



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:09 AM UTC

PDB ID : 5JVH / pdb_00005jvh
Title : The crystal structure large ribosomal subunit (50S) of *Deinococcus radiodurans* in complex with evernimicin
Authors : Yonath, A.
Deposited on : 2016-05-11
Resolution : 3.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

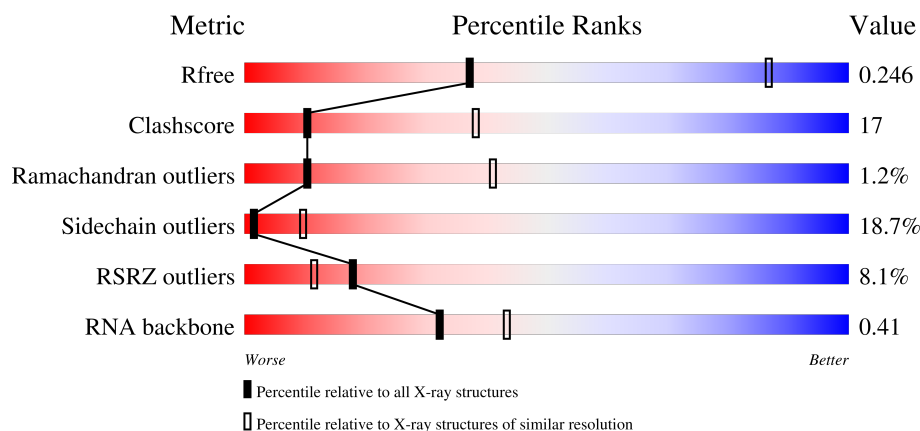
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)
RNA backbone	3983	1013 (4.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2880	5% 38% 43% 12% 8%
2	Y	123	9% 46% 41% 11% .
3	A	275	15% 39% 44% 11% 6%
4	B	211	5% 46% 39% 9% ...

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	G	174	
9	H	134	
10	I	156	
11	J	141	
12	K	116	
13	L	114	
14	M	166	
15	N	118	
16	O	100	
17	P	134	
18	Q	95	
19	R	115	
20	S	237	
21	T	91	
22	U	81	
23	V	67	
24	W	55	
25	Z	60	
26	1	54	
27	2	47	
28	3	66	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	2906	-	-	-	X
30	MG	X	2909	-	-	-	X
30	MG	X	2916	-	-	-	X
30	MG	X	2921	-	-	-	X
30	MG	X	2927	-	-	-	X
30	MG	X	2931	-	-	-	X
30	MG	X	2939	-	-	-	X
30	MG	X	2944	-	-	-	X
30	MG	X	2952	-	-	-	X
30	MG	X	2964	-	-	-	X
30	MG	X	2967	-	-	-	X
30	MG	X	2970	-	-	-	X
30	MG	X	2976	-	-	-	X
30	MG	X	2977	-	-	-	X
30	MG	X	2988	-	-	-	X
30	MG	X	2999	-	-	-	X
30	MG	X	3001	-	-	-	X
30	MG	X	3015	-	-	-	X
30	MG	X	3016	-	-	-	X
30	MG	X	3019	-	-	-	X
30	MG	X	3020	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83681 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2658	Total	C	N	O	P	0	0	0
			57052	25450	10532	18413	2657			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	259	Total	C	N	O	S	0	0	0
			1973	1226	395	349	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1078	690	196	185	7			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	108	Total	C	N	O	0	0	0
			859	537	166	156			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	179	Total	C	N	O	S	0	0	0
			1374	867	240	261	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

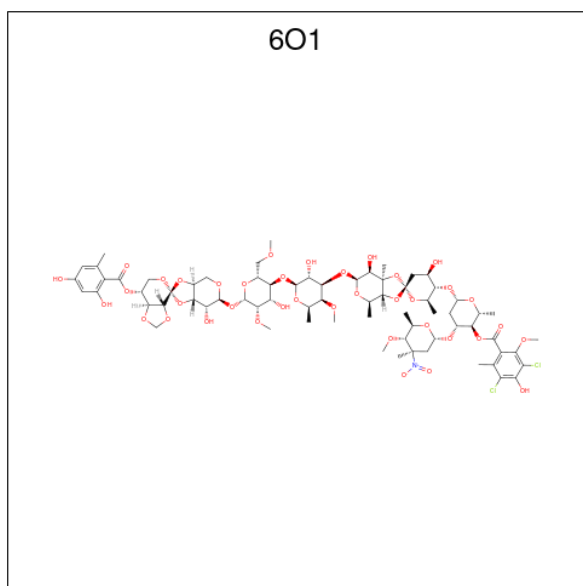
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 29 is Evernimicin (CCD ID: 6O1) (formula: $C_{70}H_{97}Cl_2NO_{38}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	Cl	N	O	0	0
			111	70	2	1	38		

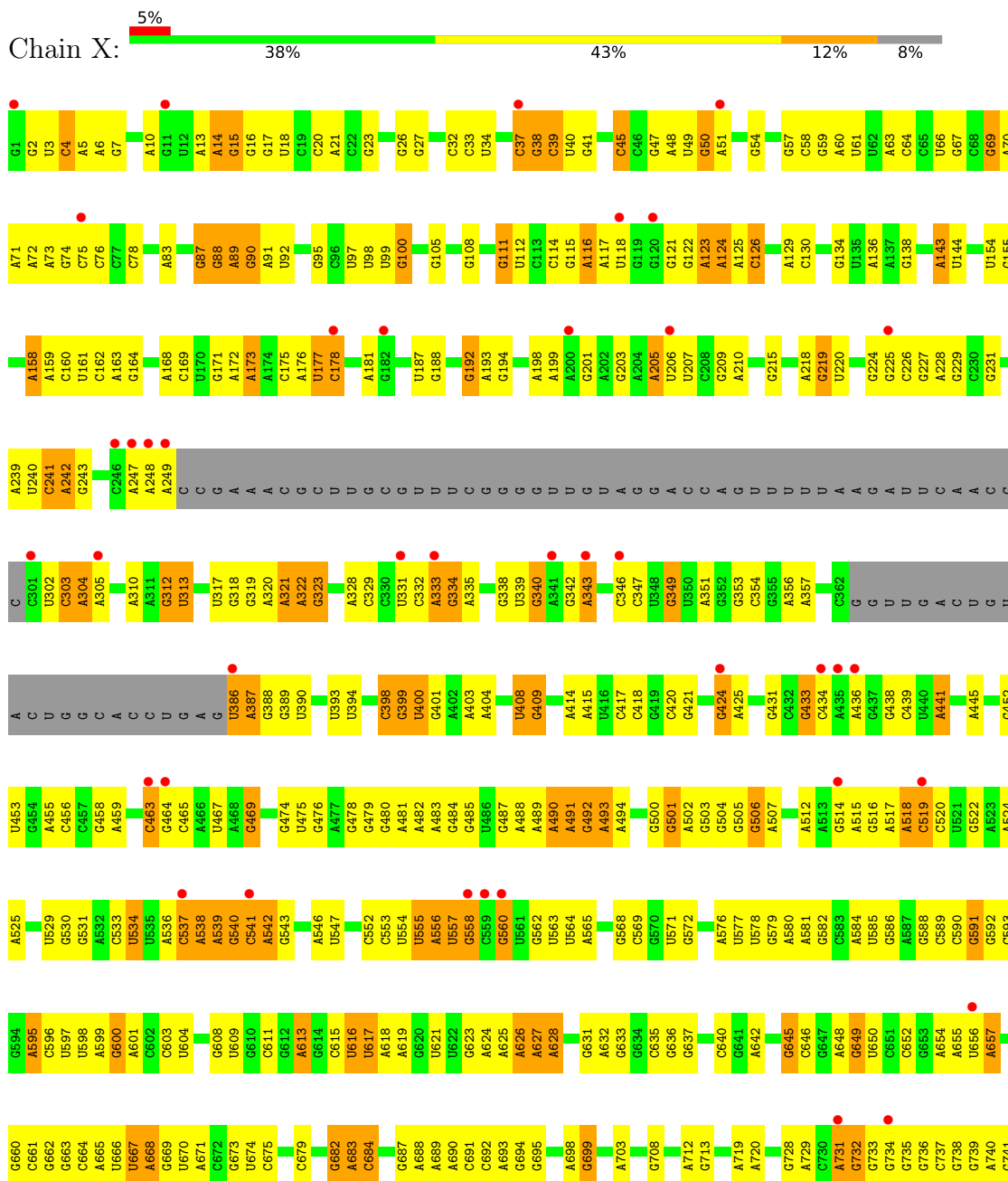
- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	119	Total	Mg	0	0
			119	119		
30	Y	1	Total	Mg	0	0
			1	1		
30	K	2	Total	Mg	0	0
			2	2		
30	M	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

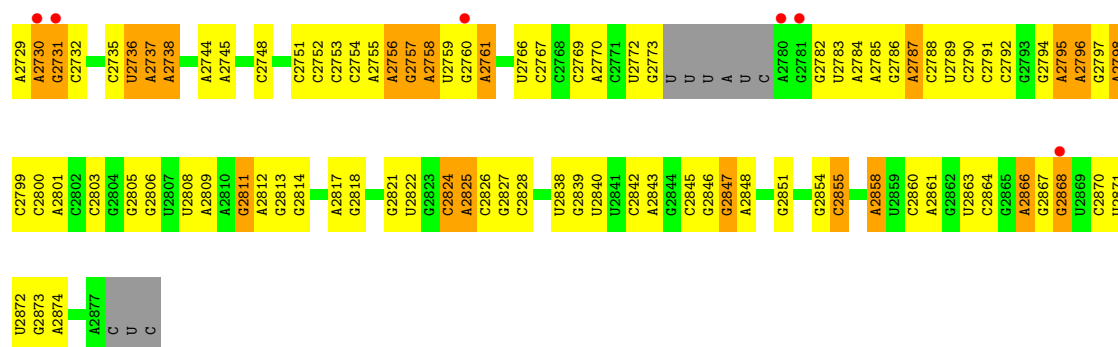
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S ribosomal RNA

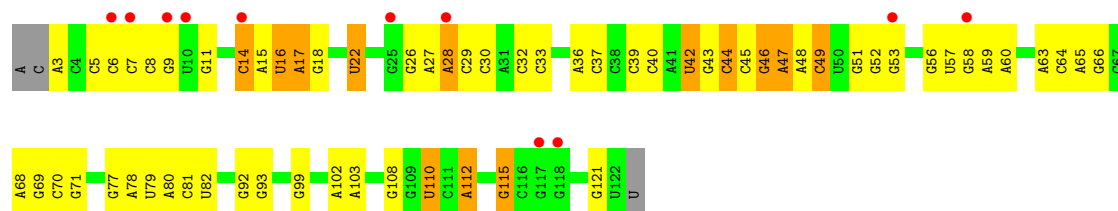


U1697	A1810	G1532	C1462	C1385	A1314	A1231	G1165	C	C1029	G951	A879	U810	G742
C1698	C1614	G1533	A1463	A1386	A1315	C1235	A1166	U	U1030	A952	C880	C811	A743
A1699	C1615	A1534	G1465	G1390	G1316	C1236	C1236	U	C1031	G953	U881	C812	A746
C1700	C1616	G1542	A1466	A1391	G1317	G1237	G1173	A	A1032	G955	U890	C813	A747
U1705	G1617	G1543	U1467	U1392	C1321	G1240	A1174	A	G1033	A956	C	C818	C750
C1623	C1623	A1544	A1468	G1393	C1322	G1241	A1175	A	U1034	G957	A	C819	G751
A1624	A1624	U1547	U1469	A1397	G1323	G1242	U1176	G	G1035	G958	G	U820	G752
A1625	A1625	G1548	G1398	G1398	U1325	A1242	C1177	A	U1036	G959	G	C822	G753
A1630	A1630	C1550	U1475	C1399	U1326	G1245	C1178	G	U1037	A964	G	G821	G754
G1713	G1713	U1551	G1476	U1403	C1327	G1246	A1180	G102	A1039	G965	G	U823	C755
A1714	A1714	C1477	U1477	C1404	U1328	U1247	G1181	C103	A1040	A966	C	U824	C756
A1831	A1831	U1476	U1476	C1404	U1329	G1248	U1182	G1104	G1041	G967	U	C825	U757
A1832	A1832	C1552	U1477	C1404	G1330	G1249	C1183	U1105	U1044	C968	C	U758	G758
C1633	C1633	G1553	G1479	G1407	G1331	A1250	G1184	A1106	A1045	U969	A	C829	G759
A1634	A1634	G1554	U1481	A1408	G1332	A1251	C1185	U1107	U1046	C970	C	C830	U760
G1635	G1635	A1555	U1482	U1409	G1333	C1252	G1186	U1108	U1047	A971	C	G831	G761
A1643	A1643	G1557	G1483	U1411	A1334	A1255	A1187	A1109	G1048	C972	A	A832	A762
G1721	G1721	C1558	C1412	C1412	G1335	C1256	A1188	G1110	U1048	G977	C	A833	A763
G1722	G1722	G1559	A1416	A1416	G1336	C1257	G1189	G1111	U1050	U978	C	A834	A764
U1723	U1723	A1560	C1487	C1417	G1337	C1258	G1191	U1112	U1051	U979	U	U835	A766
C1724	C1724	A1561	G1488	C1418	G1340	U1261	A1192	G1117	C1052	A984	C	U837	G767
A1728	A1728	G1562	C1489	C1419	G1341	U1262	G1193	C1120	G1053	G985	C	U840	U768
C1735	C1735	U1564	C1491	G1420	U1342	G1283	U1194	G1121	C1054	A986	A	G841	C769
G1742	G1742	G1565	A1492	U1421	C1343	C1284	U1195	A1122	U1055	G987	C	A842	G773
C1743	C1743	C1570	A1493	C1422	G1344	U1285	G1196	G1123	A1057	G988	C	U845	A774
G1744	G1744	C1571	G1494	C1423	G1345	C1286	U1197	U1124	G1058	C914	C	U846	A777
A1750	A1750	U1578	G1495	U1424	A1348	U1268	G1201	G1125	A1059	G989	C	A847	U778
U1752	U1752	G1573	C1496	G1425	C1349	G1289	U1202	C1126	C1063	A992	U	C847	U779
C1755	C1755	A1574	C1497	U1426	G1350	C1290	U1203	A1127	C	G993	G	A848	
A1756	A1756	G1575	G1498	G1427	G1351	C1291	A1203	G1128	A	A994	G	C849	U784
G1757	G1757	U1576	U1500	G1428	G1352	C1272	G1204	A1129	A995	A922	C	C850	U785
C1661	C1661	G1577	C1501	C1429	A1353	G1273	G1205	U1130	G	C996	G	U851	U786
A1751	A1751	U1578	G1430	U1430	A1354	C1274	G1206	G1136	A	C997	U	C852	U787
U1762	U1762	G1579	U1431	U1432	A1355	A1275	G1207	G1136	G	A998	C	C853	A787
A1669	A1669	A1582	C1506	G1432	G1356	U1276	A1208	G	C	A999	C	G854	G788
G1670	G1670	G1583	A1507	A1433	U1357	G1277	G1209	A1139	U	C1003	G	U857	G789
A1671	A1671	G1584	G1508	U1434	C1358	A1278	U1212	A1140	A1004	A928	G	U858	A790
C1672	C1672	A1585	A1509	G1435	G1359	G1279	G1213	G1142	A1005	A930	G	U859	G791
G1673	G1673	A1586	A1510	U1436	G1360	C1283	U1214	G1073	C1006	A931	G	U860	U792
C1675	C1675	A1587	G1437	G1438	A1361	G1284	A1215	G1074	A1007	G932	C	C861	G793
U1676	U1676	U1588	U1438	G1439	A1362	U1285	G1216	C1075	C1008	G933	C	A862	A795
C1677	C1677	A1594	G1440	U1441	C1363	U1286	G1217	U1076	C1009	G934	C	C863	G796
G1678	G1678	A1595	C1442	A1442	U1365	A1287	C1218	U1077	G	G938	C	C864	A797
A1682	A1682	G1520	G1443	G1443	U1370	A1288	G1219	G1079	G1013	U938	G	A865	G798
G1683	G1683	U1521	C1444	C1444	G1371	A1289	G1220	A1080	C939	C939	G	U866	C799
C1684	C1684	C1522	A1448	A1448	A1372	A1290	U1151	A1081	G940	G940	G	C870	U800
A1685	A1685	G1523	G1373	G1373	G1374	G1296	C1152	C1016	U941	U941	G	U871	A801
A1686	A1686	C1524	U1454	U1454	G1374	A1299	A1153	C1017	U942	U942	G	C872	C803
C1687	C1687	A1604	A1455	C1455	A1378	A1299	G1155	A1084	U943	U943	G	U873	G804
G1691	G1691	U1526	U1456	U1456	G1378	A1299	G1155	C	U944	U944	G	A874	G805
C1692	C1692	G1527	U1459	U1459	G1381	C1310	U1161	C	U945	U945	G	C875	A806
A1693	A1693	C1528	G1460	G1460	G1381	C1311	A1162	A	C947	C947	G	A876	A807
A1694	A1694	C1531	C1461	C1461	G1384	U1313	C1164	C	U1023	U1023	G	C877	C808

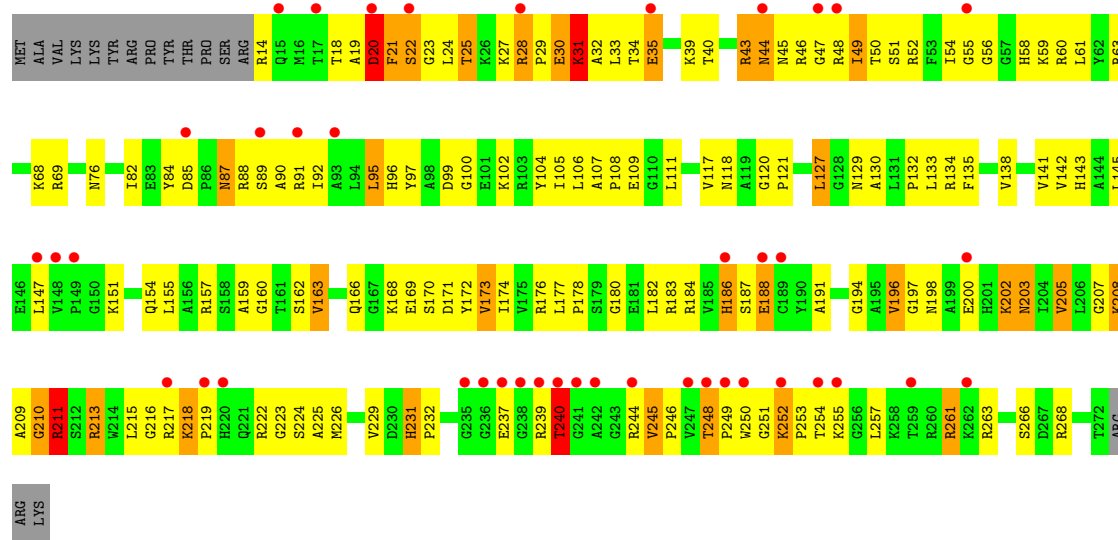




• Molecule 2: 5S ribosomal RNA

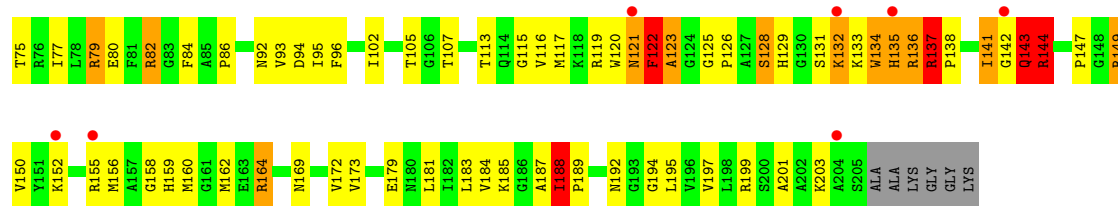


• Molecule 3: 50S ribosomal protein L2

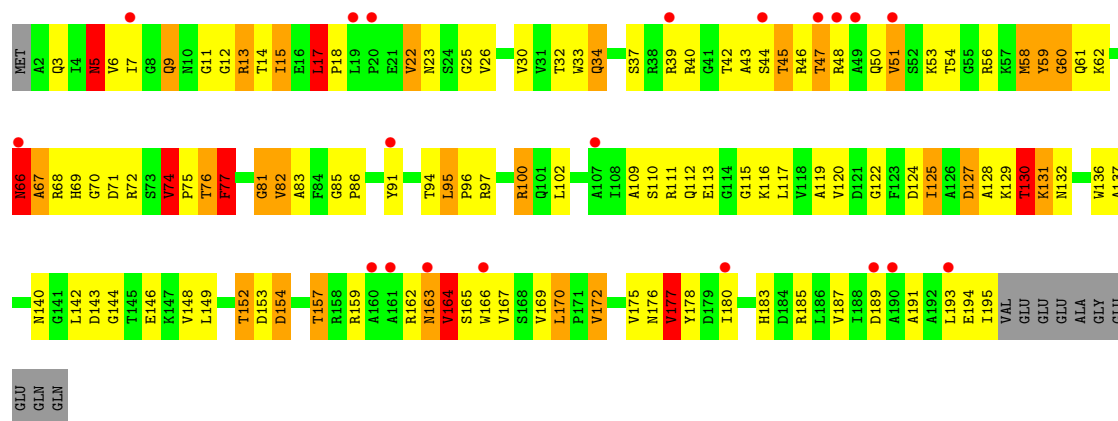


• Molecule 4: 50S ribosomal protein L3

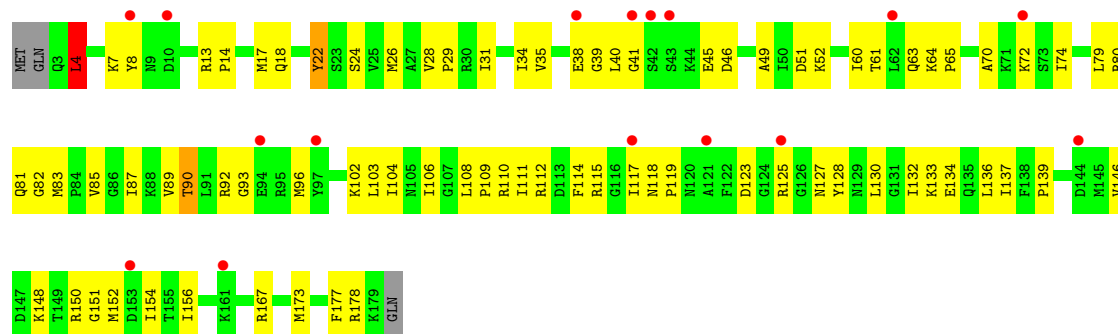




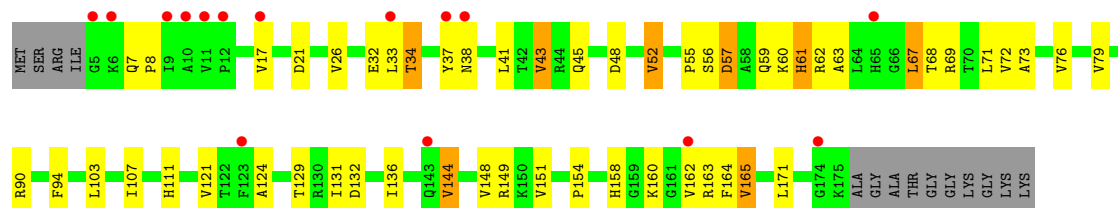
• Molecule 5: 50S ribosomal protein L4



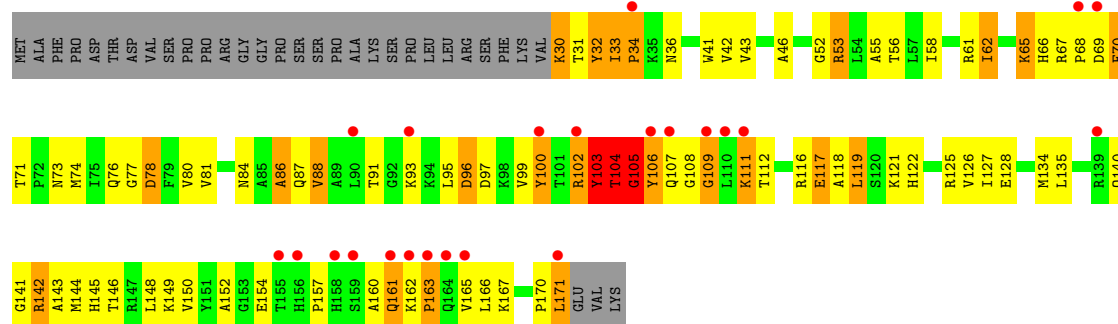
• Molecule 6: 50S ribosomal protein L5



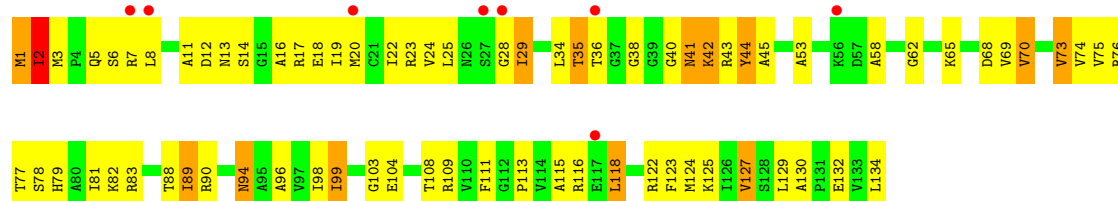
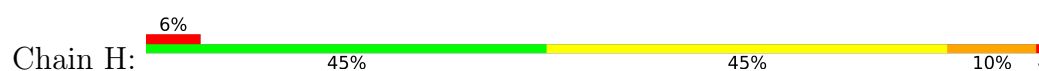
• Molecule 7: 50S ribosomal protein L6



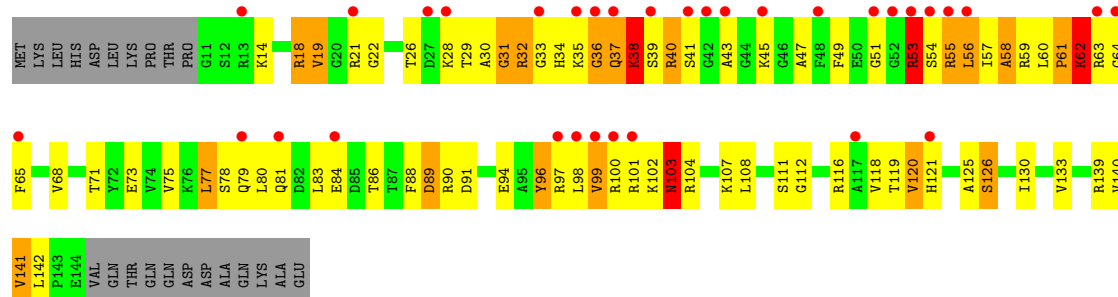
• Molecule 8: 50S ribosomal protein L13



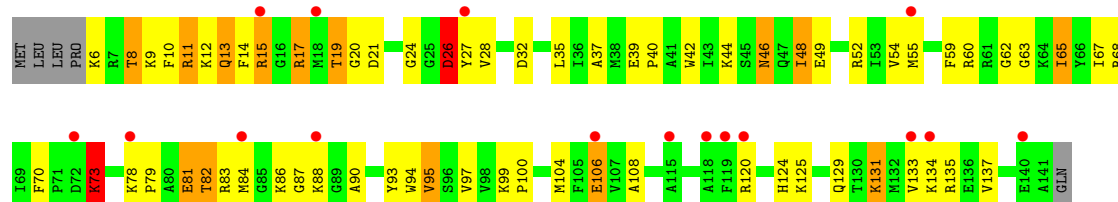
• Molecule 9: 50S ribosomal protein L14



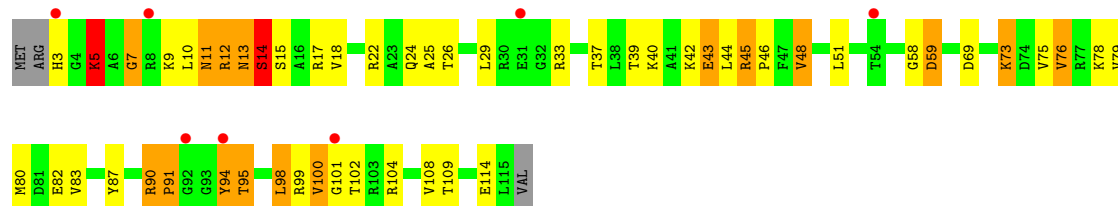
• Molecule 10: 50S ribosomal protein L15



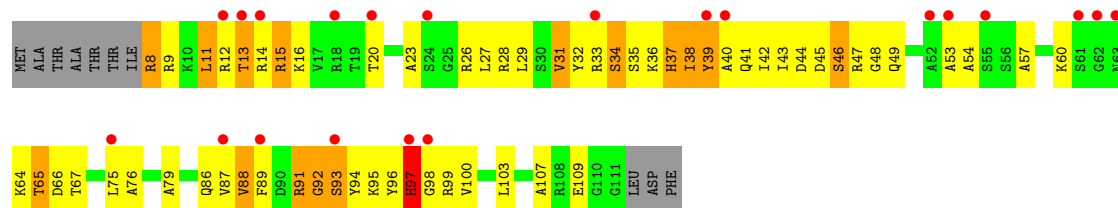
• Molecule 11: 50S ribosomal protein L16



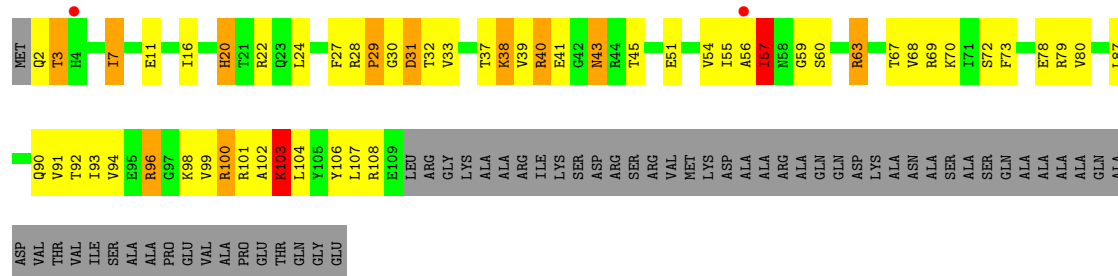
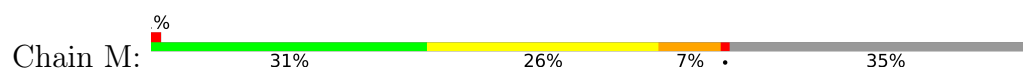
• Molecule 12: 50S ribosomal protein L17



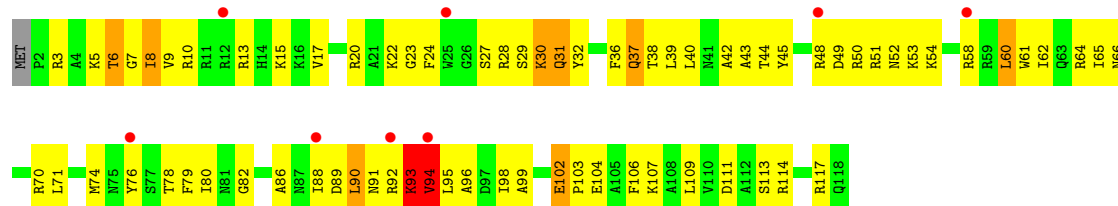
- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19

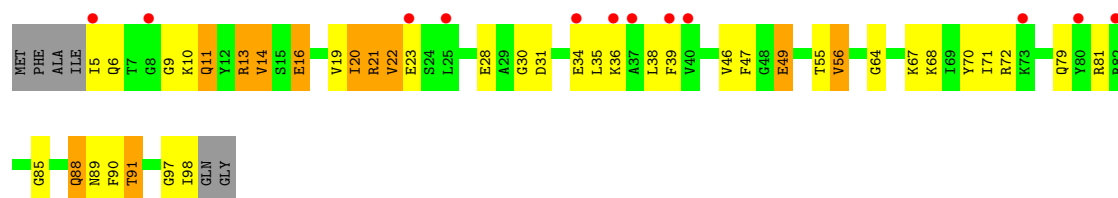


- Molecule 15: 50S ribosomal protein L20

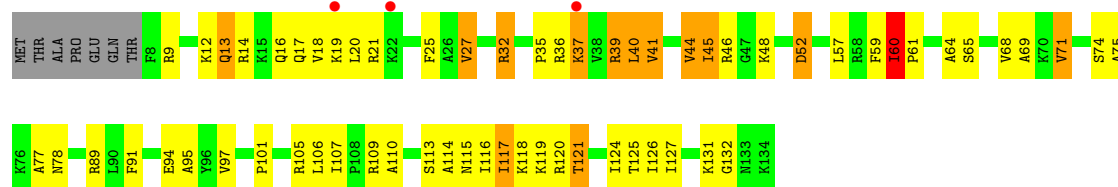


- Molecule 16: 50S ribosomal protein L21

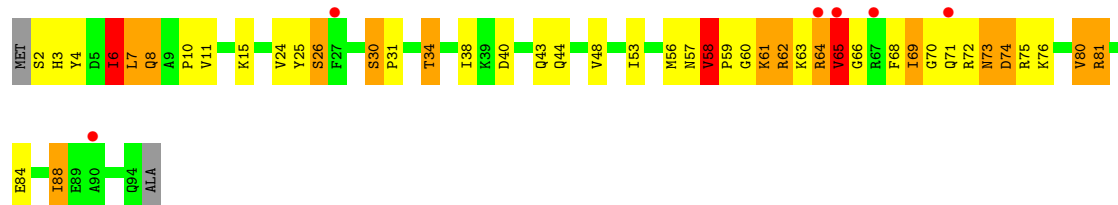




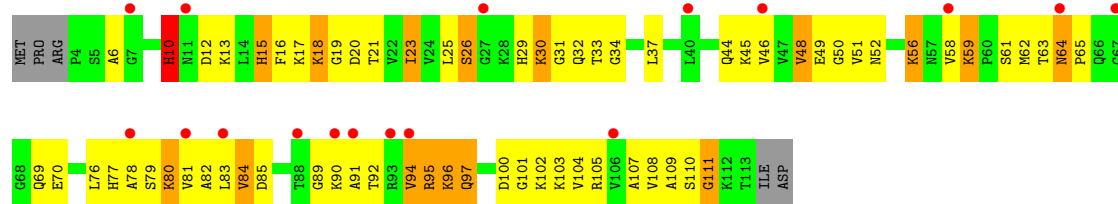
• Molecule 17: 50S ribosomal protein L22



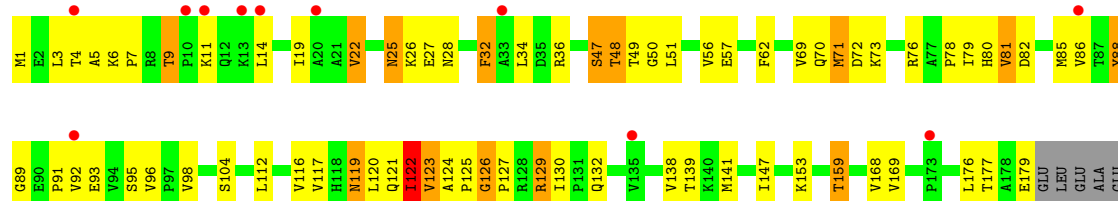
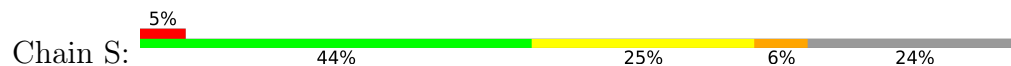
• Molecule 18: 50S ribosomal protein L23



• Molecule 19: 50S ribosomal protein L24



• Molecule 20: 50S ribosomal protein L25



VAL GLN ALA ALA ALA GLN VAL ALA GLY VAL LEU VAL ALA ALA GLY GLU LEU SER SER GLU GLU ALA ALA GLU VAL ALA VAL LEU GLY ASP ASP SER LEU GLU VAL THR ASP SER ASP ASN ASP SER ASP ALA GLN

• Molecule 21: 50S ribosomal protein L27

Chain T: 10% 51% 24% 7% 19%

MET ALA HIS LYS LYS VAL GLY SER SER LYS N12 N13 R14 D15 S16 N17 P18 K19 Y20 V23 K24 K25 F26 E29 V30 T36 L37 V38 K44 F45 K46 A47 V51 F60 D64 G65 K66 V67 V68 K72 G73 K74 G75 A76 R77 F78 I79 S80 Q85 THR

GLU VAL ALA ALA ASP

• Molecule 22: 50S ribosomal protein L28

Chain U: 14% 40% 32% 15% 11%

MET SER ARG GLU CYS TYR LEU T8 G9 L13 V14 V15 N16 S17 T19 R20 R21 R22 K23 D27 G28 G29 V30 G31 R32 K33 T34 T35 G36 L37 T38 K39 R40 V41 Q42 R43 A44 N45 L46 H47 K48 K49 A50 I51 R52 E53 K54 K58 T59 V60 W61 L62 S63 A66 L67

L70 Y75 K76 G77 I78 E79 LEU ILE

• Molecule 23: 50S ribosomal protein L29

Chain V: 3% 58% 39%

MET K2 P3 S4 E5 M6 T12 D13 F14 E17 I18 D19 A20 K22 K23 L28 R29 F30 Q31 A32 Q36 L37 R42 V43 R44 Q45 L46 R47 R48 Q52 L53 R62 Q66 GLN

• Molecule 24: 50S ribosomal protein L30

Chain W: 5% 51% 38% 11%

M1 K2 T3 K4 P5 L5 V6 R7 S8 V9 T10 G11 R12 P13 G14 T19 L23 L25 R26 K27 D30 D36 T37 P38 C33 V40 R41 Q42 M43 T46 V47 L50 L51 E52 V53 Q54 E55

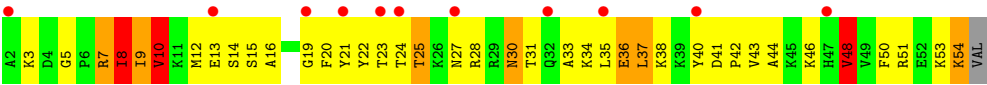
• Molecule 25: 50S ribosomal protein L32

Chain Z: 5% 37% 40% 15% 5%

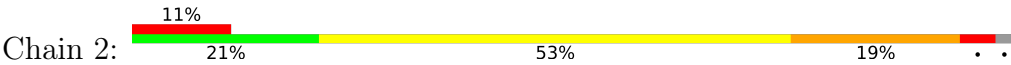
MET ALA K3 H4 P5 V6 P7 K8 K9 K10 K13 S14 K15 R16 D17 M18 R19 R20 S21 L25 T26 A27 L30 T31 E32 C33 P34 Q35 K40 L41 S42 I45 C46 C49 G50 Y51 D53 G54 R55 Q56 V57 L58 A59 VAL

• Molecule 26: 50S ribosomal protein L33

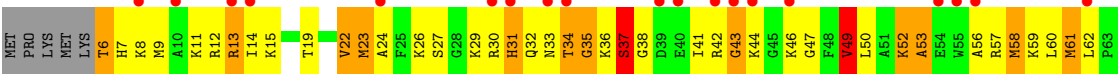
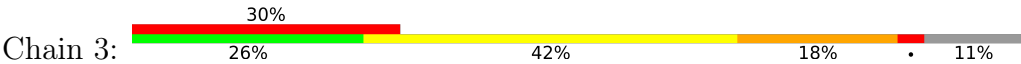
Chain 1: 20% 26% 54% 13% 6%



