Full wwPDB EM Validation Report (i)

Nov 13, 2022 – 10:05 AM EST

PDB ID	:	6WRU
EMDB ID	:	EMD-21888
Title	:	Structure of the 50S subunit of the ribosome from Methicillin Resistant Staphylococcus aureus in complex with an isomer of the tedizolid
Authors	:	Belousoff, M.J.
Deposited on	:	2020-04-30
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

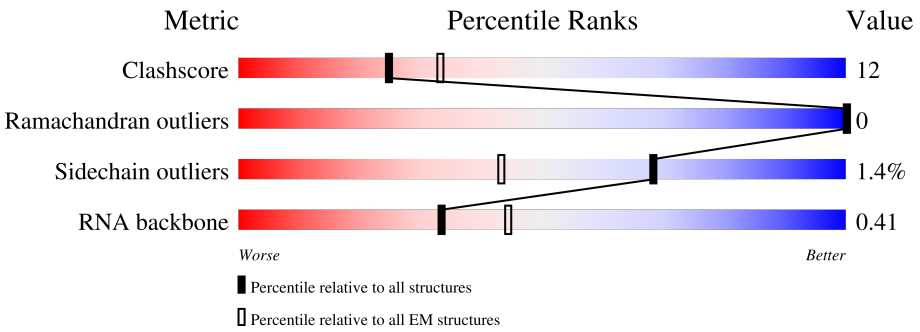
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	116	67% 28% • •
2	B	277	69% 30% •
3	C	118	73% 23% • •
4	D	105	72% 23% 5%
5	E	117	70% 24% • 5%
6	F	91	60% 35% •
7	G	105	43% 42% 15%

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Mol	Chain	Length	Quality of chain
8	H	107	52% 45% 42% 13%
9	J	62	71% 24% 5%
10	K	72	51% 29% 19%
11	L	217	77% 22%
12	M	58	72% 22%
13	N	57	72% 16% 12%
14	O	49	59% 37%
15	P	50	72% 16% 12%
16	Q	65	66% 32%
17	R	37	76% 24%
18	S	207	66% 27% 7%
19	U	175	66% 33%
20	V	145	70% 28%
21	W	122	63% 35%
22	X	146	71% 27%
23	Y	144	72% 23% 6%
24	Z	122	72% 21% 7%
25	a	119	97%
26	1	2923	42% 33% 15% 9%
27	2	115	38% 41% 17%
28	I	85	74% 16% 8%

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 81707 atoms, of which 14 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	113	915	576	184	155	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	275	2103	1309	417	372	5	0	0

- Molecule 3 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	116	943	593	189	157	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	100	785	499	139	146	1	0	0

- Molecule 5 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	111	853	532	163	155	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	110	ALA	GLY	variant	UNP A0A077UKF9

- Molecule 6 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	87	711	447	128	132	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	87	ASP	ILE	variant	UNP W8TUB4

- Molecule 7 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	89	689	437	126	125	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	54	SER	GLY	variant	UNP W8TRD5

- Molecule 8 is a protein called uL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	93	727	465	129	132	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	59	463	287	99	76	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	62	ALA	-	insertion	UNP A0A077URJ8

- Molecule 10 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	K	58	481	296	92	93	0	0

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	215	1628	1018	299	306	5	0	0

- Molecule 12 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	M	56	432	269	82	81	0	0

- Molecule 13 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	50	397	241	83	68	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	54	ALA	VAL	variant	UNP A0A077UWR7

- Molecule 14 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	47	390	233	79	73	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	44	372	228	90	53	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L35.

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

- Molecule 17 is a protein called 50S ribosomal protein L36.

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

- Molecule 18 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	192	1472	924	271	275	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	174	1360	845	249	263	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	18	SER	THR	variant	UNP W8U3X2

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	143	1138	710	209	217	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	121	911	566	173	168	4	0	0

- Molecule 22 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	X	144	1082	669	213	200	0	0

- Molecule 23 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	136	1089	698	206	181	4	0	0

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	114	899	554	175	169	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	a	116	899	560	171	168	0	0

- Molecule 26 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	1	2665	57132	25513	10463	18496	2660	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1866	A	G	conflict	GB 1760383645

- Molecule 27 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
27	2	112	2381	1066	427	777	111	0	0

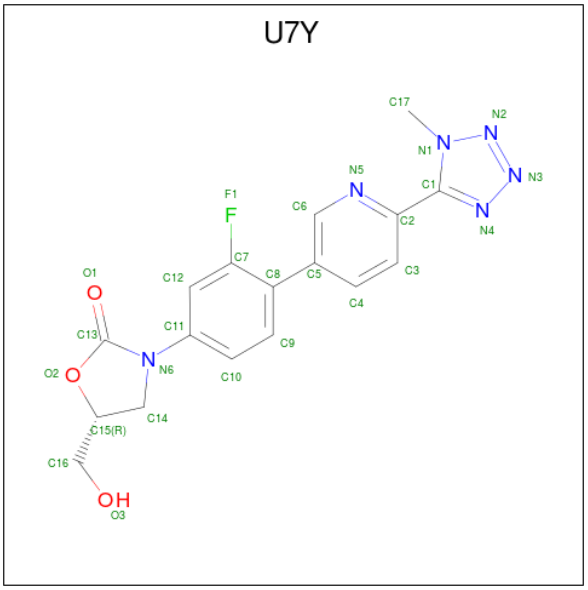
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	80	C	G	variant	GB 1750990749
2	109	C	G	variant	GB 1750990749
2	111	A	C	variant	GB 1750990749
2	112	G	A	variant	GB 1750990749

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	I	78	597	367	116	114	0	0

- Molecule 29 is Tedizolid isomer (three-letter code: U7Y) (formula: $C_{17}H_{15}FN_6O_3$) (labeled as "Ligand of Interest" by depositor).



