1.43
44	k	601	GCP	O6-C6	-2.47	1.18	1.23
44	k	601	GCP	C5-N7	-2.38	1.34	1.39
44	k	601	GCP	PB-O2B	-2.09	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	601	GCP	C5-C4-N3	-5.29	119.97	128.39
44	k	601	GCP	C2-N3-C4	4.47	119.99	112.30
44	k	601	GCP	N9-C4-N3	3.07	132.09	125.95
44	k	601	GCP	PB-O3A-PA	-3.04	122.46	132.37
44	k	601	GCP	N9-C8-N7	-2.97	107.89	113.40
44	k	601	GCP	C2-N1-C6	-2.81	120.01	125.11
44	k	601	GCP	C5-C6-N1	2.62	119.93	113.25
44	k	601	GCP	O6-C6-C5	-2.48	119.98	126.53
44	k	601	GCP	C8-N7-C5	2.21	108.20	104.26

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	k	601	GCP	PG-C3B-PB-O1B
44	k	601	GCP	PG-C3B-PB-O3A
44	k	601	GCP	C5'-O5'-PA-O3A
44	k	601	GCP	C5'-O5'-PA-O2A
44	k	601	GCP	O4'-C4'-C5'-O5'
44	k	601	GCP	C3'-C4'-C5'-O5'

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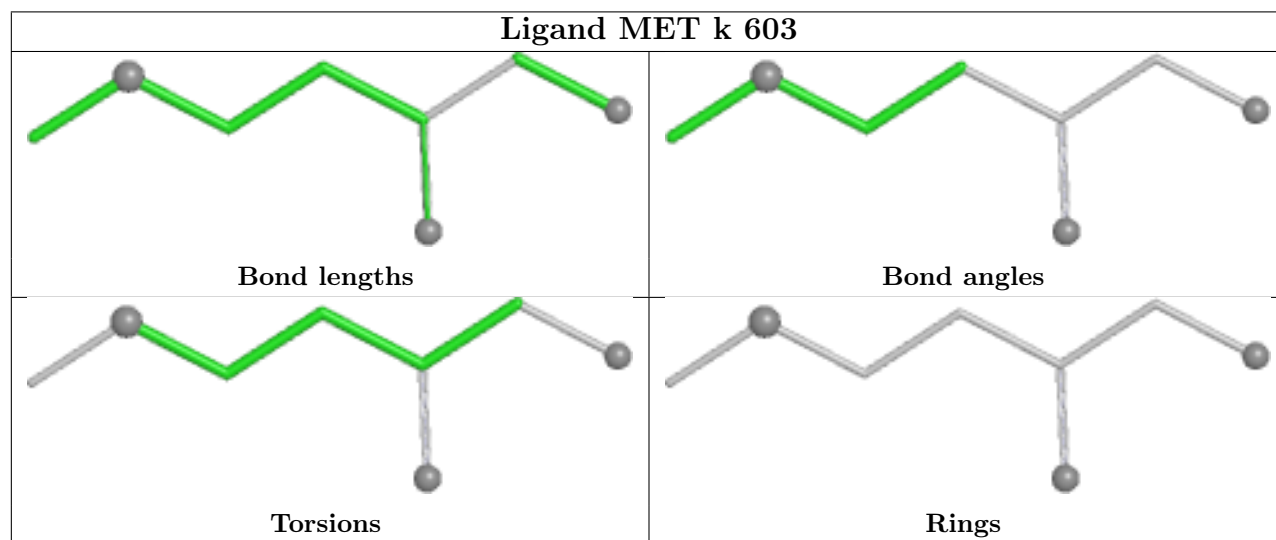
Mol	Chain	Res	Type	Atoms
44	k	601	GCP	PG-C3B-PB-O2B

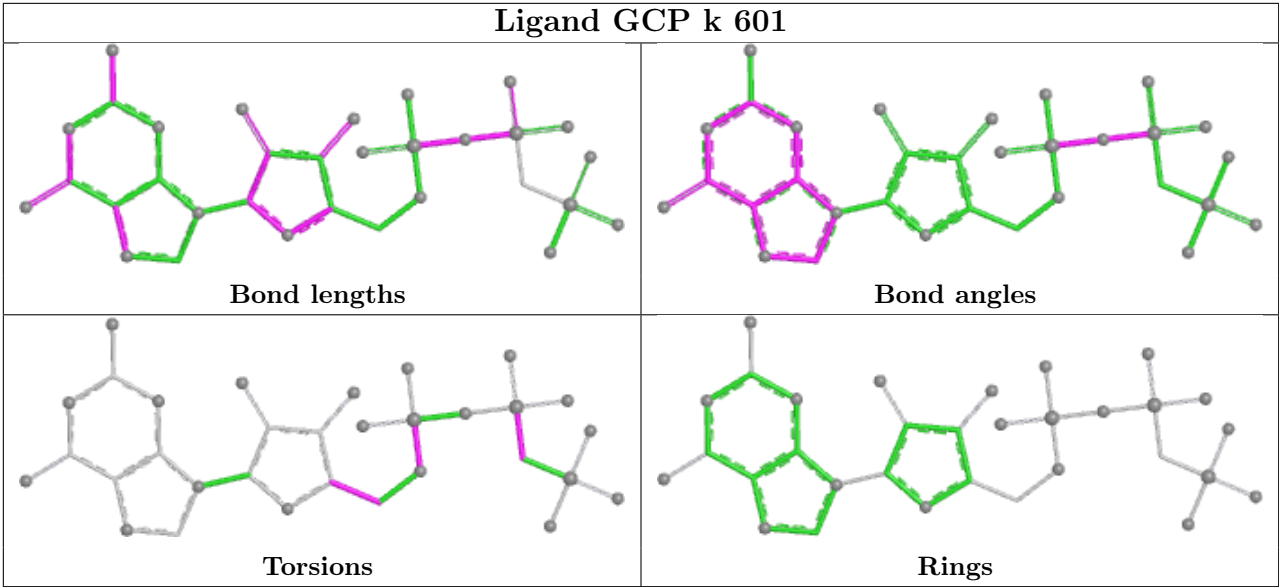
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	k	603	MET	4	0
44	k	601	GCP	4	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	8.15
1	1	63:G	O3'	64:RIA	P	4.24
1	1	16:H2U	O3'	18:G	P	3.15

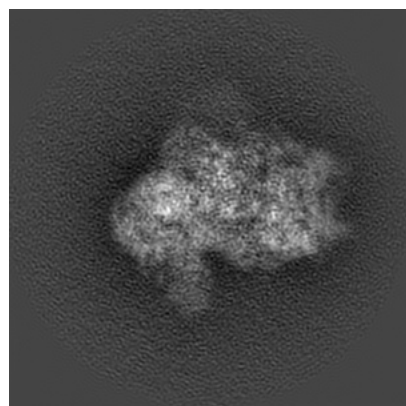
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19805. These allow visual inspection of the internal detail of the map and identification of artifacts.