• Molecule 27: 50S ribosomal protein L34



• Molecule 28: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.47Å 407.38Å 692.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.58 29.84 – 3.58	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.84-3.58) 94.2 (29.84-3.58)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.247 0.203 , 0.246	Depositor DCC
R_{free} test set	13397 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83681	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6O1, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	X	0.37	0/63887	0.56	5/99650 (0.0%)
2	Y	0.23	0/2863	0.42	0/4461
3	A	0.70	3/2011 (0.1%)	1.27	23/2708 (0.8%)
4	B	0.78	0/1567	1.29	16/2105 (0.8%)
5	C	0.67	1/1504 (0.1%)	1.26	19/2036 (0.9%)
6	D	0.40	0/1419	0.92	3/1903 (0.2%)
7	E	0.44	0/1308	0.94	2/1771 (0.1%)
8	G	0.63	0/1138	1.25	16/1539 (1.0%)
9	H	0.77	1/1007 (0.1%)	1.15	5/1352 (0.4%)
10	I	0.82	0/1022	1.45	15/1366 (1.1%)
11	J	0.66	1/1101 (0.1%)	1.22	14/1472 (1.0%)
12	K	0.88	1/886 (0.1%)	1.34	12/1188 (1.0%)
13	L	0.55	0/785	1.09	3/1048 (0.3%)
14	M	0.88	1/872 (0.1%)	1.34	11/1172 (0.9%)
15	N	0.67	0/994	1.15	9/1323 (0.7%)
16	O	0.55	0/750	1.19	6/1000 (0.6%)
17	P	0.74	0/1027	1.19	6/1373 (0.4%)
18	Q	0.66	0/737	1.41	6/988 (0.6%)
19	R	0.61	1/835 (0.1%)	1.25	15/1121 (1.3%)
20	S	0.46	0/1399	0.99	7/1902 (0.4%)
21	T	0.55	0/563	1.18	4/747 (0.5%)
22	U	0.59	0/556	1.08	2/741 (0.3%)
23	V	0.42	0/529	0.89	0/704
24	W	0.56	0/426	0.98	2/568 (0.4%)
25	Z	0.75	0/464	1.36	8/622 (1.3%)
26	1	0.67	0/434	1.39	10/579 (1.7%)
27	2	0.78	0/387	1.55	9/509 (1.8%)
28	3	0.74	0/468	1.46	9/614 (1.5%)
All	All	0.46	9/90939 (0.0%)	0.76	237/136562 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
4	B	0	1
5	C	0	2
8	G	0	4
10	I	0	5
11	J	0	1
13	L	0	1
15	N	0	2
19	R	0	1
25	Z	0	1
27	2	0	3
28	3	0	2
All	All	0	24

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	29	PRO	CA-C	9.62	1.66	1.52
3	A	20	ASP	N-CA	7.46	1.55	1.46
5	C	51	VAL	CA-CB	6.51	1.64	1.54
12	K	12	ARG	CA-C	6.32	1.61	1.52
3	A	20	ASP	CA-C	5.92	1.60	1.52
11	J	19	THR	CA-C	5.53	1.59	1.52
19	R	94	VAL	CA-CB	5.38	1.59	1.54
3	A	35	GLU	CA-C	5.25	1.58	1.53
9	H	2	ILE	CA-CB	-5.02	1.48	1.54

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	58	VAL	CA-C-N	16.57	136.47	119.24
18	Q	58	VAL	C-N-CA	16.57	136.47	119.24
3	A	35	GLU	N-CA-C	14.34	127.69	110.91
17	P	60	ILE	CA-C-N	13.30	132.86	119.82
17	P	60	ILE	C-N-CA	13.30	132.86	119.82
27	2	38	GLY	N-CA-C	-12.02	100.54	111.95
12	K	90	ARG	CA-C-N	11.42	134.11	119.84
12	K	90	ARG	C-N-CA	11.42	134.11	119.84
3	A	245	VAL	CA-C-N	11.34	134.01	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	245	VAL	C-N-CA	11.34	134.01	119.84
16	O	11	GLN	N-CA-C	10.70	123.84	108.00
10	I	47	ALA	N-CA-C	10.69	126.64	113.17
10	I	56	LEU	N-CA-C	10.53	125.70	113.38
18	Q	61	LYS	N-CA-C	10.18	122.81	110.91
10	I	22	GLY	CA-C-N	9.87	131.41	120.66
10	I	22	GLY	C-N-CA	9.87	131.41	120.66
4	B	179	GLU	N-CA-C	-9.78	100.85	113.17
14	M	57	ILE	N-CA-C	9.69	121.38	112.17
28	3	37	SER	N-CA-C	9.62	125.18	109.02
10	I	51	GLY	N-CA-C	9.42	132.20	115.80
5	C	81	GLY	N-CA-C	-9.36	97.44	111.10
11	J	81	GLU	N-CA-C	9.29	120.92	108.38
14	M	59	GLY	N-CA-C	9.26	120.75	111.95
25	Z	33	CYS	CA-C-N	9.24	128.87	119.82
25	Z	33	CYS	C-N-CA	9.24	128.87	119.82
3	A	44	ASN	N-CA-C	9.05	121.23	111.36
11	J	48	ILE	N-CA-C	-8.98	103.03	111.48
27	2	40	HIS	N-CA-C	-8.88	96.09	109.86
21	T	17	ASN	CA-C-N	8.79	128.44	119.56
21	T	17	ASN	C-N-CA	8.79	128.44	119.56
26	1	37	LEU	N-CA-C	8.79	123.16	110.24
6	D	118	ASN	CA-C-N	8.36	128.00	119.56
6	D	118	ASN	C-N-CA	8.36	128.00	119.56
14	M	28	ARG	N-CA-C	-8.36	91.34	109.81
1	X	1975	G	C2'-C3'-O3'	8.34	122.01	109.50
10	I	62	LYS	N-CA-C	8.34	122.15	109.23
3	A	31	LYS	N-CA-C	8.24	122.33	109.07
3	A	34	THR	N-CA-C	8.17	121.83	108.26
28	3	35	GLY	N-CA-C	-8.09	103.50	115.72
8	G	86	ALA	N-CA-C	-8.05	102.90	112.89
26	1	5	GLY	CA-C-N	8.05	127.71	119.82
26	1	5	GLY	C-N-CA	8.05	127.71	119.82
10	I	54	SER	N-CA-C	-7.93	103.63	113.38
28	3	43	GLY	N-CA-C	7.74	123.04	110.97
18	Q	59	PRO	N-CA-C	7.72	126.28	113.78
10	I	53	ARG	N-CA-C	7.60	120.88	108.26
21	T	14	ARG	N-CA-C	7.59	122.12	112.86
4	B	188	ILE	CA-C-N	-7.59	112.66	120.85
4	B	188	ILE	C-N-CA	-7.59	112.66	120.85
10	I	58	ALA	N-CA-C	-7.58	100.78	110.19
5	C	131	LYS	N-CA-C	-7.58	102.69	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	134	TRP	N-CA-C	-7.51	98.37	110.32
19	R	12	ASP	N-CA-C	-7.43	103.52	112.58
8	G	109	GLY	N-CA-C	-7.37	104.67	114.25
14	M	24	LEU	CA-C-N	7.36	127.41	119.90
14	M	24	LEU	C-N-CA	7.36	127.41	119.90
3	A	30	GLU	N-CA-C	7.34	119.50	110.91
19	R	26	SER	CB-CA-C	-7.24	106.33	115.89
3	A	21	PHE	N-CA-C	7.20	126.14	110.80
8	G	33	ILE	CA-C-N	-7.20	112.51	120.14
8	G	33	ILE	C-N-CA	-7.20	112.51	120.14
5	C	74	VAL	CA-C-N	7.13	127.74	119.47
5	C	74	VAL	C-N-CA	7.13	127.74	119.47
5	C	59	TYR	CB-CA-C	-7.05	107.41	115.79
13	L	53	ALA	N-CA-C	7.03	119.14	110.91
15	N	102	GLU	CA-C-N	7.01	126.49	118.85
15	N	102	GLU	C-N-CA	7.01	126.49	118.85
4	B	142	GLY	N-CA-C	7.01	121.20	112.79
28	3	41	ILE	CB-CA-C	-6.93	103.09	111.97
24	W	14	GLY	N-CA-C	6.93	120.54	112.50
26	1	7	ARG	N-CA-C	6.91	118.75	110.19
16	O	30	GLY	N-CA-C	-6.80	97.07	113.18
14	M	103	LYS	N-CA-C	6.74	121.16	112.12
8	G	117	GLU	N-CA-C	-6.71	103.89	111.07
25	Z	30	LEU	N-CA-C	6.67	118.72	110.91
3	A	120	GLY	CA-C-N	6.64	126.23	119.19
3	A	120	GLY	C-N-CA	6.64	126.23	119.19
3	A	24	LEU	N-CA-C	6.59	124.83	110.80
15	N	90	LEU	N-CA-C	-6.56	99.74	108.34
20	S	119	ASN	N-CA-C	6.56	118.59	110.91
3	A	261	ARG	N-CA-C	6.55	117.23	108.38
26	1	41	ASP	CA-C-N	6.55	128.03	119.84
26	1	41	ASP	C-N-CA	6.55	128.03	119.84
5	C	13	ARG	N-CA-C	-6.51	105.33	113.28
3	A	211	ARG	N-CA-C	-6.49	103.71	111.69
11	J	19	THR	N-CA-C	6.48	119.16	108.99
14	M	30	GLY	N-CA-C	-6.45	97.89	113.18
3	A	240	THR	N-CA-C	6.45	116.75	108.24
19	R	84	VAL	N-CA-C	6.45	116.91	107.37
12	K	7	GLY	N-CA-C	6.44	128.44	113.18
19	R	111	GLY	N-CA-C	6.43	120.15	111.72
21	T	44	LYS	N-CA-C	-6.42	104.14	112.23
16	O	11	GLN	CB-CA-C	-6.42	107.36	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	58	GLY	N-CA-C	6.41	122.31	114.69
4	B	122	PHE	CB-CA-C	-6.40	107.45	115.89
15	N	89	ASP	N-CA-C	6.38	119.64	109.24
5	C	170	LEU	CA-C-N	6.36	126.33	119.78
5	C	170	LEU	C-N-CA	6.36	126.33	119.78
8	G	103	TYR	N-CA-C	6.31	118.73	108.26
7	E	7	GLN	N-CA-C	6.29	120.78	112.35
11	J	81	GLU	CA-C-N	6.28	133.54	121.54
11	J	81	GLU	C-N-CA	6.28	133.54	121.54
27	2	42	LEU	N-CA-C	6.28	119.88	109.96
19	R	85	ASP	N-CA-C	6.24	120.71	112.35
5	C	5	ASN	N-CA-C	6.24	118.57	110.53
19	R	52	ASN	N-CA-C	6.21	118.40	109.14
5	C	144	GLY	N-CA-C	-6.19	106.78	115.32
11	J	95	VAL	N-CA-C	6.18	118.03	109.45
8	G	70	PHE	N-CA-C	6.17	120.75	113.23
9	H	99	ILE	N-CA-C	6.13	116.30	108.82
19	R	31	GLY	N-CA-C	-6.13	106.06	114.64
11	J	15	ARG	N-CA-C	6.07	117.46	108.60
26	1	48	VAL	N-CA-C	6.06	117.48	108.46
10	I	91	ASP	N-CA-C	6.03	120.63	113.28
25	Z	13	LYS	N-CA-C	-6.02	104.83	111.82
11	J	11	ARG	N-CA-C	6.00	115.76	107.73
27	2	40	HIS	CA-C-N	-6.00	112.30	123.03
27	2	40	HIS	C-N-CA	-6.00	112.30	123.03
11	J	13	GLN	N-CA-C	5.99	122.61	113.51
5	C	163	ASN	N-CA-C	-5.98	101.34	109.95
28	3	37	SER	CB-CA-C	-5.98	108.00	115.89
5	C	152	THR	N-CA-C	5.97	117.34	107.73
15	N	6	THR	N-CA-C	-5.97	105.98	113.20
27	2	38	GLY	CA-C-O	-5.97	118.34	122.22
1	X	2705	A	C4'-C3'-O3'	5.96	118.34	109.40
20	S	76	ARG	N-CA-C	-5.95	105.68	113.17
12	K	94	TYR	N-CA-C	-5.94	105.89	113.02
27	2	26	SER	N-CA-C	-5.93	104.89	111.36
27	2	30	ILE	CB-CA-C	-5.91	104.16	112.14
12	K	83	VAL	N-CA-C	5.90	116.02	110.30
4	B	143	GLN	N-CA-C	-5.84	100.53	109.41
3	A	231	HIS	CA-C-N	5.83	125.97	119.32
3	A	231	HIS	C-N-CA	5.83	125.97	119.32
26	1	36	GLU	CA-C-N	5.82	129.37	121.05
26	1	36	GLU	C-N-CA	5.82	129.37	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	31	ASP	N-CA-C	5.82	119.09	110.48
12	K	14	SER	N-CA-C	5.80	118.48	111.40
20	S	9	THR	CA-C-N	5.79	125.32	119.19
20	S	9	THR	C-N-CA	5.79	125.32	119.19
18	Q	75	ARG	N-CA-C	5.77	118.96	109.85
9	H	43	ARG	N-CA-C	5.76	117.56	111.28
5	C	165	SER	N-CA-C	-5.76	106.25	113.28
14	M	20	HIS	N-CA-C	-5.74	101.16	109.31
3	A	210	GLY	N-CA-C	-5.73	108.14	115.42
8	G	104	THR	N-CA-C	5.72	118.72	109.79
8	G	96	ASP	N-CA-C	-5.72	100.73	109.65
16	O	9	GLY	N-CA-C	5.71	121.28	111.98
15	N	43	ALA	N-CA-C	-5.70	104.76	110.97
4	B	137	ARG	CA-C-N	5.69	126.01	119.92
4	B	137	ARG	C-N-CA	5.69	126.01	119.92
3	A	22	SER	N-CA-C	5.67	116.86	108.86
4	B	23	VAL	CB-CA-C	-5.67	103.42	111.19
1	X	1391	A	C4'-C3'-O3'	5.67	117.90	109.40
5	C	77	PHE	N-CA-C	-5.66	99.38	108.55
11	J	133	VAL	N-CA-C	5.63	115.40	108.53
15	N	38	THR	CB-CA-C	-5.63	99.22	110.42
19	R	70	GLU	N-CA-C	5.60	118.11	110.55
22	U	49	LYS	N-CA-C	5.60	116.76	108.86
19	R	6	ALA	N-CA-C	5.60	122.73	110.80
1	X	2705	A	P-O3'-C3'	5.60	128.59	120.20
11	J	73	LYS	CA-C-N	-5.56	113.83	119.83
11	J	73	LYS	C-N-CA	-5.56	113.83	119.83
5	C	9	GLN	N-CA-C	5.55	117.08	110.19
4	B	172	VAL	CB-CA-C	-5.54	104.60	111.08
12	K	90	ARG	N-CA-C	5.53	117.58	110.39
28	3	23	MET	N-CA-C	5.52	117.64	108.20
11	J	87	GLY	N-CA-C	-5.50	105.04	112.14
8	G	108	GLY	N-CA-C	-5.49	100.76	111.03
9	H	44	TYR	N-CA-C	5.49	118.51	109.72
1	X	2018	G	O4'-C1'-N9	5.49	116.43	108.20
4	B	123	ALA	N-CA-C	5.49	122.49	110.80
13	L	92	GLY	N-CA-C	-5.47	104.80	112.13
3	A	20	ASP	N-CA-C	5.43	122.38	110.80
25	Z	52	TYR	CA-C-N	5.42	131.89	121.54
25	Z	52	TYR	C-N-CA	5.42	131.89	121.54
17	P	20	LEU	N-CA-C	5.40	117.22	110.91
3	A	216	GLY	CA-C-N	-5.35	111.33	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	216	GLY	C-N-CA	-5.35	111.33	121.54
15	N	37	GLN	N-CA-C	-5.34	103.84	110.41
19	R	64	ASN	CA-C-N	5.34	124.79	119.24
19	R	64	ASN	C-N-CA	5.34	124.79	119.24
5	C	17	LEU	CA-C-N	5.32	125.62	119.93
5	C	17	LEU	C-N-CA	5.32	125.62	119.93
8	G	105	GLY	CA-C-N	-5.31	115.36	122.42
8	G	105	GLY	C-N-CA	-5.31	115.36	122.42
10	I	141	VAL	N-CA-C	5.31	116.12	108.48
8	G	112	THR	N-CA-C	5.30	117.46	108.02
14	M	3	THR	CA-C-N	-5.29	115.97	122.84
14	M	3	THR	C-N-CA	-5.29	115.97	122.84
18	Q	74	ASP	N-CA-C	5.29	122.06	110.80
5	C	67	ALA	N-CA-C	5.28	115.21	108.24
28	3	49	VAL	N-CA-C	5.28	116.62	108.44
24	W	47	VAL	N-CA-C	5.26	116.59	111.91
4	B	128	SER	N-CA-C	5.25	119.84	113.38
16	O	14	VAL	N-CA-C	5.24	115.51	108.17
11	J	14	PHE	N-CA-C	5.24	115.97	108.74
22	U	54	ASN	N-CA-C	5.23	116.94	108.26
17	P	109	ARG	N-CA-C	5.22	116.91	109.14
26	1	19	GLY	N-CA-C	-5.21	101.51	112.04
19	R	10	HIS	N-CA-C	-5.19	102.77	110.46
4	B	115	GLY	N-CA-C	-5.17	104.68	112.60
20	S	126	GLY	CA-C-N	5.17	125.33	119.90
20	S	126	GLY	C-N-CA	5.17	125.33	119.90
9	H	130	ALA	CA-C-N	5.16	124.34	118.97
9	H	130	ALA	C-N-CA	5.16	124.34	118.97
5	C	60	GLY	N-CA-C	5.15	125.39	113.18
10	I	84	GLU	CB-CA-C	-5.15	109.66	115.79
4	B	201	ALA	N-CA-C	5.15	117.50	110.24
8	G	142	ARG	N-CA-C	-5.14	104.94	111.11
6	D	4	LEU	CB-CA-C	-5.13	110.25	117.23
10	I	61	PRO	CA-C-N	-5.13	113.82	122.29
10	I	61	PRO	C-N-CA	-5.13	113.82	122.29
12	K	108	VAL	CB-CA-C	-5.13	104.55	110.91
4	B	158	GLY	N-CA-C	5.13	118.03	110.80
13	L	44	ASP	N-CA-C	-5.12	104.11	110.41
10	I	61	PRO	CA-C-O	-5.12	116.01	123.07
12	K	5	LYS	CA-C-N	5.12	129.83	121.74
12	K	5	LYS	C-N-CA	5.12	129.83	121.74
3	A	20	ASP	N-CA-CB	5.12	119.14	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	111	LYS	N-CA-C	5.11	117.74	109.40
8	G	100	TYR	N-CA-C	-5.11	102.72	110.28
12	K	10	LEU	CA-CB-CG	5.08	134.08	116.30
28	3	58	MET	N-CA-C	-5.07	105.88	111.71
15	N	40	LEU	N-CA-C	-5.07	105.22	111.40
19	R	32	GLN	N-CA-C	-5.07	103.24	110.59
27	2	43	THR	N-CA-C	5.06	116.87	111.36
7	E	21	ASP	CB-CA-C	-5.06	110.35	117.23
20	S	47	SER	N-CA-C	5.06	115.49	108.00
17	P	41	VAL	CB-CA-C	-5.05	105.40	112.02
25	Z	6	VAL	CA-C-N	5.04	125.48	120.14
25	Z	6	VAL	C-N-CA	5.04	125.48	120.14
17	P	27	VAL	N-CA-C	5.03	115.90	108.45
28	3	53	ALA	N-CA-C	-5.03	105.69	111.07
3	A	216	GLY	N-CA-C	-5.03	102.92	112.27
14	M	100	ARG	N-CA-C	5.02	119.55	113.38
19	R	59	LYS	CA-C-N	5.01	124.46	119.24
19	R	59	LYS	C-N-CA	5.01	124.46	119.24

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	2	4	THR	Peptide
27	2	40	HIS	Peptide
27	2	6	GLN	Peptide
28	3	37	SER	Peptide
28	3	44	LYS	Peptide
3	A	58	HIS	Peptide
4	B	122	PHE	Peptide
5	C	176	ASN	Peptide
5	C	66	ASN	Peptide
8	G	105	GLY	Peptide
8	G	109	GLY	Peptide
8	G	111	LYS	Peptide
8	G	34	PRO	Peptide
10	I	31	GLY	Peptide
10	I	36	GLY	Peptide
10	I	38	LYS	Peptide
10	I	53	ARG	Peptide
10	I	55	ARG	Peptide
11	J	26	ASP	Peptide

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Mol	Chain	Res	Type	Group
13	L	97	HIS	Peptide
15	N	93	LYS	Peptide
15	N	94	VAL	Peptide
19	R	64	ASN	Peptide
25	Z	3	LYS	Peptide

5.2 Too-close contacts [i](#)

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	X	57052	0	28750	1266	0
2	Y	2561	0	1306	57	0
3	A	1973	0	2034	136	0
4	B	1539	0	1600	85	0
5	C	1481	0	1504	99	0
6	D	1400	0	1481	61	0
7	E	1286	0	1336	31	0
8	G	1114	0	1144	83	0
9	H	997	0	1046	58	0
10	I	1011	0	1047	77	0
11	J	1078	0	1103	48	0
12	K	878	0	930	36	0
13	L	779	0	820	50	0
14	M	859	0	872	35	0
15	N	978	0	1020	73	0
16	O	741	0	756	34	0
17	P	1014	0	1096	51	0
18	Q	726	0	753	31	0
19	R	825	0	881	59	0
20	S	1374	0	1401	48	0
21	T	556	0	579	25	0
22	U	552	0	604	43	0
23	V	525	0	546	14	0
24	W	424	0	470	17	0
25	Z	452	0	457	36	0
26	1	427	0	445	36	0
27	2	383	0	414	38	0
28	3	462	0	506	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	X	111	0	0	2	0
30	K	2	0	0	0	0
30	M	1	0	0	0	0
30	X	119	0	0	0	0
30	Y	1	0	0	0	0
All	All	83681	0	54901	2321	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 17.