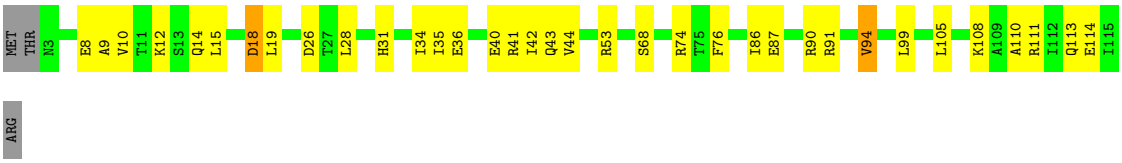
Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	H	N	O	
29	1	1	41	17	1	14	6	3	0

3 Residue-property plots (i)

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

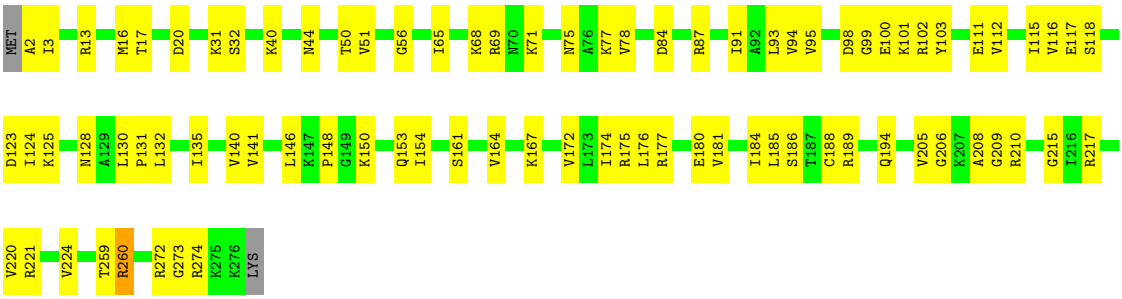
• Molecule 1: 50S ribosomal protein L19

Chain A:



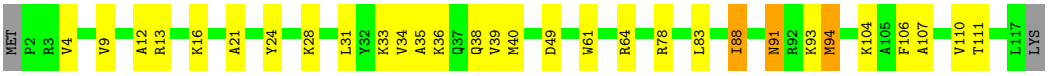
• Molecule 2: 50S ribosomal protein L2

Chain B:



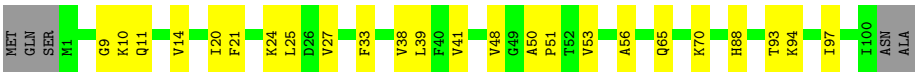
• Molecule 3: 50S ribosomal protein L20

Chain C:



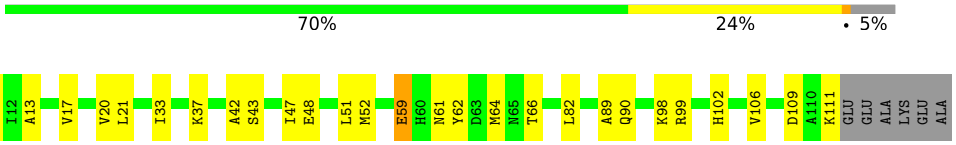
• Molecule 4: 50S ribosomal protein L21

Chain D:



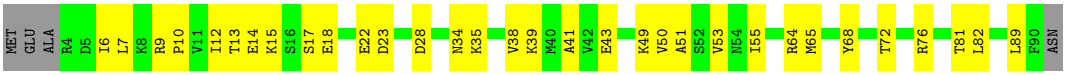
- Molecule 5: 50S ribosomal protein L22

Chain E:



- Molecule 6: 50S ribosomal protein L23

Chain F:

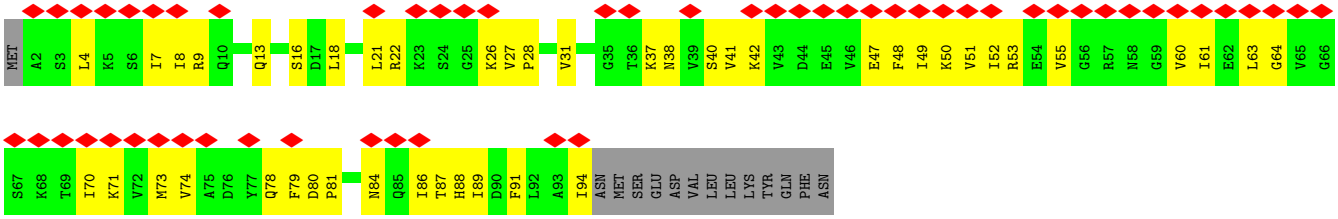


- Molecule 7: 50S ribosomal protein L24

Chain G:

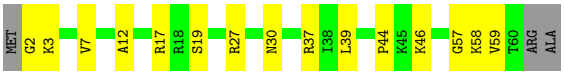
- Molecule 8: uL25

Chain H:



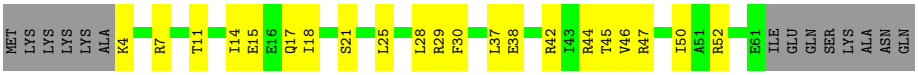
- Molecule 9: 50S ribosomal protein L28

Chain J:



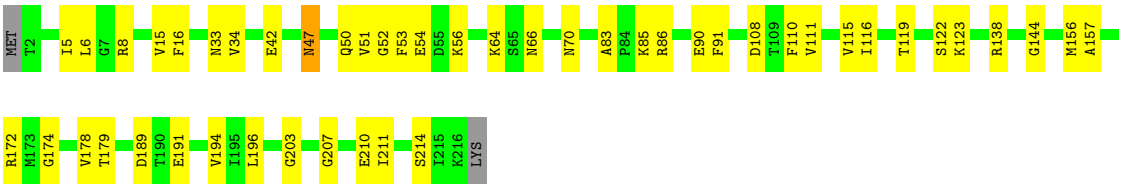
- Molecule 10: 50S ribosomal protein L29

Chain K:



- Molecule 11: 50S ribosomal protein L3

Chain L: 77% 22%

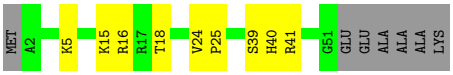


- Molecule 12: 50S ribosomal protein L30

Chain M: 72% 22%

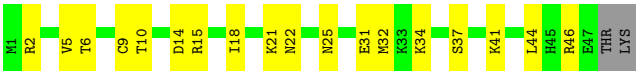
- Molecule 13: 50S ribosomal protein L32

Chain N: 72% 16% 12%



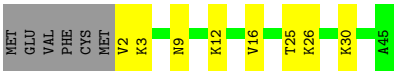
- Molecule 14: 50S ribosomal protein L33

Chain O: 59% 37%



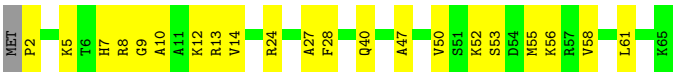
- Molecule 15: 50S ribosomal protein L34

Chain P: 72% 16% 12%



- Molecule 16: 50S ribosomal protein L35

Chain Q: 66% 32%



- Molecule 17: 50S ribosomal protein L36

Chain R: 76% 24%

- Molecule 18: 50S ribosomal protein L4

Chain S: 66% 27% 7%

MET ALA ASN TYR ASP VAL LEU LYS LEU ASP GLY THR LYS SER GLY S16 I17 E18 L19 I37 Q46 V51 K52 N53 V57 K66 Q67 K68 R74 T77 I88 V89 F90 G91 R95 R106 R107 E120 L123 E132 F139 E147 Q148 P149 K150

K151 V152 L153 V154 V155 T156 E157 N158 E159 D160 V161 E164 L165 S166 A167 R168 V173 T176 T177 A178 Q179 N182 V183 L184 T187 N188 I194 T195 E196 A197 A198 A199 K200 K201 V202 L206 G207

- Molecule 19: 50S ribosomal protein L6

Chain U: 66% 33% ••

MET S2 R3 V4 K7 I8 I9 V17 S18 F19 V24 T25 V26 K27 G28 R35 R40 M41 T42 F43 K44 Q45 E46 E47 N48 T49 I50 E51 V52 V53 S56 D57 S58 K59 R62 T63 R69 A70 L71 L72 M75 V76 Q77 G78 V79 S80 Y83 V90

A96 Q97 N98 Q99 L103 V107 E114 I115 I121 V125 E126 K127 E139 L144 I148 R149 E155 K158 R163 Y164 Q165 Y168 K175

- Molecule 20: 50S ribosomal protein L13

Chain V: 70% 28% ••

MET R2 Q3 T4 N8 E9 S10 N11 R14 V18 I19 E22 L26 V33 I36 L37 R38 G39 K40 H48 V49 G52 V57 A60 S61 K62 I63 E64 F65 K73 V74 Y75 S79 N80 S87 A90 E99 R100 L101 I102 E103 I106

P111 S112 T113 G116 Y126 H133 E139 N140 Y141 R144 GLY

- Molecule 21: 50S ribosomal protein L14

Chain W: 63% 35% ••

M1 I2 Q3 Q4 E5 L8 D12 N13 S14 R17 V24 S28 K31 T32 A33 N34 I35 C41 T42 V43 K44 N45 A46 T47 K54 V58 V61 I62 V63 R64 T65 K66 S67 G68 R71 N72 D73 I77 N82 V85 I86 I87 K91 R97

I98 F99 G100 P101 V102 A103 R104 E108 G109 N110 F111 M112 V115 V121 LEU

- Molecule 22: 50S ribosomal protein L15

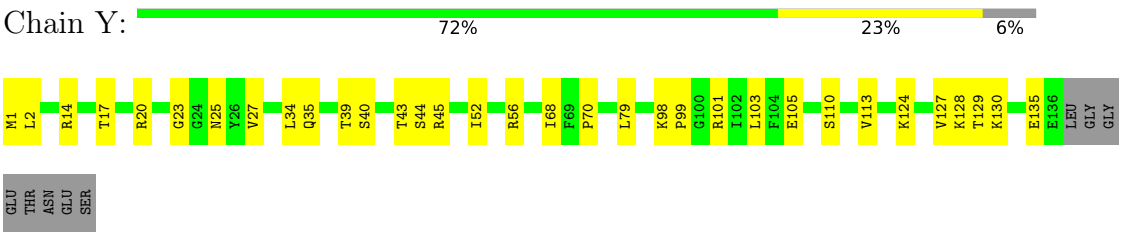
Chain X: 71% 27% •

MET K2 L3 K14 E15 G22 N27 G28 K29 T30 S31 G32 R33 F50 E51 G52 G53 Q54 R60 N68 I69 E73 N78 L79 N83 V91 T92 P93 A94 L95 L96 V97 E98 K103 S107 G108 I109 K110 N114 D118 K119 H126 K127 F128