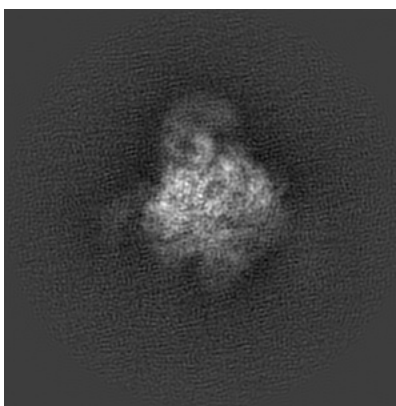
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

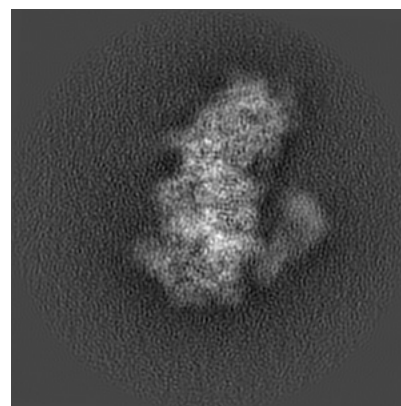
6.1.1 Primary map



X

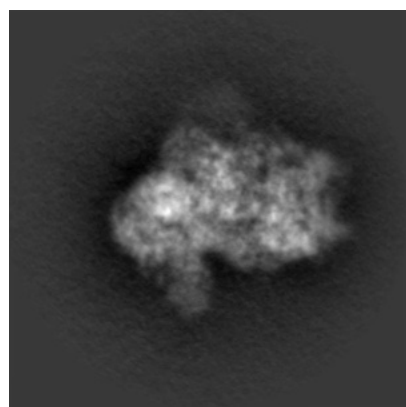


Y

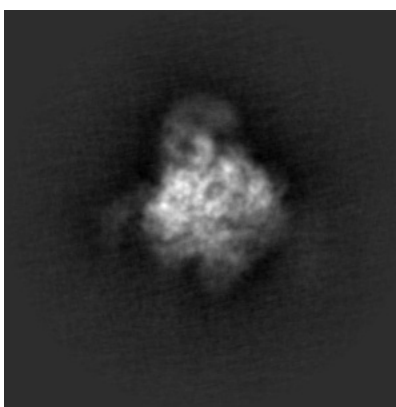


Z

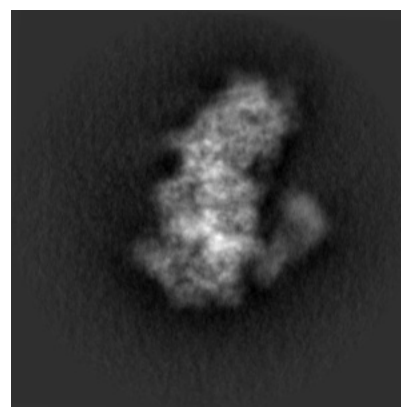
6.1.2 Raw map



X



Y

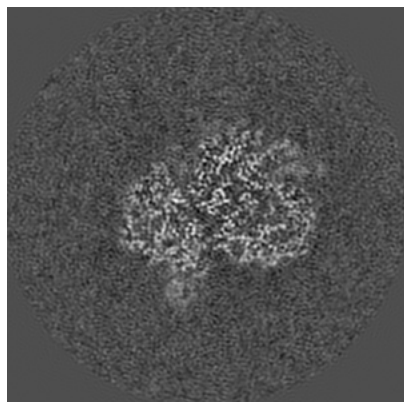


Z

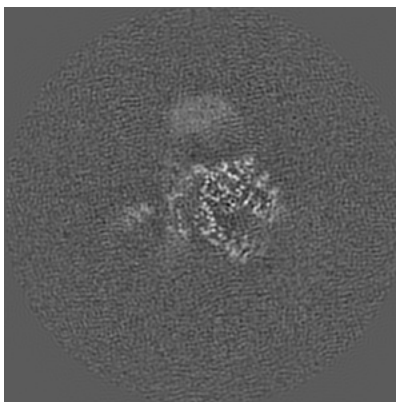
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