All (2321) 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)
8:G:100:TYR:HB2	8:G:116:ARG:HE	1.25	0.96
10:I:56:LEU:H	10:I:59:ARG:HD3	1.30	0.94
1:X:1277:G:OP1	25:Z:19:ARG:NH2	2.01	0.93
1:X:1264:C:H5''	15:N:13:ARG:HH12	1.34	0.93
15:N:66:ASN:HB3	15:N:76:TYR:HB2	1.48	0.92
1:X:608:G:H1'	10:I:21:ARG:HG3	1.52	0.91
1:X:971:A:H61	11:J:83:ARG:HH22	1.16	0.89
1:X:177:U:O2'	1:X:178:C:O5'	1.90	0.88
1:X:2033:C:H1'	4:B:156:MET:HE1	1.56	0.88
1:X:2598:C:OP1	4:B:152:LYS:NZ	2.07	0.87
1:X:1030:U:H3	1:X:1153:A:H62	1.23	0.87
1:X:2016:A:O2'	1:X:2018:G:OP2	1.94	0.85
26:1:12:MET:SD	26:1:13:GLU:N	2.50	0.85
1:X:796:A:H8	1:X:797:A:H4'	1.40	0.85
1:X:640:C:H4'	1:X:660:G:H21	1.40	0.85
4:B:77:ILE:HD13	4:B:195:LEU:HD22	1.59	0.85
1:X:538:A:O2'	1:X:539:A:O5'	1.95	0.84
1:X:1882:G:H21	1:X:1885:C:H41	1.26	0.83
17:P:45:ILE:HD11	17:P:57:LEU:HD11	1.58	0.83
1:X:1562:G:H5'	1:X:1563:U:H5'	1.61	0.82
1:X:824:U:H2'	10:I:30:ALA:HA	1.59	0.82
1:X:1322:G:H4'	27:2:7:PRO:HB2	1.61	0.82
1:X:2039:G:N2	25:Z:4:HIS:O	2.12	0.82
1:X:2757:G:H5''	1:X:2758:A:H5'	1.60	0.82
19:R:84:VAL:HG11	19:R:90:LYS:H	1.44	0.82
15:N:95:LEU:HA	15:N:98:ILE:HD13	1.62	0.81
16:O:5:ILE:HG23	16:O:10:LYS:HZ2	1.45	0.81
10:I:41:SER:OG	10:I:45:LYS:NZ	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:332:C:O2	5:C:159:ARG:NH2	2.14	0.81
1:X:2653:A:O2'	9:H:41:ASN:ND2	2.14	0.81
3:A:145:LEU:HB3	3:A:155:LEU:HB2	1.62	0.81
1:X:339:U:H4'	19:R:77:HIS:CD2	2.16	0.80
1:X:339:U:H4'	19:R:77:HIS:HD2	1.45	0.80
1:X:2218:G:H5'	3:A:249:PRO:HD3	1.62	0.80
1:X:2796:A:OP2	12:K:3:HIS:NE2	2.15	0.79
1:X:215:G:H21	1:X:632:A:H8	1.27	0.79
19:R:80:LYS:NZ	19:R:81:VAL:O	2.13	0.79
8:G:73:ASN:O	8:G:140:GLN:NE2	2.16	0.78
1:X:2638:G:OP1	7:E:158:HIS:NE2	2.17	0.78
28:3:37:SER:OG	28:3:38:GLY:N	2.16	0.78
4:B:194:GLY:HA2	14:M:2:GLN:HB3	1.65	0.78
6:D:13:ARG:HG3	6:D:28:VAL:HG21	1.63	0.78
7:E:56:SER:HG	7:E:61:HIS:HD1	1.28	0.78
1:X:596:C:N3	10:I:37:GLN:NE2	2.32	0.78
4:B:143:GLN:HB2	4:B:147:PRO:HG3	1.65	0.78
1:X:841:G:H2'	1:X:842:A:C8	2.19	0.78
1:X:1007:A:H4'	15:N:93:LYS:HZ3	1.49	0.77
1:X:89:A:O2'	1:X:91:A:N6	2.18	0.77
13:L:26:ARG:NH1	13:L:86:GLN:O	2.17	0.77
1:X:2237:C:O2'	1:X:2406:C:OP2	2.00	0.77
13:L:11:LEU:HD12	13:L:93:SER:HB3	1.65	0.77
1:X:1278:A:H2	1:X:1997:A:H62	1.32	0.77
1:X:1337:G:OP2	17:P:105:ARG:NH1	2.18	0.77
1:X:2660:C:H42	1:X:2705:A:H2	1.31	0.76
9:H:88:THR:HB	14:M:80:VAL:HB	1.67	0.76
1:X:923:A:N7	11:J:12:LYS:HG2	1.99	0.76
1:X:1617:G:OP2	18:Q:57:ASN:ND2	2.18	0.76
1:X:1834:G:O2'	3:A:244:ARG:NH2	2.19	0.76
3:A:246:PRO:HD2	3:A:251:GLY:H	1.49	0.76
9:H:29:ILE:HG21	9:H:122:ARG:HB2	1.68	0.76
10:I:33:GLY:HA2	16:O:79:GLN:HG3	1.68	0.76
19:R:59:LYS:HB3	19:R:62:MET:HB2	1.68	0.76
1:X:2029:G:OP1	25:Z:15:LYS:NZ	2.16	0.76
3:A:172:TYR:HA	3:A:186:HIS:HA	1.68	0.76
9:H:124:MET:HA	9:H:127:VAL:HB	1.68	0.75
2:Y:46:G:N3	2:Y:49:C:N4	2.34	0.75
8:G:31:THR:HG22	15:N:61:TRP:CH2	2.22	0.75
8:G:67:ARG:HB2	8:G:70:PHE:HA	1.69	0.75
16:O:34:GLU:HB2	16:O:56:VAL:HG23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2672:U:H2'	1:X:2673:G:H8	1.50	0.75
1:X:1373:G:H22	1:X:2192:U:H3	1.35	0.74
1:X:2474:G:H5''	11:J:82:THR:HA	1.69	0.74
17:P:101:PRO:O	17:P:121:THR:OG1	2.05	0.74
1:X:989:G:HO2'	1:X:1013:G:HO2'	1.29	0.74
2:Y:42:U:O2'	2:Y:47:A:N6	2.20	0.74
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.69	0.74
1:X:2043:A:H62	5:C:68:ARG:HH12	1.36	0.74
15:N:92:ARG:HB3	15:N:95:LEU:HD22	1.69	0.74
1:X:1348:C:OP2	18:Q:62:ARG:NH1	2.21	0.74
24:W:2:LYS:HB3	24:W:54:GLN:HB3	1.69	0.74
1:X:1222:G:O2'	1:X:1250:A:N6	2.21	0.74
20:S:69:VAL:HG13	20:S:81:VAL:HG22	1.70	0.73
1:X:954:U:OP2	10:I:38:LYS:NZ	2.17	0.73
3:A:205:VAL:HG12	3:A:207:GLY:H	1.50	0.73
9:H:76:ARG:NH1	9:H:113:PRO:O	2.20	0.73
3:A:108:PRO:HA	3:A:196:VAL:HA	1.71	0.73
1:X:1769:U:H2'	1:X:1775:A:H62	1.53	0.73
1:X:2551:A:H5''	1:X:2553:G:H4'	1.68	0.73
3:A:250:TRP:O	3:A:255:LYS:NZ	2.19	0.73
1:X:1283:C:H5''	1:X:1284:G:H5'	1.71	0.72
1:X:2059:U:OP2	1:X:2217:G:N2	2.20	0.72
1:X:2556:A:H5''	1:X:2557:G:H5'	1.71	0.72
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.71	0.72
1:X:492:G:O2'	1:X:517:A:N6	2.22	0.72
1:X:2170:C:H3'	1:X:2171:U:H5''	1.70	0.72
4:B:60:ASN:HB3	4:B:62:PRO:HD2	1.70	0.72
9:H:70:VAL:HG21	9:H:98:ILE:HG23	1.72	0.72
10:I:56:LEU:HB3	28:3:52:LYS:HZ2	1.55	0.72
22:U:19:ILE:HA	22:U:42:GLN:HA	1.72	0.72
2:Y:27:A:N6	2:Y:56:G:OP2	2.23	0.72
1:X:168:A:H2'	1:X:169:C:C6	2.25	0.71
1:X:558:G:H8	1:X:560:G:C8	2.08	0.71
1:X:2450:A:N3	29:X:2901:6O1:O30	2.23	0.71
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.71	0.71
3:A:45:ASN:OD1	3:A:46:ARG:NH1	2.22	0.71
9:H:113:PRO:HD3	14:M:73:PHE:HB2	1.72	0.71
1:X:1264:C:H5''	15:N:13:ARG:NH1	2.05	0.71
1:X:2545:A:H61	9:H:40:GLY:HA3	1.56	0.71
1:X:2716:G:H1	1:X:2748:C:H42	1.39	0.71
16:O:11:GLN:HE22	16:O:38:LEU:HB3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:89:A:H4'	1:X:90:G:H5'	1.73	0.71
1:X:160:C:O2'	1:X:445:A:N3	2.24	0.71
1:X:349:G:OP1	19:R:13:LYS:NZ	2.20	0.71
5:C:54:THR:HG21	5:C:72:ARG:HB2	1.72	0.71
12:K:29:LEU:HD13	12:K:79:VAL:HG11	1.73	0.71
21:T:23:VAL:HG13	21:T:38:VAL:HG23	1.71	0.71
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.56	0.71
1:X:408:U:H2'	1:X:409:G:C8	2.26	0.71
1:X:1079:G:N2	1:X:1106:A:O2'	2.24	0.71
1:X:1333:G:N2	1:X:1344:C:H41	1.88	0.70
1:X:2516:U:H2'	1:X:2517:C:C6	2.26	0.70
8:G:157:PRO:O	8:G:161:GLN:NE2	2.24	0.70
15:N:88:ILE:HG12	16:O:49:GLU:HB2	1.71	0.70
12:K:13:ASN:OD1	12:K:14:SER:N	2.24	0.70
22:U:27:ASP:HB3	22:U:32:ARG:HA	1.73	0.70
18:Q:62:ARG:O	18:Q:70:GLY:HA3	1.90	0.70
1:X:346:C:H2'	1:X:347:C:H6	1.55	0.70
1:X:2634:G:O2'	1:X:2635:U:OP2	2.09	0.70
3:A:168:LYS:HB3	3:A:173:VAL:HG13	1.73	0.70
1:X:242:A:N6	1:X:441:A:OP2	2.24	0.70
1:X:1007:A:H2'	1:X:1008:G:H8	1.55	0.70
1:X:1551:U:OP2	1:X:1553:G:N2	2.24	0.70
1:X:1922:U:OP1	1:X:2583:U:O2'	2.08	0.70
20:S:93:GLU:HG3	20:S:123:VAL:HG23	1.74	0.69
1:X:304:A:N6	1:X:356:A:N7	2.39	0.69
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.73	0.69
1:X:2400:G:N7	28:3:32:GLN:HB3	2.07	0.69
1:X:797:A:C5	3:A:229:VAL:HG21	2.27	0.69
2:Y:30:C:OP1	13:L:37:HIS:ND1	2.25	0.69
28:3:14:ILE:HD13	28:3:56:ALA:HB1	1.74	0.69
3:A:218:LYS:NZ	3:A:219:PRO:O	2.25	0.69
4:B:122:PHE:HE2	4:B:138:PRO:HB3	1.58	0.69
5:C:163:ASN:HB3	5:C:166:TRP:HB2	1.73	0.69
1:X:588:G:O2'	1:X:2002:A:OP1	2.07	0.69
2:Y:11:G:OP2	13:L:16:LYS:NZ	2.26	0.69
1:X:1422:C:H2'	1:X:1423:A:H8	1.58	0.69
10:I:18:ARG:HB3	10:I:21:ARG:HB2	1.74	0.69
1:X:854:G:H1	1:X:948:C:H42	1.39	0.69
8:G:149:LYS:NZ	8:G:160:ALA:O	2.26	0.69
17:P:25:PHE:HD1	17:P:127:ILE:HD11	1.58	0.69
1:X:1329:U:H2'	1:X:1330:G:H8	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1386:A:OP1	1:X:2191:A:N6	2.25	0.68
1:X:1810:U:OP2	3:A:157:ARG:NH1	2.25	0.68
1:X:1542:G:H22	1:X:1562:G:H1	1.39	0.68
17:P:25:PHE:HA	17:P:127:ILE:HG12	1.74	0.68
20:S:25:ASN:HB3	20:S:85:MET:HB2	1.74	0.68
22:U:53:GLU:HB3	22:U:58:LYS:H	1.57	0.68
1:X:1296:G:H22	1:X:1299:A:H5'	1.58	0.68
5:C:58:MET:HE2	5:C:59:TYR:HB2	1.75	0.68
13:L:15:ARG:HA	13:L:15:ARG:HH11	1.58	0.68
1:X:1124:U:H2'	1:X:1125:G:H8	1.58	0.68
22:U:54:ASN:HA	22:U:78:ILE:HG22	1.75	0.68
3:A:14:ARG:HH11	3:A:27:LYS:HB3	1.59	0.68
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.76	0.68
1:X:673:G:N3	10:I:21:ARG:NH2	2.41	0.68
20:S:3:LEU:HD13	20:S:32:PHE:HB3	1.75	0.68
3:A:245:VAL:HA	3:A:251:GLY:HA2	1.75	0.68
7:E:8:PRO:O	7:E:69:ARG:NH1	2.26	0.68
13:L:8:ARG:HG3	13:L:9:ARG:H	1.59	0.68
1:X:203:G:O2'	1:X:205:A:N6	2.26	0.68
1:X:2838:U:H2'	1:X:2839:G:H8	1.58	0.68
1:X:2551:A:C8	4:B:144:ARG:HG2	2.29	0.68
1:X:2659:C:H5'	4:B:189:PRO:HA	1.77	0.68
26:1:30:ASN:HD22	26:1:31:THR:H	1.41	0.67
1:X:863:C:HO2'	24:W:19:THR:HG1	1.38	0.67
1:X:2672:U:H2'	1:X:2673:G:C8	2.29	0.67
1:X:2786:G:H5''	4:B:60:ASN:HD22	1.59	0.67
1:X:346:C:H2'	1:X:347:C:C6	2.28	0.67
1:X:1054:C:H42	1:X:1123:G:H1	1.40	0.67
1:X:1850:G:O2'	1:X:1867:A:N6	2.27	0.67
1:X:2663:U:H3	1:X:2705:A:H62	1.39	0.67
8:G:41:TRP:HZ3	8:G:149:LYS:HD2	1.58	0.67
2:Y:52:G:OP1	13:L:65:THR:OG1	2.11	0.67
1:X:646:C:O2'	1:X:650:U:OP1	2.09	0.67
1:X:1678:G:H1	1:X:1982:C:H42	1.42	0.67
1:X:1684:G:O2'	1:X:1974:U:O4	2.11	0.67
1:X:1882:G:N2	1:X:1885:C:H41	1.93	0.67
1:X:64:C:OP1	18:Q:71:GLN:HB2	1.95	0.67
1:X:492:G:H1'	1:X:516:G:N2	2.10	0.67
1:X:1800:A:H4'	1:X:1801:C:OP1	1.95	0.67
10:I:18:ARG:O	10:I:18:ARG:NH2	2.27	0.67
10:I:56:LEU:HB3	28:3:52:LYS:NZ	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:76:ALA:HB2	13:L:107:ALA:HA	1.75	0.67
1:X:504:G:H4'	17:P:27:VAL:HG12	1.76	0.67
1:X:791:G:H5''	3:A:48:ARG:HB2	1.76	0.67
1:X:812:G:H3'	1:X:813:A:H2'	1.75	0.67
1:X:1340:C:O3'	12:K:104:ARG:NH2	2.28	0.67
1:X:1429:A:H1'	1:X:1603:A:C6	2.30	0.67
1:X:2372:A:H62	1:X:2401:A:H62	1.43	0.67
3:A:176:ARG:HH11	3:A:180:GLY:HA2	1.60	0.67
18:Q:63:LYS:HE3	18:Q:65:VAL:HA	1.77	0.67
1:X:712:A:H2'	1:X:713:G:O4'	1.94	0.66
1:X:953:G:O2'	1:X:1203:A:N3	2.27	0.66
6:D:72:LYS:HA	6:D:81:GLN:HA	1.77	0.66
6:D:119:PRO:HD3	6:D:178:ARG:HG3	1.77	0.66
1:X:746:G:N7	1:X:774:A:C6	2.63	0.66
2:Y:115:G:N2	13:L:48:GLY:O	2.28	0.66
5:C:136:TRP:O	5:C:140:ASN:ND2	2.27	0.66
8:G:103:TYR:C	8:G:107:GLN:HG3	2.21	0.66
3:A:244:ARG:HD2	3:A:253:PRO:HD3	1.78	0.66
2:Y:27:A:O2'	2:Y:28:A:O5'	2.12	0.66
5:C:129:LYS:O	5:C:131:LYS:N	2.28	0.66
13:L:54:ALA:H	13:L:75:LEU:HD13	1.60	0.66
1:X:1264:C:OP1	15:N:13:ARG:NH1	2.29	0.66
1:X:920:G:H21	11:J:11:ARG:HH22	1.44	0.66
15:N:74:MET:HE2	15:N:78:THR:HG22	1.77	0.66
25:Z:6:VAL:HG22	25:Z:7:PRO:HD2	1.77	0.66
1:X:761:G:H5''	17:P:110:ALA:HB2	1.78	0.66
1:X:1431:U:H4'	1:X:1604:A:H4'	1.78	0.66
4:B:131:SER:O	4:B:134:TRP:NE1	2.26	0.66
22:U:21:ARG:HA	22:U:39:LYS:HB2	1.77	0.66
1:X:88:G:H3'	1:X:89:A:H5''	1.78	0.66
1:X:83:A:H3'	19:R:17:LYS:HG2	1.78	0.65
1:X:1332:G:O2'	1:X:1333:G:H5'	1.96	0.65
1:X:1675:C:H2'	1:X:1676:U:C6	2.30	0.65
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.77	0.65
22:U:48:LYS:HE2	22:U:49:LYS:H	1.61	0.65
1:X:318:G:N2	1:X:321:A:OP2	2.28	0.65
11:J:21:ASP:HA	11:J:99:LYS:HE2	1.79	0.65
13:L:26:ARG:HH11	13:L:88:VAL:HG22	1.61	0.65
1:X:595:A:H5'	5:C:83:ALA:HB3	1.79	0.65
1:X:814:G:OP2	5:C:56:ARG:NH2	2.29	0.65
1:X:2064:U:H5'	22:U:41:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:3:GLN:H	5:C:12:GLY:HA3	1.62	0.65
8:G:100:TYR:CB	8:G:116:ARG:HE	2.06	0.65
1:X:786:U:H4'	3:A:47:GLY:HA2	1.78	0.65
3:A:43:ARG:HB3	3:A:54:ILE:HG13	1.78	0.65
21:T:26:PHE:N	21:T:29:GLU:OE1	2.29	0.65
5:C:11:GLY:O	5:C:13:ARG:NH1	2.30	0.65
10:I:80:LEU:O	10:I:116:ARG:NH2	2.30	0.65
3:A:56:GLY:H	3:A:217:ARG:HB2	1.60	0.65
15:N:61:TRP:CE2	15:N:94:VAL:HG22	2.32	0.65
1:X:540:G:C5	1:X:2005:U:H5''	2.32	0.65
1:X:1184:G:H3'	1:X:1185:C:H5''	1.79	0.65
5:C:95:LEU:O	5:C:100:ARG:NH2	2.30	0.65
1:X:679:C:H5''	10:I:49:PHE:HB3	1.77	0.65
21:T:45:PHE:HB3	21:T:77:ARG:HB2	1.79	0.65
1:X:1270:C:H5'	5:C:69:HIS:CE1	2.32	0.65
26:1:35:LEU:HA	26:1:53:LYS:HD2	1.78	0.65
1:X:692:C:H2'	1:X:693:A:H8	1.61	0.64
1:X:1342:U:H5''	1:X:1343:C:H5	1.62	0.64
10:I:88:PHE:HE1	10:I:118:VAL:HA	1.62	0.64
1:X:2481:G:H5'	1:X:2482:A:H5''	1.79	0.64
1:X:87:G:H2'	1:X:88:G:H5''	1.79	0.64
10:I:81:GLN:HG2	10:I:116:ARG:HB3	1.78	0.64
13:L:33:ARG:HH11	13:L:38:ILE:HG21	1.62	0.64
3:A:143:HIS:ND1	3:A:194:GLY:O	2.27	0.64
1:X:332:C:HO2'	1:X:351:A:HO2'	1.42	0.64
1:X:1443:G:H2'	1:X:1444:C:C6	2.33	0.64
19:R:84:VAL:HG21	19:R:89:GLY:HA2	1.78	0.64
1:X:2556:A:H1'	25:Z:4:HIS:HB3	1.79	0.64
1:X:2838:U:H2'	1:X:2839:G:C8	2.33	0.64
13:L:27:LEU:HB2	13:L:87:VAL:HG22	1.79	0.64
11:J:78:LYS:HD2	11:J:81:GLU:HA	1.80	0.64
1:X:1345:G:N7	1:X:1625:A:O2'	2.26	0.64
1:X:2766:U:OP1	4:B:69:LYS:NZ	2.28	0.64
3:A:203:ASN:OD1	3:A:203:ASN:N	2.28	0.64
1:X:1685:A:O2'	1:X:1691:G:N7	2.28	0.64
1:X:2811:G:H2'	1:X:2812:A:C8	2.32	0.64
6:D:60:ILE:HG13	6:D:61:THR:HG23	1.79	0.64
8:G:84:ASN:O	8:G:152:ALA:HA	1.97	0.64
19:R:97:GLN:HB3	19:R:101:GLY:HA2	1.80	0.64
1:X:1674:C:H2'	1:X:1675:C:C6	2.33	0.63
1:X:1744:G:N2	1:X:1747:G:OP2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1296:G:N2	1:X:1299:A:H5'	2.13	0.63
22:U:47:HIS:ND1	22:U:48:LYS:O	2.32	0.63
1:X:1007:A:H1'	16:O:6:GLN:HG3	1.80	0.63
1:X:1791:C:OP1	3:A:261:ARG:NH2	2.29	0.63
1:X:2371:A:C8	10:I:59:ARG:HG2	2.33	0.63
1:X:946:U:H2'	1:X:947:C:C6	2.33	0.63
22:U:21:ARG:HE	22:U:40:ARG:HG2	1.64	0.63
1:X:2324:G:N3	1:X:2360:C:H2'	2.14	0.63
2:Y:7:C:O2'	2:Y:29:C:O2	2.16	0.63
10:I:62:LYS:HD3	10:I:63:ARG:H	1.64	0.63
19:R:81:VAL:HG12	19:R:82:ALA:H	1.64	0.63
1:X:796:A:C8	1:X:797:A:H4'	2.28	0.63
1:X:2222:U:H2'	1:X:2223:U:C6	2.34	0.63
1:X:2796:A:H2'	1:X:2797:G:H8	1.64	0.63
1:X:876:A:H2	1:X:926:C:H41	1.46	0.63
6:D:4:LEU:HD22	6:D:173:MET:HE1	1.81	0.63
7:E:103:LEU:HD21	7:E:131:ILE:HD13	1.80	0.63
16:O:56:VAL:HG12	16:O:97:GLY:HA3	1.79	0.63
26:1:51:ARG:NH2	26:1:53:LYS:O	2.32	0.63
1:X:1003:C:H2'	1:X:1004:A:H8	1.63	0.63
1:X:1223:G:H5'	1:X:1225:G:O4'	1.98	0.63
1:X:649:G:C6	1:X:662:G:N2	2.67	0.62
1:X:938:G:H4'	1:X:939:C:H5'	1.81	0.62
1:X:2240:C:N4	21:T:14:ARG:O	2.32	0.62
20:S:138:VAL:HB	20:S:141:MET:HE2	1.81	0.62
3:A:223:GLY:HA2	3:A:226:MET:HE3	1.81	0.62
8:G:61:ARG:NH1	8:G:66:HIS:H	1.97	0.62
25:Z:18:MET:O	25:Z:21:SER:HB3	1.98	0.62
1:X:830:C:O2'	1:X:852:U:OP1	2.17	0.62
3:A:25:THR:HG23	3:A:211:ARG:HH12	1.65	0.62
4:B:37:LYS:NZ	4:B:80:GLU:OE2	2.29	0.62
4:B:117:MET:HA	4:B:121:ASN:O	1.99	0.62
19:R:16:PHE:HZ	19:R:46:VAL:HG21	1.64	0.62
19:R:48:VAL:HG13	19:R:50:GLY:H	1.64	0.62
1:X:824:U:C2'	10:I:30:ALA:HA	2.30	0.62
20:S:51:LEU:HD23	20:S:51:LEU:H	1.64	0.62
5:C:39:ARG:HH21	5:C:91:TYR:HB2	1.64	0.62
6:D:74:ILE:HA	6:D:79:LEU:HB3	1.81	0.62
1:X:564:U:H2'	1:X:565:A:C8	2.34	0.62
16:O:5:ILE:HG23	16:O:10:LYS:NZ	2.14	0.62
1:X:824:U:H2'	10:I:30:ALA:CA	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:96:HIS:HE1	3:A:100:GLY:HA2	1.65	0.62
29:X:2901:6O1:O57	29:X:2901:6O1:O52	2.15	0.62
20:S:50:GLY:HA2	20:S:130:ILE:HD12	1.82	0.62
1:X:172:A:H61	1:X:175:C:H3'	1.65	0.62
1:X:403:A:H4'	1:X:404:A:H5'	1.82	0.62
1:X:2579:A:H2'	1:X:2580:C:C6	2.35	0.62
1:X:2693:U:OP1	12:K:14:SER:HB3	2.00	0.61
21:T:64:ASP:OD1	21:T:64:ASP:N	2.32	0.61
5:C:149:LEU:HD11	5:C:170:LEU:HB2	1.83	0.61
23:V:6:MET:HE1	23:V:52:GLN:HB3	1.82	0.61
1:X:825:C:H5''	10:I:30:ALA:HB1	1.82	0.61
1:X:1052:C:N4	1:X:1053:G:N7	2.48	0.61
1:X:2372:A:H62	1:X:2401:A:N6	1.99	0.61
4:B:35:GLN:HB3	4:B:48:GLN:HB3	1.82	0.61
22:U:19:ILE:HG22	22:U:42:GLN:HG3	1.82	0.61
22:U:52:ARG:HG3	22:U:62:LEU:HD22	1.81	0.61
3:A:184:ARG:HD2	3:A:266:SER:HA	1.82	0.61
14:M:31:ASP:N	14:M:31:ASP:OD1	2.31	0.61
1:X:872:G:O2'	1:X:928:G:O6	2.17	0.61
1:X:1584:G:H5''	3:A:61:LEU:HG	1.82	0.61
11:J:49:GLU:OE2	11:J:52:ARG:NH2	2.34	0.61
20:S:104:SER:HA	20:S:139:THR:HA	1.81	0.61
2:Y:9:G:H5'	13:L:32:TYR:CE2	2.35	0.61
13:L:40:ALA:HB2	13:L:103:LEU:HD11	1.82	0.61
22:U:47:HIS:CG	22:U:48:LYS:H	2.19	0.61
1:X:171:G:H2'	1:X:172:A:O4'	2.00	0.61
1:X:517:A:H5''	1:X:518:A:H5'	1.83	0.61
1:X:1279:G:O2'	1:X:1995:G:O6	2.12	0.61
27:2:41:GLN:HA	27:2:41:GLN:NE2	2.14	0.61
1:X:943:U:O2'	1:X:944:A:O4'	2.10	0.61
1:X:1008:G:OP1	15:N:93:LYS:HB2	2.01	0.61
1:X:1182:U:H3	1:X:1192:A:H61	1.48	0.61
6:D:46:ASP:HB2	6:D:49:ALA:HB3	1.83	0.61
13:L:89:PHE:O	13:L:91:ARG:NH2	2.33	0.61
26:1:25:THR:O	26:1:27:ASN:ND2	2.34	0.61
28:3:26:LYS:HE2	28:3:43:GLY:HA3	1.81	0.61
1:X:2696:A:O2'	1:X:2697:G:H5'	2.01	0.60
8:G:70:PHE:HB3	15:N:64:ARG:HG2	1.83	0.60
20:S:9:THR:HG22	20:S:11:LYS:H	1.65	0.60
1:X:1250:A:OP1	1:X:1250:A:H4'	1.99	0.60
1:X:1468:A:C8	1:X:1468:A:H5''	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:31:THR:HG22	15:N:61:TRP:HH2	1.65	0.60
12:K:33:ARG:HG3	12:K:114:GLU:HB3	1.83	0.60
22:U:63:SER:O	22:U:67:LEU:N	2.33	0.60
25:Z:35:GLN:HG3	25:Z:51:TYR:CD2	2.36	0.60
1:X:1279:G:O5'	17:P:36:ARG:NH2	2.34	0.60
1:X:603:C:H2'	1:X:604:U:C6	2.36	0.60
1:X:2873:G:H2'	1:X:2874:A:C8	2.35	0.60
6:D:60:ILE:O	6:D:102:LYS:NZ	2.31	0.60
8:G:119:LEU:HD13	8:G:122:HIS:CE1	2.36	0.60
1:X:537:C:O2'	1:X:538:A:C4	2.54	0.60
1:X:2466:G:H2'	1:X:2467:A:H8	1.65	0.60
20:S:70:GLN:HB2	20:S:80:HIS:HB3	1.82	0.60
1:X:1196:G:H2'	1:X:1197:U:O4'	2.01	0.60
1:X:1313:U:H4'	1:X:1314:A:H5''	1.84	0.60
1:X:1915:A:H3'	1:X:1916:G:H8	1.66	0.60
1:X:2335:U:H4'	21:T:20:TYR:CD2	2.37	0.60
22:U:22:GLY:HA3	22:U:39:LYS:NZ	2.15	0.60
26:1:28:ARG:HB2	26:1:30:ASN:OD1	2.02	0.60
17:P:14:ARG:HA	17:P:17:GLN:HG2	1.82	0.60
1:X:37:C:O2	5:C:44:SER:OG	2.19	0.60
1:X:806:A:OP2	1:X:2054:A:O2'	2.20	0.60
1:X:2757:G:OP2	1:X:2761:A:O2'	2.19	0.60
2:Y:52:G:OP2	13:L:65:THR:HG21	2.02	0.60
8:G:84:ASN:HD22	8:G:87:GLN:HG3	1.66	0.60
9:H:12:ASP:OD1	9:H:14:SER:OG	2.14	0.60
1:X:478:G:OP1	27:2:33:ARG:HD2	2.01	0.60
5:C:3:GLN:HB2	5:C:116:LYS:HZ2	1.67	0.60
26:1:14:SER:HB2	26:1:22:TYR:HA	1.84	0.60
1:X:863:C:O2'	24:W:19:THR:OG1	2.13	0.60
10:I:32:ARG:HD2	10:I:32:ARG:O	2.02	0.60
18:Q:61:LYS:H	18:Q:72:ARG:HA	1.66	0.60
24:W:38:PRO:HD3	24:W:41:ARG:HH21	1.66	0.60
1:X:415:A:H61	1:X:436:A:H61	1.50	0.59
1:X:627:A:H2'	1:X:628:A:C8	2.36	0.59
5:C:76:THR:O	5:C:76:THR:OG1	2.15	0.59
9:H:28:GLY:O	9:H:35:THR:N	2.29	0.59
12:K:87:TYR:HE1	12:K:94:TYR:HD1	1.49	0.59
1:X:636:G:H5'	1:X:637:G:OP2	2.01	0.59
1:X:1422:C:H2'	1:X:1423:A:C8	2.38	0.59
1:X:1643:A:H61	1:X:1656:U:H3	1.49	0.59
1:X:2245:A:H4'	1:X:2246:A:C2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:74:ILE:HG12	6:D:80:ARG:HA	1.83	0.59
26:1:30:ASN:ND2	26:1:31:THR:H	1.99	0.59
3:A:133:LEU:HB2	3:A:187:SER:HA	1.84	0.59
14:M:56:ALA:HB3	14:M:67:THR:HB	1.84	0.59
22:U:54:ASN:CG	22:U:78:ILE:H	2.10	0.59
24:W:23:LEU:HD21	24:W:43:MET:HB3	1.84	0.59
1:X:1333:G:N7	1:X:1342:U:H5'	2.17	0.59
6:D:8:TYR:OH	6:D:31:ILE:N	2.29	0.59
6:D:8:TYR:HH	6:D:31:ILE:H	1.50	0.59
1:X:48:A:H61	1:X:154:U:H2'	1.67	0.59
1:X:417:C:H4'	1:X:418:C:H5'	1.83	0.59
1:X:1058:G:O2'	1:X:1122:A:N6	2.36	0.59
1:X:1154:A:H8	1:X:1154:A:OP1	1.85	0.59
1:X:1673:C:OP1	4:B:136:ARG:HG2	2.02	0.59
1:X:2038:C:H5'	1:X:2039:G:H5''	1.84	0.59
2:Y:17:A:H1'	2:Y:112:A:C8	2.37	0.59
2:Y:22:U:O2'	2:Y:66:G:N2	2.36	0.59
6:D:13:ARG:HA	6:D:28:VAL:HG11	1.85	0.59
1:X:742:G:C6	3:A:208:LYS:HB3	2.37	0.59
1:X:1963:G:O2'	1:X:1965:U:OP2	2.20	0.59
6:D:167:ARG:HG3	6:D:177:PHE:CZ	2.38	0.59
26:1:35:LEU:HD13	26:1:37:LEU:HD12	1.83	0.59
4:B:5:LEU:HD13	4:B:51:TYR:HB2	1.84	0.59
4:B:122:PHE:CE2	4:B:138:PRO:HB3	2.36	0.59
1:X:2226:A:H2'	1:X:2227:C:C6	2.37	0.59
6:D:132:ILE:HG13	6:D:154:ILE:HD13	1.85	0.59
3:A:14:ARG:HD2	3:A:27:LYS:HB3	1.84	0.59
9:H:77:THR:HA	9:H:94:ASN:HB3	1.84	0.59
27:2:1:MET:HG3	27:2:3:ARG:NH1	2.18	0.59
1:X:1179:A:H2'	1:X:1180:A:C8	2.37	0.58
1:X:2285:U:O4'	6:D:150:ARG:NH1	2.36	0.58
1:X:1225:G:H2'	1:X:1249:G:H22	1.68	0.58
1:X:2298:U:O2	1:X:2299:A:N6	2.36	0.58
1:X:2491:C:OP1	4:B:123:ALA:HB2	2.03	0.58
1:X:2607:C:H1'	1:X:2761:A:H2'	1.85	0.58
2:Y:9:G:H21	13:L:41:GLN:HE22	1.49	0.58
9:H:23:ARG:HG2	9:H:25:LEU:HD23	1.84	0.58
1:X:492:G:H1'	1:X:516:G:H21	1.67	0.58
3:A:60:ARG:HD3	3:A:87:ASN:HD22	1.68	0.58
1:X:1212:U:H2'	1:X:1213:U:C6	2.38	0.58
1:X:1745:C:O2	1:X:2697:G:H4'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2634:G:O2'	1:X:2643:G:N1	2.36	0.58
9:H:41:ASN:HD22	9:H:42:LYS:H	1.52	0.58
21:T:18:PRO:O	21:T:19:LYS:HG2	2.02	0.58
1:X:691:C:H2'	1:X:692:C:C6	2.39	0.58
1:X:1582:A:OP1	3:A:211:ARG:NH1	2.35	0.58
1:X:1594:U:H2'	1:X:1595:A:H8	1.68	0.58
1:X:2262:C:O2	1:X:2304:G:N2	2.26	0.58
1:X:178:C:O5'	22:U:40:ARG:NH2	2.36	0.58
1:X:834:A:H5'	1:X:835:U:C6	2.39	0.58
1:X:930:A:N3	2:Y:82:U:O2'	2.33	0.58
1:X:1264:C:OP1	15:N:10:ARG:HG3	2.02	0.58
1:X:1268:U:H2'	5:C:66:ASN:HA	1.85	0.58
1:X:1332:G:C6	1:X:1333:G:N1	2.71	0.58
3:A:209:ALA:C	3:A:211:ARG:H	2.11	0.58
1:X:1047:G:H1	1:X:1130:U:H3	1.52	0.58
1:X:1770:U:H5	1:X:1775:A:N7	2.01	0.58
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.86	0.58
1:X:774:A:H8	1:X:774:A:O5'	1.86	0.58
1:X:1261:G:C4	15:N:3:ARG:HG2	2.39	0.58
1:X:1350:G:H2'	1:X:1351:G:H8	1.69	0.58
1:X:2494:C:H42	1:X:2548:G:H1	1.50	0.58
4:B:92:ASN:HA	4:B:95:ILE:HB	1.84	0.58
11:J:48:ILE:O	11:J:52:ARG:N	2.26	0.58
15:N:74:MET:HE3	15:N:114:ARG:HG3	1.86	0.58
1:X:537:C:H1'	1:X:538:A:C6	2.39	0.58
1:X:1586:A:H2'	1:X:1587:A:C8	2.39	0.58
26:1:8:ILE:HG12	26:1:9:ILE:HG23	1.86	0.58
1:X:1919:A:H2	1:X:1926:U:H3	1.51	0.58
1:X:1922:U:H3'	1:X:1923:U:H5'	1.84	0.58
3:A:182:LEU:HB2	3:A:268:ARG:O	2.04	0.58
15:N:78:THR:HG23	15:N:117:ARG:CZ	2.34	0.58
1:X:2594:U:C6	25:Z:7:PRO:HA	2.39	0.57
3:A:231:HIS:CD2	3:A:232:PRO:HD2	2.38	0.57
6:D:134:GLU:HG2	6:D:136:LEU:H	1.69	0.57
18:Q:10:PRO:HD3	23:V:30:PHE:CD2	2.38	0.57
19:R:92:THR:HA	19:R:108:VAL:HG22	1.85	0.57
26:1:46:LYS:O	26:1:48:VAL:HG12	2.04	0.57
1:X:753:U:H2'	1:X:754:G:C8	2.39	0.57
1:X:2212:U:H2'	1:X:2213:G:C8	2.39	0.57
1:X:2772:U:H2'	1:X:2773:G:C8	2.38	0.57
6:D:70:ALA:HB3	6:D:82:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:81:GLN:HA	10:I:116:ARG:HD2	1.86	0.57
20:S:117:VAL:HG22	20:S:168:VAL:HA	1.86	0.57
1:X:636:G:O2'	1:X:669:G:H4'	2.03	0.57
1:X:1287:A:N1	1:X:1661:C:O2'	2.34	0.57
1:X:487:G:H4'	1:X:512:A:N1	2.18	0.57
1:X:829:C:H2'	1:X:830:C:C6	2.39	0.57
1:X:2234:G:H2'	1:X:2235:G:O4'	2.04	0.57
1:X:2269:G:H22	1:X:2322:U:H1'	1.70	0.57
2:Y:44:C:O2'	6:D:64:LYS:O	2.18	0.57
4:B:38:THR:HB	4:B:41:THR:HG23	1.86	0.57
6:D:111:ILE:HG12	6:D:137:ILE:HD12	1.87	0.57
10:I:90:ARG:HA	10:I:121:HIS:H	1.69	0.57
14:M:78:GLU:OE1	14:M:108:ARG:NH2	2.35	0.57
15:N:66:ASN:ND2	15:N:70:ARG:HH12	2.01	0.57
1:X:1974:U:O2'	1:X:1975:G:H5'	2.04	0.57
1:X:2398:U:H5'	26:1:24:THR:HG21	1.86	0.57
1:X:2708:U:H2'	1:X:2709:C:C6	2.39	0.57
8:G:122:HIS:ND1	8:G:122:HIS:O	2.38	0.57
1:X:408:U:H2'	1:X:409:G:H8	1.67	0.57
1:X:1886:G:H2'	1:X:1887:G:H8	1.69	0.57
1:X:398:C:H42	1:X:424:G:H1	1.52	0.57
1:X:2825:A:N7	1:X:2843:A:O2'	2.36	0.57
3:A:246:PRO:HD2	3:A:251:GLY:N	2.19	0.57
4:B:120:TRP:CD1	4:B:155:ARG:HB3	2.40	0.57
9:H:109:ARG:HA	9:H:129:LEU:HD13	1.86	0.57
26:1:13:GLU:HG2	26:1:24:THR:HA	1.86	0.57
9:H:19:ILE:O	9:H:19:ILE:HG13	2.05	0.57
15:N:17:VAL:HG21	15:N:32:TYR:HE1	1.69	0.57
1:X:1030:U:H3	1:X:1153:A:N6	1.98	0.57
1:X:1336:G:O6	1:X:1337:G:C6	2.58	0.57
1:X:2006:G:H5'	1:X:2596:C:H4'	1.86	0.57
1:X:2795:A:N3	1:X:2795:A:H2'	2.18	0.57
14:M:104:LEU:HD23	14:M:106:TYR:CE2	2.40	0.57
1:X:143:A:H2'	1:X:144:U:C6	2.39	0.56
1:X:394:U:OP2	22:U:21:ARG:NH2	2.38	0.56
1:X:1333:G:N2	1:X:1344:C:N4	2.52	0.56
1:X:2034:A:H4'	4:B:141:ILE:HG12	1.85	0.56
19:R:16:PHE:CZ	19:R:46:VAL:HG21	2.40	0.56
28:3:29:LYS:NZ	28:3:36:LYS:O	2.36	0.56
1:X:16:G:H2'	1:X:17:G:H8	1.69	0.56
1:X:1443:G:H2'	1:X:1444:C:H6	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:7:C:H2'	2:Y:8:C:H6	1.70	0.56
1:X:1046:U:H5'	7:E:59:GLN:HG2	1.87	0.56
1:X:1321:A:H5'	1:X:1322:G:OP2	2.05	0.56
1:X:1834:G:H2'	1:X:1835:C:C6	2.41	0.56
1:X:1976:U:C5'	4:B:128:SER:HB3	2.35	0.56
1:X:2020:G:H2'	1:X:2021:G:C8	2.40	0.56
4:B:14:ILE:HG12	14:M:20:HIS:CD2	2.39	0.56
9:H:2:ILE:HD12	9:H:8:LEU:HD21	1.87	0.56
17:P:37:LYS:HZ3	17:P:64:ALA:H	1.53	0.56
1:X:1831:G:H2'	1:X:1832:G:H8	1.71	0.56
1:X:2313:G:C2	13:L:13:THR:HG22	2.41	0.56
1:X:2372:A:N6	1:X:2401:A:H62	2.02	0.56
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.88	0.56
4:B:39:ALA:HB2	4:B:45:GLU:HG2	1.87	0.56
5:C:152:THR:OG1	5:C:153:ASP:N	2.39	0.56
1:X:2225:G:H2'	1:X:2226:A:H8	1.68	0.56
19:R:26:SER:O	19:R:30:LYS:HB2	2.05	0.56
20:S:3:LEU:HD23	20:S:56:VAL:HG13	1.87	0.56
1:X:693:A:H2'	1:X:694:G:C8	2.40	0.56
1:X:1223:G:H4'	1:X:1224:A:H5''	1.87	0.56
1:X:1448:A:H61	1:X:1574:A:H61	1.53	0.56
1:X:1883:A:H1'	1:X:1953:A:H2'	1.88	0.56
1:X:1919:A:H62	1:X:1946:U:H3	1.53	0.56
15:N:20:ARG:NH1	16:O:72:ARG:HD2	2.21	0.56
1:X:568:G:N2	15:N:49:ASP:OD1	2.38	0.56
1:X:992:A:N1	1:X:2010:G:O2'	2.33	0.56
1:X:1023:U:O4	8:G:56:THR:OG1	2.23	0.56
1:X:1183:C:N4	1:X:1189:G:O6	2.39	0.56
1:X:1360:G:N2	1:X:1615:C:O2	2.34	0.56
2:Y:59:A:H5'	2:Y:60:A:OP2	2.05	0.56
20:S:47:SER:OG	20:S:48:THR:N	2.20	0.56
1:X:682:G:H3'	1:X:683:A:H5''	1.88	0.56
1:X:708:G:OP1	1:X:1393:G:O2'	2.24	0.56
1:X:1792:C:OP1	3:A:263:ARG:NH2	2.39	0.56
1:X:2272:A:OP2	13:L:15:ARG:NH2	2.39	0.56
1:X:2797:G:OP2	12:K:3:HIS:NE2	2.38	0.56
8:G:65:LYS:HZ3	15:N:70:ARG:HD2	1.71	0.56
1:X:539:A:OP1	1:X:539:A:H4'	2.06	0.56
1:X:1727:C:H2'	1:X:1728:A:C8	2.40	0.56
1:X:2352:A:H2'	1:X:2353:G:C8	2.41	0.56
4:B:8:LYS:HG2	4:B:192:ASN:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1746:A:H2	1:X:2696:A:HO2'	1.54	0.56
5:C:127:ASP:OD2	5:C:129:LYS:NZ	2.39	0.56
10:I:88:PHE:HB3	10:I:90:ARG:NH2	2.21	0.56
19:R:23:ILE:HG23	19:R:33:THR:HB	1.87	0.56
20:S:72:ASP:HB2	20:S:79:ILE:HD13	1.88	0.56
1:X:319:G:N7	17:P:12:LYS:NZ	2.54	0.55
1:X:854:G:H1	1:X:948:C:N4	2.02	0.55
1:X:1250:A:H2'	1:X:1251:G:O4'	2.06	0.55
1:X:1919:A:H1'	1:X:1923:U:C2	2.41	0.55
6:D:130:LEU:HD13	6:D:132:ILE:HD11	1.88	0.55
8:G:55:ALA:C	8:G:134:MET:HE1	2.31	0.55
9:H:116:ARG:CZ	14:M:38:LYS:HD3	2.36	0.55
11:J:55:MET:HB3	11:J:65:ILE:HD11	1.88	0.55
13:L:31:VAL:HA	13:L:40:ALA:HA	1.88	0.55
1:X:27:G:N2	1:X:522:G:H1'	2.21	0.55
1:X:832:A:OP2	1:X:1201:G:N2	2.34	0.55
1:X:953:G:H5''	10:I:38:LYS:HA	1.88	0.55
1:X:2226:A:H2'	1:X:2227:C:H6	1.71	0.55
8:G:141:GLY:O	8:G:144:MET:N	2.39	0.55
9:H:89:ILE:HG23	14:M:79:ARG:HD3	1.89	0.55
1:X:642:A:O2'	10:I:65:PHE:HB2	2.06	0.55
1:X:1482:U:H2'	1:X:1483:G:H8	1.72	0.55
18:Q:73:ASN:N	18:Q:73:ASN:OD1	2.39	0.55
26:1:38:LYS:HD2	26:1:40:TYR:HE1	1.71	0.55
1:X:542:A:C2	1:X:2004:U:H2'	2.41	0.55
1:X:617:U:H5	1:X:632:A:C2	2.24	0.55
1:X:1482:U:H2'	1:X:1483:G:C8	2.41	0.55
1:X:2526:U:H2'	1:X:2527:G:H8	1.71	0.55
1:X:2705:A:H1'	1:X:2706:U:H2'	1.89	0.55
8:G:140:GLN:O	8:G:144:MET:HG3	2.07	0.55
8:G:41:TRP:CZ3	8:G:149:LYS:HD2	2.41	0.55
1:X:2708:U:H2'	1:X:2709:C:H6	1.71	0.55
2:Y:45:C:O2	6:D:92:ARG:NH2	2.40	0.55
5:C:47:THR:HG1	5:C:85:GLY:H	1.54	0.55
27:2:36:ALA:C	27:2:38:GLY:H	2.15	0.55
7:E:37:TYR:CZ	7:E:72:VAL:HG22	2.42	0.55
8:G:61:ARG:HH12	8:G:66:HIS:HB2	1.72	0.55
10:I:32:ARG:HH12	10:I:34:HIS:HE1	1.55	0.55
17:P:57:LEU:HD13	17:P:69:ALA:HB2	1.88	0.55
18:Q:34:THR:O	18:Q:38:ILE:HG12	2.06	0.55
1:X:75:C:H2'	1:X:76:C:H6	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:603:C:H4'	28:3:61:MET:HG2	1.88	0.55
1:X:787:A:H2	1:X:800:U:HO2'	1.53	0.55
1:X:2195:C:H5'	1:X:2196:U:OP1	2.07	0.55
8:G:103:TYR:HB3	8:G:107:GLN:CG	2.37	0.55
17:P:95:ALA:HB2	17:P:126:ILE:HG13	1.89	0.55
1:X:1398:G:O2'	1:X:1399:C:O4'	2.21	0.55
1:X:2469:G:H8	1:X:2469:G:OP2	1.89	0.55
2:Y:39:C:H5'	2:Y:40:C:OP2	2.08	0.55
6:D:4:LEU:HD11	6:D:7:LYS:HB2	1.88	0.55
1:X:219:G:N2	1:X:231:G:H2'	2.22	0.54
1:X:617:U:C5	1:X:632:A:C2	2.96	0.54
1:X:793:G:H21	1:X:796:A:H62	1.54	0.54
1:X:954:U:P	10:I:38:LYS:HZ3	2.29	0.54
1:X:1630:A:O2'	1:X:1631:C:OP1	2.24	0.54
1:X:1785:A:H2'	1:X:1786:C:C6	2.41	0.54
1:X:1809:G:H3'	3:A:157:ARG:HH12	1.71	0.54
5:C:58:MET:HG2	5:C:70:GLY:O	2.07	0.54
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.88	0.54
7:E:154:PRO:HA	7:E:160:LYS:O	2.07	0.54
14:M:43:ASN:OD1	14:M:43:ASN:N	2.39	0.54
1:X:2674:C:H2'	1:X:2675:U:H6	1.73	0.54
1:X:2756:A:H3'	1:X:2756:A:OP1	2.07	0.54
2:Y:46:G:H1'	2:Y:49:C:H41	1.72	0.54
3:A:168:LYS:HA	3:A:173:VAL:HA	1.89	0.54
8:G:67:ARG:HG3	8:G:70:PHE:CD1	2.42	0.54
14:M:102:ALA:C	14:M:103:LYS:HD2	2.32	0.54
19:R:56:LYS:HA	19:R:69:GLN:HG2	1.88	0.54
1:X:224:G:H4'	1:X:399:G:C5	2.43	0.54
1:X:834:A:H5'	1:X:835:U:H6	1.72	0.54
1:X:1005:U:H1'	16:O:21:ARG:HH22	1.72	0.54
1:X:1288:A:H4'	1:X:1289:A:OP1	2.06	0.54
1:X:1547:U:H3	1:X:1556:A:H61	1.55	0.54
1:X:1973:C:H2'	1:X:1974:U:O4'	2.07	0.54
1:X:2753:C:H5''	4:B:164:ARG:HG2	1.88	0.54
2:Y:51:G:H2'	2:Y:52:G:H8	1.73	0.54
10:I:34:HIS:O	10:I:35:LYS:HD3	2.07	0.54
10:I:89:ASP:HB2	10:I:120:VAL:HG12	1.88	0.54
20:S:116:VAL:HG12	20:S:117:VAL:HG13	1.90	0.54
1:X:14:A:H5''	1:X:15:G:OP2	2.06	0.54
1:X:20:C:H2'	1:X:21:A:H8	1.72	0.54
1:X:1687:C:O2	4:B:129:HIS:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:40:C:H5'	13:L:97:HIS:CE1	2.43	0.54
6:D:103:LEU:HG	6:D:108:LEU:HG	1.89	0.54
1:X:320:A:N3	1:X:340:G:O2'	2.37	0.54
1:X:475:U:O3'	27:2:12:ARG:NH2	2.41	0.54
1:X:2368:G:H5''	1:X:2369:U:H5'	1.89	0.54
1:X:2522:G:H2'	1:X:2523:G:C8	2.42	0.54
1:X:2572:U:H2'	1:X:2573:C:H6	1.71	0.54
2:Y:7:C:H2'	2:Y:8:C:C6	2.43	0.54
1:X:1261:G:C5	15:N:3:ARG:HG2	2.42	0.54
1:X:2528:G:H2'	1:X:2529:G:H8	1.73	0.54
9:H:28:GLY:HA3	9:H:34:LEU:HD22	1.88	0.54
16:O:89:ASN:OD1	16:O:89:ASN:N	2.40	0.54
17:P:40:LEU:HB3	25:Z:25:LEU:HD22	1.90	0.54
18:Q:6:ILE:HA	18:Q:30:SER:OG	2.07	0.54
1:X:847:C:H2'	1:X:848:A:H8	1.72	0.54
1:X:1329:U:H2'	1:X:1330:G:C8	2.40	0.54
1:X:2466:G:H2'	1:X:2467:A:C8	2.41	0.54
1:X:2597:G:H21	4:B:150:VAL:HG21	1.73	0.54
1:X:2736:U:H1'	1:X:2737:A:H5''	1.88	0.54
11:J:99:LYS:HE3	11:J:100:PRO:HD2	1.90	0.54
12:K:39:THR:O	12:K:42:LYS:N	2.41	0.54
1:X:530:G:H2'	1:X:531:G:H8	1.72	0.54
1:X:613:A:H8	1:X:636:G:H21	1.54	0.54
1:X:758:G:H2'	1:X:759:C:H5'	1.90	0.54
1:X:1782:A:O2'	3:A:207:GLY:O	2.18	0.54
1:X:1845:A:N6	1:X:1871:G:O2'	2.41	0.54
1:X:1856:U:OP1	1:X:2389:G:O2'	2.21	0.54
3:A:43:ARG:HB3	3:A:54:ILE:O	2.08	0.54
17:P:39:ARG:HD2	17:P:97:VAL:HB	1.90	0.54
19:R:92:THR:O	19:R:92:THR:OG1	2.17	0.54
20:S:25:ASN:H	20:S:25:ASN:HD22	1.56	0.54
24:W:12:ARG:HG2	24:W:12:ARG:HH11	1.72	0.54
1:X:356:A:O2'	1:X:357:A:H8	1.91	0.54
1:X:1991:C:H2'	1:X:1992:G:H8	1.73	0.54
1:X:2043:A:H62	5:C:68:ARG:NH1	2.04	0.54
1:X:2729:A:N1	1:X:2730:A:N6	2.56	0.54
3:A:134:ARG:HG3	3:A:135:PHE:CD2	2.43	0.54
18:Q:11:VAL:HB	18:Q:26:SER:HB2	1.90	0.54
28:3:6:THR:HG23	28:3:8:LYS:H	1.73	0.54
1:X:356:A:HO2'	1:X:357:A:H8	1.55	0.54
1:X:1121:G:H2'	1:X:1122:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2293:G:H5'	6:D:35:VAL:HG11	1.89	0.54
1:X:2579:A:H2'	1:X:2580:C:H6	1.71	0.54
1:X:2767:C:H1'	4:B:62:PRO:HG3	1.89	0.54
7:E:43:VAL:HA	7:E:52:VAL:HG22	1.90	0.54
9:H:16:ALA:HB3	9:H:98:ILE:HD11	1.90	0.54
1:X:177:U:H1'	1:X:178:C:OP1	2.08	0.53
1:X:1496:G:H4'	1:X:1497:C:OP1	2.07	0.53
1:X:2195:C:H2'	1:X:2196:U:C5	2.44	0.53
1:X:2806:G:OP1	4:B:57:ARG:NH1	2.41	0.53
3:A:44:ASN:HA	3:A:49:ILE:HA	1.90	0.53
3:A:160:GLY:N	3:A:196:VAL:O	2.41	0.53
13:L:46:SER:OG	13:L:47:ARG:N	2.38	0.53
1:X:388:G:H2'	1:X:389:G:H8	1.73	0.53
1:X:852:U:H1'	1:X:1205:G:H1'	1.91	0.53
1:X:1816:G:OP1	3:A:52:ARG:HD3	2.07	0.53
1:X:1820:G:OP2	3:A:239:ARG:NH2	2.41	0.53
1:X:2591:C:O2'	1:X:2592:U:OP1	2.25	0.53
1:X:611:C:O2	1:X:615:C:H4'	2.09	0.53
1:X:667:U:O2'	1:X:668:A:H8	1.91	0.53
1:X:691:C:H2'	1:X:692:C:H6	1.71	0.53
2:Y:57:U:O2'	6:D:24:SER:OG	2.17	0.53
13:L:95:LYS:HG3	13:L:96:TYR:H	1.73	0.53
21:T:46:LYS:NZ	21:T:76:ALA:HA	2.24	0.53
21:T:46:LYS:HB2	21:T:78:PHE:CE2	2.43	0.53
1:X:492:G:OP2	19:R:56:LYS:HG2	2.09	0.53
1:X:1744:G:OP1	14:M:100:ARG:HD2	2.08	0.53
5:C:129:LYS:C	5:C:131:LYS:H	2.16	0.53
1:X:608:G:H2'	1:X:609:U:H6	1.73	0.53
1:X:1385:C:H2'	1:X:1386:A:O4'	2.09	0.53
1:X:1674:C:H2'	1:X:1675:C:H6	1.74	0.53
1:X:1693:A:H2'	1:X:1694:A:O4'	2.08	0.53
1:X:2526:U:H2'	1:X:2527:G:C8	2.44	0.53
11:J:32:ASP:H	11:J:108:ALA:HB2	1.74	0.53
14:M:29:PRO:HB2	14:M:99:VAL:HG11	1.91	0.53
14:M:103:LYS:O	14:M:104:LEU:HB2	2.08	0.53
1:X:742:G:H2'	1:X:1766:U:H1'	1.90	0.53
1:X:1777:A:H1'	1:X:1921:A:N6	2.24	0.53
1:X:1884:A:O2'	3:A:244:ARG:HD3	2.08	0.53
1:X:2043:A:H1'	1:X:2481:G:H1'	1.89	0.53
4:B:33:ILE:HD11	4:B:86:PRO:HB2	1.91	0.53
8:G:67:ARG:CB	8:G:70:PHE:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:90:ARG:HD2	12:K:94:TYR:HB2	1.90	0.53
19:R:16:PHE:HE2	19:R:80:LYS:HZ3	1.57	0.53
22:U:49:LYS:HD3	22:U:61:TRP:CE2	2.44	0.53
28:3:13:ARG:HG3	28:3:14:ILE:HG13	1.90	0.53
1:X:1046:U:H4'	7:E:60:LYS:HE2	1.91	0.53
1:X:1517:C:H4'	3:A:96:HIS:NE2	2.24	0.53
1:X:2245:A:H4'	1:X:2246:A:N3	2.24	0.53
1:X:70:A:H4'	1:X:71:A:H5''	1.90	0.53
1:X:1059:A:H2	1:X:1123:G:H21	1.55	0.53
1:X:1184:G:O6	1:X:1190:C:N4	2.41	0.53
1:X:1479:G:H2'	1:X:1480:G:C8	2.44	0.53
3:A:246:PRO:HG2	3:A:248:THR:O	2.09	0.53
5:C:125:ILE:HG12	5:C:157:THR:HA	1.91	0.53
5:C:154:ASP:HB3	5:C:157:THR:HB	1.91	0.53
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.91	0.53
13:L:32:TYR:HB3	13:L:39:TYR:HB2	1.89	0.53
28:3:52:LYS:O	28:3:56:ALA:HB2	2.08	0.53
1:X:965:G:O2'	1:X:2253:A:N1	2.36	0.53
1:X:1692:C:N3	4:B:128:SER:OG	2.39	0.53
1:X:2054:A:H2'	1:X:2055:G:H8	1.73	0.53
3:A:111:LEU:HD23	3:A:127:LEU:HD13	1.91	0.53
26:1:9:ILE:O	26:1:10:VAL:HB	2.08	0.53
1:X:99:U:H3'	1:X:100:G:H5'	1.91	0.53
1:X:857:U:H2'	1:X:858:G:O4'	2.09	0.53
1:X:1177:U:H2'	1:X:1178:C:O4'	2.09	0.53
1:X:1418:C:H2'	1:X:1419:G:C8	2.44	0.53
12:K:100:VAL:HG12	12:K:101:GLY:N	2.24	0.53
14:M:29:PRO:HA	14:M:54:VAL:HG13	1.91	0.53
1:X:1342:U:H5''	1:X:1343:C:C5	2.43	0.52
1:X:1816:G:H21	3:A:252:LYS:HG3	1.73	0.52
1:X:1819:U:H2'	1:X:1820:G:O4'	2.08	0.52
1:X:863:C:H42	1:X:940:G:H1	1.57	0.52
1:X:2639:A:H2'	1:X:2640:G:O4'	2.09	0.52
10:I:77:LEU:HD12	10:I:108:LEU:HD11	1.92	0.52
16:O:19:VAL:HG13	16:O:90:PHE:CD1	2.44	0.52
27:2:26:SER:O	27:2:30:ILE:HG13	2.09	0.52
1:X:1204:G:H2'	1:X:1205:G:C8	2.45	0.52
1:X:1781:C:H4'	3:A:209:ALA:HB2	1.90	0.52
1:X:2440:C:H2'	1:X:2441:U:C6	2.44	0.52
5:C:76:THR:O	5:C:77:PHE:HD1	1.92	0.52
8:G:103:TYR:HB3	8:G:107:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:29:ILE:HD13	9:H:123:PHE:CE1	2.44	0.52
10:I:62:LYS:CB	28:3:12:ARG:HA	2.39	0.52
19:R:84:VAL:CG1	19:R:90:LYS:H	2.17	0.52
24:W:46:THR:HG22	24:W:47:VAL:HG13	1.91	0.52
1:X:469:G:N2	1:X:480:G:H2'	2.25	0.52
1:X:1870:U:P	1:X:1871:G:H22	2.32	0.52
3:A:186:HIS:HB2	3:A:188:GLU:HG2	1.92	0.52
5:C:6:VAL:HG12	5:C:7:ILE:HG12	1.91	0.52
14:M:70:LYS:HE2	14:M:72:SER:HB3	1.90	0.52
1:X:394:U:OP1	22:U:19:ILE:HG12	2.10	0.52