A135 K139 H143 E144 V145 ILE

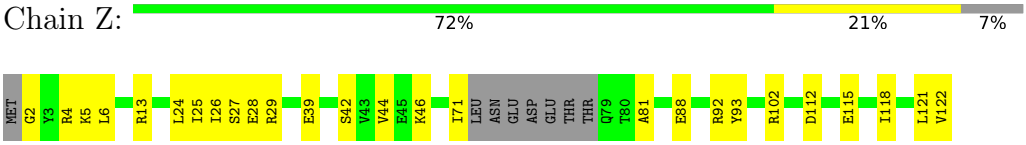
- Molecule 23: 50S ribosomal protein L16

Chain Y:



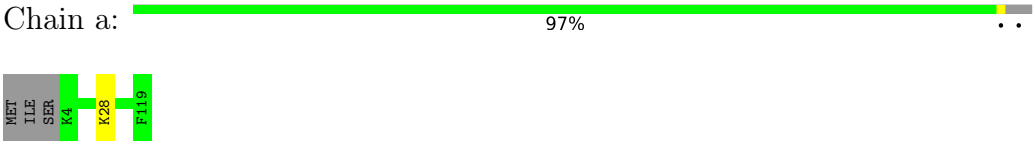
- Molecule 24: 50S ribosomal protein L17

Chain Z:



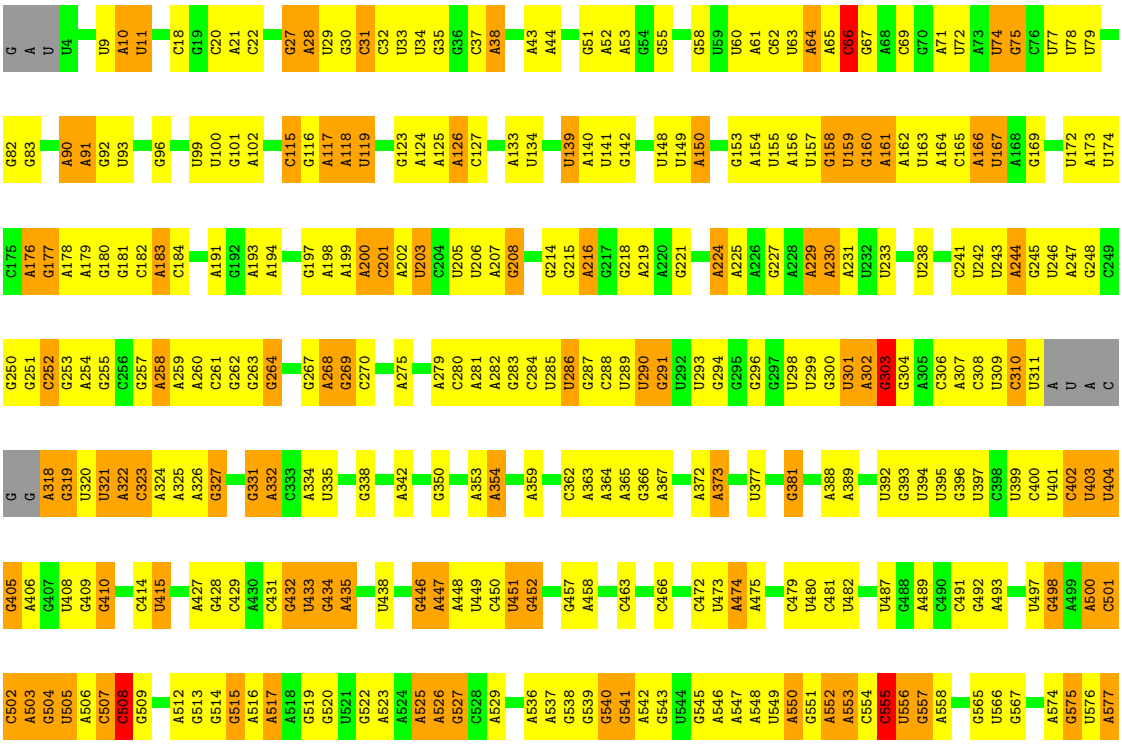
- Molecule 25: 50S ribosomal protein L18

Chain a:

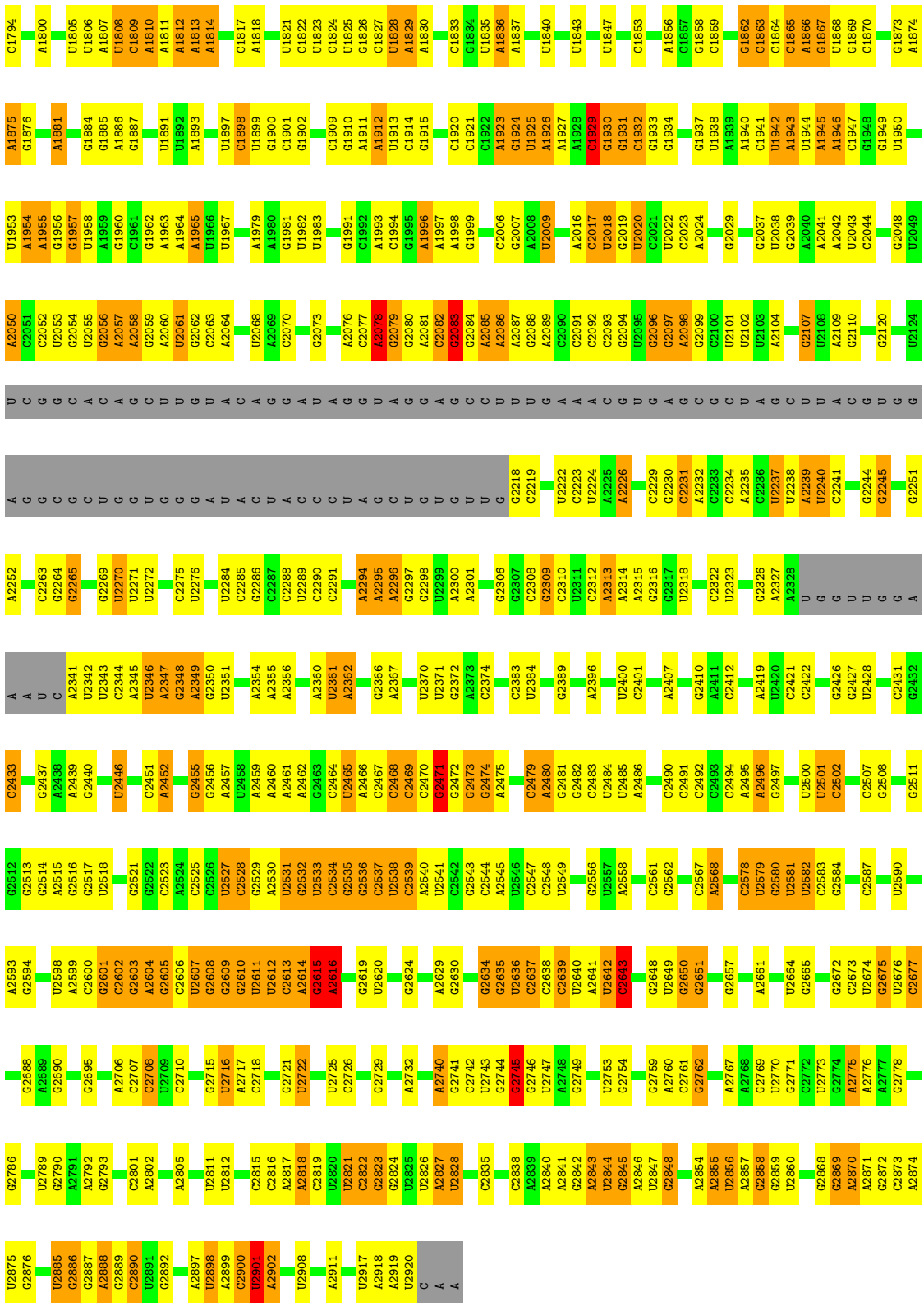


- Molecule 26: 23S rRNA

Chain 1:

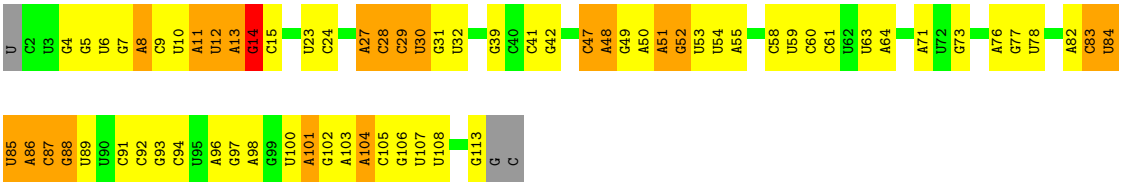


C1716 G1717 G1718 C1719 A1720 A1721 A1722 A1723 U1724 G1725 A1726 C1727 C1730 U1737 C1738 G1739 G1740 G1741 A1742 A1745 G1746 G1749 U1750 G1751 C1752 U1756 U1757 A1758 G1759 G1760 G1761 U1762 U A A C G C1768 C1769 G1772 A1773 A1774 G1780 C1781 A1782 G1783 A1788 A1789 G1790 G1791 C1792 C1793
U A G1638 G1639 U1640 G1645 U1646 A1647 G1650 C1651 A1652 A1653 A1654 C1655 A1660 G1663 G1664 U1665 A1666 G1667 U1668 C1669 U1674 G1675 A1676 G1677 A1678 A1679 U1680 U1681 C1682 U1683 A1684 A1685 G1686 A1690 G1691 C1692 G1693 C1696 G1697 A1698 A1699 U1703 A1709 G1710 G1711 A1712 A1713 C1714 U1715
G1566 A1567 U1568 G1569 G1570 G1571 G1572 A1573 G1574 A1575 A1576 G1577 A1578 C1579 A1580 U1581 U1582 G1583 U1584 G1585 U1586 C1587 U1588 U1589 C1590 G1591 A1592 G1593 U1594 C1595 G1596 U1597 U1598 G1599 A1600 U1601 A1605 C1606 C1612 G1613 A1614 G1615 A1616 A1617 A1618 C1624 U1625 A1626 G1627 A U A G A A A G1556 C1557 U1558 G1559 A1560 G1561 C1562 U1563 G1564 U1565
U1504 G1505 C1506 A1507 C1508 G1509 U1510 C1511 U1512 A1513 A1514 G1515 C1516 A1517 G1518 U1519 A1520 A1521 G1522 G1523 C U U G A G U A U U A A A G U U C G U U U A A1459 G1462 A1463 U1464 G1469 G1470 A1471 C1472 G1476 U1477 A1478 G1479 G1480 A1481 U1482 A1483 G1484 G1485 C1486 G1487 A1488 A1489 G1490 C1491 G1492 U1493 A1497 U1498 U1499 G1500 G1501 A1502 U1503
U1428 G1429 A1430 U1431 A1432 U1433 U1434 A1443 C1444 A1447 U1448 A A U C G U U U A A1459 G1462 A1463 U1464 G1469 G1470 A1471 C1472 G1476 U1477 A1478 G1479 G1480 A1481 U1482 A1483 G1484 G1485 C1486 G1487 A1488 A1489 G1490 C1491 G1492 U1493 A1497 U1498 U1499 G1500 G1501 A1502 U1503
G1329 U1330 G1336 A1337 U1338 U1339 U1343 A1344 A1345 G1346 G1347 U1348 U1349 U1350 C1351 C1352 A1353 G1354 A1355 G1356 G1357 A1358 A1359 G1360 G1361 C1364 G1365 U1366 G1375 U1378 A1379 G1380 U1389 A1390 A1391 G1401 A1402 C1403 A1404 G1405 G1414 A1415 U1416 A1421 A1422 C1423 A1424 G1425 G1426 U1427
A1231 G1232 U1238 A1241 A1242 G1245 C1246 A1251 A1252 G1253 C1254 G1257 A1258 A1263 U1272 G1273 G1274 A1275 G1276 C1277 G1278 A1285 G1286 U1287 G1288 A1289 G1290 A1291 A1292 U1293 G1294 C1295 G1300 A1303 G1304 U1305 A1306 G1307 C1308 G1309 A1310 A1311 A1312 G1313 G1320 A1323 A1324 U1325
A G1156 A1159 C1160 G1166 C1167 C1168 G1169 A1170 A1171 A1172 A1173 U1176 A1177 C1178 C1179 U1185 A1186 A1187 A1188 C1189 A1190 U1191 A1195 C1196 C1197 G1201 C1202 U1203 G1207 A1208 U1209 U1210 G1211 U1212 C1213 C1214 U1215 U1216 U1217 G1218 G1219 A1220 C1221 A1222 A1223 U1224 G1225 G1226 U1227 A1228 G1229 G1230
A C U A G G A U U G U U C C A A G C A G C C A U C A U U U A A U U A G C G U A A G G A U C A C U C A C G A A G A C A
A1001 U1002 A1003 A1004 G1005 U1013 U1014 A1018 A1024 A1025 C1026 A1027 G1028 C1029 A1040 A1044 A1045 C1051 A1055 U1056 A1057 U1058 A1059 U1063 A1064 A1065 G1066 U1067 G1068 G1069 A1070 A1071 A1072 A1073 G1074 U1077 G1078 U1079 G1083 U1084 U1085 G1086 C1087 C1088 C A G A C A
G G G G C C C U C U C G G G U U A C C G A A U U948 C949 A950 G951 A955 A962 A963 U964 G965 C966 C967 A968 A969 U970 U971 A972 A973 U974 U975 U976 A977 G982 G983 G984 A985 A989 G990 A991 A992 U999 G1000
C831 C832 A833 A834 U835 C836 G837 A838 A839 G846 A847 U848 A849 G850 G854 U855 U856 C857 U858 C859 C870 U871 U872 U873 G877 C878 C883 G888 U889 G890 A891 U892 G893 A894 U895 U896 A897 U898 U899 G900 G901 A902 G903 G904 U905 G909 C910 A911 A920 C921 G A
G749 A750 A751 G752 U753 U754 C755 A756 G757 A760 A761 C762 A763 C764 U765 A768 A772 G773 G774 A775 G778 C781 U787 A788 U791 U792 G793 A794 A795 A796 A797 A801 G802 G805 A806 U807 G808 A809 A819 G820 C821 G822 G823 A824 G825 A826 A827 A828 U829 U830
G665 A666 G667 C668 A672 G673 C674 G675 A678 G679 C680 G681 A682 G683 U684 C685 U686 G687 A688 A689 U690 A691 G692 G693 G694 C695 G696 U697 U698 U699 A700 G701 U702 A703 U704 U705 U712 G719 A720 A721 A722 C723 C724 A730 U731 C732 U738 U739 A744 G745 G746 U747 U748
G578 U579 A583 C587 G588 U589 U590 A591 A592 U593 G594 U597 G598 A599 U600 G604 U605 G606 G613 U614 A615 G616 A617 A618 U619 G620 A621 A622 C623 A629 G630 U631 U632 A633 A646 G647 G648 U649 U650 A651 A652 G653 C654 A655 G656 U657 A658 A659 A660 U661 G662 U663 G664