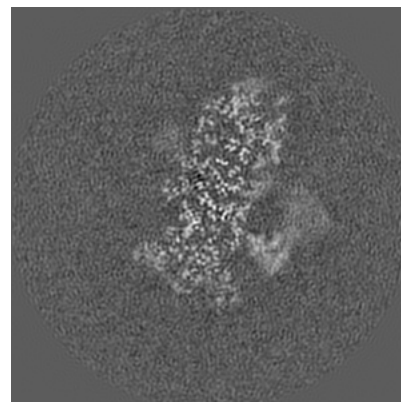
6.2.1 Primary map



X Index: 150

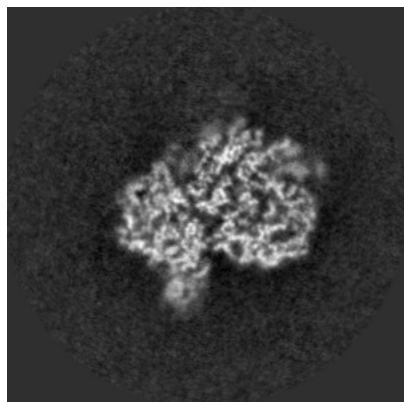


Y Index: 150

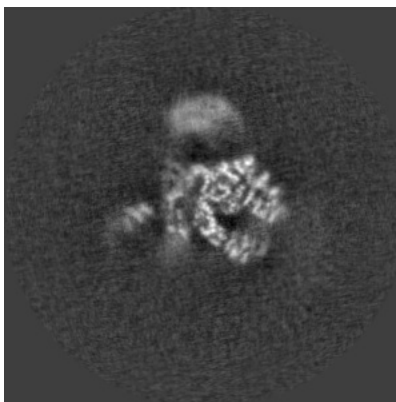


Z Index: 150

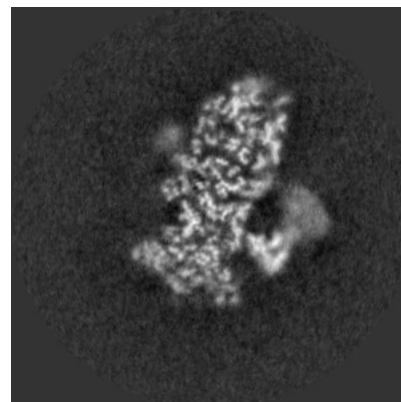
6.2.2 Raw map



X Index: 150



Y Index: 150

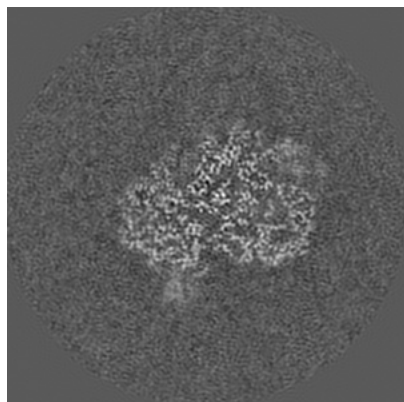


Z Index: 150

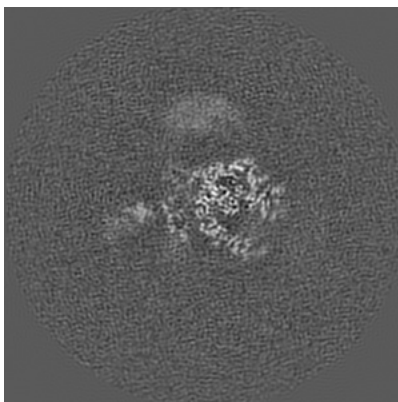
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

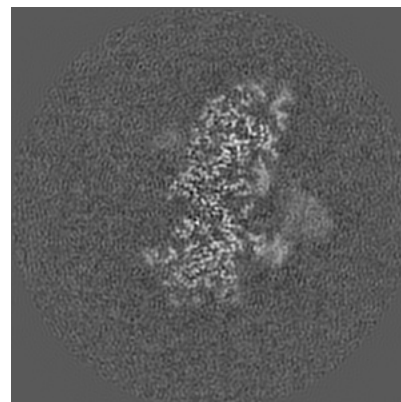
6.3.1 Primary map



X Index: 151

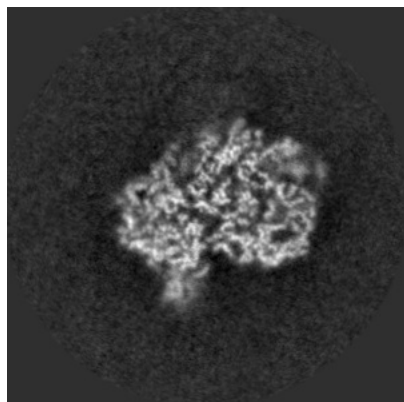


Y Index: 148

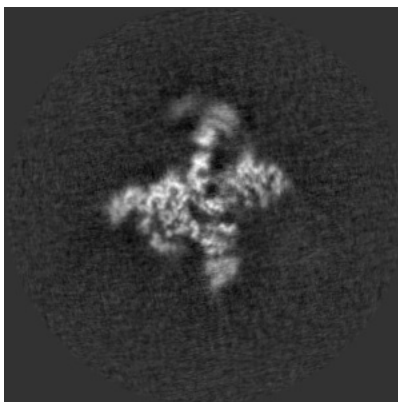


Z Index: 146

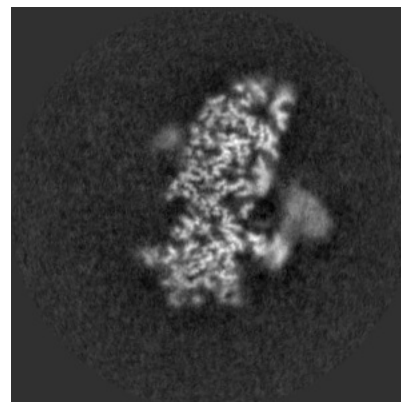
6.3.2 Raw map



X Index: 151



Y Index: 125

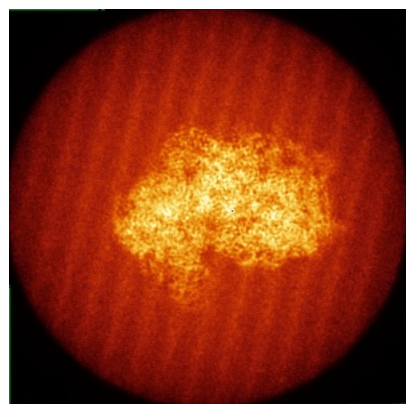


Z Index: 146

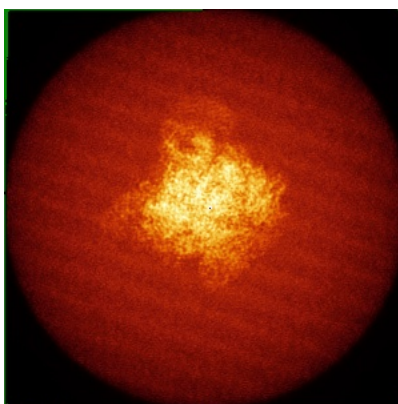
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