1:X:503:G:H2'	1:X:504:G:O4'	2.10	0.52
1:X:692:C:H2'	1:X:693:A:C8	2.43	0.52
1:X:2855:C:H1'	12:K:91:PRO:HB2	1.92	0.52
10:I:62:LYS:HD3	10:I:63:ARG:N	2.24	0.52
1:X:502:A:H2'	1:X:503:G:O4'	2.10	0.52
1:X:1223:G:H5''	1:X:1224:A:H3'	1.92	0.52
1:X:1454:U:H2'	1:X:1455:C:C6	2.44	0.52
10:I:78:SER:HB3	10:I:112:GLY:HA3	1.92	0.52
11:J:42:TRP:CD1	11:J:97:VAL:HG12	2.44	0.52
13:L:75:LEU:O	13:L:79:ALA:N	2.42	0.52
18:Q:7:LEU:H	18:Q:7:LEU:HD22	1.75	0.52
19:R:105:ARG:NH2	19:R:111:GLY:O	2.42	0.52
22:U:17:SER:OG	22:U:45:ASN:N	2.42	0.52
1:X:47:G:N2	1:X:154:U:OP2	2.29	0.52
1:X:761:G:H2'	1:X:763:A:N7	2.25	0.52
1:X:940:G:H4'	24:W:37:THR:HG21	1.92	0.52
1:X:1673:C:H5''	4:B:136:ARG:HB3	1.91	0.52
1:X:2441:U:H1'	1:X:2470:U:O4	2.09	0.52
1:X:2824:C:H4'	1:X:2825:A:O5'	2.10	0.52
2:Y:9:G:H5'	13:L:32:TYR:CZ	2.45	0.52
8:G:46:ALA:HB1	8:G:88:VAL:HG23	1.92	0.52
9:H:83:ARG:HG2	14:M:40:ARG:NH2	2.24	0.52
13:L:27:LEU:C	13:L:87:VAL:HG13	2.35	0.52
15:N:66:ASN:HB3	15:N:76:TYR:CB	2.33	0.52
23:V:32:ALA:HB2	23:V:37:LEU:HD13	1.92	0.52
1:X:580:A:H4'	1:X:581:A:OP1	2.10	0.52
1:X:615:C:H41	10:I:100:ARG:NH1	2.07	0.52
1:X:2078:G:H1	1:X:2177:U:H3	1.57	0.52
1:X:2668:U:P	1:X:2699:G:H22	2.33	0.52
9:H:73:VAL:HG21	9:H:123:PHE:CE2	2.44	0.52
11:J:46:ASN:C	11:J:48:ILE:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:15:VAL:HA	22:U:45:ASN:O	2.10	0.52
1:X:538:A:H2'	1:X:538:A:N3	2.24	0.52
1:X:1004:A:H1'	16:O:88:GLN:HG3	1.92	0.52
1:X:1558:C:H2'	1:X:1559:G:O4'	2.10	0.52
1:X:2451:G:H22	1:X:2456:U:H5'	1.74	0.52
1:X:2716:G:H1	1:X:2748:C:N4	2.07	0.52
5:C:47:THR:HA	5:C:82:VAL:HG13	1.90	0.52
10:I:102:LYS:C	10:I:104:ARG:H	2.18	0.52
13:L:37:HIS:HD2	13:L:57:ALA:HA	1.75	0.52
1:X:1787:U:H2'	1:X:1788:C:C6	2.44	0.52
5:C:26:VAL:HG11	5:C:102:LEU:HD22	1.91	0.52
6:D:65:PRO:HA	6:D:89:VAL:HG22	1.92	0.52
9:H:99:ILE:HD12	9:H:103:GLY:HA2	1.91	0.52
15:N:58:ARG:O	15:N:62:ILE:HG13	2.10	0.52
15:N:86:ALA:HB1	15:N:88:ILE:HB	1.92	0.52
20:S:19:ILE:HD11	20:S:36:ARG:HG3	1.91	0.52
26:1:12:MET:HG3	26:1:54:LYS:HB3	1.92	0.52
1:X:2269:G:N2	1:X:2322:U:H1'	2.24	0.51
9:H:73:VAL:HG21	9:H:123:PHE:HE2	1.75	0.51
10:I:56:LEU:HD22	28:3:52:LYS:HZ2	1.75	0.51
19:R:29:HIS:NE2	19:R:51:VAL:HG13	2.25	0.51
20:S:7:PRO:HB2	20:S:9:THR:H	1.74	0.51
1:X:1033:G:H4'	1:X:1034:U:H5'	1.92	0.51
1:X:1128:G:H3'	1:X:1129:A:H5''	1.93	0.51
2:Y:16:U:O2'	2:Y:17:A:OP2	2.28	0.51
24:W:40:VAL:HA	24:W:43:MET:HE3	1.92	0.51
1:X:608:G:H2'	1:X:609:U:C6	2.45	0.51
1:X:1825:C:O2	1:X:1955:G:N2	2.35	0.51
5:C:45:THR:HG23	5:C:47:THR:H	1.74	0.51
7:E:17:VAL:HG13	7:E:26:VAL:HG22	1.91	0.51
7:E:41:LEU:HD22	7:E:68:THR:HG21	1.93	0.51
8:G:68:PRO:HD2	8:G:76:GLN:HB3	1.91	0.51
19:R:77:HIS:CG	19:R:78:ALA:H	2.29	0.51
1:X:346:C:C6	1:X:347:C:H5	2.29	0.51
1:X:967:G:N2	1:X:971:A:OP2	2.43	0.51
1:X:1429:A:H1'	1:X:1603:A:C5	2.46	0.51
1:X:2692:A:H5''	1:X:2693:U:OP2	2.10	0.51
6:D:110:ARG:O	6:D:111:ILE:HG13	2.10	0.51
24:W:4:LYS:HG2	24:W:52:GLU:HB3	1.92	0.51
26:1:30:ASN:HD22	26:1:31:THR:HG23	1.75	0.51
1:X:224:G:OP2	1:X:226:C:N4	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:977:G:H1'	1:X:2246:A:H62	1.75	0.51
1:X:1599:G:C2	1:X:1600:U:H1'	2.45	0.51
1:X:1714:A:O2'	1:X:1961:A:OP1	2.23	0.51
1:X:1886:G:H2'	1:X:1887:G:C8	2.45	0.51
8:G:33:ILE:HB	8:G:34:PRO:HD2	1.92	0.51
17:P:35:PRO:HD3	17:P:121:THR:O	2.10	0.51
1:X:334:G:C8	5:C:164:VAL:HG13	2.46	0.51
1:X:845:U:OP1	10:I:41:SER:HB3	2.11	0.51
1:X:1686:A:H5''	1:X:1687:C:OP2	2.10	0.51
1:X:1769:U:H2'	1:X:1775:A:N6	2.24	0.51
4:B:102:ILE:N	4:B:169:ASN:O	2.43	0.51
14:M:60:SER:HB3	14:M:63:ARG:HH12	1.75	0.51
15:N:7:GLY:O	15:N:8:ILE:HG12	2.11	0.51
15:N:39:LEU:HA	15:N:42:ALA:HB3	1.93	0.51
20:S:6:LYS:HE2	20:S:56:VAL:HG11	1.93	0.51
25:Z:4:HIS:HB2	25:Z:5:PRO:HD3	1.92	0.51
1:X:617:U:H5	1:X:632:A:H2	1.58	0.51
1:X:938:G:O2'	1:X:939:C:O5'	2.28	0.51
1:X:1101:U:H2'	1:X:1102:G:C8	2.45	0.51
1:X:1724:C:N3	1:X:1747:G:C6	2.79	0.51
5:C:119:ALA:HB3	5:C:189:ASP:HA	1.92	0.51
1:X:542:A:H5'	15:N:28:ARG:HH21	1.74	0.51
1:X:1770:U:C2	1:X:1774:A:N7	2.79	0.51
1:X:2043:A:N3	1:X:2481:G:C4	2.79	0.51
1:X:2371:A:H8	10:I:59:ARG:HG2	1.76	0.51
1:X:2594:U:H2'	1:X:2595:C:H6	1.75	0.51
1:X:836:G:H2'	1:X:837:U:H6	1.76	0.51
1:X:1846:A:H2'	1:X:1847:G:O4'	2.11	0.51
1:X:2270:U:H2'	1:X:2271:C:C6	2.46	0.51
2:Y:44:C:N3	6:D:90:THR:OG1	2.40	0.51
3:A:170:SER:OG	3:A:171:ASP:N	2.35	0.51
4:B:41:THR:OG1	4:B:42:ASP:N	2.41	0.51
8:G:96:ASP:HB3	8:G:97:ASP:OD1	2.10	0.51
8:G:128:GLU:HG3	8:G:150:VAL:HG21	1.93	0.51
9:H:13:ASN:HD21	9:H:109:ARG:HG2	1.75	0.51
1:X:455:A:H1'	1:X:1215:A:O4'	2.11	0.51
1:X:590:C:H2'	1:X:591:G:H8	1.76	0.51
1:X:1173:G:H5''	16:O:22:VAL:HG22	1.93	0.51
1:X:1348:C:H2'	1:X:1349:A:H8	1.76	0.51
1:X:1469:U:H5'	1:X:1470:G:OP2	2.11	0.51
3:A:88:ARG:HG3	3:A:90:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:59:PHE:CD1	25:Z:41:LEU:HD22	2.45	0.51
26:1:8:ILE:O	26:1:9:ILE:HG12	2.11	0.51
1:X:1486:A:H2'	1:X:1487:C:C6	2.46	0.50
3:A:108:PRO:HB3	3:A:143:HIS:CE1	2.46	0.50
5:C:153:ASP:OD1	5:C:172:VAL:HA	2.11	0.50
10:I:94:GLU:HA	10:I:97:ARG:NE	2.25	0.50
20:S:88:TYR:O	20:S:127:PRO:HB3	2.11	0.50
28:3:22:VAL:HG21	28:3:53:ALA:HA	1.92	0.50
1:X:50:G:H4'	1:X:51:A:H5'	1.93	0.50
1:X:558:G:OP2	1:X:558:G:N2	2.42	0.50
1:X:1048:U:H3	1:X:1129:A:H61	1.59	0.50
1:X:1919:A:H1'	1:X:1923:U:N3	2.25	0.50
1:X:2372:A:H5''	10:I:61:PRO:HB3	1.92	0.50
1:X:2474:G:H5''	11:J:82:THR:CA	2.40	0.50
1:X:2640:G:H2'	1:X:2641:A:C8	2.46	0.50
6:D:34:ILE:HD12	6:D:156:ILE:HG12	1.92	0.50
1:X:740:A:C6	1:X:741:G:C6	2.99	0.50
1:X:875:G:H2'	1:X:876:A:O4'	2.11	0.50
1:X:1935:A:N3	1:X:2539:C:O2'	2.38	0.50
1:X:2283:G:O2'	6:D:130:LEU:O	2.28	0.50
1:X:2558:C:H2'	1:X:2559:U:O4'	2.10	0.50
7:E:33:LEU:HD22	7:E:136:ILE:HG22	1.92	0.50
1:X:399:G:H5'	1:X:401:G:H22	1.75	0.50
1:X:489:A:O3'	19:R:45:LYS:NZ	2.44	0.50
1:X:518:A:O2'	1:X:519:C:OP1	2.28	0.50
1:X:754:G:H2'	1:X:755:C:H6	1.77	0.50
1:X:1573:G:H3'	1:X:1574:A:H5''	1.92	0.50
1:X:1997:A:H2'	1:X:1998:A:C8	2.47	0.50
1:X:2620:G:P	8:G:102:ARG:HH21	2.34	0.50
1:X:2705:A:C8	1:X:2706:U:H2'	2.47	0.50
5:C:47:THR:OG1	5:C:85:GLY:N	2.38	0.50
6:D:63:GLN:NE2	6:D:90:THR:O	2.24	0.50
8:G:67:ARG:HB2	8:G:76:GLN:NE2	2.26	0.50
20:S:91:PRO:HG2	20:S:125:PRO:HD2	1.93	0.50
26:1:14:SER:HB3	26:1:50:PHE:CD2	2.47	0.50
27:2:34:ARG:HG2	27:2:40:HIS:HD2	1.75	0.50
1:X:719:A:H2'	1:X:720:A:O4'	2.12	0.50
1:X:1850:G:H1'	1:X:1867:A:H62	1.77	0.50
10:I:88:PHE:HB3	10:I:90:ARG:CZ	2.41	0.50
12:K:11:ASN:ND2	12:K:11:ASN:H	2.07	0.50
1:X:761:G:C8	1:X:763:A:C8	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:877:G:H1	1:X:924:C:H42	1.58	0.50
1:X:1441:A:H4'	1:X:1442:C:O5'	2.12	0.50
1:X:1495:G:OP1	1:X:1576:G:O2'	2.28	0.50
1:X:1578:U:H2'	1:X:1579:G:H8	1.77	0.50
1:X:1870:U:O5'	1:X:1871:G:N2	2.45	0.50
15:N:90:LEU:O	15:N:92:ARG:HG3	2.11	0.50
1:X:409:G:H1'	22:U:45:ASN:ND2	2.27	0.50
1:X:734:G:H2'	1:X:735:G:H8	1.76	0.50
1:X:1427:G:N1	1:X:1603:A:OP1	2.45	0.50
1:X:2262:C:H2'	1:X:2263:C:O4'	2.11	0.50
1:X:2627:G:O2'	9:H:38:GLY:HA2	2.12	0.50
10:I:86:THR:OG1	10:I:116:ARG:NE	2.45	0.50
15:N:49:ASP:HA	15:N:52:ASN:HB2	1.92	0.50
17:P:97:VAL:HG22	17:P:124:ILE:HG23	1.94	0.50
18:Q:2:SER:OG	18:Q:3:HIS:N	2.45	0.50
19:R:90:LYS:HG3	19:R:108:VAL:HG21	1.93	0.50
28:3:34:THR:OG1	28:3:35:GLY:N	2.43	0.50
1:X:123:A:H1'	27:2:14:LYS:HD3	1.93	0.50
1:X:919:U:O3'	11:J:24:GLY:HA3	2.12	0.50
1:X:1614:C:H2'	1:X:1615:C:H6	1.77	0.50
3:A:244:ARG:HG2	3:A:244:ARG:O	2.12	0.50
5:C:112:GLN:OE1	5:C:112:GLN:HA	2.08	0.50
17:P:52:ASP:OD1	17:P:52:ASP:N	2.43	0.50
25:Z:56:GLN:OE1	25:Z:56:GLN:N	2.45	0.50
1:X:615:C:O2	1:X:670:U:O2'	2.30	0.50
1:X:971:A:H61	11:J:83:ARG:NH2	1.98	0.50
1:X:1235:C:H42	1:X:1240:G:H1	1.60	0.50
1:X:1481:U:O2'	1:X:1562:G:H1'	2.12	0.50
8:G:31:THR:OG1	8:G:32:TYR:N	2.37	0.50
1:X:332:C:H5''	1:X:333:A:OP2	2.12	0.49
1:X:399:G:H5'	1:X:401:G:N2	2.28	0.49
1:X:542:A:H8	15:N:28:ARG:NH2	2.10	0.49
1:X:542:A:C5'	15:N:28:ARG:HH21	2.26	0.49
1:X:825:C:H1'	1:X:1263:G:C2	2.46	0.49
1:X:1949:A:H1'	1:X:2572:U:H5'	1.93	0.49
1:X:2036:G:H5'	4:B:144:ARG:O	2.12	0.49
9:H:70:VAL:CG2	9:H:98:ILE:HG23	2.38	0.49
1:X:558:G:H8	1:X:560:G:N7	2.10	0.49
1:X:667:U:H2'	1:X:668:A:H5''	1.94	0.49
1:X:922:A:N7	1:X:923:A:C6	2.80	0.49
1:X:1223:G:N2	1:X:1249:G:O2'	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:42:U:HO2'	2:Y:47:A:N6	2.10	0.49
3:A:85:ASP:CG	3:A:92:ILE:HD12	2.37	0.49
5:C:53:LYS:O	5:C:54:THR:OG1	2.23	0.49
10:I:18:ARG:HB3	10:I:21:ARG:CB	2.42	0.49
11:J:44:LYS:HA	11:J:95:VAL:HG12	1.92	0.49
24:W:25:LEU:HD23	24:W:30:ASP:HB3	1.94	0.49
27:2:22:MET:HA	27:2:28:ARG:HD3	1.94	0.49
1:X:592:G:O5'	15:N:10:ARG:NH1	2.45	0.49
1:X:1236:G:O6	16:O:70:TYR:OH	2.29	0.49
1:X:1390:G:H8	1:X:1390:G:O5'	1.95	0.49
1:X:1750:A:C8	1:X:2675:U:H1'	2.47	0.49
1:X:2498:U:C5	1:X:2520:A:C6	3.00	0.49
1:X:2854:G:H4'	1:X:2855:C:OP1	2.12	0.49
2:Y:14:C:P	21:T:72:LYS:HZ3	2.35	0.49
5:C:47:THR:OG1	5:C:82:VAL:HG22	2.12	0.49
15:N:82:GLY:HA3	15:N:113:SER:OG	2.12	0.49
19:R:15:HIS:N	19:R:15:HIS:CD2	2.81	0.49
1:X:1006:C:N3	8:G:31:THR:HG23	2.26	0.49
1:X:1805:G:N3	3:A:50:THR:OG1	2.44	0.49
1:X:2335:U:H2'	1:X:2336:G:C8	2.48	0.49
5:C:5:ASN:ND2	5:C:9:GLN:HG3	2.27	0.49
9:H:83:ARG:HH12	14:M:38:LYS:HE2	1.77	0.49
17:P:35:PRO:O	17:P:39:ARG:HD3	2.12	0.49
19:R:33:THR:OG1	19:R:34:GLY:N	2.43	0.49
27:2:41:GLN:HA	27:2:41:GLN:HE21	1.76	0.49
1:X:420:C:H2'	1:X:421:G:C8	2.47	0.49
1:X:946:U:H2'	1:X:947:C:H6	1.73	0.49
1:X:1034:U:OP2	1:X:1036:G:O2'	2.31	0.49
1:X:1468:A:C8	1:X:1468:A:OP2	2.66	0.49
1:X:1827:G:H1'	1:X:1914:U:C2	2.48	0.49
1:X:2018:G:H4'	1:X:2019:C:OP2	2.13	0.49
1:X:2314:A:O2'	1:X:2316:G:N7	2.32	0.49
6:D:115:ARG:HH22	6:D:178:ARG:HH12	1.59	0.49
8:G:78:ASP:OD1	8:G:78:ASP:N	2.45	0.49
8:G:84:ASN:C	8:G:86:ALA:H	2.20	0.49
22:U:22:GLY:HA3	22:U:39:LYS:HZ1	1.77	0.49
22:U:60:VAL:O	22:U:61:TRP:HD1	1.95	0.49
27:2:38:GLY:O	27:2:40:HIS:N	2.45	0.49
1:X:585:U:H4'	1:X:2481:G:C8	2.48	0.49
1:X:746:G:C8	1:X:774:A:N1	2.80	0.49
1:X:871:U:O2	1:X:2247:A:H2'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1816:G:H2'	1:X:1817:U:C6	2.48	0.49
1:X:1918:G:H1'	1:X:1947:G:N2	2.28	0.49
1:X:2311:U:O2'	1:X:2315:A:N7	2.45	0.49
1:X:2500:C:H2'	1:X:2501:U:C6	2.47	0.49
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.95	0.49
1:X:386:U:H5'	1:X:436:A:N3	2.27	0.49
1:X:1834:G:H2'	1:X:1835:C:H6	1.77	0.49
1:X:2084:G:H2'	1:X:2085:G:C8	2.47	0.49
8:G:58:ILE:HG12	8:G:80:VAL:HG11	1.95	0.49
14:M:104:LEU:HA	14:M:106:TYR:CE2	2.48	0.49
25:Z:57:VAL:HG12	25:Z:58:LEU:HD23	1.95	0.49
1:X:635:C:O2'	1:X:670:U:OP1	2.29	0.49
1:X:645:G:H2'	1:X:646:C:C6	2.47	0.49
1:X:687:G:H4'	5:C:68:ARG:O	2.13	0.49
1:X:1675:C:H2'	1:X:1676:U:H6	1.76	0.49
1:X:1974:U:C2'	1:X:1975:G:H5'	2.42	0.49
1:X:2206:C:H2'	1:X:2207:G:O4'	2.12	0.49
8:G:43:VAL:HB	8:G:167:LYS:HG2	1.94	0.49
1:X:227:G:OP2	28:3:8:LYS:HG2	2.13	0.49
1:X:493:A:H4'	19:R:56:LYS:HG3	1.95	0.49
1:X:1004:A:OP1	15:N:50:ARG:NH1	2.41	0.49
1:X:1023:U:C4	8:G:53:ARG:HG3	2.47	0.49
1:X:1742:G:H2'	1:X:1743:C:C6	2.47	0.49
1:X:1746:A:C2	1:X:2696:A:H1'	2.47	0.49
1:X:1779:C:H2'	1:X:1780:A:C8	2.48	0.49
1:X:2598:C:O2'	1:X:2599:U:H5'	2.12	0.49
3:A:76:ASN:HA	3:A:118:ASN:HA	1.94	0.49
5:C:22:VAL:HG22	5:C:110:SER:HA	1.94	0.49
5:C:60:GLY:C	5:C:62:LYS:H	2.21	0.49
11:J:60:ARG:HA	11:J:60:ARG:HE	1.77	0.49
23:V:2:LYS:HB2	23:V:3:PRO:HD3	1.95	0.49
1:X:58:C:H1'	1:X:72:A:H2'	1.93	0.49
1:X:870:C:H5''	21:T:77:ARG:HH22	1.78	0.49
1:X:1225:G:O6	17:P:12:LYS:HB2	2.12	0.49
1:X:1272:G:H2'	1:X:1273:G:C8	2.48	0.49
1:X:1350:G:H2'	1:X:1351:G:C8	2.46	0.49
1:X:1448:A:N6	1:X:1574:A:H61	2.11	0.49
1:X:1578:U:H2'	1:X:1579:G:C8	2.48	0.49
1:X:1791:C:OP2	3:A:183:ARG:NH1	2.44	0.49
1:X:2326:C:OP1	1:X:2326:C:H4'	2.13	0.49
1:X:2572:U:H2'	1:X:2573:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:128:ALA:O	5:C:130:THR:N	2.38	0.49
12:K:73:LYS:O	12:K:76:VAL:HG12	2.13	0.49
13:L:33:ARG:NH1	13:L:38:ILE:HG21	2.28	0.49
20:S:80:HIS:NE2	20:S:82:ASP:OD2	2.43	0.49
1:X:38:G:O2'	1:X:39:C:O5'	2.23	0.48
1:X:89:A:H4'	1:X:90:G:C5'	2.40	0.48
1:X:321:A:C6	1:X:323:G:C4	3.01	0.48
1:X:591:G:C6	1:X:592:G:C6	3.00	0.48
1:X:1468:A:OP2	1:X:1468:A:H8	1.96	0.48
1:X:2516:U:H2'	1:X:2517:C:H6	1.75	0.48
2:Y:3:A:N6	2:Y:121:G:O6	2.46	0.48
3:A:29:PRO:HB2	3:A:30:GLU:CD	2.38	0.48
7:E:61:HIS:C	7:E:63:ALA:H	2.21	0.48
8:G:62:ILE:O	8:G:77:GLY:HA3	2.13	0.48
8:G:71:THR:N	8:G:76:GLN:HE22	2.10	0.48
22:U:17:SER:HB2	22:U:44:ALA:HA	1.95	0.48
1:X:5:A:H2'	1:X:6:A:C8	2.48	0.48
1:X:40:U:H2'	1:X:41:G:C8	2.48	0.48
1:X:70:A:H5''	1:X:71:A:H2'	1.95	0.48
1:X:121:G:H2'	1:X:122:G:O4'	2.13	0.48
1:X:590:C:H2'	1:X:591:G:C8	2.48	0.48
1:X:865:A:H5'	24:W:42:GLY:HA3	1.94	0.48
1:X:977:G:C1'	1:X:2246:A:H62	2.26	0.48
1:X:1699:A:H61	1:X:1723:U:H3	1.61	0.48
1:X:2211:U:OP1	22:U:43:ARG:NH1	2.22	0.48
1:X:2225:G:H2'	1:X:2226:A:C8	2.47	0.48
1:X:2619:G:OP1	8:G:125:ARG:NH2	2.46	0.48
1:X:2796:A:H4'	4:B:162:MET:SD	2.53	0.48
4:B:16:LYS:H	4:B:21:ILE:HD11	1.78	0.48
16:O:10:LYS:HE2	16:O:13:ARG:NH2	2.27	0.48
17:P:71:VAL:HG13	17:P:126:ILE:HG22	1.95	0.48
22:U:23:LYS:HB2	22:U:35:THR:HG23	1.94	0.48
1:X:318:G:N1	1:X:321:A:OP2	2.45	0.48
1:X:577:U:H2'	1:X:579:G:OP2	2.12	0.48
1:X:596:C:C4	1:X:684:C:C2	3.02	0.48
1:X:824:U:H2'	10:I:30:ALA:N	2.29	0.48
1:X:1269:G:N3	1:X:1269:G:H2'	2.28	0.48
1:X:2240:C:C2'	1:X:2241:U:H5'	2.43	0.48
1:X:2370:G:O6	1:X:2406:C:H1'	2.13	0.48
1:X:2596:C:H2'	1:X:2597:G:H8	1.77	0.48
4:B:119:ARG:HA	4:B:160:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:26:VAL:O	5:C:30:VAL:HG23	2.12	0.48
14:M:32:THR:O	14:M:51:GLU:HA	2.13	0.48
1:X:1466:C:H2'	1:X:1467:U:C1'	2.43	0.48
1:X:1510:A:H2'	1:X:1511:A:O4'	2.13	0.48
1:X:1630:A:OP1	1:X:1633:C:N4	2.40	0.48
1:X:1982:C:O2	1:X:2666:U:O2'	2.29	0.48
1:X:2031:A:H2'	1:X:2032:G:O4'	2.13	0.48
1:X:2571:G:C6	1:X:2572:U:N3	2.82	0.48
11:J:11:ARG:NE	11:J:15:ARG:HH12	2.11	0.48
20:S:3:LEU:HD22	20:S:32:PHE:CD2	2.48	0.48
23:V:31:GLN:O	23:V:36:GLN:HB3	2.12	0.48
1:X:154:U:H3'	1:X:155:G:H8	1.78	0.48
1:X:331:U:H2'	5:C:130:THR:HG21	1.93	0.48
1:X:343:A:O2'	1:X:346:C:N4	2.42	0.48
1:X:540:G:C6	1:X:2005:U:H5''	2.48	0.48
1:X:1075:C:H2'	1:X:1076:U:O4'	2.13	0.48
1:X:1678:G:H1	1:X:1982:C:N4	2.07	0.48
1:X:2200:G:H2'	1:X:2201:G:C8	2.47	0.48
1:X:2691:C:O2'	1:X:2693:U:H5'	2.14	0.48
6:D:13:ARG:O	6:D:17:MET:HG3	2.13	0.48
7:E:121:VAL:HG11	7:E:144:VAL:HG21	1.95	0.48
9:H:62:GLY:O	9:H:65:LYS:NZ	2.36	0.48
11:J:15:ARG:HD3	11:J:73:LYS:HE3	1.96	0.48
16:O:11:GLN:HA	16:O:38:LEU:O	2.13	0.48
25:Z:16:ARG:HD3	25:Z:20:ARG:CZ	2.44	0.48
1:X:1029:C:H42	1:X:1155:G:H1	1.62	0.48
1:X:1151:U:O4	8:G:93:LYS:HE3	2.14	0.48
1:X:1310:C:H2'	1:X:1311:C:H6	1.79	0.48
1:X:1705:U:O2	1:X:1717:A:H5'	2.13	0.48
1:X:2670:C:H2'	1:X:2671:C:H6	1.79	0.48
1:X:2751:C:H2'	1:X:2752:C:C6	2.48	0.48
1:X:2787:A:H2'	1:X:2788:C:H6	1.78	0.48
3:A:14:ARG:NH1	3:A:27:LYS:O	2.47	0.48
8:G:67:ARG:HD3	8:G:70:PHE:C	2.39	0.48
26:1:37:LEU:HD23	26:1:51:ARG:HA	1.96	0.48
1:X:438:G:H2'	1:X:439:C:C6	2.49	0.48
1:X:507:A:OP2	17:P:19:LYS:NZ	2.36	0.48
1:X:546:A:H2'	1:X:547:U:C6	2.48	0.48
1:X:810:U:H2'	1:X:811:G:O4'	2.12	0.48
1:X:1603:A:H8	1:X:1603:A:OP2	1.96	0.48
1:X:2738:A:C5	7:E:67:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:17:MET:HG2	6:D:22:TYR:HB2	1.94	0.48
7:E:67:LEU:O	7:E:71:LEU:HG	2.13	0.48
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.29	0.48
15:N:76:TYR:CZ	15:N:80:ILE:HG13	2.48	0.48
22:U:32:ARG:HE	22:U:32:ARG:N	2.10	0.48
1:X:303:C:H3'	1:X:304:A:H5''	1.95	0.48
1:X:542:A:H2	1:X:2004:U:H2'	1.78	0.48
1:X:649:G:C5	1:X:650:U:C5	3.01	0.48
1:X:688:A:H4'	5:C:61:GLN:OE1	2.12	0.48
1:X:736:G:H2'	1:X:737:C:O4'	2.13	0.48
1:X:1148:G:O2'	8:G:134:MET:HG3	2.13	0.48
1:X:1269:G:O3'	5:C:69:HIS:CE1	2.67	0.48
1:X:1276:U:O4'	25:Z:10:LYS:HG3	2.13	0.48
1:X:1426:U:H2'	1:X:1427:G:O4'	2.14	0.48
1:X:1563:U:H2'	1:X:1564:U:C6	2.48	0.48
1:X:1984:A:H2'	1:X:1985:G:O4'	2.14	0.48
5:C:71:ASP:OD1	5:C:72:ARG:N	2.44	0.48
5:C:117:LEU:HB3	5:C:187:VAL:HA	1.94	0.48
19:R:18:LYS:HE2	19:R:19:GLY:N	2.28	0.48
1:X:115:G:OP2	1:X:117:A:O2'	2.32	0.48
1:X:227:G:C6	1:X:228:A:C6	3.02	0.48
1:X:401:G:OP1	22:U:35:THR:HB	2.13	0.48
1:X:536:A:N6	1:X:2605:C:H4'	2.28	0.48
1:X:1202:U:H2'	1:X:1203:A:H8	1.78	0.48
1:X:1442:C:O2'	1:X:1585:A:OP2	2.22	0.48
1:X:1782:A:N3	3:A:208:LYS:HE2	2.29	0.48
1:X:1816:G:H2'	1:X:1817:U:H6	1.78	0.48
1:X:1816:G:N2	3:A:252:LYS:HG3	2.28	0.48
1:X:2370:G:C6	1:X:2406:C:H1'	2.49	0.48
2:Y:63:A:H2'	2:Y:64:C:H6	1.79	0.48
6:D:14:PRO:HA	6:D:17:MET:HB2	1.96	0.48
11:J:42:TRP:HB3	11:J:95:VAL:HG11	1.95	0.48
20:S:168:VAL:HG12	20:S:169:VAL:HG23	1.95	0.48
28:3:15:LYS:HB2	28:3:23:MET:HB2	1.96	0.48
1:X:69:G:H1'	1:X:72:A:H1'	1.95	0.48
1:X:240:U:H2'	1:X:241:C:O4'	2.14	0.48
1:X:613:A:N6	1:X:668:A:O4'	2.46	0.48
1:X:809:C:H2'	1:X:810:U:C6	2.49	0.48
1:X:1163:C:H2'	1:X:1164:C:H6	1.78	0.48
1:X:1337:G:N2	1:X:1344:C:C2	2.82	0.48
1:X:2551:A:N7	4:B:144:ARG:HG2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2674:C:H2'	1:X:2675:U:C6	2.49	0.48
1:X:2784:A:C6	1:X:2866:A:C8	3.02	0.48
1:X:2821:G:H2'	1:X:2822:U:O4'	2.14	0.48
3:A:208:LYS:O	3:A:211:ARG:HB3	2.14	0.48
5:C:149:LEU:HB2	5:C:183:HIS:ND1	2.29	0.48
11:J:131:LYS:HB2	11:J:131:LYS:NZ	2.28	0.48
13:L:60:LYS:HD2	13:L:60:LYS:HA	1.58	0.48
15:N:49:ASP:O	15:N:53:LYS:HG2	2.14	0.48
15:N:92:ARG:O	15:N:93:LYS:HD3	2.12	0.48
16:O:5:ILE:N	16:O:10:LYS:HD3	2.28	0.48
1:X:469:G:H5'	27:2:39:ARG:O	2.14	0.47
1:X:785:U:H2'	1:X:786:U:H6	1.78	0.47
1:X:1003:C:H2'	1:X:1004:A:C8	2.46	0.47
1:X:1024:G:N2	1:X:1161:U:O2	2.47	0.47
1:X:1054:C:N4	1:X:1123:G:H1	2.10	0.47
1:X:1653:C:H2'	1:X:1654:A:C8	2.49	0.47
1:X:1845:A:N3	1:X:2212:U:O2'	2.43	0.47
1:X:2015:G:OP2	1:X:2433:G:O2'	2.26	0.47
1:X:2060:A:H2'	1:X:2061:C:H6	1.78	0.47
1:X:2378:G:H1	1:X:2396:C:H42	1.61	0.47
12:K:3:HIS:HB3	12:K:5:LYS:HD2	1.96	0.47
13:L:47:ARG:C	13:L:49:GLN:H	2.20	0.47
16:O:11:GLN:HB2	16:O:13:ARG:HH21	1.78	0.47
18:Q:31:PRO:HA	18:Q:76:LYS:CB	2.44	0.47
21:T:17:ASN:HA	21:T:18:PRO:HD3	1.64	0.47
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.47	0.47
26:1:13:GLU:O	26:1:14:SER:OG	2.27	0.47
1:X:824:U:H2'	10:I:30:ALA:H	1.78	0.47
1:X:2492:G:H2'	1:X:2493:U:C6	2.48	0.47
1:X:2798:A:C5	1:X:2799:C:C5	3.02	0.47
4:B:4:ILE:HG22	4:B:96:PHE:HE1	1.79	0.47
8:G:81:VAL:HG21	8:G:161:GLN:HG2	1.96	0.47
12:K:11:ASN:O	12:K:12:ARG:HG2	2.13	0.47
15:N:79:PHE:HE2	15:N:95:LEU:HD21	1.79	0.47
19:R:10:HIS:HD2	19:R:44:GLN:NE2	2.12	0.47
1:X:125:A:H5''	1:X:126:C:O4'	2.14	0.47
1:X:1357:U:H4'	1:X:1397:A:C6	2.49	0.47
1:X:1988:A:H5''	1:X:1989:C:OP2	2.14	0.47
1:X:2614:A:O2'	4:B:48:GLN:NE2	2.47	0.47
4:B:38:THR:HG22	4:B:40:GLN:H	1.79	0.47
7:E:56:SER:OG	7:E:61:HIS:ND1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:82:THR:HG23	11:J:84:MET:H	1.79	0.47
17:P:94:GLU:HG3	17:P:127:ILE:HB	1.96	0.47
18:Q:31:PRO:HA	18:Q:76:LYS:HB2	1.97	0.47
1:X:557:U:O4	1:X:560:G:N2	2.47	0.47
1:X:1348:C:H2'	1:X:1349:A:C8	2.49	0.47
1:X:1854:G:H1	1:X:1863:U:H3	1.62	0.47
1:X:1976:U:H5''	4:B:128:SER:HB3	1.96	0.47
1:X:2382:C:N4	1:X:2393:G:H1	2.11	0.47
1:X:2477:C:H5'	1:X:2477:C:H6	1.79	0.47
1:X:2610:G:O2'	1:X:2785:A:N1	2.42	0.47
3:A:96:HIS:HB2	3:A:102:LYS:NZ	2.29	0.47
3:A:198:ASN:O	3:A:198:ASN:ND2	2.48	0.47
5:C:43:ALA:HB3	5:C:86:PRO:HB2	1.96	0.47
21:T:38:VAL:HG21	21:T:45:PHE:CE1	2.50	0.47
1:X:830:C:O2'	1:X:852:U:H5''	2.15	0.47
1:X:1779:C:H2'	1:X:1780:A:H8	1.78	0.47
1:X:1884:A:OP2	3:A:252:LYS:HE3	2.14	0.47
1:X:2797:G:O2'	1:X:2799:C:OP2	2.30	0.47
1:X:2826:C:H2'	1:X:2827:G:O4'	2.15	0.47
1:X:2860:C:H2'	1:X:2861:A:O4'	2.14	0.47
1:X:2871:U:H2'	1:X:2872:U:C6	2.49	0.47
8:G:162:LYS:N	8:G:163:PRO:HD2	2.30	0.47
11:J:137:VAL:HG11	20:S:71:MET:SD	2.55	0.47
19:R:59:LYS:HD2	19:R:62:MET:HG3	1.96	0.47
20:S:25:ASN:OD1	20:S:27:GLU:HB2	2.14	0.47
20:S:122:ILE:HB	20:S:123:VAL:H	1.58	0.47
1:X:87:G:C2'	1:X:88:G:H5''	2.43	0.47
1:X:485:G:C6	1:X:520:C:N4	2.83	0.47
1:X:661:C:OP1	28:3:19:THR:OG1	2.20	0.47
1:X:788:G:C4	1:X:807:A:C8	3.02	0.47
1:X:792:U:OP1	3:A:48:ARG:HA	2.14	0.47
1:X:1260:A:C6	1:X:1262:U:C2	3.02	0.47
1:X:1283:C:H5''	1:X:1284:G:C5'	2.44	0.47
1:X:1348:C:H4'	18:Q:64:ARG:HH12	1.79	0.47
1:X:1399:C:OP2	1:X:1409:U:N3	2.46	0.47
1:X:1494:G:H2'	1:X:1495:G:H8	1.78	0.47
1:X:1746:A:H2	1:X:2696:A:H1'	1.80	0.47
1:X:1785:A:H2'	1:X:1786:C:H6	1.79	0.47
1:X:2691:C:O2'	1:X:2692:A:OP2	2.31	0.47
4:B:188:ILE:HG12	4:B:189:PRO:HD2	1.96	0.47
5:C:18:PRO:HD2	5:C:109:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:25:GLY:HA3	10:I:18:ARG:NH1	2.30	0.47
11:J:8:THR:HG23	11:J:70:PHE:HE2	1.79	0.47
17:P:59:PHE:CG	25:Z:30:LEU:HD21	2.50	0.47
18:Q:53:ILE:HD13	18:Q:80:VAL:HG13	1.97	0.47
22:U:31:GLY:HA2	22:U:32:ARG:HE	1.80	0.47
1:X:105:G:H21	1:X:357:A:H61	1.62	0.47
1:X:239:A:H5''	1:X:621:U:H5'	1.96	0.47
1:X:340:G:O4'	1:X:488:A:H1'	2.15	0.47
1:X:474:G:N2	1:X:476:G:H3'	2.30	0.47
1:X:597:U:H2'	1:X:598:U:C6	2.49	0.47
1:X:624:A:O2'	1:X:626:A:OP2	2.28	0.47
1:X:652:C:H42	1:X:657:A:H61	1.63	0.47
1:X:836:G:H2'	1:X:837:U:C6	2.49	0.47
1:X:865:A:H2'	1:X:866:U:C6	2.50	0.47
1:X:875:G:O2'	2:Y:80:A:N3	2.47	0.47
1:X:1330:G:O6	1:X:1349:A:N6	2.48	0.47
1:X:1349:A:H2'	1:X:1350:G:H8	1.79	0.47
1:X:1437:A:H2'	1:X:1438:G:C8	2.49	0.47
1:X:2067:U:H2'	1:X:2068:C:C6	2.49	0.47
1:X:2084:G:H1	1:X:2171:U:H3	1.62	0.47
1:X:2258:G:O6	21:T:14:ARG:HG3	2.15	0.47
2:Y:36:A:N6	2:Y:46:G:H2'	2.29	0.47
3:A:108:PRO:HG2	3:A:111:LEU:HB2	1.95	0.47
3:A:246:PRO:CD	3:A:251:GLY:H	2.21	0.47
4:B:37:LYS:HD2	4:B:42:ASP:OD1	2.14	0.47
4:B:96:PHE:CD2	4:B:102:ILE:HG21	2.48	0.47
5:C:5:ASN:N	5:C:5:ASN:OD1	2.47	0.47
8:G:116:ARG:NH1	8:G:126:VAL:HG13	2.29	0.47
9:H:17:ARG:H	9:H:58:ALA:HA	1.78	0.47
10:I:107:LYS:HG3	10:I:125:ALA:HA	1.96	0.47
11:J:137:VAL:HG21	20:S:71:MET:SD	2.54	0.47
12:K:98:LEU:HD13	12:K:98:LEU:HA	1.60	0.47
14:M:55:ILE:O	14:M:103:LYS:O	2.32	0.47
15:N:45:TYR:O	15:N:49:ASP:HB2	2.15	0.47
19:R:29:HIS:CG	19:R:51:VAL:HG22	2.50	0.47
19:R:45:LYS:HA	19:R:76:LEU:O	2.15	0.47
21:T:38:VAL:HG21	21:T:45:PHE:CZ	2.49	0.47
1:X:37:C:O2'	5:C:44:SER:HB3	2.15	0.47
1:X:768:U:H2'	1:X:769:C:O4'	2.15	0.47
1:X:876:A:O2'	1:X:877:G:H5'	2.14	0.47
1:X:1219:C:H2'	1:X:1220:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1631:C:H2'	1:X:1631:C:O2	2.15	0.47
1:X:1975:G:O2'	1:X:1976:U:OP2	2.24	0.47
1:X:2171:U:H4'	1:X:2171:U:OP1	2.15	0.47
1:X:2284:U:H3'	1:X:2286:G:N2	2.29	0.47
1:X:2537:C:H2'	1:X:2538:C:O4'	2.14	0.47
2:Y:80:A:H2'	2:Y:81:C:O4'	2.15	0.47
4:B:84:PHE:O	4:B:86:PRO:HD3	2.14	0.47
7:E:94:PHE:HB3	7:E:107:ILE:HG22	1.95	0.47
13:L:33:ARG:NH2	13:L:103:LEU:HB2	2.29	0.47
16:O:39:PHE:HE2	16:O:46:VAL:HB	1.78	0.47
19:R:15:HIS:CD2	19:R:15:HIS:H	2.33	0.47
1:X:17:G:H2'	1:X:18:U:C6	2.50	0.47
1:X:39:C:H1'	5:C:42:THR:HG21	1.96	0.47
1:X:187:U:H2'	1:X:188:G:C8	2.50	0.47
1:X:321:A:N6	1:X:323:G:N3	2.63	0.47
1:X:353:G:H2'	1:X:354:C:C6	2.50	0.47
1:X:469:G:H3'	27:2:39:ARG:O	2.14	0.47
1:X:1669:A:OP1	12:K:9:LYS:HE2	2.15	0.47
1:X:1757:C:O2'	1:X:1758:C:H5'	2.15	0.47
1:X:2817:A:H2'	1:X:2818:G:O4'	2.15	0.47
28:3:26:LYS:HG2	28:3:43:GLY:O	2.15	0.47
1:X:825:C:H5''	10:I:30:ALA:CB	2.45	0.47
1:X:2367:A:N7	1:X:2368:G:C6	2.83	0.47
1:X:2660:C:C2	1:X:2704:U:O4	2.68	0.47
1:X:2766:U:O2'	4:B:62:PRO:O	2.24	0.47
1:X:2769:C:H1'	1:X:2866:A:H2	1.79	0.47
3:A:163:VAL:HG22	3:A:177:LEU:HA	1.97	0.47
11:J:62:GLY:N	11:J:63:GLY:HA2	2.30	0.47
19:R:61:SER:HA	19:R:65:PRO:HG3	1.97	0.47
20:S:3:LEU:HB3	20:S:56:VAL:HA	1.96	0.47
25:Z:40:LYS:HD3	25:Z:46:CYS:HB2	1.97	0.47
1:X:757:U:H2'	1:X:758:G:O4'	2.14	0.46
4:B:183:LEU:HD21	14:M:16:ILE:HG12	1.97	0.46
6:D:111:ILE:HG22	6:D:114:PHE:HB2	1.96	0.46
14:M:57:ILE:H	14:M:57:ILE:HD12	1.81	0.46
22:U:20:ARG:HE	22:U:20:ARG:HB2	1.47	0.46
1:X:494:A:O4'	19:R:56:LYS:HB2	2.14	0.46
1:X:956:A:C4	1:X:2427:A:C2	3.03	0.46
1:X:2265:A:OP1	26:1:31:THR:OG1	2.21	0.46
3:A:63:ARG:HG3	3:A:85:ASP:OD1	2.15	0.46
3:A:188:GLU:HG2	3:A:188:GLU:H	1.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:65:LYS:NZ	15:N:70:ARG:HD2	2.30	0.46
20:S:95:SER:HB3	20:S:119:ASN:HB3	1.97	0.46
23:V:62:ARG:O	23:V:66:GLN:N	2.45	0.46
1:X:32:C:O2'	1:X:33:C:H5'	2.16	0.46
1:X:811:G:OP2	5:C:56:ARG:HG2	2.15	0.46
1:X:1584:G:H4'	3:A:59:LYS:HG3	1.97	0.46
1:X:1673:C:H2'	1:X:1674:C:H6	1.80	0.46
1:X:1802:A:H2'	1:X:1803:G:O4'	2.15	0.46
1:X:1827:G:H1	1:X:1888:C:H42	1.63	0.46
1:X:2394:G:C2	1:X:2395:C:C2	3.03	0.46
1:X:2629:U:H2'	1:X:2630:C:H6	1.81	0.46
2:Y:51:G:OP1	13:L:99:ARG:N	2.41	0.46
3:A:91:ARG:O	3:A:107:ALA:N	2.33	0.46
3:A:245:VAL:HB	3:A:249:PRO:HA	1.97	0.46
6:D:104:ILE:HG12	6:D:108:LEU:HD12	1.98	0.46
11:J:54:VAL:HG21	11:J:125:LYS:HE3	1.97	0.46
15:N:102:GLU:HA	15:N:103:PRO:HD3	1.69	0.46
21:T:47:ALA:HB1	21:T:51:VAL:HB	1.96	0.46
1:X:224:G:H4'	1:X:399:G:C6	2.50	0.46
1:X:623:G:H21	1:X:626:A:H2	1.61	0.46
1:X:765:C:OP2	27:2:1:MET:HE2	2.15	0.46
1:X:1609:G:H2'	1:X:1610:A:O4'	2.16	0.46
1:X:1761:G:C5	1:X:1762:C:C5	3.03	0.46
2:Y:14:C:H4'	2:Y:17:A:H62	1.79	0.46
4:B:14:ILE:HA	14:M:20:HIS:CD2	2.49	0.46
6:D:17:MET:HE3	6:D:22:TYR:HB3	1.98	0.46
6:D:112:ARG:CZ	6:D:137:ILE:HG22	2.46	0.46
7:E:34:THR:O	7:E:34:THR:OG1	2.34	0.46
8:G:34:PRO:HA	8:G:69:ASP:CG	2.41	0.46
11:J:79:PRO:CD	11:J:88:LYS:HD2	2.45	0.46
22:U:20:ARG:HD2	22:U:43:ARG:NE	2.30	0.46
9:H:134:LEU:HA	9:H:134:LEU:HD23	1.78	0.46
11:J:20:GLY:O	11:J:99:LYS:HG2	2.16	0.46
15:N:66:ASN:HD22	15:N:70:ARG:HH12	1.63	0.46
18:Q:4:TYR:CE2	23:V:23:LYS:HB2	2.51	0.46
19:R:81:VAL:HG12	19:R:82:ALA:N	2.30	0.46
1:X:670:U:H2'	1:X:671:A:C8	2.50	0.46
1:X:753:U:H2'	1:X:754:G:H8	1.80	0.46
1:X:1046:U:C5'	7:E:59:GLN:HG2	2.45	0.46
1:X:1925:C:H2'	1:X:1926:U:C5	2.50	0.46
1:X:2309:G:H2'	1:X:2310:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2663:U:H3	1:X:2705:A:N6	2.09	0.46
1:X:2707:G:H2'	1:X:2708:U:C6	2.50	0.46
2:Y:46:G:H1'	2:Y:49:C:N4	2.31	0.46
3:A:117:VAL:HG13	3:A:129:ASN:HD22	1.80	0.46
4:B:188:ILE:HG12	4:B:189:PRO:CD	2.46	0.46
6:D:133:LYS:O	6:D:151:GLY:HA3	2.15	0.46
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.97	0.46
15:N:86:ALA:C	15:N:88:ILE:N	2.74	0.46
17:P:44:VAL:HG21	25:Z:27:ALA:HB2	1.98	0.46
19:R:18:LYS:H	19:R:18:LYS:HD3	1.79	0.46
19:R:61:SER:HA	19:R:65:PRO:HB3	1.97	0.46
27:2:28:ARG:HD2	27:2:28:ARG:HA	1.75	0.46
1:X:388:G:H2'	1:X:389:G:C8	2.51	0.46
1:X:529:U:H2'	1:X:530:G:H8	1.80	0.46
1:X:568:G:H2'	1:X:569:C:O4'	2.16	0.46
1:X:1004:A:N3	16:O:88:GLN:NE2	2.63	0.46
1:X:1104:G:H1'	1:X:1110:G:N2	2.31	0.46
1:X:1231:A:C2	1:X:1245:G:C2	3.04	0.46
1:X:1349:A:H2'	1:X:1350:G:C8	2.50	0.46
1:X:2272:A:P	13:L:15:ARG:HH21	2.38	0.46
3:A:244:ARG:NH1	3:A:253:PRO:HG3	2.31	0.46
7:E:90:ARG:CZ	7:E:163:ARG:HD2	2.46	0.46
8:G:140:GLN:O	8:G:143:ALA:HB3	2.15	0.46
26:1:42:PRO:HG3	26:1:50:PHE:CE1	2.51	0.46
1:X:20:C:H2'	1:X:21:A:C8	2.50	0.46
1:X:162:C:H2'	1:X:163:A:C8	2.51	0.46
1:X:742:G:C5	3:A:208:LYS:HB3	2.50	0.46
1:X:1361:G:H2'	1:X:1362:A:C8	2.51	0.46
1:X:1606:C:N4	1:X:1607:A:H62	2.14	0.46
1:X:2057:U:H2'	1:X:2058:U:C6	2.51	0.46
1:X:2363:G:OP2	1:X:2363:G:H8	1.99	0.46
1:X:2474:G:H2'	1:X:2475:C:O4'	2.16	0.46
2:Y:70:C:H2'	2:Y:71:G:O4'	2.15	0.46
2:Y:77:G:H1'	20:S:22:VAL:HG21	1.97	0.46
3:A:55:GLY:C	3:A:217:ARG:HD3	2.40	0.46
3:A:218:LYS:HA	3:A:218:LYS:HD2	1.60	0.46
8:G:42:VAL:HA	8:G:166:LEU:O	2.16	0.46
8:G:170:PRO:O	8:G:171:LEU:HB2	2.15	0.46
13:L:15:ARG:HA	13:L:15:ARG:HD3	1.70	0.46
16:O:36:LYS:HZ1	16:O:56:VAL:HG13	1.80	0.46
16:O:36:LYS:NZ	16:O:56:VAL:HG13	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:67:LYS:HG3	16:O:68:LYS:N	2.30	0.46
27:2:18:PHE:H	27:2:44:VAL:CG2	2.29	0.46
1:X:464:G:H2'	1:X:465:C:C6	2.51	0.46
1:X:627:A:H2'	1:X:628:A:H8	1.78	0.46
1:X:1583:A:H2	3:A:31:LYS:HE2	1.80	0.46
1:X:1987:G:C5	1:X:1988:A:C8	3.04	0.46
1:X:2448:A:H2'	1:X:2449:G:O4'	2.16	0.46
1:X:2845:C:C4	1:X:2846:G:N7	2.84	0.46
9:H:23:ARG:HG3	9:H:24:VAL:N	2.31	0.46
13:L:8:ARG:HG3	13:L:9:ARG:N	2.30	0.46
1:X:18:U:O2'	15:N:23:GLY:HA2	2.16	0.46
1:X:334:G:OP1	1:X:349:G:N2	2.47	0.46
1:X:1439:G:H2'	1:X:1440:G:C8	2.51	0.46
1:X:1494:G:C4	1:X:1495:G:C8	3.04	0.46
1:X:1710:U:H5''	1:X:1711:C:H5	1.81	0.46
1:X:2039:G:C2	1:X:2040:A:C8	3.04	0.46
1:X:2200:G:H2'	1:X:2201:G:H8	1.80	0.46
1:X:2707:G:H2'	1:X:2708:U:H6	1.81	0.46
1:X:2796:A:H2'	1:X:2797:G:C8	2.47	0.46
2:Y:78:A:H2'	2:Y:79:U:O4'	2.16	0.46
9:H:29:ILE:CG2	9:H:122:ARG:HB2	2.44	0.46
13:L:20:THR:HG21	13:L:23:ALA:HB3	1.97	0.46
15:N:62:ILE:HG23	15:N:76:TYR:CE1	2.51	0.46
17:P:89:ARG:HD3	17:P:132:GLY:HA2	1.98	0.46
18:Q:66:GLY:HA3	18:Q:68:PHE:CD2	2.51	0.46
27:2:1:MET:HG3	27:2:3:ARG:HH12	1.80	0.46
27:2:21:ARG:HE	27:2:43:THR:HG21	1.81	0.46
1:X:78:C:O2'	1:X:357:A:N3	2.46	0.45
1:X:562:G:C6	1:X:563:U:C4	3.04	0.45
1:X:732:G:H2'	1:X:733:G:C8	2.51	0.45
1:X:750:C:H2'	1:X:751:G:H5'	1.98	0.45
1:X:849:G:C5	1:X:850:C:C4	3.04	0.45
1:X:1407:G:C6	1:X:1408:A:N6	2.84	0.45
1:X:2197:U:H5'	1:X:2198:U:OP1	2.16	0.45
1:X:2447:G:OP1	11:J:120:ARG:NH2	2.49	0.45
6:D:112:ARG:N	6:D:112:ARG:HD2	2.31	0.45
9:H:11:ALA:O	9:H:111:PHE:N	2.41	0.45
1:X:746:G:C8	1:X:774:A:C6	3.04	0.45
1:X:938:G:H2'	1:X:940:G:N7	2.32	0.45
1:X:1008:G:H5'	15:N:93:LYS:HG3	1.98	0.45
1:X:1459:U:O2	1:X:1475:U:H5''	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1715:A:C8	1:X:1717:A:O4'	2.70	0.45
1:X:1981:A:O2'	1:X:2704:U:O2'	2.23	0.45
1:X:2229:G:C6	11:J:83:ARG:HG2	2.52	0.45
1:X:2468:G:C6	1:X:2469:G:C6	3.05	0.45
1:X:2495:G:O2'	1:X:2496:C:H5'	2.16	0.45
3:A:222:ARG:HH11	3:A:225:ALA:HB2	1.81	0.45
7:E:45:GLN:NE2	7:E:48:ASP:O	2.48	0.45
7:E:69:ARG:HH21	7:E:73:ALA:HB2	1.81	0.45
8:G:66:HIS:CD2	15:N:71:LEU:HD13	2.51	0.45
8:G:154:GLU:C	8:G:157:PRO:HD2	2.41	0.45
20:S:62:PHE:HB3	20:S:85:MET:HE2	1.99	0.45
1:X:66:U:H2'	1:X:67:G:H8	1.82	0.45
1:X:595:A:N1	1:X:822:G:O2'	2.39	0.45
1:X:1745:C:C5	1:X:1746:A:C5	3.04	0.45
1:X:2262:C:OP1	26:1:7:ARG:NH1	2.48	0.45
1:X:2422:C:H2'	1:X:2423:G:H8	1.81	0.45
1:X:2594:U:N1	25:Z:7:PRO:HA	2.31	0.45
2:Y:27:A:HO2'	2:Y:28:A:P	2.38	0.45
5:C:128:ALA:C	5:C:130:THR:H	2.24	0.45
9:H:3:MET:O	9:H:6:SER:HB3	2.16	0.45
9:H:124:MET:HB3	9:H:124:MET:HE3	1.66	0.45
10:I:75:VAL:HG22	10:I:99:VAL:HG21	1.97	0.45
11:J:6:LYS:HE2	11:J:6:LYS:HB3	1.69	0.45
19:R:96:LYS:O	19:R:104:VAL:HA	2.16	0.45
25:Z:18:MET:HE3	25:Z:18:MET:HB2	1.86	0.45
28:3:13:ARG:HD2	28:3:24:ALA:HA	1.98	0.45
1:X:400:U:H4'	1:X:401:G:O5'	2.16	0.45
1:X:764:A:C6	1:X:802:A:C5	3.04	0.45
1:X:1121:G:H2'	1:X:1122:A:C8	2.52	0.45
1:X:1164:C:H2'	1:X:1165:G:O4'	2.17	0.45
1:X:1781:C:OP1	3:A:219:PRO:HB2	2.16	0.45
1:X:1922:U:H5''	1:X:1922:U:O2	2.16	0.45
1:X:2058:U:H2'	1:X:2217:G:N2	2.32	0.45
1:X:2401:A:N3	1:X:2401:A:H2'	2.31	0.45
1:X:2442:C:H2'	1:X:2443:C:C6	2.52	0.45
1:X:2662:C:H2'	1:X:2663:U:C6	2.52	0.45
3:A:96:HIS:NE2	3:A:97:TYR:O	2.49	0.45
3:A:169:GLU:N	3:A:172:TYR:O	2.34	0.45
3:A:169:GLU:OE2	3:A:184:ARG:NH1	2.49	0.45
5:C:191:ALA:HA	5:C:194:GLU:HB2	1.99	0.45
9:H:29:ILE:HB	9:H:123:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:25:ALA:HB1	12:K:48:VAL:HG23	1.99	0.45
17:P:89:ARG:HG2	17:P:131:LYS:H	1.81	0.45
18:Q:8:GLN:O	23:V:29:ARG:HD2	2.16	0.45
25:Z:51:TYR:CE1	25:Z:55:ARG:HG2	2.52	0.45
1:X:824:U:H1'	1:X:1264:C:O4'	2.15	0.45
1:X:1374:G:N2	1:X:1384:G:H1'	2.31	0.45
4:B:5:LEU:H	4:B:5:LEU:HD12	1.80	0.45
4:B:32:PRO:O	4:B:49:ILE:HA	2.17	0.45
27:2:4:THR:O	27:2:4:THR:OG1	2.34	0.45
1:X:88:G:C3'	1:X:89:A:H5''	2.45	0.45
1:X:969:U:O4'	11:J:17:ARG:NH1	2.50	0.45
1:X:999:A:OP1	24:W:7:ARG:HD3	2.16	0.45
1:X:1007:A:H2'	1:X:1008:G:C8	2.44	0.45
1:X:1008:G:C2	1:X:1009:C:C5	3.05	0.45
1:X:1227:A:H4'	1:X:1252:C:H4'	1.98	0.45
1:X:1462:C:H2'	1:X:1463:A:C8	2.52	0.45
1:X:1935:A:C6	1:X:1936:A:N1	2.85	0.45
1:X:2255:G:H2'	1:X:2256:G:H8	1.82	0.45
1:X:2576:G:C6	1:X:2577:A:N6	2.84	0.45
3:A:96:HIS:CE1	3:A:100:GLY:HA2	2.47	0.45
7:E:57:ASP:HB3	7:E:62:ARG:HH11	1.82	0.45
13:L:97:HIS:HB3	13:L:98:GLY:H	1.60	0.45
17:P:114:ALA:O	17:P:115:ASN:ND2	2.43	0.45
26:1:28:ARG:O	26:1:33:ALA:HB2	2.17	0.45
1:X:111:G:H8	1:X:111:G:OP2	2.00	0.45
1:X:177:U:O2'	1:X:178:C:O4'	2.35	0.45
1:X:746:G:N7	1:X:774:A:C5	2.85	0.45
1:X:1050:G:H1	1:X:1127:C:H42	1.64	0.45
1:X:1330:G:C6	1:X:1349:A:C6	3.05	0.45
1:X:2014:A:C6	1:X:2477:C:H1'	2.52	0.45
1:X:2067:U:H2'	1:X:2068:C:H6	1.82	0.45
1:X:2309:G:N2	1:X:2365:U:C2	2.85	0.45
1:X:2371:A:C4	1:X:2408:G:C6	3.05	0.45
4:B:137:ARG:HG3	4:B:138:PRO:HD2	1.99	0.45
5:C:97:ARG:O	5:C:100:ARG:HG2	2.15	0.45
6:D:93:GLY:H	6:D:96:MET:HE2	1.82	0.45
10:I:31:GLY:HA2	10:I:34:HIS:HB2	1.99	0.45
11:J:124:HIS:CD2	11:J:124:HIS:H	2.34	0.45
15:N:92:ARG:CA	15:N:95:LEU:HB2	2.46	0.45
17:P:35:PRO:HB2	17:P:39:ARG:NH1	2.32	0.45
17:P:75:ALA:HB2	17:P:126:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:17:GLY:O	27:2:21:ARG:HG2	2.17	0.45
27:2:36:ALA:C	27:2:38:GLY:N	2.73	0.45
28:3:29:LYS:HD2	28:3:33:ASN:O	2.17	0.45
1:X:750:C:C2'	1:X:751:G:H5'	2.47	0.45
1:X:1189:G:H2'	1:X:1190:C:C6	2.51	0.45
1:X:1652:G:H2'	1:X:1653:C:H6	1.82	0.45
1:X:1818:G:OP1	3:A:224:SER:OG	2.27	0.45
1:X:1949:A:H1'	1:X:2572:U:C5'	2.47	0.45
1:X:2727:G:O6	1:X:2735:C:H5''	2.17	0.45
3:A:89:SER:O	3:A:159:ALA:HB2	2.17	0.45
3:A:143:HIS:CD2	3:A:196:VAL:HG13	2.52	0.45
3:A:200:GLU:HG3	3:A:202:LYS:HG3	1.97	0.45
10:I:32:ARG:HH22	10:I:34:HIS:CE1	2.34	0.45
11:J:35:LEU:HD12	11:J:131:LYS:O	2.17	0.45
12:K:80:MET:HE2	12:K:80:MET:HB2	1.61	0.45
25:Z:3:LYS:O	25:Z:4:HIS:C	2.60	0.45
27:2:1:MET:HG3	27:2:3:ARG:CZ	2.46	0.45
28:3:11:LYS:HD2	28:3:11:LYS:N	2.32	0.45
1:X:469:G:H22	1:X:480:G:H2'	1.82	0.45