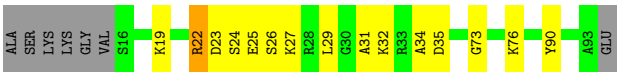
- Molecule 27: 5S rRNA

Chain 2: 38% 41% 17%



• Molecule 28: 50S ribosomal protein L27

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	11.419	Depositor
Minimum map value	-7.604	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.292	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	419.04, 419.04, 419.04	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: U7Y

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	A	0.47	0/927	0.59	0/1239
2	B	0.48	0/2138	0.55	0/2869
3	C	0.56	0/955	0.58	0/1265
4	D	0.45	0/795	0.55	0/1062
5	E	0.44	0/861	0.58	0/1159
6	F	0.45	0/719	0.57	0/959
7	G	0.36	0/695	0.48	0/926
8	H	0.28	0/735	0.45	0/986
9	J	0.42	0/469	0.52	0/625
10	K	0.47	0/482	0.58	0/642
11	L	0.53	0/1652	0.64	0/2216
12	M	0.58	0/434	0.64	0/585
13	N	0.50	0/404	0.53	0/537
14	O	0.39	0/393	0.54	0/523
15	P	0.53	0/376	0.56	0/491
16	Q	0.50	0/526	0.55	0/690
17	R	0.43	0/299	0.54	0/393
18	S	0.47	0/1494	0.58	0/2018
19	U	0.37	0/1378	0.53	0/1853
20	V	0.50	0/1160	0.54	0/1563
21	W	0.48	0/918	0.58	0/1232
22	X	0.45	0/1096	0.56	0/1461
23	Y	0.47	0/1113	0.52	0/1493
24	Z	0.46	0/902	0.55	0/1202
25	a	0.37	0/908	0.50	0/1215
26	1	0.84	0/63978	1.00	90/99764 (0.1%)
27	2	0.57	0/2662	0.95	1/4146 (0.0%)
28	I	0.53	0/603	0.60	0/801
All	All	0.75	0/89072	0.92	91/133915 (0.1%)