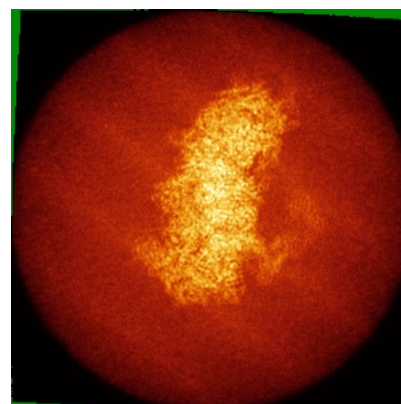
6.4.1 Primary map



X

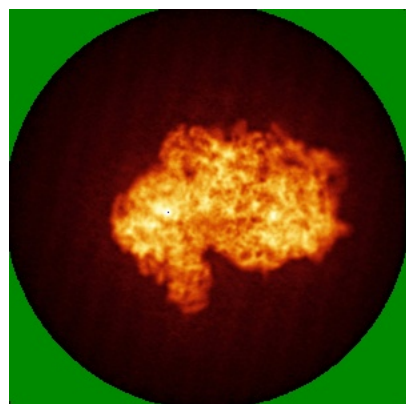


Y

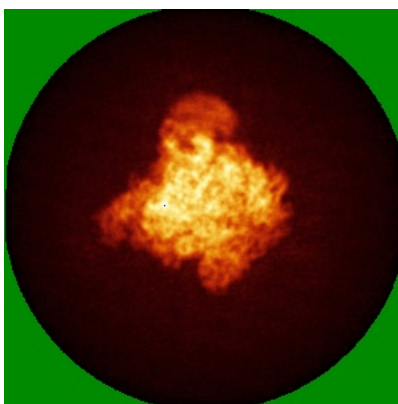


Z

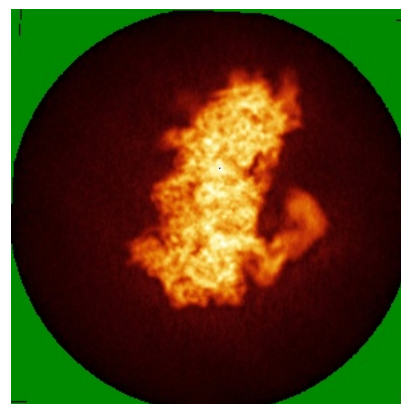
6.4.2 Raw map



X



Y

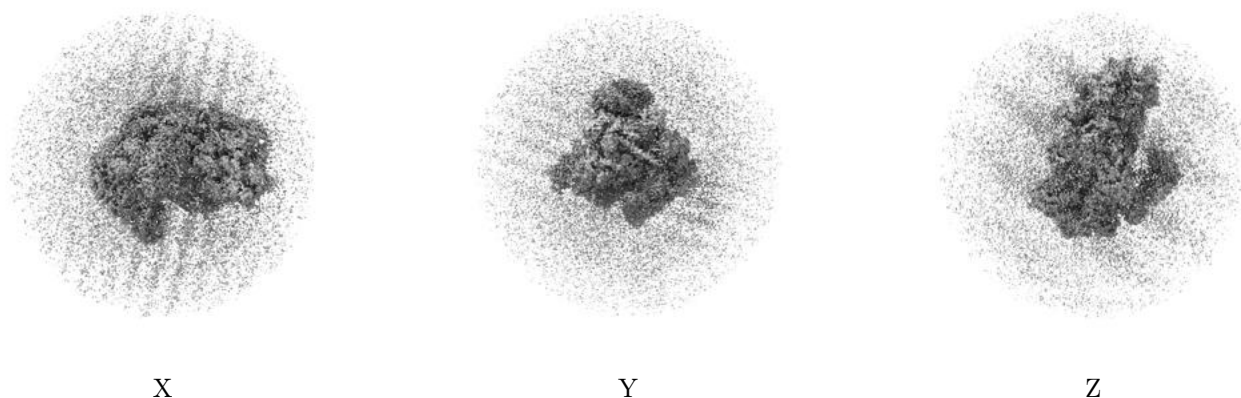


Z

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.

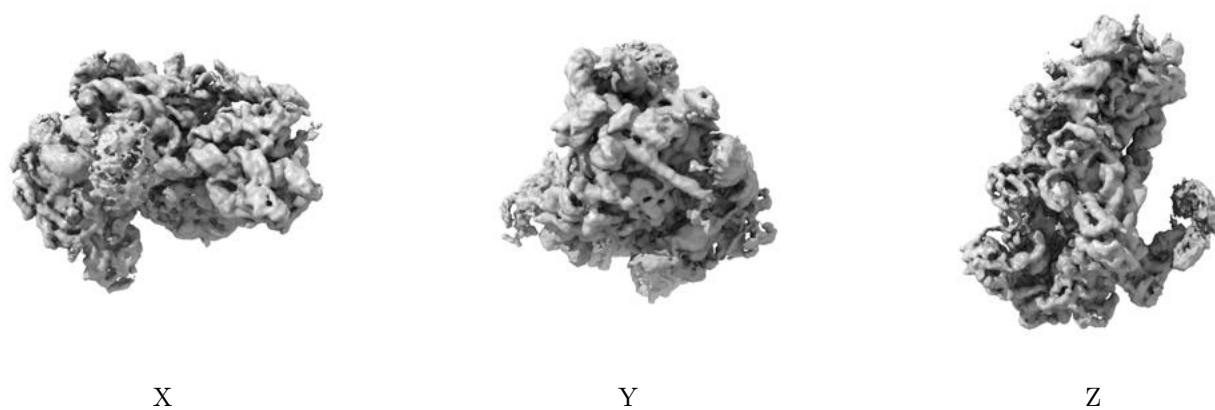
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

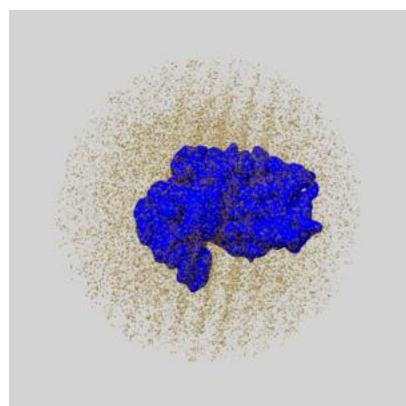
6.6 Mask visualisation [i](#)

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

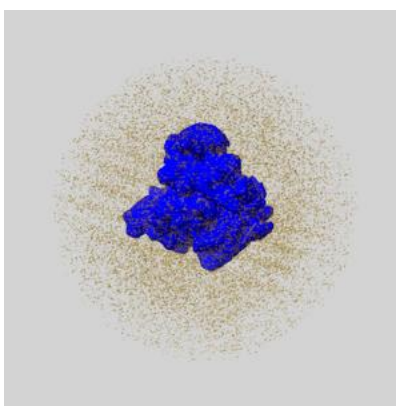
A mask typically either:

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

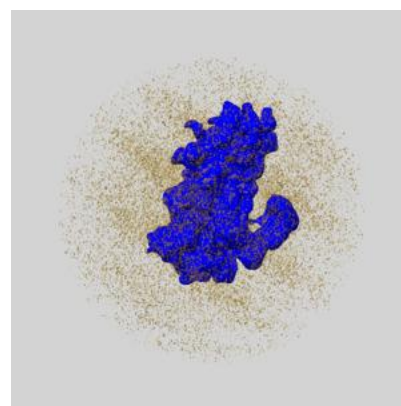
6.6.1 emd_19805_msk_1.map [i](#)