1:X:481:A:C6	1:X:482:A:C6	3.05	0.45
1:X:603:C:H2'	1:X:604:U:H6	1.82	0.45
1:X:920:G:P	11:J:24:GLY:HA3	2.57	0.45
1:X:938:G:O2'	1:X:939:C:P	2.75	0.45
1:X:978:U:H2'	1:X:979:A:C8	2.52	0.45
1:X:2340:C:O5'	28:3:27:SER:OG	2.35	0.45
1:X:2579:A:O2'	1:X:2580:C:H5'	2.16	0.45
1:X:2754:C:H2'	1:X:2755:A:O4'	2.17	0.45
1:X:2827:G:H2'	1:X:2828:C:O4'	2.17	0.45
7:E:107:ILE:HD11	7:E:151:VAL:HG12	1.99	0.45
8:G:97:ASP:O	8:G:99:VAL:HG23	2.16	0.45
11:J:46:ASN:HA	11:J:49:GLU:HB2	1.99	0.45
1:X:389:G:H2'	1:X:390:U:C6	2.52	0.45
1:X:481:A:N3	1:X:481:A:H2'	2.32	0.45
1:X:576:A:H4'	1:X:821:A:OP1	2.16	0.45
1:X:1398:G:O2'	1:X:1399:C:O5'	2.34	0.45
1:X:1517:C:H4'	3:A:96:HIS:CE1	2.52	0.45
1:X:1692:C:N4	1:X:1976:U:O4'	2.49	0.45
1:X:2662:C:H2'	1:X:2663:U:H6	1.81	0.45
1:X:2691:C:O2'	1:X:2692:A:P	2.75	0.45
2:Y:5:C:H2'	2:Y:6:C:O4'	2.16	0.45
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:8:ARG:HB2	13:L:8:ARG:CZ	2.46	0.45
13:L:35:SER:OG	13:L:36:LYS:N	2.50	0.45
14:M:32:THR:HG22	14:M:93:ILE:HA	1.99	0.45
18:Q:6:ILE:HG22	18:Q:7:LEU:HD13	1.99	0.45
20:S:153:LYS:HA	20:S:153:LYS:HD3	1.79	0.45
21:T:66:LYS:HB3	21:T:66:LYS:HE2	1.78	0.45
1:X:854:G:N2	1:X:948:C:N3	2.58	0.44
1:X:1479:G:H2'	1:X:1480:G:H8	1.81	0.44
1:X:1552:C:O2	1:X:1553:G:N2	2.50	0.44
1:X:1778:U:H2'	1:X:1779:C:H6	1.82	0.44
1:X:1786:C:O2	3:A:252:LYS:HD2	2.17	0.44
1:X:2344:G:H4'	21:T:60:PHE:CE1	2.52	0.44
1:X:2398:U:H4'	26:1:13:GLU:OE1	2.17	0.44
1:X:2543:A:C6	1:X:2544:A:N1	2.85	0.44
2:Y:64:C:H2'	2:Y:65:A:H8	1.82	0.44
3:A:31:LYS:HE3	3:A:32:ALA:H	1.82	0.44
5:C:177:VAL:HB	5:C:178:TYR:H	1.59	0.44
8:G:67:ARG:HD3	8:G:70:PHE:HA	1.99	0.44
8:G:118:ALA:O	8:G:121:LYS:HB3	2.17	0.44
9:H:75:VAL:HG22	9:H:96:ALA:HA	1.98	0.44
9:H:83:ARG:HG2	14:M:40:ARG:HH22	1.83	0.44
12:K:75:VAL:O	12:K:79:VAL:HG13	2.17	0.44
13:L:11:LEU:HA	13:L:14:ARG:NH1	2.32	0.44
13:L:27:LEU:HD13	13:L:87:VAL:HG22	1.99	0.44
18:Q:60:GLY:HA3	18:Q:73:ASN:H	1.81	0.44
19:R:84:VAL:HG11	19:R:90:LYS:N	2.23	0.44
22:U:42:GLN:OE1	22:U:42:GLN:N	2.51	0.44
1:X:353:G:H2'	1:X:354:C:H6	1.82	0.44
1:X:596:C:N4	10:I:36:GLY:HA3	2.32	0.44
1:X:934:G:H1'	21:T:26:PHE:CD1	2.52	0.44
1:X:1032:A:H62	1:X:1151:U:H3	1.65	0.44
1:X:1658:A:H2'	1:X:1659:G:O4'	2.17	0.44
1:X:2339:A:P	28:3:49:VAL:HG11	2.57	0.44
1:X:2396:C:H2'	1:X:2397:A:O4'	2.17	0.44
1:X:2526:U:C4	1:X:2545:A:N7	2.85	0.44
1:X:2630:C:H2'	1:X:2631:C:C6	2.52	0.44
2:Y:63:A:H2'	2:Y:64:C:C6	2.53	0.44
3:A:121:PRO:HA	3:A:132:PRO:HD2	1.98	0.44
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.99	0.44
11:J:37:ALA:O	11:J:100:PRO:HA	2.17	0.44
11:J:39:GLU:HA	11:J:40:PRO:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:107:LEU:HD23	14:M:107:LEU:HA	1.73	0.44
17:P:106:LEU:HD23	17:P:106:LEU:O	2.17	0.44
1:X:75:C:H2'	1:X:76:C:C6	2.52	0.44
1:X:321:A:N1	1:X:323:G:H1'	2.32	0.44
1:X:1212:U:H2'	1:X:1213:U:H6	1.81	0.44
1:X:1353:A:H2'	18:Q:56:MET:SD	2.57	0.44
1:X:1430:G:H2'	1:X:1431:U:C6	2.52	0.44
1:X:1713:G:C5	1:X:1714:A:C8	3.06	0.44
1:X:2024:U:H2'	1:X:2025:A:O4'	2.18	0.44
1:X:2701:A:H2'	1:X:2702:G:O4'	2.16	0.44
1:X:2848:A:N3	12:K:7:GLY:N	2.61	0.44
2:Y:11:G:OP1	13:L:28:ARG:NH1	2.50	0.44
11:J:68:ARG:HE	11:J:106:GLU:CD	2.26	0.44
12:K:59:ASP:OD2	12:K:59:ASP:N	2.51	0.44
13:L:88:VAL:HG12	13:L:89:PHE:H	1.82	0.44
15:N:37:GLN:C	15:N:39:LEU:H	2.25	0.44
25:Z:41:LEU:HD13	25:Z:41:LEU:HA	1.70	0.44
25:Z:58:LEU:O	25:Z:58:LEU:HG	2.16	0.44
28:3:30:ARG:HB3	28:3:31:HIS:ND1	2.33	0.44
28:3:57:ARG:HG3	28:3:58:MET:HE2	2.00	0.44
1:X:433:G:N2	1:X:434:C:H1'	2.32	0.44
1:X:490:A:H1'	1:X:491:A:H5''	2.00	0.44
1:X:836:G:C5	1:X:837:U:C5	3.05	0.44
1:X:1727:C:H2'	1:X:1728:A:H8	1.81	0.44
1:X:1847:G:H2'	1:X:1848:U:C6	2.52	0.44
1:X:1919:A:OP2	1:X:1944:C:N4	2.46	0.44
1:X:2633:A:N1	1:X:2644:A:H5''	2.32	0.44
2:Y:59:A:C6	6:D:26:MET:HE3	2.52	0.44
3:A:23:GLY:HA3	3:A:205:VAL:HG11	1.99	0.44
3:A:39:LYS:HD2	3:A:39:LYS:HA	1.66	0.44
4:B:173:VAL:HG23	4:B:185:LYS:HB2	1.98	0.44
5:C:122:GLY:O	5:C:125:ILE:HB	2.18	0.44
8:G:104:THR:OG1	8:G:105:GLY:N	2.48	0.44
12:K:43:GLU:O	12:K:46:PRO:HD2	2.17	0.44
15:N:50:ARG:HA	15:N:53:LYS:HD3	1.99	0.44
20:S:36:ARG:HH21	20:S:78:PRO:HD2	1.83	0.44
1:X:593:C:OP2	15:N:6:THR:OG1	2.36	0.44
1:X:2010:G:C6	1:X:2011:U:C4	3.06	0.44
1:X:2529:G:C6	1:X:2530:C:C4	3.06	0.44
1:X:2630:C:H2'	1:X:2631:C:H6	1.83	0.44
2:Y:51:G:H2'	2:Y:52:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:52:G:C2	2:Y:53:G:C8	3.06	0.44
6:D:128:TYR:HB3	6:D:156:ILE:HB	1.98	0.44
8:G:141:GLY:O	8:G:145:HIS:HD2	2.00	0.44
15:N:27:SER:HB2	15:N:31:GLN:HG3	1.98	0.44
15:N:60:LEU:O	15:N:64:ARG:HG3	2.17	0.44
17:P:45:ILE:HD11	17:P:57:LEU:CD1	2.40	0.44
1:X:54:G:O2'	1:X:125:A:N1	2.47	0.44
1:X:452:G:H2'	1:X:453:U:O4'	2.17	0.44
1:X:1316:G:N2	1:X:1317:G:H1'	2.33	0.44
1:X:1919:A:H2	1:X:1926:U:N3	2.15	0.44
1:X:1998:A:N3	25:Z:6:VAL:HG23	2.32	0.44
1:X:2261:G:H5''	1:X:2262:C:O4'	2.17	0.44
1:X:2545:A:H61	9:H:40:GLY:CA	2.28	0.44
1:X:2595:C:H5''	1:X:2596:C:OP2	2.17	0.44
1:X:2736:U:H4'	1:X:2737:A:OP1	2.18	0.44
7:E:68:THR:O	7:E:72:VAL:HG23	2.18	0.44
8:G:52:GLY:O	8:G:55:ALA:HB3	2.18	0.44
15:N:61:TRP:O	15:N:65:ILE:HG12	2.17	0.44
16:O:20:ILE:HG13	16:O:21:ARG:N	2.27	0.44
1:X:21:A:C6	1:X:530:G:C6	3.05	0.44
1:X:530:G:H2'	1:X:531:G:C8	2.51	0.44
1:X:703:A:O2'	1:X:793:G:OP1	2.36	0.44
1:X:1018:C:OP2	1:X:1019:U:O2'	2.15	0.44
1:X:1041:G:OP2	11:J:129:GLN:NE2	2.50	0.44
1:X:1430:G:H2'	1:X:1431:U:H6	1.83	0.44
1:X:1594:U:H2'	1:X:1595:A:C8	2.52	0.44
1:X:2265:A:H61	26:1:25:THR:HG21	1.83	0.44
1:X:2285:U:H2'	1:X:2286:G:H5'	1.98	0.44
6:D:108:LEU:HD22	6:D:117:ILE:HD11	1.99	0.44
14:M:27:PHE:HA	14:M:96:ARG:NH2	2.33	0.44
18:Q:63:LYS:HB2	18:Q:69:ILE:C	2.43	0.44
19:R:23:ILE:O	19:R:80:LYS:HB2	2.17	0.44
20:S:70:GLN:CB	20:S:80:HIS:HB3	2.48	0.44
20:S:96:VAL:O	20:S:119:ASN:HA	2.17	0.44
22:U:54:ASN:HD21	22:U:77:GLY:HA2	1.82	0.44
1:X:66:U:H2'	1:X:67:G:C8	2.52	0.44
1:X:187:U:H2'	1:X:188:G:H8	1.82	0.44
1:X:386:U:H5'	1:X:436:A:C2	2.52	0.44
1:X:1775:A:H4'	1:X:1776:A:O5'	2.18	0.44
1:X:2418:A:N1	1:X:2564:U:O2'	2.48	0.44
1:X:2839:G:H2'	1:X:2840:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:59:VAL:HG12	4:B:64:GLN:HG3	1.99	0.44
9:H:1:MET:HB2	9:H:44:TYR:HB3	1.98	0.44
9:H:83:ARG:HD2	9:H:89:ILE:HD11	1.99	0.44
23:V:21:ARG:NH1	23:V:53:LEU:HD11	2.33	0.44
1:X:178:C:P	22:U:40:ARG:CZ	3.06	0.44
1:X:778:G:H2'	1:X:779:U:H6	1.83	0.44
1:X:998:C:H2'	1:X:999:A:O4'	2.18	0.44
1:X:1175:A:C2	1:X:1176:U:C2	3.06	0.44
1:X:1193:G:H2'	1:X:1194:U:C6	2.53	0.44
1:X:1652:G:H2'	1:X:1653:C:C6	2.53	0.44
1:X:1966:C:H4'	1:X:2585:C:H4'	2.00	0.44
1:X:2399:C:H41	28:3:31:HIS:HB2	1.82	0.44
1:X:2491:C:H2'	1:X:2492:G:O4'	2.18	0.44
1:X:2610:G:N2	1:X:2767:C:O2	2.44	0.44
17:P:13:GLN:O	17:P:16:GLN:HG2	2.18	0.44
17:P:41:VAL:O	17:P:44:VAL:HG12	2.18	0.44
18:Q:25:TYR:CZ	18:Q:88:ILE:HG23	2.53	0.44
1:X:14:A:C6	1:X:536:A:C2	3.06	0.43
1:X:504:G:H4'	17:P:27:VAL:CG1	2.47	0.43
1:X:556:A:O2'	1:X:557:U:OP2	2.32	0.43
1:X:661:C:O2	1:X:662:G:N2	2.51	0.43
1:X:2010:G:H1	1:X:2019:C:H42	1.66	0.43
1:X:2295:C:O2'	6:D:125:ARG:NH2	2.50	0.43
1:X:2609:G:H2'	1:X:2610:G:C8	2.52	0.43
1:X:2812:A:H2'	1:X:2813:G:C8	2.53	0.43
2:Y:16:U:O2'	2:Y:110:U:O2	2.36	0.43
4:B:14:ILE:HG12	14:M:20:HIS:NE2	2.32	0.43
5:C:17:LEU:HD12	5:C:17:LEU:HA	1.73	0.43
5:C:50:GLN:NE2	5:C:56:ARG:HH12	2.16	0.43
11:J:13:GLN:HE21	11:J:90:ALA:HB1	1.82	0.43
15:N:92:ARG:HB3	15:N:95:LEU:HB2	2.00	0.43
16:O:35:LEU:HD23	16:O:55:THR:HG22	1.98	0.43
17:P:60:ILE:HA	17:P:61:PRO:HD3	1.45	0.43
26:1:9:ILE:HG22	26:1:30:ASN:OD1	2.17	0.43
26:1:14:SER:HB2	26:1:23:THR:H	1.82	0.43
1:X:463:C:P	5:C:46:ARG:HG2	2.59	0.43
1:X:540:G:N1	1:X:2005:U:OP1	2.51	0.43
1:X:814:G:OP1	5:C:50:GLN:HB2	2.17	0.43
1:X:1635:G:O2'	27:2:1:MET:HB2	2.17	0.43
1:X:2069:U:H2'	1:X:2070:G:C8	2.52	0.43
1:X:2222:U:H2'	1:X:2223:U:H6	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2787:A:H2'	1:X:2788:C:C6	2.53	0.43
2:Y:14:C:O5'	21:T:72:LYS:NZ	2.51	0.43
4:B:38:THR:HB	4:B:41:THR:H	1.83	0.43
5:C:45:THR:HB	5:C:86:PRO:O	2.17	0.43
8:G:36:ASN:HB3	8:G:74:MET:HG3	2.00	0.43
10:I:62:LYS:HB3	28:3:12:ARG:HA	2.00	0.43
13:L:89:PHE:HZ	13:L:100:VAL:HG22	1.83	0.43
25:Z:19:ARG:O	25:Z:21:SER:N	2.51	0.43
26:1:44:ALA:C	26:1:46:LYS:H	2.26	0.43
1:X:1216:G:C6	1:X:1217:U:C4	3.06	0.43
1:X:1228:G:C6	1:X:1229:C:C4	3.05	0.43
1:X:1672:A:C6	1:X:1673:C:C2	3.06	0.43
1:X:1721:G:H2'	1:X:1722:G:O4'	2.18	0.43
1:X:1810:U:O2'	3:A:154:GLN:O	2.30	0.43
1:X:2758:A:HO2'	1:X:2760:G:HO2'	1.57	0.43
4:B:122:PHE:HE2	4:B:138:PRO:CB	2.30	0.43
5:C:50:GLN:CD	5:C:56:ARG:HH12	2.26	0.43
9:H:1:MET:HE3	9:H:79:HIS:CD2	2.52	0.43
10:I:103:ASN:O	10:I:103:ASN:ND2	2.52	0.43
14:M:87:LEU:HD23	14:M:87:LEU:HA	1.61	0.43
1:X:5:A:O2'	8:G:162:LYS:HE3	2.18	0.43
1:X:662:G:H2'	1:X:663:G:O4'	2.19	0.43
1:X:2077:G:N2	1:X:2179:C:H1'	2.33	0.43
1:X:2169:A:H2'	1:X:2170:C:C6	2.53	0.43
1:X:2504:G:C2	1:X:2518:C:C2	3.07	0.43
1:X:2657:G:H2'	1:X:2658:A:O4'	2.18	0.43
1:X:2681:A:OP1	12:K:73:LYS:NZ	2.52	0.43
3:A:186:HIS:CD2	3:A:186:HIS:H	2.34	0.43
4:B:10:GLY:O	4:B:25:VAL:HG23	2.19	0.43
5:C:97:ARG:HA	5:C:100:ARG:HD3	1.99	0.43
5:C:111:ARG:O	5:C:115:GLY:O	2.37	0.43
6:D:14:PRO:O	6:D:18:GLN:HG2	2.17	0.43
8:G:84:ASN:HD21	8:G:154:GLU:HG2	1.84	0.43
9:H:115:ALA:O	9:H:118:LEU:HB2	2.19	0.43
15:N:86:ALA:C	15:N:88:ILE:H	2.27	0.43
17:P:17:GLN:HG3	17:P:18:VAL:HG23	2.01	0.43
20:S:121:GLN:C	20:S:122:ILE:HG13	2.43	0.43
27:2:21:ARG:HD2	27:2:30:ILE:HD12	2.00	0.43
27:2:24:THR:OG1	27:2:25:LYS:N	2.51	0.43
28:3:24:ALA:N	28:3:47:GLY:O	2.37	0.43
1:X:26:G:H1'	1:X:524:A:N6	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:125:A:H5''	1:X:126:C:C1'	2.49	0.43
1:X:328:A:H2'	1:X:329:C:C6	2.53	0.43
1:X:1507:A:O4'	3:A:99:ASP:HB3	2.18	0.43
1:X:2424:G:O2'	1:X:2425:G:H5'	2.18	0.43
1:X:2576:G:C6	1:X:2577:A:C6	3.07	0.43
1:X:2751:C:H2'	1:X:2752:C:H6	1.84	0.43
3:A:217:ARG:HG2	3:A:218:LYS:HB2	2.00	0.43
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.18	0.43
12:K:45:ARG:HD3	12:K:95:THR:HG22	2.01	0.43
16:O:64:GLY:HA3	16:O:90:PHE:CZ	2.54	0.43
17:P:45:ILE:HG21	17:P:45:ILE:HD13	1.77	0.43
19:R:77:HIS:C	19:R:79:SER:H	2.27	0.43
22:U:63:SER:HB2	22:U:66:ALA:H	1.84	0.43
1:X:393:U:H2'	1:X:394:U:C6	2.53	0.43
1:X:494:A:H5''	19:R:58:VAL:HG22	2.00	0.43
1:X:518:A:H5''	1:X:518:A:N3	2.34	0.43
1:X:608:G:H1'	10:I:21:ARG:CG	2.36	0.43
1:X:1586:A:C6	1:X:1587:A:C6	3.07	0.43
1:X:1693:A:C2	1:X:1976:U:H5'	2.53	0.43
1:X:1699:A:C2	1:X:1700:C:C2	3.07	0.43
1:X:1944:C:H2'	1:X:1945:C:O4'	2.18	0.43
1:X:2788:C:H2'	1:X:2789:U:H6	1.84	0.43
4:B:159:HIS:NE2	4:B:162:MET:HE2	2.33	0.43
8:G:67:ARG:HD3	8:G:70:PHE:O	2.18	0.43
8:G:67:ARG:CG	8:G:70:PHE:HA	2.49	0.43
8:G:106:TYR:HD1	8:G:106:TYR:HA	1.50	0.43
19:R:108:VAL:HB	19:R:109:ALA:H	1.66	0.43
26:1:9:ILE:HG13	26:1:10:VAL:N	2.34	0.43
26:1:42:PRO:HG3	26:1:50:PHE:HE1	1.82	0.43
28:3:13:ARG:HH12	28:3:49:VAL:CG2	2.32	0.43
1:X:116:A:N3	1:X:155:G:H1'	2.34	0.43
1:X:694:G:H2'	1:X:695:G:O4'	2.18	0.43
1:X:1746:A:H2	1:X:2696:A:O2'	2.00	0.43
1:X:2528:G:C2	1:X:2529:G:N7	2.87	0.43
3:A:177:LEU:HB3	3:A:178:PRO:HD2	2.00	0.43
4:B:79:ARG:HA	4:B:79:ARG:HD3	1.71	0.43
7:E:76:VAL:HA	7:E:79:VAL:HG22	2.00	0.43
8:G:71:THR:N	8:G:76:GLN:NE2	2.67	0.43
17:P:32:ARG:C	17:P:32:ARG:HE	2.27	0.43
20:S:127:PRO:C	20:S:129:ARG:H	2.27	0.43
24:W:7:ARG:HB2	24:W:50:LEU:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:19:ARG:C	25:Z:21:SER:H	2.27	0.43
28:3:9:MET:SD	28:3:59:LYS:HG3	2.58	0.43
1:X:618:A:H2'	1:X:619:A:C8	2.54	0.43
1:X:861:G:N3	1:X:944:A:H1'	2.34	0.43
1:X:874:A:H2'	1:X:875:G:O4'	2.18	0.43
1:X:914:C:H2'	1:X:915:C:C6	2.54	0.43
1:X:1954:A:H1'	3:A:240:THR:HA	2.01	0.43
1:X:2033:C:H2'	1:X:2034:A:O4'	2.19	0.43
1:X:2048:C:H2'	1:X:2049:C:C6	2.54	0.43
1:X:2271:C:H2'	1:X:2272:A:C8	2.53	0.43
3:A:56:GLY:N	3:A:217:ARG:HB2	2.29	0.43
3:A:223:GLY:HA2	3:A:226:MET:HG3	2.01	0.43
5:C:102:LEU:O	5:C:102:LEU:HD23	2.18	0.43
10:I:43:ALA:O	10:I:45:LYS:HG2	2.17	0.43
11:J:26:ASP:HB2	11:J:68:ARG:HH22	1.84	0.43
13:L:47:ARG:C	13:L:49:GLN:N	2.76	0.43
15:N:36:PHE:O	15:N:39:LEU:HB2	2.18	0.43
23:V:2:LYS:HB3	23:V:52:GLN:HE22	1.84	0.43
1:X:589:C:H2'	1:X:590:C:C6	2.54	0.43
1:X:687:G:H21	5:C:68:ARG:NH2	2.15	0.43
1:X:699:G:C6	27:2:12:ARG:HA	2.53	0.43
1:X:764:A:C6	1:X:802:A:C6	3.06	0.43
1:X:824:U:C4	10:I:29:THR:HB	2.53	0.43
1:X:1174:G:H2'	1:X:1175:A:H8	1.84	0.43
1:X:1198:C:OP1	24:W:26:ARG:NH1	2.52	0.43
1:X:1371:G:O2'	1:X:1386:A:N6	2.47	0.43
1:X:1419:G:H2'	1:X:1420:A:C8	2.54	0.43
1:X:1646:G:C5	1:X:1647:U:N3	2.87	0.43
1:X:2442:C:H2'	1:X:2443:C:H6	1.84	0.43
1:X:2687:G:H2'	1:X:2688:G:H8	1.83	0.43
4:B:44:TYR:HB2	4:B:82:ARG:NH1	2.34	0.43
19:R:29:HIS:CE1	19:R:51:VAL:HA	2.54	0.43
1:X:589:C:H4'	15:N:31:GLN:NE2	2.34	0.43
1:X:599:A:O2'	1:X:600:G:H5'	2.19	0.43
1:X:1278:A:H2	1:X:1997:A:N6	2.08	0.43
1:X:1751:A:H2'	1:X:1752:U:C6	2.53	0.43
1:X:1774:A:C2	1:X:2566:A:C5	3.07	0.43
1:X:2000:U:H4'	25:Z:8:LYS:O	2.18	0.43
1:X:2304:G:P	1:X:2304:G:H8	2.41	0.43
4:B:59:VAL:CG1	4:B:64:GLN:HG3	2.49	0.43
6:D:130:LEU:HA	6:D:130:LEU:HD23	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:103:TYR:HB3	8:G:107:GLN:HG3	2.01	0.43
16:O:23:GLU:HG3	16:O:91:THR:OG1	2.19	0.43
19:R:23:ILE:HD11	19:R:84:VAL:HG21	2.01	0.43
19:R:77:HIS:CG	19:R:78:ALA:N	2.87	0.43
26:1:16:ALA:HB2	26:1:50:PHE:HA	2.01	0.43
1:X:661:C:C2	1:X:662:G:N1	2.87	0.42
1:X:689:A:H1'	1:X:2422:C:H1'	2.01	0.42
1:X:760:U:C4	1:X:2592:U:C4	3.06	0.42
1:X:1246:G:C5	1:X:1247:U:C5	3.07	0.42
1:X:1351:G:H2'	1:X:1352:G:C8	2.54	0.42
1:X:1407:G:O6	1:X:1408:A:N6	2.52	0.42
1:X:1583:A:C2	3:A:31:LYS:HE2	2.54	0.42
1:X:2863:U:H2'	1:X:2864:C:O4'	2.18	0.42
3:A:166:GLN:HB2	3:A:174:ILE:HB	2.00	0.42
3:A:250:TRP:N	3:A:250:TRP:CD1	2.87	0.42
4:B:21:ILE:H	4:B:21:ILE:HG12	1.60	0.42
4:B:31:CYS:HA	4:B:32:PRO:HD3	1.79	0.42
4:B:59:VAL:HG21	4:B:74:PRO:HB3	2.01	0.42
5:C:54:THR:CG2	5:C:72:ARG:HB2	2.46	0.42
8:G:141:GLY:O	8:G:142:ARG:C	2.62	0.42
10:I:14:LYS:HD2	10:I:14:LYS:HA	1.90	0.42
10:I:119:THR:HG22	10:I:139:ARG:HB3	2.01	0.42
19:R:97:GLN:CB	19:R:101:GLY:HA2	2.49	0.42
1:X:123:A:O5'	27:2:19:ARG:HG2	2.19	0.42
1:X:555:U:H3'	1:X:556:A:H8	1.84	0.42
1:X:1370:U:H2'	1:X:1371:G:C8	2.54	0.42
1:X:1544:A:C4	1:X:1560:A:C6	3.08	0.42
1:X:1647:U:H6	1:X:1649:A:OP2	2.02	0.42
1:X:1710:U:H5''	1:X:1711:C:C5	2.54	0.42
1:X:1810:U:H2'	3:A:157:ARG:HD3	2.01	0.42
1:X:2006:G:H4'	1:X:2596:C:O3'	2.19	0.42
1:X:2052:G:C2	1:X:2053:G:C8	3.08	0.42
1:X:2371:A:H2	1:X:2403:C:H42	1.67	0.42
3:A:31:LYS:HA	3:A:31:LYS:HD2	1.72	0.42
10:I:57:ILE:N	10:I:58:ALA:O	2.52	0.42
1:X:500:G:C2	1:X:501:G:H1'	2.54	0.42
1:X:571:U:C2	1:X:581:A:C8	3.07	0.42
1:X:699:G:C2	27:2:12:ARG:HB2	2.55	0.42
1:X:733:G:H2'	1:X:734:G:H8	1.84	0.42
1:X:1466:C:H2'	1:X:1467:U:H1'	1.99	0.42
1:X:1777:A:C4	1:X:1921:A:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1859:A:H2'	1:X:1860:A:C8	2.54	0.42
6:D:17:MET:HG2	6:D:22:TYR:CB	2.49	0.42
8:G:67:ARG:O	8:G:70:PHE:CG	2.72	0.42
9:H:68:ASP:O	9:H:70:VAL:HG12	2.19	0.42
10:I:60:LEU:HA	10:I:61:PRO:HD3	1.85	0.42
15:N:94:VAL:C	15:N:96:ALA:N	2.77	0.42
22:U:27:ASP:OD2	22:U:32:ARG:HG3	2.19	0.42
26:1:8:ILE:HD13	26:1:8:ILE:H	1.84	0.42
1:X:320:A:H1'	1:X:340:G:N3	2.33	0.42
1:X:524:A:H2'	1:X:525:A:O4'	2.19	0.42
1:X:859:U:O2'	1:X:860:U:O5'	2.30	0.42
1:X:954:U:OP2	10:I:38:LYS:HG2	2.20	0.42
1:X:1429:A:H2'	1:X:1429:A:N3	2.34	0.42
1:X:1548:U:H2'	1:X:1549:C:C6	2.54	0.42
1:X:1630:A:N6	17:P:113:SER:O	2.48	0.42
1:X:1698:C:O2	1:X:1753:A:H2'	2.19	0.42
1:X:1982:C:H5''	1:X:2703:C:O2'	2.19	0.42
1:X:1991:C:H2'	1:X:1992:G:C8	2.53	0.42
1:X:2046:C:O2	1:X:2430:A:C2	2.72	0.42
1:X:2328:G:OP2	28:3:42:ARG:HG3	2.18	0.42
1:X:2350:G:C2	1:X:2351:G:C5	3.07	0.42
1:X:2664:G:C2'	1:X:2665:G:H5'	2.49	0.42
1:X:2800:C:H3'	1:X:2801:A:H8	1.85	0.42
4:B:96:PHE:CE2	4:B:102:ILE:HG21	2.54	0.42
4:B:149:ARG:HG3	4:B:150:VAL:N	2.34	0.42
5:C:74:VAL:HG23	5:C:76:THR:H	1.83	0.42
5:C:187:VAL:HG12	5:C:189:ASP:HB2	2.02	0.42
15:N:74:MET:HE1	15:N:113:SER:OG	2.19	0.42
1:X:491:A:N3	1:X:491:A:H2'	2.34	0.42
1:X:552:C:H2'	1:X:553:C:H5''	2.02	0.42
1:X:1013:G:C5	1:X:1014:G:C8	3.07	0.42
1:X:1164:C:H2'	1:X:1165:G:C8	2.53	0.42
1:X:1349:A:H5'	18:Q:64:ARG:NH2	2.35	0.42
1:X:1766:U:H2'	1:X:1767:G:O4'	2.19	0.42
1:X:1956:G:C6	1:X:1957:C:N4	2.87	0.42
1:X:2039:G:H22	25:Z:4:HIS:HA	1.85	0.42
1:X:2505:G:N1	1:X:2517:C:C2	2.88	0.42
1:X:2805:G:O2'	1:X:2858:A:N1	2.49	0.42
2:Y:58:G:H4'	2:Y:59:A:C5'	2.49	0.42
3:A:19:ALA:O	3:A:20:ASP:CG	2.62	0.42
3:A:109:GLU:OE1	3:A:197:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:35:PRO:HD2	17:P:120:ARG:HB2	2.00	0.42
18:Q:57:ASN:O	18:Q:58:VAL:HG23	2.19	0.42
19:R:107:ALA:HB2	19:R:111:GLY:HA3	2.02	0.42
20:S:4:THR:HA	20:S:57:GLU:HG3	2.02	0.42
1:X:346:C:H5''	19:R:91:ALA:HB2	2.02	0.42
1:X:507:A:P	17:P:21:ARG:HE	2.42	0.42
1:X:538:A:N3	1:X:538:A:C2'	2.82	0.42
1:X:540:G:C2	1:X:2005:U:OP1	2.73	0.42
1:X:699:G:N2	27:2:12:ARG:HB2	2.35	0.42
1:X:753:U:O4'	1:X:1964:A:C4	2.73	0.42
1:X:1102:G:N2	1:X:1112:U:H1'	2.35	0.42
1:X:1187:A:H2'	1:X:1188:A:C8	2.55	0.42
1:X:1416:A:H2'	1:X:1417:C:C6	2.55	0.42
1:X:1755:G:C6	1:X:1972:G:C2	3.08	0.42
1:X:2054:A:H2'	1:X:2055:G:C8	2.54	0.42
1:X:2861:A:O2'	25:Z:31:THR:HG23	2.19	0.42
4:B:134:TRP:O	4:B:135:HIS:C	2.63	0.42
6:D:80:ARG:HD3	6:D:83:MET:CB	2.49	0.42
6:D:119:PRO:HB2	6:D:167:ARG:HH22	1.83	0.42
10:I:62:LYS:HB2	28:3:12:ARG:HA	2.02	0.42
10:I:133:VAL:HG11	10:I:140:VAL:HG23	2.01	0.42
11:J:19:THR:HG23	11:J:99:LYS:HD3	2.01	0.42
22:U:9:GLY:H	22:U:14:VAL:HG21	1.85	0.42
24:W:27:LYS:HE2	24:W:27:LYS:HB3	1.83	0.42
1:X:114:C:O2'	1:X:124:A:N3	2.45	0.42
1:X:175:C:H5'	1:X:2223:U:OP1	2.18	0.42
1:X:585:U:H2'	1:X:586:G:C8	2.55	0.42
1:X:615:C:H1'	1:X:670:U:H1'	2.00	0.42
1:X:731:A:H2'	1:X:732:G:H4'	2.02	0.42
1:X:777:A:H5'	3:A:210:GLY:HA3	2.01	0.42
1:X:820:U:P	10:I:40:ARG:NH2	2.93	0.42
1:X:1336:G:H2'	1:X:1337:G:H5'	2.00	0.42
1:X:1480:G:N3	1:X:1561:A:H2	2.18	0.42
1:X:2284:U:P	1:X:2286:G:H22	2.42	0.42
1:X:2293:G:H2'	1:X:2294:U:C6	2.54	0.42
1:X:2796:A:C4	1:X:2797:G:C8	3.07	0.42
3:A:45:ASN:C	3:A:46:ARG:HD2	2.45	0.42
4:B:11:MET:HE2	4:B:11:MET:HB3	1.84	0.42
5:C:59:TYR:HE1	5:C:67:ALA:HA	1.85	0.42
9:H:7:ARG:HD3	9:H:18:GLU:OE2	2.19	0.42
11:J:83:ARG:HD3	11:J:83:ARG:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:14:VAL:N	16:O:16:GLU:OE2	2.53	0.42
25:Z:52:TYR:HB3	25:Z:56:GLN:NE2	2.34	0.42
1:X:60:A:C6	1:X:61:U:C4	3.08	0.42
1:X:2284:U:H3	6:D:39:GLY:HA3	1.84	0.42
1:X:2355:A:H8	1:X:2355:A:OP1	2.03	0.42
1:X:2471:U:H2'	1:X:2472:U:C6	2.55	0.42
1:X:2604:G:H2'	1:X:2605:C:C6	2.55	0.42
1:X:2729:A:C6	1:X:2730:A:N6	2.88	0.42
3:A:30:GLU:HB2	3:A:82:ILE:O	2.20	0.42
3:A:69:ARG:NH1	3:A:130:ALA:HB2	2.35	0.42
4:B:132:LYS:HB2	4:B:132:LYS:HE3	1.71	0.42
5:C:125:ILE:HD12	5:C:125:ILE:HA	1.87	0.42
9:H:104:GLU:HG3	9:H:125:LYS:HG3	2.02	0.42
10:I:96:TYR:HD2	10:I:96:TYR:HA	1.65	0.42
13:L:12:ARG:HG3	13:L:92:GLY:HA2	2.02	0.42
17:P:25:PHE:CD2	17:P:25:PHE:C	2.97	0.42
27:2:38:GLY:O	27:2:39:ARG:C	2.61	0.42
28:3:9:MET:HE1	28:3:59:LYS:HG3	2.02	0.42
1:X:674:U:H2'	1:X:675:C:O4'	2.20	0.42
1:X:788:G:C5	1:X:807:A:C8	3.08	0.42
1:X:1147:G:H2'	1:X:1148:G:C8	2.55	0.42
1:X:2080:U:H2'	1:X:2081:U:C6	2.55	0.42
2:Y:33:C:H1'	2:Y:56:G:N2	2.35	0.42
2:Y:103:A:O5'	2:Y:103:A:H8	2.03	0.42
3:A:130:ALA:HA	3:A:191:ALA:O	2.19	0.42
8:G:34:PRO:HA	8:G:69:ASP:CB	2.49	0.42
9:H:22:ILE:H	9:H:53:ALA:HA	1.84	0.42
19:R:25:LEU:HD12	19:R:80:LYS:C	2.44	0.42
19:R:95:ARG:HB2	19:R:104:VAL:HB	2.02	0.42
20:S:71:MET:HB2	20:S:78:PRO:HA	2.01	0.42
20:S:89:GLY:O	20:S:126:GLY:HA2	2.20	0.42
20:S:123:VAL:HG13	20:S:124:ALA:HB3	2.01	0.42
1:X:88:G:OP2	1:X:89:A:H3'	2.20	0.42
1:X:161:U:H1'	1:X:194:G:O2'	2.20	0.42
1:X:333:A:H5'	1:X:351:A:H1'	2.01	0.42
1:X:984:A:O4'	1:X:1202:U:C6	2.73	0.42
1:X:1005:U:H3'	15:N:54:LYS:HE3	2.02	0.42
1:X:1745:C:H5	1:X:1746:A:C5	2.37	0.42
2:Y:92:G:N7	2:Y:93:G:H1'	2.35	0.42
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.54	0.42
15:N:107:LYS:HE3	15:N:111:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:48:VAL:HG12	19:R:51:VAL:H	1.85	0.42
27:2:25:LYS:HA	27:2:25:LYS:HD3	1.72	0.42
1:X:617:U:H3'	1:X:617:U:O2	2.20	0.41
1:X:673:G:H21	10:I:21:ARG:HG2	1.84	0.41
1:X:876:A:H2	1:X:926:C:N4	2.16	0.41
1:X:987:G:C2	1:X:988:G:C8	3.08	0.41
1:X:1794:A:O2'	3:A:257:LEU:HD12	2.20	0.41
1:X:1796:A:N3	3:A:50:THR:HB	2.35	0.41
1:X:1865:C:H2'	1:X:1866:G:O4'	2.20	0.41
1:X:2019:C:O2'	1:X:2020:G:H5'	2.20	0.41
5:C:23:ASN:ND2	5:C:26:VAL:HG23	2.34	0.41
5:C:33:TRP:CZ3	5:C:34:GLN:HG2	2.55	0.41
5:C:47:THR:HG1	5:C:85:GLY:N	2.15	0.41
5:C:50:GLN:OE1	5:C:56:ARG:NH1	2.53	0.41
7:E:55:PRO:HB2	7:E:61:HIS:CE1	2.55	0.41
10:I:126:SER:O	10:I:130:ILE:HG13	2.19	0.41
11:J:93:TYR:CE1	11:J:95:VAL:HG13	2.55	0.41
12:K:15:SER:O	12:K:18:VAL:HB	2.20	0.41
12:K:73:LYS:HE2	12:K:73:LYS:HB3	1.86	0.41
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.30	0.41
1:X:226:C:OP2	1:X:2373:C:O2'	2.38	0.41
1:X:741:G:O2'	1:X:743:A:H8	2.03	0.41
1:X:1269:G:O3'	5:C:69:HIS:HE1	2.03	0.41
1:X:1290:A:OP1	12:K:40:LYS:NZ	2.53	0.41
1:X:1314:A:O2'	1:X:1315:A:H3'	2.19	0.41
1:X:1476:G:C6	1:X:1477:C:C4	3.08	0.41
1:X:2490:U:H2'	1:X:2491:C:C6	2.55	0.41
1:X:2495:G:C6	1:X:2496:C:N4	2.88	0.41
3:A:50:THR:OG1	3:A:51:SER:N	2.53	0.41
4:B:102:ILE:O	4:B:102:ILE:HG13	2.19	0.41
5:C:47:THR:HA	5:C:82:VAL:H	1.85	0.41
5:C:146:GLU:HG3	5:C:185:ARG:HH22	1.84	0.41
8:G:103:TYR:CE1	8:G:107:GLN:O	2.73	0.41
20:S:49:THR:HB	20:S:132:GLN:HA	2.02	0.41
28:3:26:LYS:CE	28:3:43:GLY:HA3	2.46	0.41
1:X:129:A:H2'	1:X:130:C:C6	2.56	0.41
1:X:649:G:N1	1:X:660:G:N1	2.68	0.41
1:X:732:G:H2'	1:X:733:G:H8	1.86	0.41
1:X:1216:G:C5	1:X:1217:U:C5	3.08	0.41
1:X:1332:G:C2	1:X:1333:G:C2	3.09	0.41
1:X:1499:A:H2'	1:X:1500:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1509:A:H8	1:X:1510:A:N7	2.18	0.41
1:X:1656:U:C2'	1:X:1657:A:H5''	2.50	0.41
1:X:1837:G:H2'	1:X:1838:G:C8	2.55	0.41
1:X:2277:A:H2'	1:X:2278:A:O4'	2.20	0.41
1:X:2394:G:H4'	10:I:64:GLY:O	2.21	0.41
1:X:2394:G:C6	1:X:2395:C:C4	3.09	0.41
1:X:2659:C:H1'	4:B:187:ALA:HB1	2.02	0.41
3:A:31:LYS:NZ	3:A:84:TYR:H	2.19	0.41
27:2:20:ALA:HA	27:2:23:LYS:HD2	2.03	0.41
1:X:13:A:N3	1:X:15:G:C6	2.87	0.41
1:X:14:A:C5	1:X:536:A:C2	3.08	0.41
1:X:616:U:O2'	1:X:671:A:H4'	2.19	0.41
1:X:1016:C:C2	1:X:1154:A:C5	3.08	0.41
1:X:1329:U:C2	1:X:1330:G:C8	3.09	0.41
1:X:1355:A:N1	1:X:1358:C:C2	2.88	0.41
1:X:1408:A:C6	1:X:1411:C:C2	3.08	0.41
1:X:1448:A:H61	1:X:1574:A:N6	2.18	0.41
1:X:1497:C:H42	1:X:1527:G:H1	1.69	0.41
1:X:1682:A:O2'	9:H:1:MET:N	2.50	0.41
1:X:1788:C:H5'	3:A:254:THR:HA	2.01	0.41
1:X:2628:C:O3'	9:H:35:THR:HG21	2.20	0.41
3:A:25:THR:CG2	3:A:211:ARG:HH12	2.31	0.41
4:B:6:GLY:HA3	4:B:28:ALA:HA	2.02	0.41
4:B:25:VAL:HG12	4:B:181:LEU:HD22	2.01	0.41
4:B:126:PRO:HG2	4:B:131:SER:HB3	2.01	0.41
5:C:13:ARG:H	5:C:13:ARG:HD2	1.85	0.41
5:C:95:LEU:HD23	5:C:96:PRO:HD2	2.03	0.41
5:C:124:ASP:OD1	5:C:136:TRP:NE1	2.49	0.41
8:G:70:PHE:CA	8:G:76:GLN:HE22	2.33	0.41
10:I:31:GLY:O	10:I:32:ARG:HG3	2.20	0.41
12:K:22:ARG:HG2	12:K:69:ASP:HB3	2.03	0.41
12:K:78:LYS:O	12:K:82:GLU:HB2	2.20	0.41
12:K:99:ARG:HG2	12:K:99:ARG:HH11	1.86	0.41
15:N:91:ASN:O	15:N:93:LYS:HB3	2.20	0.41
1:X:91:A:H2'	1:X:92:U:C6	2.56	0.41
1:X:539:A:C2	1:X:2006:G:C8	3.09	0.41
1:X:958:G:H2'	1:X:959:C:C6	2.55	0.41
1:X:1776:A:C8	1:X:1778:U:C5	3.08	0.41
1:X:2208:U:H2'	1:X:2209:G:C8	2.56	0.41
1:X:2331:A:C4	1:X:2345:A:C2	3.08	0.41
1:X:2509:A:H2'	1:X:2510:A:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2702:G:H2'	1:X:2703:C:O4'	2.20	0.41
3:A:32:ALA:O	3:A:33:LEU:HB3	2.20	0.41
5:C:15:ILE:HD11	5:C:195:ILE:H	1.84	0.41
6:D:41:GLY:HA2	6:D:45:GLU:HB2	2.01	0.41
6:D:79:LEU:HD23	6:D:79:LEU:HA	1.86	0.41
10:I:58:ALA:C	10:I:60:LEU:H	2.29	0.41
16:O:11:GLN:CB	16:O:13:ARG:HH21	2.34	0.41
17:P:57:LEU:HD13	17:P:69:ALA:CB	2.49	0.41
20:S:25:ASN:H	20:S:25:ASN:ND2	2.16	0.41
25:Z:3:LYS:HA	25:Z:3:LYS:HD2	1.63	0.41
1:X:463:C:OP2	5:C:46:ARG:HG2	2.20	0.41
1:X:474:G:C6	1:X:478:G:O6	2.74	0.41
1:X:738:G:C6	1:X:739:G:N1	2.89	0.41
1:X:787:A:H2	1:X:800:U:O2'	2.02	0.41
1:X:792:U:P	3:A:48:ARG:HA	2.61	0.41
1:X:945:G:C4	1:X:946:U:C5	3.09	0.41
1:X:951:G:N3	1:X:1205:G:H4'	2.35	0.41
1:X:1313:U:H4'	1:X:1314:A:C5'	2.51	0.41
1:X:1412:C:OP1	18:Q:81:ARG:NH1	2.54	0.41
1:X:1623:C:H4'	1:X:1624:A:O5'	2.21	0.41
1:X:2039:G:H2'	1:X:2039:G:N3	2.36	0.41
1:X:2402:U:OP2	26:1:3:LYS:HG3	2.20	0.41
1:X:2450:A:N6	1:X:2451:G:C2	2.89	0.41
6:D:52:LYS:HD2	6:D:148:LYS:HE2	2.02	0.41
12:K:76:VAL:O	12:K:79:VAL:HG22	2.20	0.41
15:N:44:THR:O	15:N:48:ARG:HG3	2.21	0.41
18:Q:43:GLN:HG2	18:Q:48:VAL:O	2.20	0.41
21:T:19:LYS:O	21:T:20:TYR:CG	2.73	0.41
28:3:6:THR:HG23	28:3:8:LYS:N	2.35	0.41
1:X:1372:A:H2'	1:X:1373:G:O4'	2.21	0.41
1:X:1583:A:H2'	3:A:84:TYR:HE1	1.85	0.41
1:X:1685:A:H5''	9:H:5:GLN:HG2	2.02	0.41
1:X:2324:G:H4'	1:X:2325:A:H5''	2.03	0.41
1:X:2391:A:H2'	1:X:2392:G:H8	1.85	0.41
1:X:2511:G:H2'	1:X:2512:A:O4'	2.21	0.41
1:X:2564:U:H4'	1:X:2565:C:OP2	2.18	0.41
16:O:23:GLU:HB2	16:O:91:THR:HG21	2.02	0.41
17:P:44:VAL:O	17:P:48:LYS:HD3	2.19	0.41
17:P:59:PHE:CZ	25:Z:40:LYS:HA	2.55	0.41
19:R:100:ASP:OD1	19:R:102:LYS:HB3	2.20	0.41
21:T:25:LYS:HA	21:T:25:LYS:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:45:PHE:CD1	21:T:45:PHE:N	2.87	0.41
1:X:26:G:C6	1:X:27:G:N1	2.89	0.41
1:X:1235:C:N4	1:X:1240:G:H1	2.19	0.41
1:X:1781:C:H4'	3:A:209:ALA:CB	2.50	0.41
1:X:2279:G:N2	1:X:2295:C:O2	2.33	0.41
1:X:2631:C:C2	1:X:2648:G:C2	3.09	0.41
1:X:2791:C:O2'	1:X:2792:C:H5'	2.21	0.41
1:X:2870:C:H2'	1:X:2871:U:C6	2.56	0.41
2:Y:48:A:H2'	2:Y:49:C:O4'	2.20	0.41
5:C:75:PRO:HA	5:C:81:GLY:O	2.19	0.41
6:D:28:VAL:HA	6:D:29:PRO:HD3	1.96	0.41
8:G:36:ASN:HB2	8:G:74:MET:HE2	2.03	0.41
9:H:28:GLY:O	9:H:34:LEU:HA	2.20	0.41
12:K:39:THR:O	12:K:40:LYS:C	2.63	0.41
17:P:117:ILE:HD13	17:P:117:ILE:HA	1.63	0.41
1:X:45:C:OP2	1:X:192:G:H2'	2.21	0.41
1:X:158:A:H2'	1:X:159:A:C8	2.55	0.41
1:X:538:A:C2	1:X:2025:A:C6	3.09	0.41
1:X:699:G:N1	27:2:12:ARG:HB2	2.35	0.41
1:X:822:G:C6	1:X:823:U:C4	3.09	0.41
1:X:870:C:C2'	1:X:871:U:H5'	2.51	0.41
1:X:881:U:C4	1:X:882:C:N4	2.89	0.41
1:X:1007:A:H4'	15:N:93:LYS:NZ	2.29	0.41
1:X:1237:G:O3'	16:O:85:GLY:HA3	2.21	0.41
1:X:1255:A:H2'	1:X:1256:C:H6	1.86	0.41
1:X:1270:C:H4'	5:C:77:PHE:CE1	2.56	0.41
1:X:1418:C:H2'	1:X:1419:G:H8	1.85	0.41
1:X:1469:U:H5''	1:X:1470:G:N7	2.35	0.41
1:X:1533:G:H2'	1:X:1534:A:H8	1.85	0.41
1:X:1564:U:H2'	1:X:1565:G:H8	1.86	0.41
1:X:1742:G:H2'	1:X:1743:C:H6	1.86	0.41
1:X:2262:C:C2	1:X:2368:G:C2	3.09	0.41
1:X:2310:G:H2'	1:X:2311:U:O4'	2.20	0.41
1:X:2557:G:N2	1:X:2558:C:C2	2.89	0.41
1:X:2790:C:H42	1:X:2806:G:H1	1.66	0.41
1:X:2847:G:C2	1:X:2848:A:N6	2.88	0.41
2:Y:53:G:C5'	13:L:64:LYS:HG3	2.51	0.41
4:B:125:GLY:O	4:B:126:PRO:C	2.61	0.41
5:C:34:GLN:O	5:C:37:SER:OG	2.34	0.41
5:C:62:LYS:HD3	5:C:62:LYS:HA	1.87	0.41
6:D:123:ASP:HB3	6:D:127:ASN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:62:ILE:HG21	8:G:135:LEU:HD11	2.02	0.41
8:G:128:GLU:HG2	8:G:148:LEU:HD23	2.03	0.41
9:H:1:MET:H3	9:H:1:MET:HG3	1.55	0.41
10:I:31:GLY:O	10:I:32:ARG:NH2	2.54	0.41
14:M:7:ILE:HD12	14:M:7:ILE:HA	1.88	0.41
14:M:90:GLN:OE1	14:M:91:VAL:N	2.42	0.41
18:Q:66:GLY:HA3	18:Q:68:PHE:CE2	2.56	0.41
19:R:103:LYS:HE2	19:R:103:LYS:HB3	1.92	0.41
20:S:3:LEU:HD11	20:S:5:ALA:O	2.21	0.41
20:S:89:GLY:HA2	20:S:127:PRO:HB3	2.03	0.41
20:S:123:VAL:HG12	20:S:159:THR:H	1.86	0.41
23:V:13:ASP:O	23:V:17:GLU:HG2	2.21	0.41
24:W:4:LYS:HE3	24:W:52:GLU:HB3	2.03	0.41
25:Z:45:ILE:HD11	25:Z:56:GLN:HG2	2.02	0.41
1:X:506:G:C6	1:X:507:A:C4	3.09	0.41
1:X:533:C:H2'	1:X:534:U:O4'	2.21	0.41
1:X:540:G:H4'	1:X:541:C:OP1	2.21	0.41
1:X:661:C:C2	1:X:662:G:C2	3.09	0.41
1:X:699:G:N2	27:2:7:PRO:O	2.53	0.41
1:X:941:U:H2'	1:X:942:U:O4'	2.21	0.41
1:X:1039:A:N6	1:X:1136:G:H2'	2.36	0.41
1:X:1179:A:H2'	1:X:1180:A:H8	1.85	0.41
1:X:1500:U:H2'	1:X:1501:C:C6	2.56	0.41
1:X:1814:G:H2'	1:X:1815:G:H8	1.86	0.41
1:X:2794:G:C2	1:X:2803:C:C2	3.09	0.41
6:D:106:ILE:O	6:D:109:PRO:HD2	2.20	0.41
7:E:94:PHE:CB	7:E:107:ILE:HG22	2.50	0.41
8:G:93:LYS:HA	8:G:93:LYS:HD3	1.80	0.41
10:I:77:LEU:HB2	10:I:111:SER:H	1.85	0.41
23:V:43:VAL:O	23:V:47:ARG:HG2	2.21	0.41
25:Z:14:SER:O	25:Z:18:MET:HB2	2.21	0.41
26:1:34:LYS:HG3	26:1:35:LEU:H	1.85	0.41
28:3:13:ARG:HB2	28:3:23:MET:O	2.21	0.41
1:X:163:A:H2'	1:X:164:G:H8	1.87	0.40
1:X:312:G:C4	1:X:313:U:C5	3.10	0.40
1:X:580:A:C8	1:X:2013:A:N6	2.89	0.40
1:X:1204:G:H2'	1:X:1205:G:H8	1.84	0.40
1:X:1500:U:H3	1:X:1520:G:H1	1.69	0.40
1:X:1669:A:N7	1:X:1670:G:C6	2.89	0.40
1:X:1839:A:O2'	1:X:1840:A:H8	2.04	0.40
1:X:2867:G:H4'	1:X:2868:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:95:LEU:HG	3:A:105:ILE:HD12	2.02	0.40
7:E:124:ALA:HB3	7:E:132:ASP:HB2	2.02	0.40
7:E:148:VAL:HG12	7:E:162:VAL:HG11	2.03	0.40
15:N:99:ALA:HB2	15:N:106:PHE:CD1	2.56	0.40
21:T:23:VAL:HA	21:T:38:VAL:HG23	2.03	0.40
22:U:47:HIS:CG	22:U:48:LYS:N	2.89	0.40
22:U:51:ILE:O	22:U:52:ARG:NH2	2.37	0.40
27:2:37:LYS:HG2	27:2:37:LYS:O	2.21	0.40
1:X:322:A:H62	1:X:339:U:H2'	1.86	0.40
1:X:698:A:H5''	1:X:801:A:H62	1.85	0.40
1:X:734:G:H2'	1:X:735:G:C8	2.56	0.40
1:X:841:G:N2	1:X:2225:G:O2'	2.46	0.40
1:X:1273:G:H2'	1:X:1274:C:O4'	2.21	0.40
1:X:2001:G:C6	1:X:2002:A:C6	3.08	0.40
1:X:2043:A:C2	1:X:2481:G:C5	3.09	0.40
1:X:2422:C:H2'	1:X:2423:G:C8	2.56	0.40
1:X:2482:A:H4'	1:X:2483:U:OP1	2.20	0.40
1:X:2658:A:H2'	1:X:2659:C:O4'	2.20	0.40
4:B:122:PHE:HB3	4:B:123:ALA:H	1.64	0.40
8:G:30:LYS:O	8:G:31:THR:OG1	2.26	0.40
8:G:100:TYR:CD2	8:G:119:LEU:HD12	2.55	0.40
11:J:73:LYS:H	11:J:94:TRP:HD1	1.69	0.40
15:N:104:GLU:N	15:N:104:GLU:OE2	2.54	0.40
16:O:68:LYS:HE3	16:O:70:TYR:CZ	2.56	0.40
17:P:68:VAL:HG22	17:P:124:ILE:HG21	2.02	0.40
22:U:13:LEU:O	22:U:14:VAL:HG13	2.22	0.40
23:V:14:PHE:O	23:V:18:ILE:HG13	2.21	0.40
25:Z:8:LYS:O	25:Z:9:LYS:HD2	2.21	0.40
1:X:317:U:H2'	1:X:318:G:O4'	2.22	0.40
1:X:478:G:H2'	1:X:479:G:O4'	2.20	0.40
1:X:932:G:H2'	1:X:933:G:H8	1.86	0.40
1:X:1915:A:N1	1:X:1956:G:H1'	2.36	0.40
1:X:2166:G:H2'	1:X:2167:A:C8	2.57	0.40
1:X:2594:U:C2	1:X:2595:C:C5	3.08	0.40
3:A:176:ARG:NH1	3:A:180:GLY:HA2	2.31	0.40
4:B:54:LYS:HD3	4:B:59:VAL:HG22	2.03	0.40
5:C:3:GLN:HB2	5:C:116:LYS:NZ	2.34	0.40
15:N:30:LYS:HA	15:N:30:LYS:HD2	1.82	0.40
16:O:36:LYS:HE2	16:O:56:VAL:HG22	2.03	0.40
19:R:10:HIS:ND1	19:R:10:HIS:N	2.69	0.40
20:S:71:MET:CB	20:S:78:PRO:HA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:3:U:O2'	1:X:4:C:P	2.80	0.40
1:X:173:A:H2'	1:X:173:A:N3	2.36	0.40
1:X:505:G:O2'	17:P:78:ASN:HB3	2.22	0.40
1:X:625:A:H4'	1:X:626:A:OP1	2.21	0.40
1:X:1424:U:H2'	1:X:1425:G:C8	2.57	0.40
1:X:1643:A:N6	1:X:1656:U:H3	2.18	0.40
1:X:1671:A:H1'	1:X:2798:A:H5'	2.02	0.40
1:X:1697:U:N3	1:X:1755:G:OP2	2.55	0.40
1:X:2039:G:N2	1:X:2040:A:N9	2.70	0.40
1:X:2060:A:H2'	1:X:2061:C:C6	2.57	0.40
1:X:2597:G:O2'	4:B:149:ARG:HB2	2.21	0.40
1:X:2617:G:O2'	1:X:2755:A:N1	2.50	0.40
1:X:2730:A:O2'	1:X:2731:G:N2	2.54	0.40
5:C:112:GLN:HE22	5:C:116:LYS:NZ	2.20	0.40
10:I:73:GLU:OE2	10:I:101:ARG:HB2	2.21	0.40
13:L:34:SER:HB3	13:L:35:SER:H	1.77	0.40
18:Q:63:LYS:HG3	18:Q:64:ARG:C	2.46	0.40
27:2:36:ALA:O	27:2:38:GLY:N	2.54	0.40
1:X:57:G:O2'	1:X:72:A:N1	2.53	0.40
1:X:387:A:H2'	1:X:387:A:N3	2.36	0.40
1:X:475:U:O2'	27:2:16:HIS:NE2	2.50	0.40
1:X:540:G:O2'	1:X:542:A:C2	2.63	0.40
1:X:787:A:C2	1:X:800:U:O2'	2.74	0.40
1:X:861:G:N2	1:X:943:U:H1'	2.36	0.40
1:X:977:G:H5'	1:X:2251:U:O2	2.22	0.40
1:X:1208:A:H2'	1:X:1209:G:O4'	2.21	0.40
1:X:1267:A:H5''	1:X:1268:U:H5''	2.03	0.40
1:X:1327:C:H42	1:X:1351:G:H1	1.69	0.40
1:X:1465:G:N3	1:X:1466:C:O2	2.54	0.40
1:X:1919:A:N6	1:X:1946:U:N3	2.69	0.40
1:X:2691:C:H2'	1:X:2694:G:H5''	2.03	0.40
1:X:2728:A:C6	1:X:2729:A:C6	3.10	0.40
1:X:2867:G:O5'	1:X:2867:G:H8	2.04	0.40
3:A:28:ARG:HA	3:A:29:PRO:HD3	1.85	0.40
5:C:154:ASP:O	5:C:157:THR:N	2.54	0.40
12:K:45:ARG:HD3	12:K:95:THR:CG2	2.51	0.40
15:N:5:LYS:C	15:N:7:GLY:H	2.28	0.40
17:P:74:SER:HA	17:P:77:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	257/275 (94%)	219 (85%)	37 (14%)	1 (0%)	30	60
4	B	203/211 (96%)	183 (90%)	15 (7%)	5 (2%)	4	28
5	C	192/205 (94%)	161 (84%)	25 (13%)	6 (3%)	3	25
6	D	175/180 (97%)	151 (86%)	24 (14%)	0	100	100
7	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	21	54
8	G	140/174 (80%)	124 (89%)	15 (11%)	1 (1%)	18	51
9	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	16	49
10	I	132/156 (85%)	98 (74%)	30 (23%)	4 (3%)	3	25
11	J	134/141 (95%)	117 (87%)	16 (12%)	1 (1%)	18	51
12	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	14	46
13	L	102/114 (90%)	80 (78%)	22 (22%)	0	100	100
14	M	106/166 (64%)	100 (94%)	6 (6%)	0	100	100
15	N	115/118 (98%)	100 (87%)	13 (11%)	2 (2%)	7	35
16	O	92/100 (92%)	83 (90%)	9 (10%)	0	100	100
17	P	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
18	Q	91/95 (96%)	69 (76%)	19 (21%)	3 (3%)	3	23
19	R	108/115 (94%)	80 (74%)	28 (26%)	0	100	100
20	S	177/237 (75%)	150 (85%)	25 (14%)	2 (1%)	11	43
21	T	72/91 (79%)	63 (88%)	9 (12%)	0	100	100
22	U	70/81 (86%)	51 (73%)	17 (24%)	2 (3%)	3	25
23	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
24	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
25	Z	55/60 (92%)	45 (82%)	10 (18%)	0	100	100
26	1	51/54 (94%)	36 (71%)	12 (24%)	3 (6%)	1	13
27	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	3	57/66 (86%)	44 (77%)	11 (19%)	2 (4%)	3	23
All	All	3026/3377 (90%)	2598 (86%)	391 (13%)	37 (1%)	10	41

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	94	VAL
18	Q	6	ILE
5	C	177	VAL
20	S	122	ILE
26	1	9	ILE
26	1	10	VAL
4	B	136	ARG
11	J	82	THR
22	U	60	VAL
27	2	5	TYR
3	A	21	PHE
4	B	144	ARG
5	C	130	THR
7	E	165	VAL
10	I	103	ASN
12	K	91	PRO
18	Q	69	ILE
22	U	15	VAL
4	B	121	ASN
5	C	113	GLU
5	C	164	VAL
10	I	38	LYS
27	2	8	ASN
4	B	137	ARG
9	H	42	LYS
18	Q	65	VAL
28	3	13	ARG
28	3	61	MET
8	G	163	PRO
4	B	73	ALA
5	C	15	ILE
15	N	8	ILE
26	1	8	ILE
5	C	22	VAL
10	I	19	VAL
10	I	68	VAL

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Mol	Chain	Res	Type
20	S	81	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	200/216 (93%)	161 (80%)	39 (20%)	1	9
4	B	155/157 (99%)	122 (79%)	33 (21%)	1	7
5	C	154/163 (94%)	119 (77%)	35 (23%)	1	6
6	D	153/156 (98%)	145 (95%)	8 (5%)	21	48
7	E	136/144 (94%)	121 (89%)	15 (11%)	6	27
8	G	118/146 (81%)	99 (84%)	19 (16%)	2	15
9	H	103/103 (100%)	83 (81%)	20 (19%)	1	9
10	I	101/121 (84%)	77 (76%)	24 (24%)	1	5
11	J	108/115 (94%)	90 (83%)	18 (17%)	2	14
12	K	90/93 (97%)	71 (79%)	19 (21%)	1	7
13	L	74/82 (90%)	51 (69%)	23 (31%)	0	2
14	M	92/134 (69%)	69 (75%)	23 (25%)	0	4
15	N	96/97 (99%)	87 (91%)	9 (9%)	8	32
16	O	75/79 (95%)	61 (81%)	14 (19%)	1	10
17	P	109/115 (95%)	88 (81%)	21 (19%)	1	9
18	Q	75/76 (99%)	55 (73%)	20 (27%)	0	3
19	R	91/96 (95%)	74 (81%)	17 (19%)	1	10
20	S	152/192 (79%)	127 (84%)	25 (16%)	2	14
21	T	55/67 (82%)	46 (84%)	9 (16%)	2	14
22	U	57/66 (86%)	42 (74%)	15 (26%)	0	4
23	V	53/55 (96%)	50 (94%)	3 (6%)	18	46
24	W	48/48 (100%)	38 (79%)	10 (21%)	1	7
25	Z	51/53 (96%)	39 (76%)	12 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	1	45/47 (96%)	34 (76%)	11 (24%)	1	5
27	2	39/40 (98%)	30 (77%)	9 (23%)	1	6
28	3	46/52 (88%)	35 (76%)	11 (24%)	1	5
All	All	2476/2713 (91%)	2014 (81%)	462 (19%)	1	10