X



Y

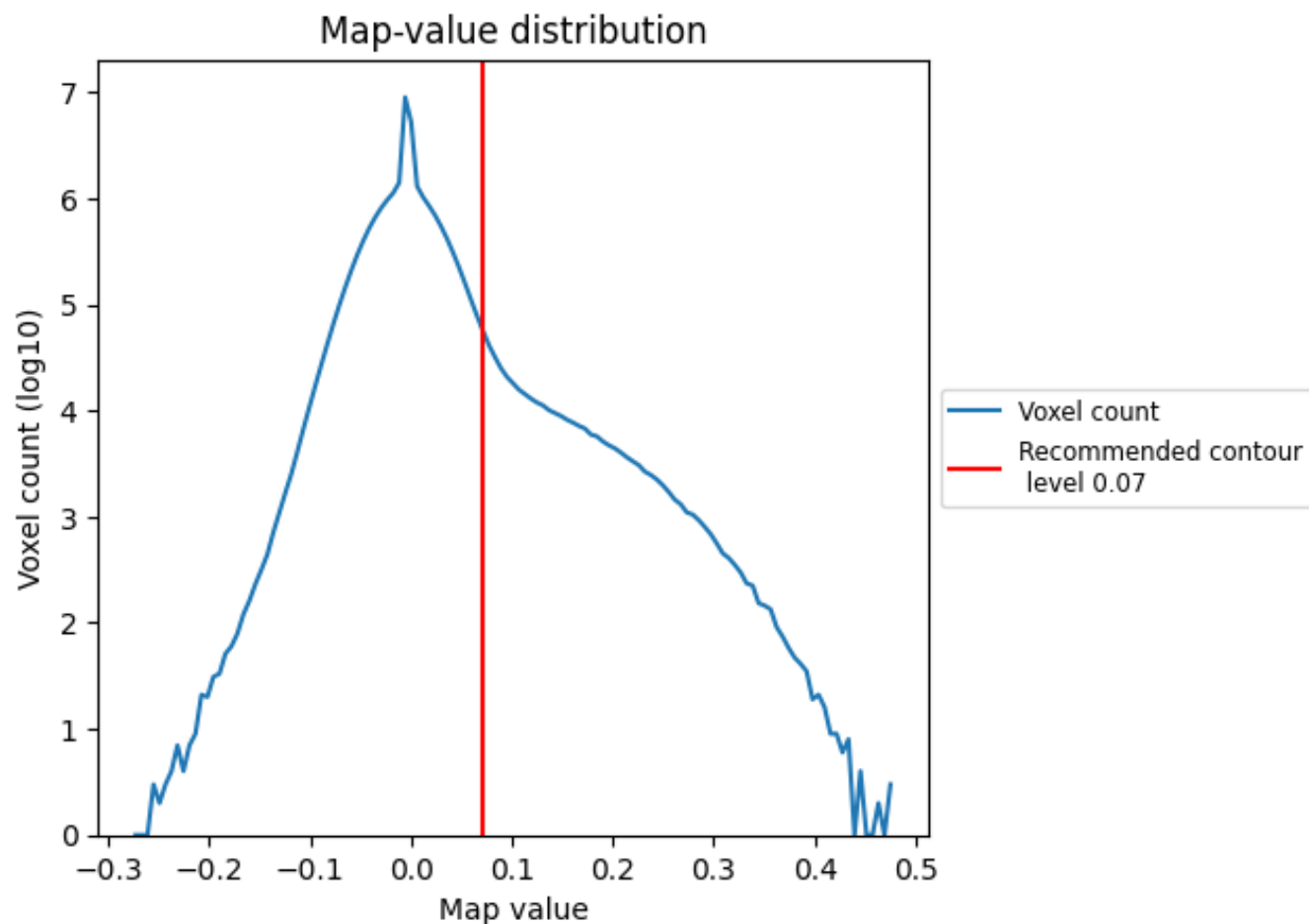


Z

7 Map analysis [i](#)

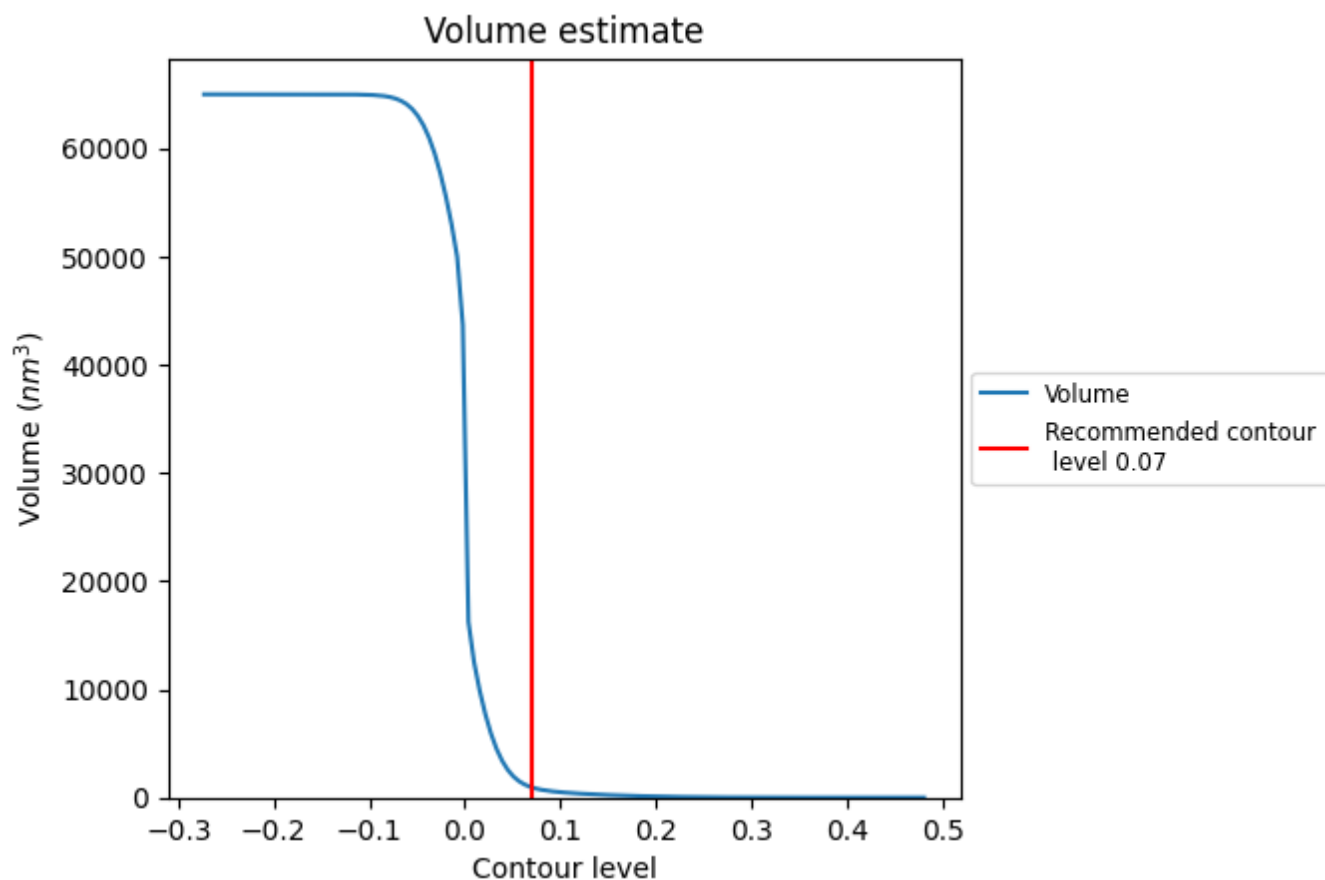
This section contains the results of statistical analysis of the map.