All (462) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	THR
3	A	20	ASP
3	A	22	SER
3	A	25	THR
3	A	28	ARG
3	A	31	LYS
3	A	35	GLU
3	A	40	THR
3	A	43	ARG
3	A	49	ILE
3	A	68	LYS
3	A	87	ASN
3	A	95	LEU
3	A	104	TYR
3	A	106	LEU
3	A	127	LEU
3	A	138	VAL
3	A	141	VAL
3	A	142	VAL
3	A	147	LEU
3	A	151	LYS
3	A	162	SER
3	A	163	VAL
3	A	173	VAL
3	A	186	HIS
3	A	188	GLU
3	A	196	VAL
3	A	202	LYS
3	A	203	ASN
3	A	205	VAL
3	A	208	LYS
3	A	211	ARG
3	A	213	ARG

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Mol	Chain	Res	Type
3	A	215	LEU
3	A	218	LYS
3	A	237	GLU
3	A	240	THR
3	A	248	THR
3	A	252	LYS
4	B	5	LEU
4	B	14	ILE
4	B	21	ILE
4	B	23	VAL
4	B	24	THR
4	B	25	VAL
4	B	34	VAL
4	B	38	THR
4	B	41	THR
4	B	49	ILE
4	B	72	VAL
4	B	75	THR
4	B	79	ARG
4	B	82	ARG
4	B	93	VAL
4	B	94	ASP
4	B	105	THR
4	B	107	THR
4	B	113	THR
4	B	116	VAL
4	B	132	LYS
4	B	133	LYS
4	B	135	HIS
4	B	141	ILE
4	B	143	GLN
4	B	144	ARG
4	B	149	ARG
4	B	164	ARG
4	B	184	VAL
4	B	188	ILE
4	B	197	VAL
4	B	199	ARG
4	B	203	LYS
5	C	5	ASN
5	C	14	THR
5	C	17	LEU

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Mol	Chain	Res	Type
5	C	32	THR
5	C	34	GLN
5	C	40	ARG
5	C	45	THR
5	C	47	THR
5	C	58	MET
5	C	66	ASN
5	C	74	VAL
5	C	76	THR
5	C	77	PHE
5	C	82	VAL
5	C	94	THR
5	C	95	LEU
5	C	100	ARG
5	C	120	VAL
5	C	125	ILE
5	C	127	ASP
5	C	130	THR
5	C	132	ASN
5	C	143	ASP
5	C	148	VAL
5	C	154	ASP
5	C	157	THR
5	C	162	ARG
5	C	164	VAL
5	C	167	VAL
5	C	169	VAL
5	C	172	VAL
5	C	175	VAL
5	C	177	VAL
5	C	180	ILE
5	C	193	LEU
6	D	4	LEU
6	D	22	TYR
6	D	40	LEU
6	D	51	ASP
6	D	85	VAL
6	D	90	THR
6	D	146	VAL
6	D	152	MET
7	E	32	GLU
7	E	34	THR

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Mol	Chain	Res	Type
7	E	38	ASN
7	E	43	VAL
7	E	52	VAL
7	E	57	ASP
7	E	61	HIS
7	E	67	LEU
7	E	111	HIS
7	E	129	THR
7	E	144	VAL
7	E	149	ARG
7	E	164	PHE
7	E	165	VAL
7	E	171	LEU
8	G	30	LYS
8	G	32	TYR
8	G	53	ARG
8	G	62	ILE
8	G	65	LYS
8	G	78	ASP
8	G	88	VAL
8	G	91	THR
8	G	95	LEU
8	G	102	ARG
8	G	103	TYR
8	G	104	THR
8	G	106	TYR
8	G	117	GLU
8	G	119	LEU
8	G	146	THR
8	G	161	GLN
8	G	165	VAL
8	G	171	LEU
9	H	1	MET
9	H	2	ILE
9	H	20	MET
9	H	29	ILE
9	H	35	THR
9	H	36	THR
9	H	41	ASN
9	H	69	VAL
9	H	70	VAL
9	H	73	VAL

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Mol	Chain	Res	Type
9	H	74	VAL
9	H	78	SER
9	H	81	ILE
9	H	82	LYS
9	H	89	ILE
9	H	90	ARG
9	H	94	ASN
9	H	108	THR
9	H	118	LEU
9	H	127	VAL
10	I	18	ARG
10	I	19	VAL
10	I	26	THR
10	I	28	LYS
10	I	32	ARG
10	I	37	GLN
10	I	39	SER
10	I	40	ARG
10	I	53	ARG
10	I	55	ARG
10	I	62	LYS
10	I	71	THR
10	I	77	LEU
10	I	79	GLN
10	I	83	LEU
10	I	89	ASP
10	I	96	TYR
10	I	98	LEU
10	I	99	VAL
10	I	103	ASN
10	I	120	VAL
10	I	126	SER
10	I	141	VAL
10	I	142	LEU
11	J	8	THR
11	J	9	LYS
11	J	10	PHE
11	J	17	ARG
11	J	26	ASP
11	J	27	TYR
11	J	28	VAL
11	J	46	ASN

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Mol	Chain	Res	Type
11	J	59	PHE
11	J	65	ILE
11	J	67	ILE
11	J	73	LYS
11	J	86	LYS
11	J	104	MET
11	J	106	GLU
11	J	131	LYS
11	J	134	LYS
11	J	135	ARG
12	K	5	LYS
12	K	11	ASN
12	K	13	ASN
12	K	14	SER
12	K	17	ARG
12	K	26	THR
12	K	37	THR
12	K	43	GLU
12	K	45	ARG
12	K	48	VAL
12	K	51	LEU
12	K	59	ASP
12	K	73	LYS
12	K	76	VAL
12	K	95	THR
12	K	98	LEU
12	K	100	VAL
12	K	102	THR
12	K	109	THR
13	L	8	ARG
13	L	11	LEU
13	L	13	THR
13	L	15	ARG
13	L	29	LEU
13	L	31	VAL
13	L	34	SER
13	L	37	HIS
13	L	38	ILE
13	L	39	TYR
13	L	42	ILE
13	L	43	ILE
13	L	45	ASP

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Mol	Chain	Res	Type
13	L	46	SER
13	L	65	THR
13	L	66	ASP
13	L	67	THR
13	L	88	VAL
13	L	91	ARG
13	L	93	SER
13	L	94	TYR
13	L	97	HIS
13	L	109	GLU
14	M	3	THR
14	M	7	ILE
14	M	11	GLU
14	M	22	ARG
14	M	31	ASP
14	M	33	VAL
14	M	37	THR
14	M	38	LYS
14	M	39	VAL
14	M	40	ARG
14	M	41	GLU
14	M	43	ASN
14	M	45	THR
14	M	57	ILE
14	M	63	ARG
14	M	68	VAL
14	M	69	ARG
14	M	92	THR
14	M	94	VAL
14	M	96	ARG
14	M	98	LYS
14	M	101	ARG
14	M	103	LYS
15	N	9	VAL
15	N	15	LYS
15	N	22	LYS
15	N	30	LYS
15	N	31	GLN
15	N	51	ARG
15	N	60	LEU
15	N	93	LYS
15	N	109	LEU

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Mol	Chain	Res	Type
16	O	13	ARG
16	O	16	GLU
16	O	20	ILE
16	O	21	ARG
16	O	22	VAL
16	O	28	GLU
16	O	47	PHE
16	O	49	GLU
16	O	56	VAL
16	O	71	ILE
16	O	81	ARG
16	O	88	GLN
16	O	91	THR
16	O	98	ILE
17	P	9	ARG
17	P	13	GLN
17	P	32	ARG
17	P	37	LYS
17	P	39	ARG
17	P	40	LEU
17	P	44	VAL
17	P	45	ILE
17	P	46	ARG
17	P	52	ASP
17	P	60	ILE
17	P	65	SER
17	P	71	VAL
17	P	91	PHE
17	P	107	ILE
17	P	116	ILE
17	P	117	ILE
17	P	118	LYS
17	P	119	LYS
17	P	121	THR
17	P	125	THR
18	Q	6	ILE
18	Q	7	LEU
18	Q	8	GLN
18	Q	15	LYS
18	Q	24	VAL
18	Q	26	SER
18	Q	30	SER

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Mol	Chain	Res	Type
18	Q	34	THR
18	Q	40	ASP
18	Q	44	GLN
18	Q	58	VAL
18	Q	62	ARG
18	Q	64	ARG
18	Q	65	VAL
18	Q	73	ASN
18	Q	74	ASP
18	Q	80	VAL
18	Q	81	ARG
18	Q	84	GLU
18	Q	88	ILE
19	R	10	HIS
19	R	15	HIS
19	R	18	LYS
19	R	20	ASP
19	R	21	THR
19	R	23	ILE
19	R	30	LYS
19	R	48	VAL
19	R	56	LYS
19	R	63	THR
19	R	80	LYS
19	R	83	LEU
19	R	94	VAL
19	R	95	ARG
19	R	96	LYS
19	R	97	GLN
19	R	110	SER
20	S	1	MET
20	S	14	LEU
20	S	22	VAL
20	S	25	ASN
20	S	26	LYS
20	S	28	ASN
20	S	32	PHE
20	S	34	LEU
20	S	48	THR
20	S	71	MET
20	S	73	LYS
20	S	86	VAL

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Mol	Chain	Res	Type
20	S	88	TYR
20	S	92	VAL
20	S	98	VAL
20	S	112	LEU
20	S	120	LEU
20	S	122	ILE
20	S	123	VAL
20	S	129	ARG
20	S	147	ILE
20	S	159	THR
20	S	176	LEU
20	S	177	THR
20	S	179	GLU
21	T	30	VAL
21	T	36	ILE
21	T	37	LEU
21	T	38	VAL
21	T	45	PHE
21	T	64	ASP
21	T	67	VAL
21	T	68	VAL
21	T	80	SER
22	U	14	VAL
22	U	17	SER
22	U	19	ILE
22	U	21	ARG
22	U	27	ASP
22	U	32	ARG
22	U	35	THR
22	U	37	ILE
22	U	49	LYS
22	U	53	GLU
22	U	54	ASN
22	U	58	LYS
22	U	70	LEU
22	U	75	TYR
22	U	78	ILE
23	V	12	THR
23	V	19	ASP
23	V	28	LEU
24	W	1	MET
24	W	2	LYS

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Mol	Chain	Res	Type
24	W	3	ILE
24	W	4	LYS
24	W	9	VAL
24	W	10	ILE
24	W	12	ARG
24	W	36	ASP
24	W	46	THR
24	W	50	LEU
25	Z	3	LYS
25	Z	6	VAL
25	Z	10	LYS
25	Z	21	SER
25	Z	25	LEU
25	Z	41	LEU
25	Z	42	SER
25	Z	49	CYS
25	Z	51	TYR
25	Z	53	ASP
25	Z	55	ARG
25	Z	57	VAL
26	1	8	ILE
26	1	10	VAL
26	1	15	SER
26	1	20	PHE
26	1	21	TYR
26	1	25	THR
26	1	30	ASN
26	1	36	GLU
26	1	43	VAL
26	1	48	VAL
26	1	54	LYS
27	2	1	MET
27	2	6	GLN
27	2	7	PRO
27	2	14	LYS
27	2	15	THR
27	2	23	LYS
27	2	31	LEU
27	2	43	THR
27	2	45	SER
28	3	6	THR
28	3	7	HIS

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Mol	Chain	Res	Type
28	3	22	VAL
28	3	31	HIS
28	3	34	THR
28	3	46	LYS
28	3	49	VAL
28	3	50	LEU
28	3	52	LYS
28	3	60	LEU
28	3	62	LEU

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

Mol	Chain	Res	Type
3	A	87	ASN
3	A	129	ASN
3	A	164	GLN
3	A	166	GLN
3	A	198	ASN
4	B	60	ASN
4	B	129	HIS
4	B	135	HIS
5	C	28	HIS
5	C	101	GLN
5	C	112	GLN
5	C	163	ASN
6	D	118	ASN
6	D	135	GLN
7	E	20	GLN
7	E	38	ASN
7	E	74	ASN
7	E	111	HIS
8	G	39	GLN
8	G	76	GLN
8	G	84	ASN
8	G	87	GLN
8	G	140	GLN
8	G	145	HIS
8	G	156	HIS
8	G	158	HIS
9	H	41	ASN
10	I	34	HIS
10	I	103	ASN

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Mol	Chain	Res	Type
11	J	13	GLN
11	J	47	GLN
11	J	58	HIS
11	J	114	GLN
11	J	124	HIS
12	K	11	ASN
12	K	35	GLN
13	L	41	GLN
13	L	97	HIS
14	M	20	HIS
15	N	31	GLN
15	N	52	ASN
15	N	66	ASN
15	N	72	HIS
16	O	6	GLN
16	O	11	GLN
17	P	10	ASN
19	R	10	HIS
19	R	77	HIS
20	S	146	HIS
21	T	12	ASN
22	U	45	ASN
23	V	52	GLN
23	V	54	ASN
24	W	49	HIS
24	W	54	GLN
25	Z	23	HIS
25	Z	44	HIS
26	1	30	ASN
27	2	29	ASN
27	2	41	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2650/2880 (92%)	581 (21%)	49 (1%)
2	Y	119/123 (96%)	23 (19%)	1 (0%)
All	All	2769/3003 (92%)	604 (21%)	50 (1%)

All (604) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	7	G
1	X	10	A
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U
1	X	37	C
1	X	39	C
1	X	45	C
1	X	49	U
1	X	50	G
1	X	59	G
1	X	63	A
1	X	69	G
1	X	73	A
1	X	74	G
1	X	87	G
1	X	88	G
1	X	89	A
1	X	90	G
1	X	95	G
1	X	97	U
1	X	98	U
1	X	100	G
1	X	108	G
1	X	111	G
1	X	112	U
1	X	116	A
1	X	118	U
1	X	123	A
1	X	124	A
1	X	126	C
1	X	134	G
1	X	136	A
1	X	138	G
1	X	143	A
1	X	158	A
1	X	173	A
1	X	176	A
1	X	177	U
1	X	178	C

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Mol	Chain	Res	Type
1	X	181	A
1	X	192	G
1	X	193	A
1	X	198	A
1	X	199	A
1	X	201	G
1	X	205	A
1	X	206	U
1	X	207	U
1	X	209	G
1	X	210	A
1	X	218	A
1	X	219	G
1	X	220	U
1	X	225	G
1	X	229	G
1	X	241	C
1	X	242	A
1	X	243	G
1	X	247	A
1	X	248	A
1	X	249	A
1	X	302	U
1	X	303	C
1	X	304	A
1	X	305	A
1	X	310	A
1	X	312	G
1	X	313	U
1	X	321	A
1	X	322	A
1	X	323	G
1	X	333	A
1	X	334	G
1	X	335	A
1	X	338	G
1	X	340	G
1	X	342	G
1	X	343	A
1	X	349	G
1	X	387	A
1	X	398	C

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Mol	Chain	Res	Type
1	X	399	G
1	X	400	U
1	X	408	U
1	X	409	G
1	X	414	A
1	X	424	G
1	X	425	A
1	X	431	G
1	X	433	G
1	X	441	A
1	X	456	C
1	X	459	A
1	X	463	C
1	X	467	U
1	X	469	G
1	X	483	A
1	X	484	G
1	X	491	A
1	X	492	G
1	X	493	A
1	X	501	G
1	X	506	G
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	534	U
1	X	537	C
1	X	538	A
1	X	539	A
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	556	A
1	X	557	U
1	X	558	G
1	X	560	G
1	X	572	G
1	X	578	U
1	X	582	G

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Mol	Chain	Res	Type
1	X	584	A
1	X	591	G
1	X	595	A
1	X	601	A
1	X	613	A
1	X	616	U
1	X	617	U
1	X	626	A
1	X	627	A
1	X	628	A
1	X	631	G
1	X	633	G
1	X	645	G
1	X	648	A
1	X	649	G
1	X	654	A
1	X	655	A
1	X	656	U
1	X	657	A
1	X	664	C
1	X	665	A
1	X	666	U
1	X	667	U
1	X	668	A
1	X	682	G
1	X	683	A
1	X	684	C
1	X	690	A
1	X	699	G
1	X	728	G
1	X	729	A
1	X	731	A
1	X	732	G
1	X	743	A
1	X	747	A
1	X	753	U
1	X	760	U
1	X	761	G
1	X	766	A
1	X	773	G
1	X	774	A
1	X	777	A

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Mol	Chain	Res	Type
1	X	784	U
1	X	788	G
1	X	789	G
1	X	790	A
1	X	792	U
1	X	795	A
1	X	796	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	805	G
1	X	818	G
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	846	A
1	X	859	U
1	X	871	U
1	X	872	G
1	X	879	A
1	X	922	A
1	X	926	C
1	X	931	G
1	X	939	C
1	X	940	G
1	X	941	U
1	X	943	U
1	X	944	A
1	X	952	A
1	X	957	G
1	X	964	A
1	X	970	A
1	X	972	C
1	X	985	G
1	X	994	A
1	X	996	C
1	X	999	A
1	X	1006	C
1	X	1007	A
1	X	1014	G

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Mol	Chain	Res	Type
1	X	1016	C
1	X	1018	C
1	X	1020	A
1	X	1021	A
1	X	1022	A
1	X	1023	U
1	X	1031	C
1	X	1032	A
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1044	U
1	X	1046	U
1	X	1049	C
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1058	G
1	X	1073	G
1	X	1076	U
1	X	1077	U
1	X	1081	A
1	X	1082	G
1	X	1083	C
1	X	1108	U
1	X	1120	C
1	X	1121	G
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1139	A
1	X	1141	U
1	X	1142	G
1	X	1145	C
1	X	1146	G
1	X	1149	G
1	X	1152	C
1	X	1153	A
1	X	1154	A
1	X	1166	A
1	X	1167	A

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Mol	Chain	Res	Type
1	X	1176	U
1	X	1183	C
1	X	1185	C
1	X	1189	G
1	X	1192	A
1	X	1194	U
1	X	1207	G
1	X	1240	G
1	X	1242	A
1	X	1249	G
1	X	1250	A
1	X	1263	G
1	X	1266	G
1	X	1267	A
1	X	1269	G
1	X	1278	A
1	X	1284	G
1	X	1285	A
1	X	1286	U
1	X	1289	A
1	X	1313	U
1	X	1314	A
1	X	1324	G
1	X	1325	U
1	X	1334	A
1	X	1342	U
1	X	1344	C
1	X	1345	G
1	X	1351	G
1	X	1363	C
1	X	1372	A
1	X	1378	A
1	X	1381	G
1	X	1391	A
1	X	1392	U
1	X	1398	G
1	X	1403	U
1	X	1404	C
1	X	1409	U
1	X	1428	G
1	X	1429	A
1	X	1430	G

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Mol	Chain	Res	Type
1	X	1432	G
1	X	1433	A
1	X	1435	G
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1475	U
1	X	1476	G
1	X	1482	U
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1506	C
1	X	1524	C
1	X	1525	A
1	X	1526	U
1	X	1528	C
1	X	1531	C
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1570	C
1	X	1574	A
1	X	1575	C
1	X	1582	A
1	X	1585	A
1	X	1594	U
1	X	1602	G
1	X	1603	A
1	X	1608	U
1	X	1614	C
1	X	1623	C
1	X	1624	A
1	X	1625	A

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Mol	Chain	Res	Type
1	X	1630	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1648	C
1	X	1656	U
1	X	1657	A
1	X	1661	C
1	X	1665	C
1	X	1671	A
1	X	1685	A
1	X	1686	A
1	X	1691	G
1	X	1710	U
1	X	1714	A
1	X	1717	A
1	X	1718	A
1	X	1735	G
1	X	1743	C
1	X	1747	G
1	X	1754	G
1	X	1755	G
1	X	1760	G
1	X	1764	A
1	X	1767	G
1	X	1775	A
1	X	1782	A
1	X	1788	C
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1801	C
1	X	1802	A
1	X	1807	A
1	X	1808	C
1	X	1819	U
1	X	1821	A
1	X	1822	C
1	X	1824	C
1	X	1825	C

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Mol	Chain	Res	Type
1	X	1830	C
1	X	1831	G
1	X	1840	A
1	X	1850	G
1	X	1861	G
1	X	1864	G
1	X	1867	A
1	X	1868	A
1	X	1882	G
1	X	1886	G
1	X	1910	A
1	X	1912	G
1	X	1919	A
1	X	1920	A
1	X	1921	A
1	X	1922	U
1	X	1923	U
1	X	1924	C
1	X	1937	G
1	X	1938	U
1	X	1943	A
1	X	1946	U
1	X	1947	G
1	X	1949	A
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1979	C
1	X	1980	A
1	X	1988	A
1	X	2003	A
1	X	2006	G
1	X	2011	U
1	X	2014	A
1	X	2015	G
1	X	2016	A
1	X	2017	U
1	X	2018	G

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Mol	Chain	Res	Type
1	X	2026	C
1	X	2032	G
1	X	2034	A
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2063	A
1	X	2076	G
1	X	2083	G
1	X	2089	C
1	X	2171	U
1	X	2173	G
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2192	U
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2198	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2217	G
1	X	2218	G
1	X	2222	U
1	X	2241	U
1	X	2247	A
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2290	A

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Mol	Chain	Res	Type
1	X	2298	U
1	X	2299	A
1	X	2301	A
1	X	2306	A
1	X	2311	U
1	X	2313	G
1	X	2314	A
1	X	2315	A
1	X	2316	G
1	X	2322	U
1	X	2326	C
1	X	2330	G
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2370	G
1	X	2375	G
1	X	2381	A
1	X	2386	G
1	X	2398	U
1	X	2401	A
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2408	G
1	X	2410	U
1	X	2414	A
1	X	2420	C
1	X	2422	C
1	X	2424	G
1	X	2426	G
1	X	2427	A
1	X	2452	U
1	X	2455	A
1	X	2457	A
1	X	2463	G
1	X	2469	G
1	X	2473	G
1	X	2477	C
1	X	2480	C

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Mol	Chain	Res	Type
1	X	2481	G
1	X	2484	G
1	X	2485	U
1	X	2492	G
1	X	2497	A
1	X	2499	C
1	X	2522	G
1	X	2535	C
1	X	2545	A
1	X	2546	G
1	X	2551	A
1	X	2552	C
1	X	2556	A
1	X	2564	U
1	X	2565	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2590	U
1	X	2591	C
1	X	2592	U
1	X	2594	U
1	X	2595	C
1	X	2600	A
1	X	2608	A
1	X	2609	G
1	X	2613	A
1	X	2618	A
1	X	2633	A
1	X	2634	G
1	X	2640	G
1	X	2642	G
1	X	2650	G
1	X	2664	G
1	X	2666	U
1	X	2668	U
1	X	2683	C
1	X	2684	A
1	X	2691	C
1	X	2692	A
1	X	2693	U
1	X	2705	A

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Mol	Chain	Res	Type
1	X	2706	U
1	X	2713	A
1	X	2730	A
1	X	2731	G
1	X	2732	C
1	X	2737	A
1	X	2738	A
1	X	2744	A
1	X	2745	A
1	X	2756	A
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2761	A
1	X	2770	A
1	X	2782	G
1	X	2783	U
1	X	2787	A
1	X	2795	A
1	X	2796	A
1	X	2798	A
1	X	2808	U
1	X	2809	A
1	X	2811	G
1	X	2814	G
1	X	2824	C
1	X	2825	A
1	X	2842	C
1	X	2847	G
1	X	2851	G
1	X	2855	C
1	X	2858	A
1	X	2866	A
1	X	2868	G
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	22	U
2	Y	26	G
2	Y	28	A
2	Y	32	C

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Mol	Chain	Res	Type
2	Y	37	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	49	C
2	Y	68	A
2	Y	69	G
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	110	U
2	Y	112	A
2	Y	115	G

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	G
1	X	49	U
1	X	177	U
1	X	219	G
1	X	334	G
1	X	386	U
1	X	458	G
1	X	490	A
1	X	518	A
1	X	540	G
1	X	557	U
1	X	600	G
1	X	683	A
1	X	788	G
1	X	789	G
1	X	797	A
1	X	824	U
1	X	938	G
1	X	1019	U
1	X	1031	C
1	X	1053	G
1	X	1055	A
1	X	1182	U

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Mol	Chain	Res	Type
1	X	1223	G
1	X	1313	U
1	X	1391	A
1	X	1441	A
1	X	1475	U
1	X	1496	G
1	X	1607	A
1	X	1630	A
1	X	1792	C
1	X	1800	A
1	X	1923	U
1	X	1975	G
1	X	2015	G
1	X	2016	A
1	X	2043	A
1	X	2190	A
1	X	2204	A
1	X	2312	A
1	X	2409	A
1	X	2485	U
1	X	2564	U
1	X	2591	C
1	X	2705	A
1	X	2736	U
1	X	2756	A
1	X	2824	C
2	Y	16	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 124 ligands modelled in this entry, 123 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
29	6O1	X	2901	-	117,123,123	1.63	14 (11%)	155,191,191	1.84	30 (19%)

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
29	6O1	X	2901	-	-	10/50/234/234	0/13/13/13

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	6O1	O71-N65	6.73	1.36	1.22
29	X	2901	6O1	C08-C05	-6.08	1.39	1.51
29	X	2901	6O1	C62-C61	-5.64	1.40	1.51
29	X	2901	6O1	O53-C49	5.39	1.45	1.40
29	X	2901	6O1	C04-C09	-4.43	1.40	1.50
29	X	2901	6O1	C56-C55	-3.90	1.41	1.50
29	X	2901	6O1	O51-C54	3.51	1.47	1.41
29	X	2901	6O1	C22-C23	3.41	1.55	1.53
29	X	2901	6O1	O20-C16	2.89	1.44	1.41
29	X	2901	6O1	C51-C50	-2.85	1.48	1.53
29	X	2901	6O1	O25-C16	2.83	1.46	1.41
29	X	2901	6O1	O50-C54	2.68	1.45	1.41
29	X	2901	6O1	C65-N65	-2.55	1.47	1.52
29	X	2901	6O1	O26-C22	2.23	1.47	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	6O1	O50-C50-C51	-10.43	97.90	106.63
29	X	2901	6O1	O51-C51-C50	-6.40	98.11	106.41
29	X	2901	6O1	C44-O44-C36	-5.05	105.27	114.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	6O1	C36-C37-C38	-5.03	102.16	110.37
29	X	2901	6O1	C06-C01-C02	4.13	122.20	117.78
29	X	2901	6O1	C29-O33-C33	-3.69	107.33	113.63
29	X	2901	6O1	C03-C02-CL1	3.18	123.84	118.95
29	X	2901	6O1	C29-C30-C31	-3.17	104.61	110.11
29	X	2901	6O1	O47-C47-C46	-3.11	98.50	103.54
29	X	2901	6O1	C15-C14-C13	-3.01	108.91	113.39
29	X	2901	6O1	O53-C49-O47	2.91	114.45	109.99
29	X	2901	6O1	C13-O13-C09	-2.89	112.64	117.24
29	X	2901	6O1	C30-C31-C32	-2.86	105.28	111.72
29	X	2901	6O1	C16-O20-C20	-2.86	109.56	112.16
29	X	2901	6O1	C48-C47-C46	-2.76	107.37	112.56
29	X	2901	6O1	C01-C02-C03	-2.59	117.25	120.68
29	X	2901	6O1	C28-C26-C25	-2.52	108.52	113.55
29	X	2901	6O1	C01-C06-C05	-2.51	119.97	122.65
29	X	2901	6O1	C69-O66-C66	-2.39	110.42	114.46
29	X	2901	6O1	C34-O32-C32	-2.26	108.67	114.47
29	X	2901	6O1	C10-O19-C19	-2.26	110.22	114.72
29	X	2901	6O1	O31-C31-C32	2.25	113.14	107.42
29	X	2901	6O1	C53-O53-C49	-2.24	110.07	111.59
29	X	2901	6O1	C42-C40-C39	-2.19	108.06	113.35
29	X	2901	6O1	O57-C57-C56	-2.15	117.17	121.14
29	X	2901	6O1	O20-C20-C21	2.10	108.50	105.94
29	X	2901	6O1	O39-C29-O33	2.10	116.21	110.69
29	X	2901	6O1	O40-C40-C42	-2.00	102.73	106.69
29	X	2901	6O1	C21-C20-C19	-2.00	110.42	113.39
29	X	2901	6O1	O25-C25-C26	2.00	112.14	108.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

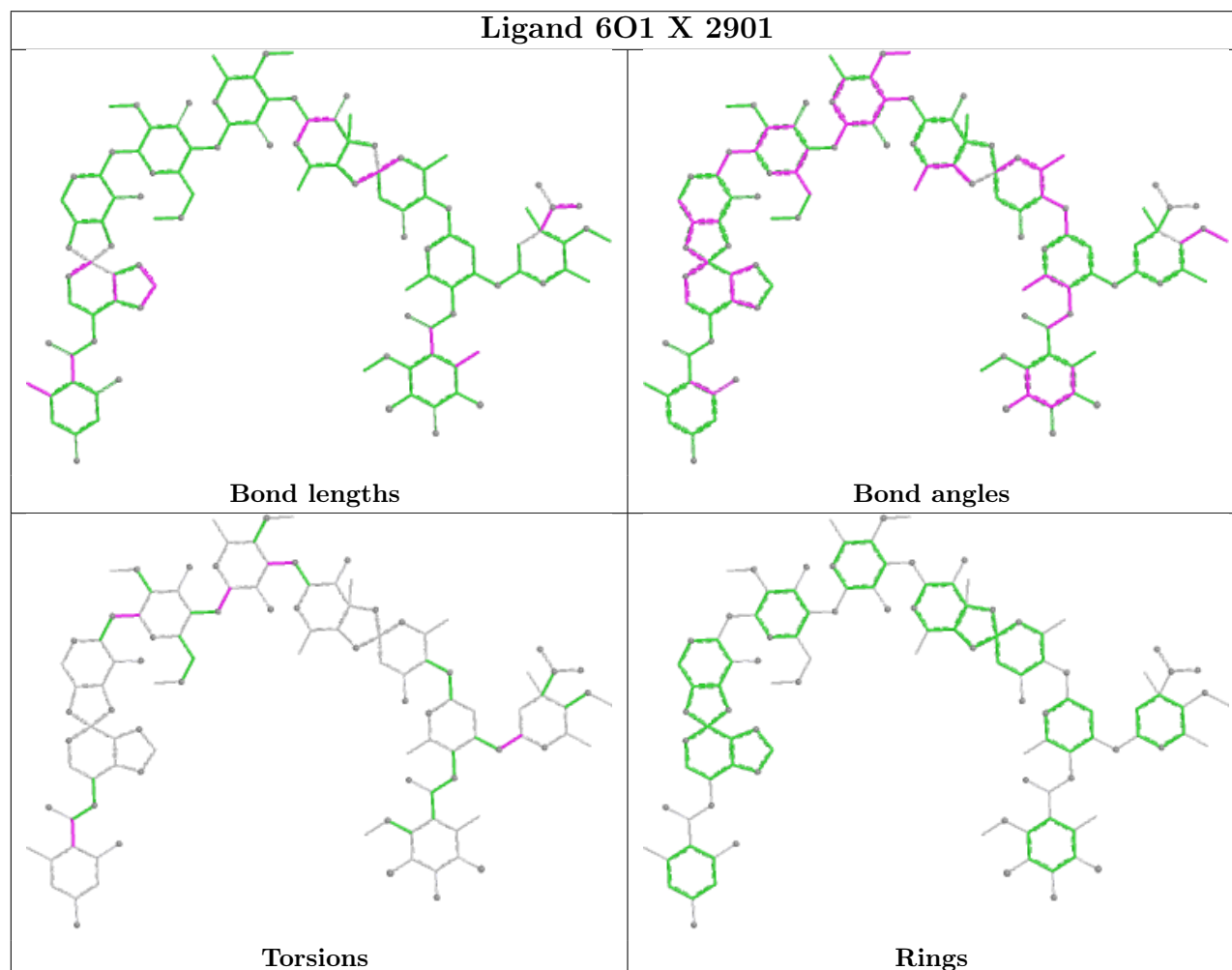
Mol	Chain	Res	Type	Atoms
29	X	2901	6O1	O67-C63-O12-C12
29	X	2901	6O1	O33-C29-O39-C39
29	X	2901	6O1	O40-C36-O44-C44
29	X	2901	6O1	C37-C36-O44-C44
29	X	2901	6O1	O55-C55-C56-C61
29	X	2901	6O1	O52-C55-C56-C61
29	X	2901	6O1	C30-C31-O31-C22
29	X	2901	6O1	O55-C55-C56-C57
29	X	2901	6O1	C32-C31-O31-C22
29	X	2901	6O1	O52-C55-C56-C57

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	2901	6O1	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2658/2880 (92%)	0.16	131 (4%) 35 19	30, 77, 204, 337	0
2	Y	120/123 (97%)	0.54	11 (9%) 14 9	80, 150, 187, 207	0
3	A	259/275 (94%)	0.82	42 (16%) 4 4	50, 105, 160, 212	0
4	B	205/211 (97%)	0.13	10 (4%) 35 19	30, 51, 113, 199	0
5	C	194/205 (94%)	0.59	20 (10%) 12 8	35, 103, 180, 254	0
6	D	177/180 (98%)	0.49	16 (9%) 15 10	128, 183, 249, 280	0
7	E	171/185 (92%)	0.41	15 (8%) 15 10	70, 142, 203, 254	0
8	G	142/174 (81%)	0.88	23 (16%) 4 4	38, 78, 188, 245	0
9	H	134/134 (100%)	0.13	8 (5%) 27 16	40, 55, 108, 175	0
10	I	134/156 (85%)	1.23	33 (24%) 2 2	50, 120, 191, 236	0
11	J	136/141 (96%)	0.57	16 (11%) 9 7	65, 106, 170, 225	0
12	K	113/116 (97%)	0.33	7 (6%) 26 15	30, 37, 91, 200	0
13	L	104/114 (91%)	1.19	21 (20%) 3 3	120, 154, 189, 241	0
14	M	108/166 (65%)	-0.02	2 (1%) 66 38	37, 50, 117, 169	0
15	N	117/118 (99%)	0.51	8 (6%) 23 14	42, 82, 136, 279	0
16	O	94/100 (94%)	0.57	12 (12%) 7 6	48, 101, 170, 216	0
17	P	127/134 (94%)	-0.06	3 (2%) 59 34	34, 53, 105, 192	0
18	Q	93/95 (97%)	0.28	6 (6%) 25 15	49, 88, 174, 215	0
19	R	110/115 (95%)	0.68	17 (15%) 5 5	62, 117, 213, 259	0
20	S	179/237 (75%)	0.49	11 (6%) 27 15	97, 158, 213, 289	0
21	T	74/91 (81%)	0.61	9 (12%) 8 7	67, 104, 157, 206	0
22	U	72/81 (88%)	0.87	11 (15%) 5 5	70, 125, 187, 215	0
23	V	65/67 (97%)	0.20	2 (3%) 51 28	83, 125, 197, 216	0
24	W	55/55 (100%)	0.01	3 (5%) 30 17	68, 90, 135, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/60 (95%)	0.20	3 (5%) 32 18	32, 43, 104, 182	0
26	1	53/54 (98%)	1.37	11 (20%) 2 3	101, 129, 224, 259	0
27	2	46/47 (97%)	0.68	5 (10%) 10 8	44, 59, 103, 162	0
28	3	59/66 (89%)	1.71	20 (33%) 1 1	72, 100, 161, 239	0
All	All	5856/6380 (91%)	0.37	476 (8%) 18 11	30, 91, 201, 337	0

All (476) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	G	109	GLY	14.7
8	G	110	LEU	11.7
3	A	220	HIS	8.4
8	G	156	HIS	8.1
27	2	46	ASP	8.0
13	L	53	ALA	7.8
10	I	63	ARG	7.7
1	X	248	A	7.5
21	T	16	SER	7.5
18	Q	64	ARG	7.4
8	G	111	LYS	7.3
5	C	19	LEU	7.1
13	L	12	ARG	6.9
10	I	33	GLY	6.8
28	3	14	ILE	6.7
3	A	249	PRO	6.7
21	T	14	ARG	6.6
11	J	84	MET	6.6
28	3	42	ARG	6.4
3	A	236	GLY	6.3
6	D	43	SER	6.2
3	A	250	TRP	6.2
5	C	189	ASP	6.2
3	A	244	ARG	6.2
6	D	42	SER	5.9
3	A	22	SER	5.8
10	I	100	ARG	5.7
10	I	51	GLY	5.7
3	A	242	ALA	5.6
1	X	1	G	5.6
12	K	94	TYR	5.6
5	C	47	THR	5.5

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Mol	Chain	Res	Type	RSRZ
10	I	48	PHE	5.4
3	A	237	GLU	5.4
13	L	52	ALA	5.4
5	C	166	TRP	5.4
15	N	12	ARG	5.4
13	L	97	HIS	5.3
1	X	519	C	5.3
10	I	45	LYS	5.3
16	O	36	LYS	5.3
3	A	239	ARG	5.2
1	X	1913	G	5.1
15	N	48	ARG	5.0
8	G	158	HIS	5.0
1	X	514	G	4.9
28	3	54	GLU	4.9
8	G	68	PRO	4.9
5	C	66	ASN	4.9
21	T	73	GLY	4.8
1	X	1553	G	4.8
16	O	23	GLU	4.8
2	Y	25	G	4.8
10	I	21	ARG	4.7
10	I	36	GLY	4.7
1	X	435	A	4.7
10	I	97	ARG	4.7
20	S	92	VAL	4.6
1	X	1515	U	4.6
1	X	1084	A	4.6
5	C	163	ASN	4.5
26	1	13	GLU	4.4
1	X	1073	G	4.4
1	X	1117	G	4.4
3	A	149	PRO	4.4
1	X	2385	U	4.4
5	C	44	SER	4.4
15	N	25	TRP	4.4
20	S	14	LEU	4.3
5	C	48	ARG	4.3
28	3	30	ARG	4.3
13	L	40	ALA	4.2
1	X	1523	A	4.2
3	A	91	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
22	U	46	LEU	4.2
22	U	52	ARG	4.2
3	A	55	GLY	4.2
13	L	13	THR	4.2
1	X	2780	A	4.2
1	X	1951	G	4.2
13	L	98	GLY	4.2
22	U	39	LYS	4.2
20	S	4	THR	4.1
1	X	656	U	4.1
1	X	537	C	4.1
19	R	93	ARG	4.1
9	H	28	GLY	4.1
28	3	55	TRP	4.1
4	B	135	HIS	4.1
5	C	193	LEU	4.1
11	J	27	TYR	4.0
26	1	23	THR	4.0
3	A	85	ASP	4.0
25	Z	4	HIS	4.0
7	E	17	VAL	4.0
7	E	37	TYR	4.0
1	X	1845	A	3.9
4	B	34	VAL	3.9
3	A	241	GLY	3.9
8	G	163	PRO	3.8
3	A	17	THR	3.8
22	U	62	LEU	3.8
16	O	80	TYR	3.8
13	L	33	ARG	3.8
28	3	39	ASP	3.8
26	1	47	HIS	3.8
8	G	107	GLN	3.8
4	B	155	ARG	3.8
8	G	100	TYR	3.8
28	3	40	GLU	3.8
19	R	58	VAL	3.8
9	H	27	SER	3.7
13	L	93	SER	3.7
10	I	53	ARG	3.7
6	D	38	GLU	3.7
1	X	1074	G	3.7

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Mol	Chain	Res	Type	RSRZ
7	E	174	GLY	3.7
24	W	6	VAL	3.7
3	A	188	GLU	3.7
1	X	249	A	3.6
12	K	8	ARG	3.6
1	X	1477	C	3.6
3	A	248	THR	3.6
20	S	20	ALA	3.6
7	E	65	HIS	3.6
1	X	247	A	3.6
10	I	52	GLY	3.6
6	D	117	ILE	3.6
22	U	47	HIS	3.6
1	X	1182	U	3.6
5	C	161	ALA	3.6
1	X	1687	C	3.5
5	C	20	PRO	3.5
21	T	20	TYR	3.5
1	X	1037	U	3.5
1	X	2608	A	3.5
13	L	75	LEU	3.5
28	3	31	HIS	3.5
1	X	1939	U	3.5
26	1	27	ASN	3.5
23	V	48	ARG	3.4
28	3	44	LYS	3.4
1	X	541	C	3.4
13	L	61	SER	3.4
13	L	14	ARG	3.4
13	L	18	ARG	3.4
16	O	39	PHE	3.4
1	X	911	A	3.4
1	X	2287	G	3.4
1	X	463	C	3.4
2	Y	6	C	3.4
1	X	1846	A	3.4
1	X	1937	G	3.3
6	D	72	LYS	3.3
21	T	19	LYS	3.3
13	L	62	GLY	3.3
10	I	37	GLN	3.3
7	E	123	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
15	N	94	VAL	3.3
26	1	35	LEU	3.3
7	E	5	GLY	3.2
3	A	252	LYS	3.2
10	I	28	LYS	3.2
5	C	91	TYR	3.2
10	I	64	GLY	3.2
19	R	106	VAL	3.2
5	C	180	ILE	3.1
16	O	82	ARG	3.1
1	X	2868	G	3.1
3	A	189	CYS	3.1
20	S	173	PRO	3.1
3	A	262	LYS	3.1
1	X	1588	A	3.1
1	X	1888	C	3.1
12	K	3	HIS	3.1
10	I	84	GLU	3.1
1	X	1552	C	3.1
15	N	58	ARG	3.0
1	X	2609	G	3.0
1	X	2037	A	3.0
1	X	559	C	3.0
3	A	219	PRO	3.0
25	Z	56	GLN	3.0
1	X	1847	G	3.0
9	H	20	MET	3.0
1	X	436	A	3.0
1	X	2393	G	3.0
1	X	434	C	3.0
12	K	92	GLY	3.0
19	R	27	GLY	3.0
18	Q	65	VAL	3.0
1	X	2564	U	3.0
22	U	16	ASN	2.9
1	X	774	A	2.9
10	I	13	ARG	2.9
1	X	2731	G	2.9
11	J	119	PHE	2.9
18	Q	71	GLN	2.9
28	3	64	ARG	2.9
11	J	88	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
27	2	42	LEU	2.9
16	O	34	GLU	2.9
8	G	164	GLN	2.9
9	H	56	LYS	2.9
1	X	2004	U	2.9
15	N	88	ILE	2.9
19	R	64	ASN	2.9
1	X	1469	U	2.9
20	S	135	VAL	2.9
27	2	22	MET	2.9
3	A	254	THR	2.8
22	U	8	THR	2.8
28	3	13	ARG	2.8
4	B	142	GLY	2.8
16	O	73	LYS	2.8
28	3	8	LYS	2.8
1	X	182	G	2.8
1	X	558	G	2.8
1	X	1559	G	2.8
1	X	1803	G	2.8
1	X	2781	G	2.8
19	R	46	VAL	2.8
1	X	2189	A	2.8
1	X	331	U	2.8
26	1	21	TYR	2.8
12	K	31	GLU	2.8
1	X	560	G	2.8
1	X	1410	U	2.8
10	I	98	LEU	2.7
19	R	83	LEU	2.7
3	A	148	VAL	2.7
19	R	91	ALA	2.7
1	X	1522	C	2.7
6	D	153	ASP	2.7
13	L	20	THR	2.7
2	Y	10	U	2.7
8	G	69	ASP	2.7
1	X	75	C	2.7
1	X	178	C	2.7
2	Y	7	C	2.7
3	A	259	THR	2.7
1	X	1078	A	2.7

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Mol	Chain	Res	Type	RSRZ
8	G	159	SER	2.7
10	I	39	SER	2.7
1	X	1121	G	2.7
4	B	121	ASN	2.7
21	T	15	ASP	2.6
1	X	120	G	2.6
1	X	1947	G	2.6
23	V	4	SER	2.6
10	I	99	VAL	2.6
1	X	1461	C	2.6
28	3	33	ASN	2.6
1	X	797	A	2.6
1	X	1081	A	2.6
10	I	55	ARG	2.6
3	A	186	HIS	2.6
20	S	33	ALA	2.6
6	D	41	GLY	2.6
26	1	19	GLY	2.6
28	3	62	LEU	2.6
8	G	155	THR	2.6
21	T	26	PHE	2.6
1	X	1686	A	2.6
1	X	2730	A	2.6
1	X	118	U	2.6
1	X	206	U	2.6
18	Q	67	ARG	2.6
1	X	2202	G	2.6
10	I	65	PHE	2.6
9	H	36	THR	2.6
3	A	217	ARG	2.6
16	O	40	VAL	2.6
1	X	1516	A	2.6
1	X	1934	U	2.6
3	A	238	GLY	2.6
3	A	200	GLU	2.5
1	X	1940	C	2.5
1	X	1076	U	2.5
1	X	1080	A	2.5
8	G	171	LEU	2.5
5	C	160	ALA	2.5
5	C	190	ALA	2.5
3	A	247	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	X	225	G	2.5
1	X	2529	G	2.5
2	Y	118	G	2.5
1	X	1935	A	2.5
1	X	1954	A	2.5
28	3	34	THR	2.5
26	1	40	TYR	2.5
4	B	61	LYS	2.5
17	P	19	LYS	2.5
2	Y	53	G	2.5
1	X	1044	U	2.5
1	X	305	A	2.5
1	X	1492	A	2.5
3	A	255	LYS	2.5
28	3	56	ALA	2.5
12	K	54	THR	2.5
11	J	18	MET	2.5
3	A	35	GLU	2.4
3	A	15	GLN	2.4
7	E	143	GLN	2.4
11	J	118	ALA	2.4
3	A	235	GLY	2.4
1	X	1945	C	2.4
2	Y	14	C	2.4
11	J	55	MET	2.4
11	J	72	ASP	2.4
1	X	1601	U	2.4
3	A	89	SER	2.4
1	X	333	A	2.4
1	X	343	A	2.4
1	X	1058	G	2.4
1	X	2437	G	2.4
17	P	37	LYS	2.4
6	D	94	GLU	2.4
21	T	37	LEU	2.4
26	1	24	THR	2.4
11	J	133	VAL	2.4
7	E	9	ILE	2.4
9	H	117	GLU	2.4
10	I	56	LEU	2.4
14	M	4	HIS	2.4
19	R	40	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
24	W	50	LEU	2.4
1	X	1365	U	2.4
11	J	15	ARG	2.4
1	X	1753	A	2.4
11	J	134	LYS	2.4
6	D	8	TYR	2.4
5	C	107	ALA	2.4
6	D	125	ARG	2.4
20	S	10	PRO	2.4
1	X	1936	A	2.4
15	N	92	ARG	2.4
4	B	62	PRO	2.4
22	U	48	LYS	2.4
10	I	41	SER	2.4
8	G	139	ARG	2.4
1	X	200	A	2.3
1	X	1554	G	2.3
1	X	1602	G	2.3
10	I	27	ASP	2.3
10	I	35	LYS	2.3
13	L	55	SER	2.3
22	U	29	GLY	2.3
9	H	7	ARG	2.3
1	X	346	C	2.3
1	X	2040	A	2.3
8	G	161	GLN	2.3
10	I	79	GLN	2.3
10	I	81	GLN	2.3
19	R	67	GLY	2.3
8	G	162	LYS	2.3
11	J	120	ARG	2.3
1	X	2313	G	2.3
1	X	2760	G	2.3
1	X	1556	A	2.3
1	X	1920	A	2.3
10	I	117	ALA	2.3
11	J	115	ALA	2.3
15	N	76	TYR	2.3
21	T	74	LYS	2.3
3	A	44	ASN	2.3
2	Y	58	G	2.3
7	E	33	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	386	U	2.3
8	G	106	TYR	2.3
7	E	162	VAL	2.3
8	G	102	ARG	2.3
10	I	101	ARG	2.3
22	U	34	THR	2.2
10	I	43	ALA	2.2
13	L	39	TYR	2.2
27	2	41	GLN	2.2
4	B	132	LYS	2.2
8	G	165	VAL	2.2
1	X	2283	G	2.2
7	E	38	ASN	2.2
19	R	11	ASN	2.2
1	X	922	A	2.2
3	A	93	ALA	2.2
1	X	301	C	2.2
1	X	1489	C	2.2
13	L	24	SER	2.2
5	C	39	ARG	2.2
7	E	11	VAL	2.2
11	J	140	GLU	2.2
13	L	87	VAL	2.2
16	O	8	GLY	2.2
3	A	20	ASP	2.2
18	Q	27	PHE	2.2
1	X	1478	U	2.2
1	X	464	G	2.2
1	X	1435	G	2.2
1	X	341	A	2.2
1	X	731	A	2.2
2	Y	28	A	2.2
1	X	1517	C	2.2
27	2	14	LYS	2.2
1	X	969	U	2.2
4	B	204	ALA	2.2
5	C	49	ALA	2.2
1	X	11	G	2.2
19	R	94	VAL	2.2
1	X	1524	C	2.2
6	D	121	ALA	2.1
28	3	10	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	1547	U	2.1
6	D	97	TYR	2.1
8	G	34	PRO	2.1
20	S	13	LYS	2.1
28	3	43	GLY	2.1
3	A	240	THR	2.1
19	R	88	THR	2.1
1	X	2363	G	2.1
7	E	10	ALA	2.1
1	X	1570	C	2.1
10	I	121	HIS	2.1
20	S	86	VAL	2.1
28	3	46	LYS	2.1
7	E	12	PRO	2.1
1	X	1077	U	2.1
8	G	90	LEU	2.1
3	A	48	ARG	2.1
19	R	78	ALA	2.1
26	1	32	GLN	2.1
7	E	6	LYS	2.1
1	X	1509	A	2.1
19	R	7	GLY	2.1
6	D	62	LEU	2.1
2	Y	9	G	2.1
2	Y	117	G	2.1
24	W	1	MET	2.1
5	C	7	ILE	2.1
22	U	37	ILE	2.1
4	B	152	LYS	2.1
6	D	161	LYS	2.1
8	G	93	LYS	2.1
6	D	144	ASP	2.1
10	I	42	GLY	2.1
16	O	25	LEU	2.1
11	J	106	GLU	2.1
3	A	28	ARG	2.1
26	1	2	ALA	2.1
5	C	51	VAL	2.1
3	A	147	LEU	2.1
1	X	246	C	2.1
1	X	1844	C	2.1
1	X	1432	G	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	47	GLY	2.1
17	P	22	LYS	2.1
10	I	54	SER	2.1
18	Q	90	ALA	2.1
28	3	24	ALA	2.1
13	L	63	ASN	2.1
1	X	51	A	2.0
1	X	1802	A	2.0
1	X	1921	A	2.0
12	K	101	GLY	2.0
20	S	11	LYS	2.0
13	L	89	PHE	2.0
1	X	37	C	2.0
9	H	8	LEU	2.0
1	X	424	G	2.0
1	X	734	G	2.0
11	J	78	LYS	2.0
16	O	5	ILE	2.0
19	R	90	LYS	2.0
6	D	10	ASP	2.0
16	O	37	ALA	2.0
25	Z	8	LYS	2.0
14	M	56	ALA	2.0
19	R	81	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3020	1/1	0.40	0.66	64,64,64,64	0
30	MG	X	3015	1/1	0.47	0.55	98,98,98,98	0
30	MG	X	2994	1/1	0.53	0.40	77,77,77,77	0
30	MG	X	2977	1/1	0.56	0.60	78,78,78,78	0
30	MG	X	2914	1/1	0.57	0.39	43,43,43,43	0
30	MG	X	2906	1/1	0.58	0.52	42,42,42,42	0
30	MG	X	2967	1/1	0.63	0.50	55,55,55,55	0
30	MG	X	2944	1/1	0.67	0.51	37,37,37,37	0
30	MG	X	2976	1/1	0.67	0.49	53,53,53,53	0
30	MG	X	2952	1/1	0.67	0.51	54,54,54,54	0
30	MG	X	3011	1/1	0.69	0.28	58,58,58,58	0
30	MG	X	2960	1/1	0.69	0.36	34,34,34,34	0
30	MG	X	2964	1/1	0.69	0.43	60,60,60,60	0
30	MG	X	2970	1/1	0.72	0.72	63,63,63,63	0
30	MG	X	2909	1/1	0.72	0.43	36,36,36,36	0
30	MG	X	3005	1/1	0.72	0.39	66,66,66,66	0
30	MG	X	2981	1/1	0.73	0.33	99,99,99,99	0
30	MG	X	2921	1/1	0.73	1.07	37,37,37,37	0
30	MG	X	2922	1/1	0.73	0.34	35,35,35,35	0
30	MG	X	2927	1/1	0.74	0.48	57,57,57,57	0
30	MG	X	3016	1/1	0.75	0.60	74,74,74,74	0
30	MG	X	3019	1/1	0.75	0.52	46,46,46,46	0
30	MG	X	3001	1/1	0.75	0.56	86,86,86,86	0
30	MG	X	2931	1/1	0.76	0.47	32,32,32,32	0
30	MG	X	2999	1/1	0.77	0.49	74,74,74,74	0
30	MG	X	2958	1/1	0.77	0.36	38,38,38,38	0
30	MG	X	2916	1/1	0.78	0.72	51,51,51,51	0
30	MG	X	2939	1/1	0.78	0.41	30,30,30,30	0
30	MG	X	2986	1/1	0.78	0.37	46,46,46,46	0
30	MG	X	2988	1/1	0.79	0.59	55,55,55,55	0
30	MG	M	201	1/1	0.80	0.70	35,35,35,35	0
30	MG	X	2979	1/1	0.81	0.32	46,46,46,46	0
30	MG	X	2961	1/1	0.82	0.36	68,68,68,68	0
30	MG	X	2908	1/1	0.82	0.46	34,34,34,34	0
30	MG	X	2995	1/1	0.82	0.47	83,83,83,83	0
30	MG	X	2957	1/1	0.82	0.40	42,42,42,42	0
30	MG	X	2989	1/1	0.83	0.40	56,56,56,56	0
30	MG	X	2969	1/1	0.83	0.31	43,43,43,43	0
30	MG	X	2954	1/1	0.83	0.42	41,41,41,41	0
30	MG	X	2959	1/1	0.84	0.72	54,54,54,54	0
30	MG	X	2926	1/1	0.84	0.33	32,32,32,32	0
30	MG	X	3017	1/1	0.84	0.32	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3003	1/1	0.84	0.28	63,63,63,63	0
30	MG	X	2912	1/1	0.84	0.26	34,34,34,34	0
30	MG	Y	201	1/1	0.84	0.86	77,77,77,77	0
30	MG	X	2924	1/1	0.84	0.43	30,30,30,30	0
30	MG	X	2913	1/1	0.85	0.44	36,36,36,36	0
30	MG	X	2941	1/1	0.86	0.37	55,55,55,55	0
30	MG	X	2907	1/1	0.86	0.88	49,49,49,49	0
30	MG	X	2972	1/1	0.87	0.32	36,36,36,36	0
30	MG	X	2911	1/1	0.87	0.33	46,46,46,46	0
30	MG	X	2997	1/1	0.87	0.32	38,38,38,38	0
30	MG	X	2953	1/1	0.88	0.36	38,38,38,38	0
30	MG	X	2930	1/1	0.88	0.33	46,46,46,46	0
30	MG	X	3004	1/1	0.88	0.32	54,54,54,54	0
29	6O1	X	2901	111/111	0.88	0.11	106,116,136,139	0
30	MG	X	2915	1/1	0.88	0.26	36,36,36,36	0
30	MG	X	2965	1/1	0.88	0.34	40,40,40,40	0
30	MG	X	2923	1/1	0.89	0.27	30,30,30,30	0
30	MG	X	3013	1/1	0.89	0.39	47,47,47,47	0
30	MG	X	2984	1/1	0.89	0.39	49,49,49,49	0
30	MG	X	2998	1/1	0.89	0.48	35,35,35,35	0
30	MG	X	2910	1/1	0.89	0.56	34,34,34,34	0
30	MG	X	2917	1/1	0.89	0.20	33,33,33,33	0
30	MG	X	2978	1/1	0.89	0.24	49,49,49,49	0
30	MG	X	2991	1/1	0.89	0.38	72,72,72,72	0
30	MG	X	2936	1/1	0.89	0.24	53,53,53,53	0
30	MG	X	2962	1/1	0.90	0.31	41,41,41,41	0
30	MG	X	2946	1/1	0.90	0.26	34,34,34,34	0
30	MG	X	2987	1/1	0.90	0.28	43,43,43,43	0
30	MG	X	2932	1/1	0.90	0.17	53,53,53,53	0
30	MG	X	2935	1/1	0.90	0.54	41,41,41,41	0
30	MG	X	2983	1/1	0.90	0.20	63,63,63,63	0
30	MG	X	3007	1/1	0.91	0.28	40,40,40,40	0
30	MG	X	3009	1/1	0.91	0.18	41,41,41,41	0
30	MG	X	2903	1/1	0.91	0.41	37,37,37,37	0
30	MG	X	2955	1/1	0.91	0.41	31,31,31,31	0
30	MG	X	2947	1/1	0.91	0.44	52,52,52,52	0
30	MG	X	2948	1/1	0.91	0.28	30,30,30,30	0
30	MG	X	3002	1/1	0.91	0.25	44,44,44,44	0
30	MG	X	2950	1/1	0.91	0.44	36,36,36,36	0
30	MG	X	2940	1/1	0.91	0.33	34,34,34,34	0
30	MG	X	2945	1/1	0.91	0.53	55,55,55,55	0
30	MG	X	3006	1/1	0.91	0.34	34,34,34,34	0

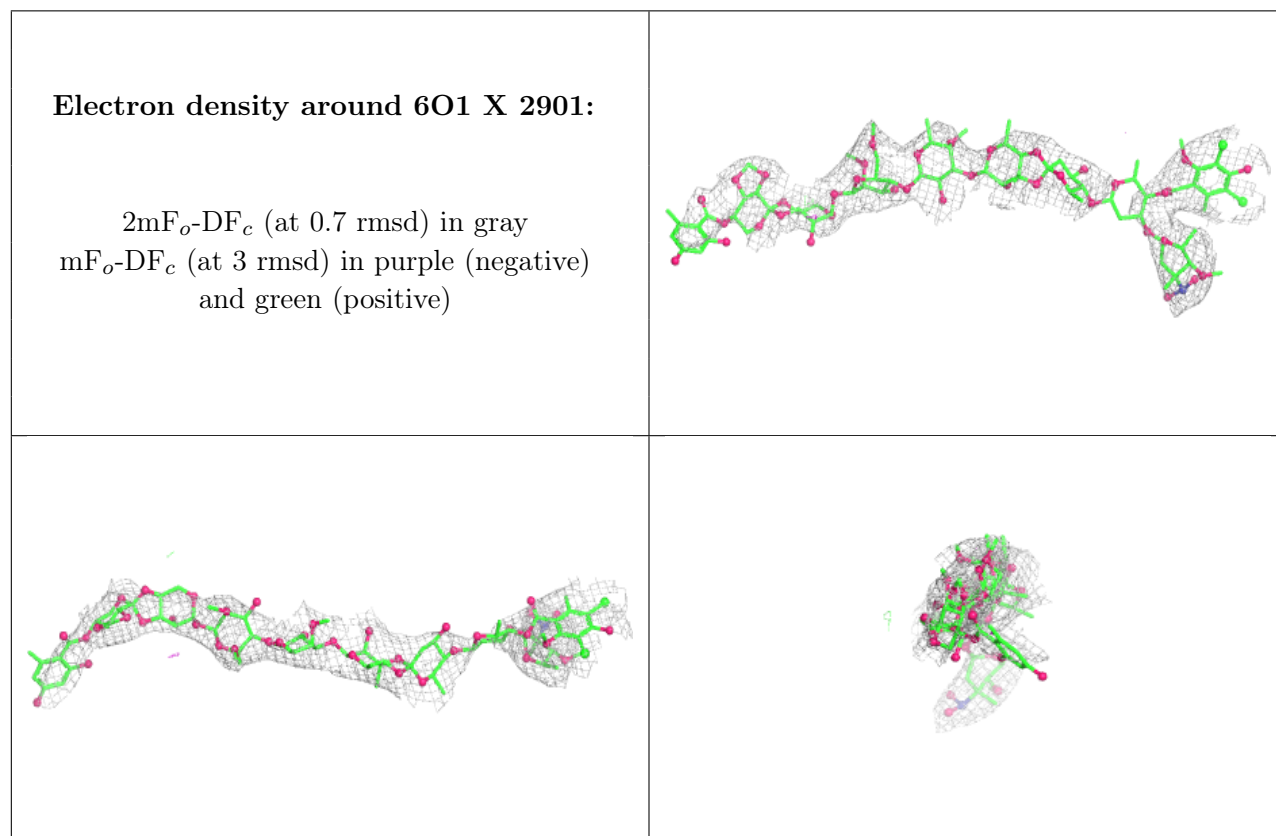
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3014	1/1	0.92	0.17	43,43,43,43	0
30	MG	X	2928	1/1	0.92	0.21	41,41,41,41	0
30	MG	X	2904	1/1	0.92	0.68	32,32,32,32	0
30	MG	X	2951	1/1	0.92	0.19	35,35,35,35	0
30	MG	X	2971	1/1	0.92	0.28	33,33,33,33	0
30	MG	X	2938	1/1	0.92	0.21	36,36,36,36	0
30	MG	X	2993	1/1	0.92	0.16	44,44,44,44	0
30	MG	K	201	1/1	0.92	0.36	31,31,31,31	0
30	MG	X	2942	1/1	0.92	0.16	31,31,31,31	0
30	MG	X	2949	1/1	0.93	0.23	32,32,32,32	0
30	MG	X	2982	1/1	0.93	0.61	31,31,31,31	0
30	MG	X	2920	1/1	0.93	0.52	34,34,34,34	0
30	MG	X	2937	1/1	0.93	0.48	32,32,32,32	0
30	MG	X	2985	1/1	0.93	0.24	55,55,55,55	0
30	MG	X	2902	1/1	0.93	0.68	32,32,32,32	0
30	MG	K	202	1/1	0.93	0.37	31,31,31,31	0
30	MG	X	2980	1/1	0.93	0.26	49,49,49,49	0
30	MG	X	2996	1/1	0.94	0.17	43,43,43,43	0
30	MG	X	2918	1/1	0.94	0.34	45,45,45,45	0
30	MG	X	2990	1/1	0.94	0.39	39,39,39,39	0
30	MG	X	2925	1/1	0.94	0.45	43,43,43,43	0
30	MG	X	2919	1/1	0.95	0.14	33,33,33,33	0
30	MG	X	2943	1/1	0.95	0.17	33,33,33,33	0
30	MG	X	3000	1/1	0.95	0.10	39,39,39,39	0
30	MG	X	3018	1/1	0.95	0.23	32,32,32,32	0
30	MG	X	2974	1/1	0.95	0.48	30,30,30,30	0
30	MG	X	3010	1/1	0.95	0.21	41,41,41,41	0
30	MG	X	2934	1/1	0.95	0.56	39,39,39,39	0
30	MG	X	3012	1/1	0.95	0.31	52,52,52,52	0
30	MG	X	2905	1/1	0.95	0.47	30,30,30,30	0
30	MG	X	2963	1/1	0.95	0.35	71,71,71,71	0
30	MG	X	2956	1/1	0.96	0.36	32,32,32,32	0
30	MG	X	3008	1/1	0.96	0.75	39,39,39,39	0
30	MG	X	2929	1/1	0.96	0.56	39,39,39,39	0
30	MG	X	2933	1/1	0.97	0.49	38,38,38,38	0
30	MG	X	2975	1/1	0.97	0.81	49,49,49,49	0
30	MG	X	2992	1/1	0.97	0.59	34,34,34,34	0
30	MG	X	2968	1/1	0.97	0.15	35,35,35,35	0
30	MG	X	2966	1/1	0.97	0.24	37,37,37,37	0
30	MG	X	2973	1/1	0.98	0.17	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.