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.

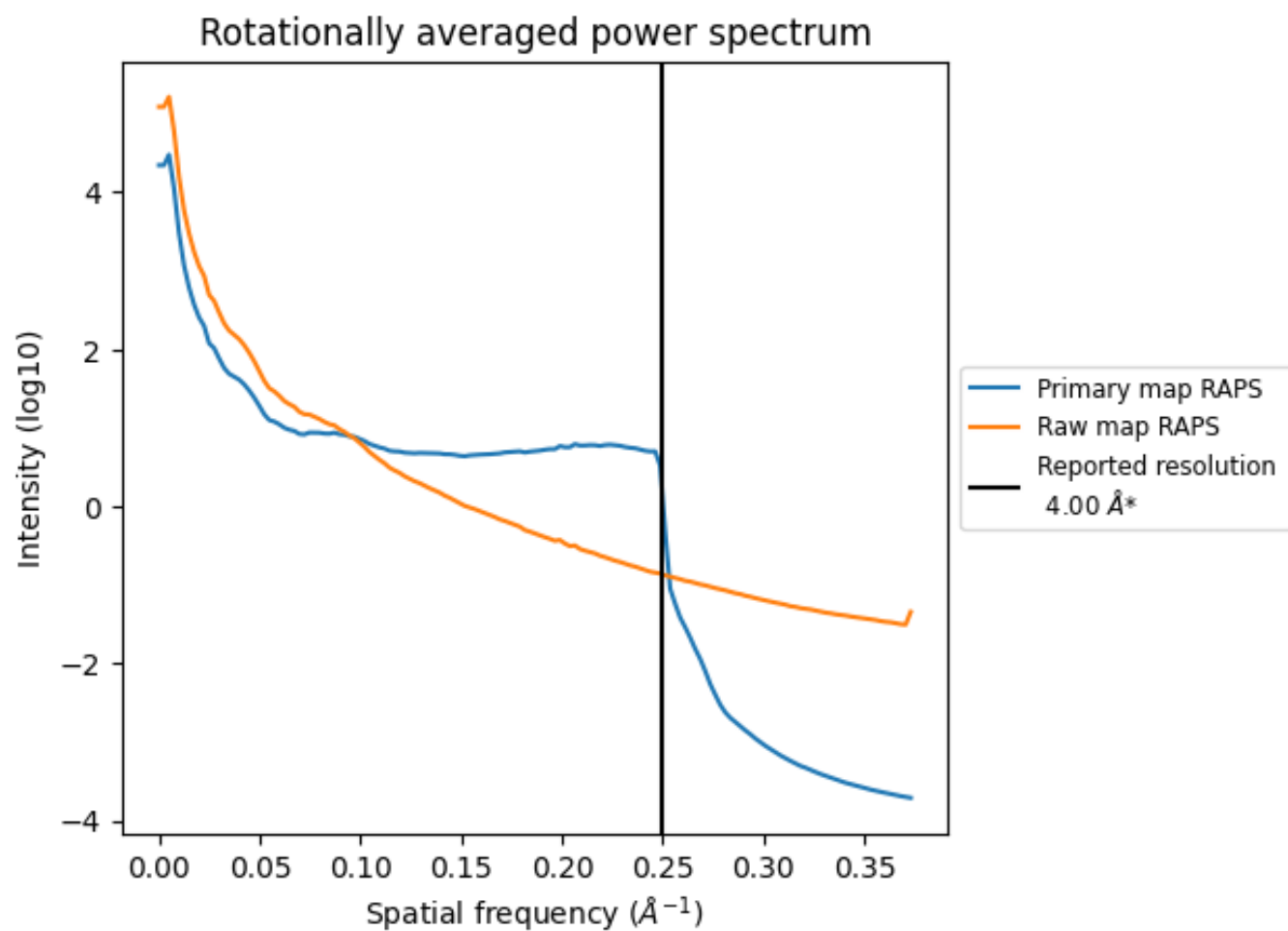
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 951 nm³; this corresponds to an approximate mass of 859 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 ⓘ

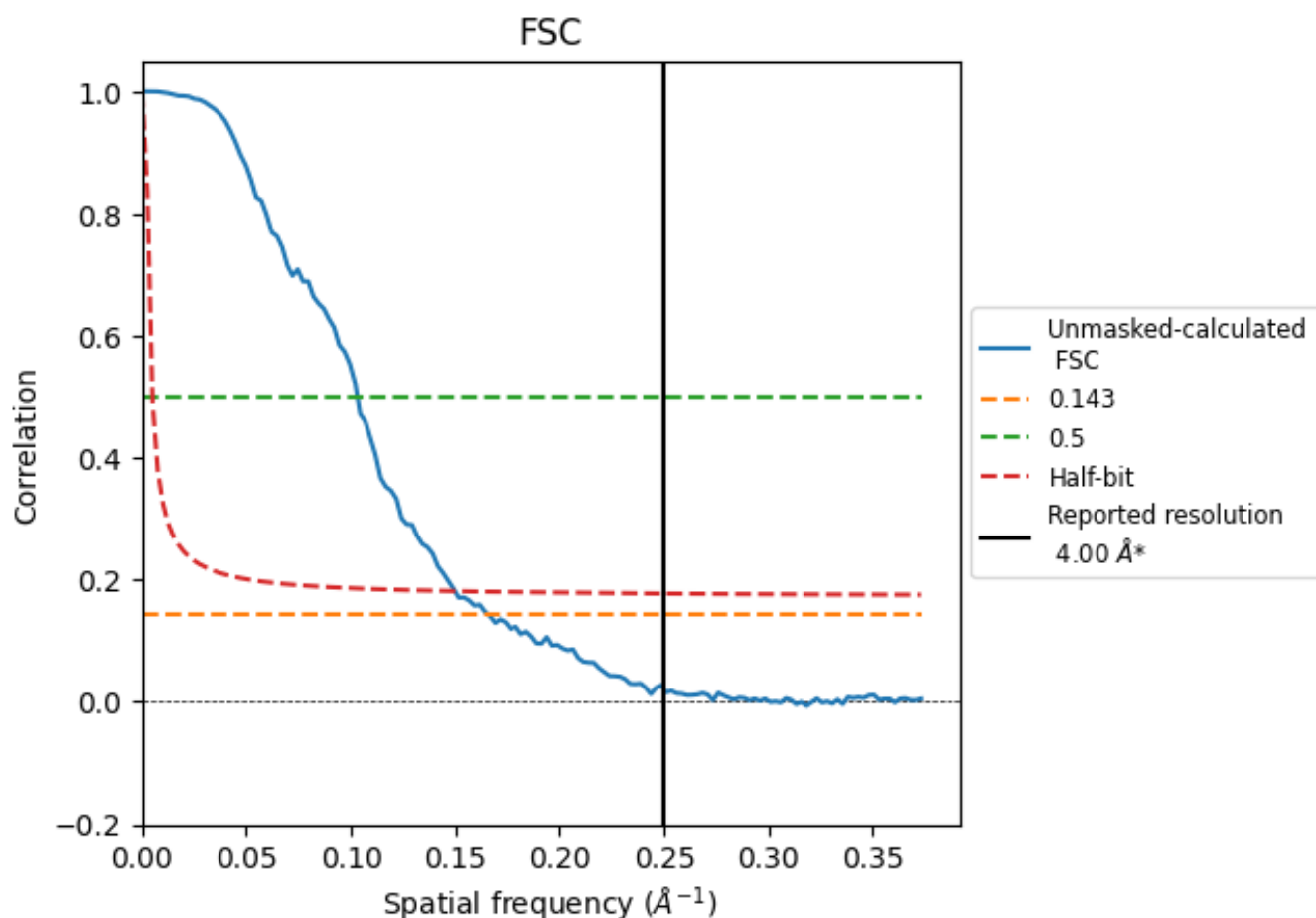


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 $0.250 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

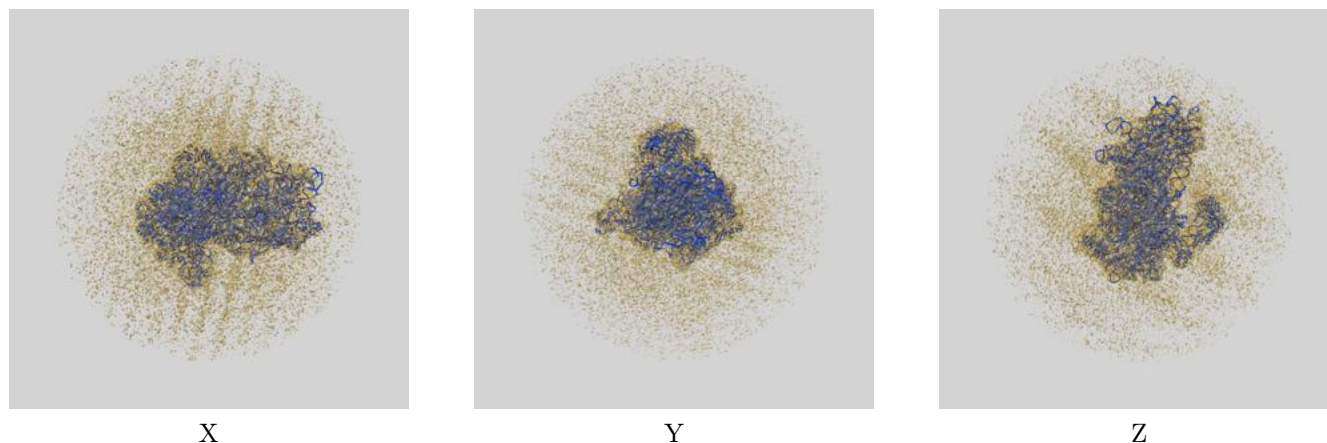
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.04	9.70	6.67

*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 6.04 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

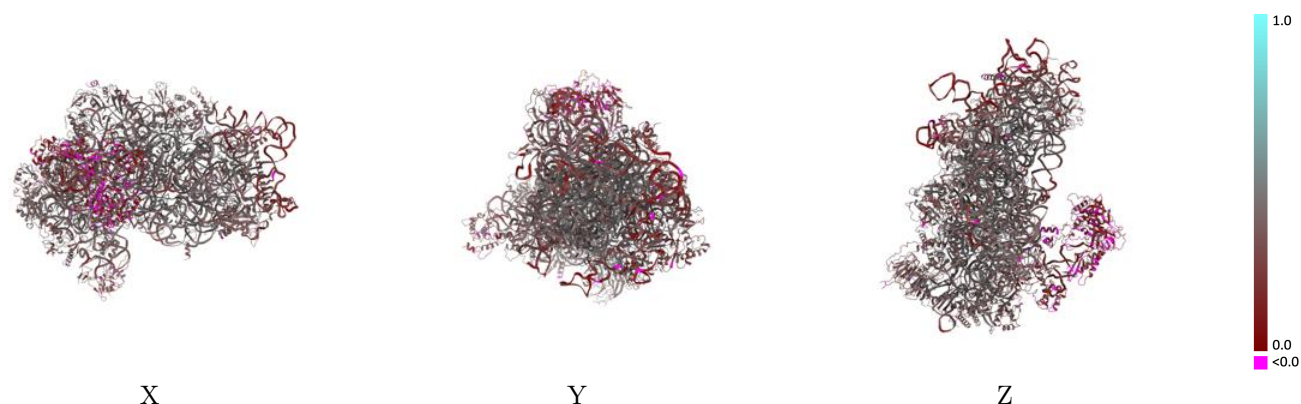
This section contains information regarding the fit between EMDB map EMD-19805 and PDB model 8S8H. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



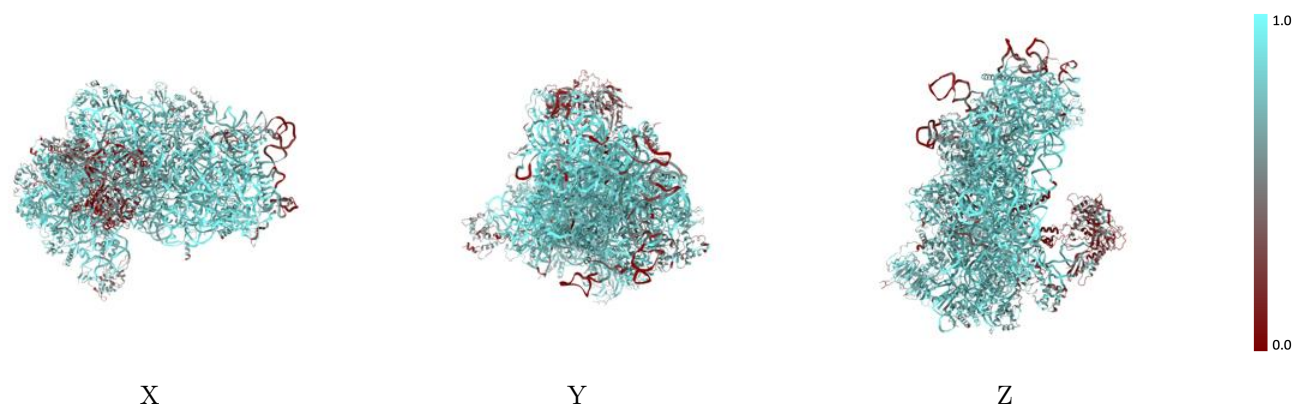
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



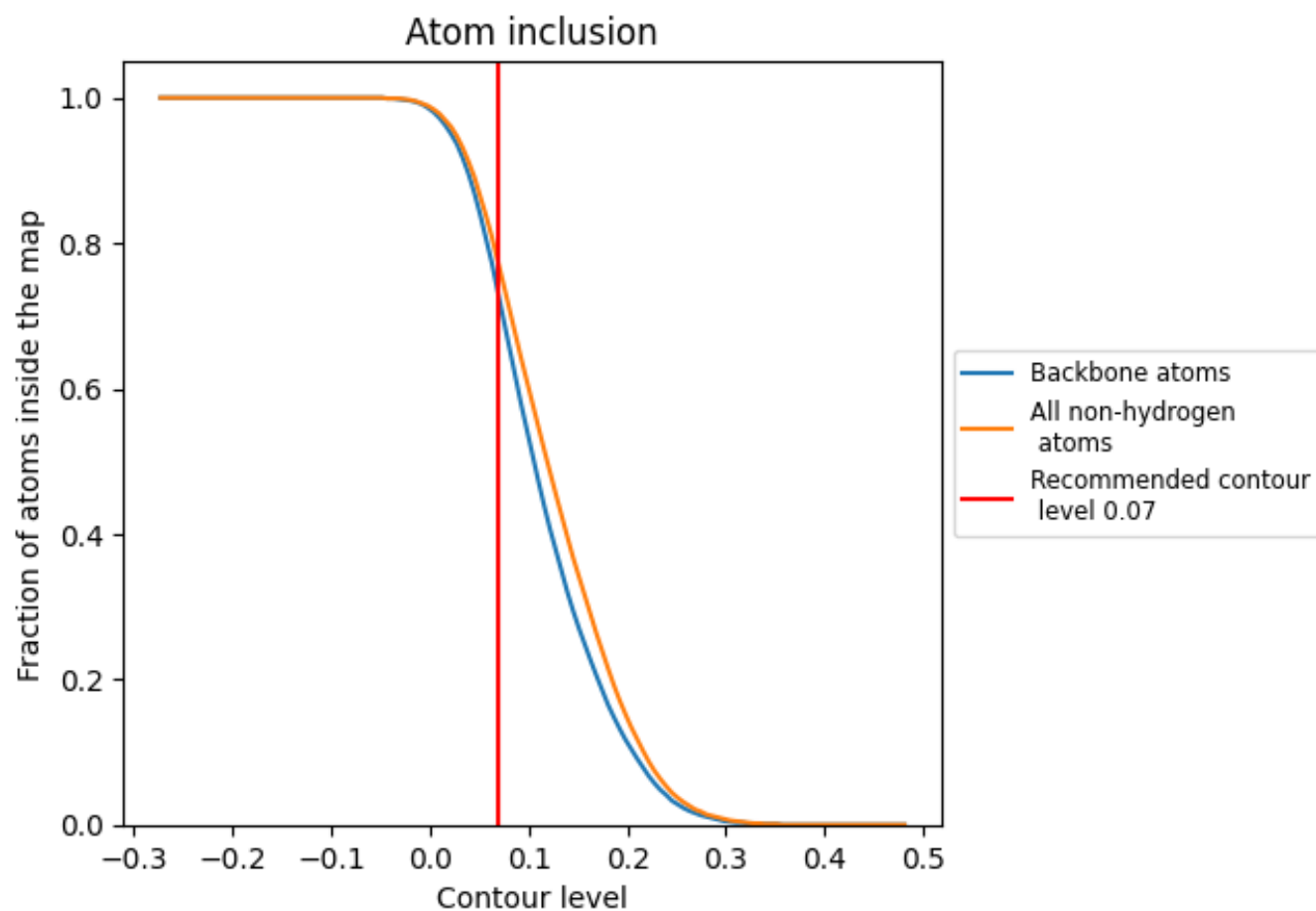
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 77% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.3600
1	 0.8750	 0.2670
2	 0.8740	 0.3730
3	 0.4320	 0.3120
A	 0.7700	 0.3900
B	 0.7600	 0.3840
C	 0.8050	 0.4320
D	 0.7640	 0.4040
E	 0.8160	 0.4340
F	 0.7730	 0.3950
G	 0.7800	 0.3580
H	 0.6280	 0.3480
I	 0.7840	 0.3970
J	 0.8170	 0.4180
K	 0.7570	 0.3530
L	 0.7580	 0.4190
M	 0.4450	 0.2470
N	 0.8070	 0.4080
O	 0.8250	 0.4080
P	 0.7800	 0.3670
Q	 0.8290	 0.4100
R	 0.6870	 0.3790
S	 0.7940	 0.3720
T	 0.8510	 0.3950
U	 0.6990	 0.3760
V	 0.8500	 0.4260
W	 0.8020	 0.4390
X	 0.8040	 0.4480
Y	 0.8290	 0.3960
Z	 0.5770	 0.3290
a	 0.8130	 0.4410
b	 0.7790	 0.3950
c	 0.8080	 0.4470
d	 0.8620	 0.4410
e	 0.7360	 0.4030



Continued on next page...

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Chain	Atom inclusion	Q-score
f	 0.5600	 0.2890
g	 0.7600	 0.3510
h	 0.1510	 0.2840
i	 0.4220	 0.3510
j	 0.4830	 0.1980
k	 0.2870	 0.1220
l	 0.1120	 0.1070