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	2902	A	N9-C1'-C2'	-8.91	102.20	112.00
26	1	2539	C	N1-C1'-C2'	-8.10	103.09	112.00
26	1	1522	G	C4'-C3'-O3'	7.63	128.25	113.00
26	1	675	G	N9-C1'-C2'	-7.37	103.89	112.00
26	1	167	U	N1-C1'-C2'	-7.19	104.09	112.00
26	1	1522	G	N9-C1'-C2'	-7.19	104.09	112.00
26	1	513	G	N9-C1'-C2'	-7.15	104.13	112.00
26	1	2643	C	C4'-C3'-O3'	7.12	127.25	113.00
26	1	2245	G	N9-C1'-C2'	-6.83	104.49	112.00
26	1	831	C	C1'-C2'-O2'	-6.78	90.28	110.60
26	1	1391	A	N9-C1'-C2'	-6.62	104.72	112.00
26	1	2745	G	C4'-C3'-O3'	6.57	126.13	113.00
26	1	1275	A	C2'-C3'-O3'	-6.55	95.08	109.50
26	1	1225	G	N9-C1'-C2'	-6.54	104.81	112.00
26	1	303	G	C4'-C3'-O3'	6.49	125.97	113.00
26	1	2245	G	C4'-C3'-O3'	6.45	125.91	113.00
26	1	652	A	N9-C1'-C2'	-6.44	104.91	112.00
26	1	831	C	C4'-C3'-O3'	6.44	125.88	113.00
26	1	1225	G	C4'-C3'-O3'	6.40	125.80	113.00
26	1	2745	G	N9-C1'-C2'	-6.39	104.97	112.00
26	1	2619	G	N3-C4-N9	6.31	129.78	126.00
26	1	1576	A	C4'-C3'-O3'	6.24	125.48	113.00
26	1	327	G	N9-C1'-C2'	-6.15	105.23	112.00
26	1	1230	G	C4'-C3'-O3'	6.11	125.22	113.00
26	1	2651	G	C4'-C3'-O3'	6.09	125.18	113.00
26	1	1167	C	C4'-C3'-O3'	6.09	125.17	113.00
26	1	31	C	C4'-C3'-O3'	6.05	125.11	113.00
26	1	1493	U	C4'-C3'-O3'	6.01	125.02	113.00
26	1	2079	G	N9-C1'-C2'	-5.96	105.44	112.00
26	1	2616	A	N9-C1'-C2'	-5.95	105.46	112.00
26	1	723	C	C4'-C3'-O3'	5.90	124.81	113.00
26	1	739	U	N1-C1'-C2'	-5.90	105.51	112.00
26	1	203	U	N1-C1'-C2'	-5.90	105.51	112.00
26	1	500	A	P-O3'-C3'	5.83	126.70	119.70
26	1	203	U	C4'-C3'-O3'	5.83	124.67	113.00
26	1	1547	C	C4'-C3'-O3'	5.80	124.61	113.00
26	1	668	C	C4'-C3'-O3'	5.79	124.58	113.00
26	1	2539	C	C4'-C3'-O3'	5.75	124.50	113.00
26	1	2078	A	C4'-C3'-O3'	-5.75	97.33	109.40
26	1	2902	A	C4'-C3'-O3'	5.72	124.43	113.00
26	1	2538	U	N1-C1'-C2'	-5.66	105.78	112.00
26	1	513	G	C4'-C3'-O3'	5.66	124.31	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	1230	G	N9-C1'-C2'	-5.65	105.78	112.00
26	1	2722	U	N1-C1'-C2'	-5.64	105.80	112.00
26	1	224	A	P-O3'-C3'	5.63	126.45	119.70
26	1	2538	U	C4'-C3'-O3'	5.62	124.25	113.00
26	1	1188	A	C4'-C3'-O3'	5.58	124.16	113.00
26	1	2643	C	N1-C1'-C2'	-5.58	105.86	112.00
26	1	31	C	N1-C1'-C2'	-5.58	105.86	112.00
26	1	831	C	N1-C1'-C2'	-5.56	105.89	112.00
26	1	2858	G	C4'-C3'-O3'	5.55	124.10	113.00
26	1	1722	A	N9-C1'-C2'	-5.55	105.90	112.00
26	1	264	G	N9-C1'-C2'	-5.54	105.90	112.00
26	1	31	C	C1'-C2'-O2'	-5.53	94.01	110.60
26	1	1167	C	N1-C1'-C2'	-5.53	105.92	112.00
26	1	723	C	N1-C1'-C2'	-5.43	106.03	112.00
26	1	897	A	N9-C1'-C2'	-5.42	106.04	112.00
26	1	2901	U	C4'-C3'-O3'	5.39	123.78	113.00
26	1	224	A	C2'-C3'-O3'	-5.38	97.65	109.50
26	1	683	G	N9-C1'-C2'	-5.38	106.09	112.00
26	1	1510	U	C2'-C3'-O3'	5.36	122.28	113.70
26	1	2858	G	N9-C1'-C2'	-5.33	106.14	112.00
26	1	303	G	N9-C1'-C2'	-5.31	106.16	112.00
26	1	2615	G	N9-C1'-C2'	-5.31	106.16	112.00
26	1	650	U	N1-C1'-C2'	-5.30	106.17	112.00
26	1	745	G	N9-C1'-C2'	-5.29	106.19	112.00
26	1	1722	A	C4'-C3'-O3'	5.28	123.56	113.00
26	1	666	A	N9-C1'-C2'	-5.27	106.21	112.00
26	1	858	U	N1-C1'-C2'	-5.25	106.22	112.00
26	1	1929	C	N1-C1'-C2'	-5.23	106.24	112.00
26	1	1867	G	C4'-C3'-O3'	5.23	123.46	113.00
26	1	1275	A	P-O3'-C3'	5.23	125.97	119.70
26	1	66	C	C4'-C3'-O3'	5.21	123.42	113.00
26	1	1521	A	N9-C1'-C2'	-5.21	106.27	112.00
26	1	415	U	N1-C1'-C2'	-5.21	106.27	112.00
26	1	1252	A	N9-C1'-C2'	-5.18	106.30	112.00
26	1	1203	U	N1-C1'-C2'	-5.17	106.31	112.00
26	1	2651	G	N9-C1'-C2'	-5.16	106.32	112.00
26	1	675	G	C4'-C3'-O3'	5.14	123.29	113.00
26	1	2471	G	N9-C1'-C2'	-5.12	106.36	112.00
26	1	2080	G	N9-C1'-C2'	-5.12	106.37	112.00
26	1	1867	G	N9-C1'-C2'	-5.12	106.37	112.00
26	1	2083	G	N9-C1'-C2'	-5.11	106.38	112.00
26	1	555	C	N1-C1'-C2'	-5.11	106.38	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	1391	A	C4'-C3'-O3'	5.09	123.17	113.00
26	1	264	G	C4'-C3'-O3'	5.06	123.11	113.00
26	1	1510	U	C4'-C3'-O3'	-5.05	98.80	109.40
26	1	1254	C	N1-C1'-C2'	-5.03	106.47	112.00
26	1	1547	C	N1-C1'-C2'	-5.01	106.49	112.00
26	1	508	C	C4'-C3'-O3'	5.01	123.01	113.00
27	2	14	G	N9-C1'-C2'	-5.00	106.50	112.00

There are no chirality outliers.

There are no planarity outliers.

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	A	915	0	987	30	0
2	B	2103	0	2218	74	0
3	C	943	0	1014	24	0
4	D	785	0	825	21	0
5	E	853	0	912	21	0
6	F	711	0	743	23	0
7	G	689	0	748	36	0
8	H	727	0	777	46	0
9	J	463	0	501	11	0
10	K	481	0	508	15	0
11	L	1628	0	1667	38	0
12	M	432	0	472	11	0
13	N	397	0	407	7	0
14	O	390	0	396	19	0
15	P	372	0	420	6	0
16	Q	521	0	586	14	0
17	R	296	0	340	5	0
18	S	1472	0	1520	48	0
19	U	1360	0	1390	54	0
20	V	1138	0	1130	30	0
21	W	911	0	970	38	0
22	X	1082	0	1119	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Y	1089	0	1155	25	0
24	Z	899	0	954	22	0
25	a	899	0	940	0	0
26	1	57132	0	28744	938	0
27	2	2381	0	1209	41	0
28	I	597	0	607	12	0
29	1	27	14	0	1	0
All	All	81693	14	53259	1522	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1522) 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)
26:1:275:A:H62	26:1:296:G:N2	1.53	1.05
10:K:17:GLN:O	10:K:21:SER:HB2	1.59	1.03
26:1:699:U:H4'	26:1:700:A:H5'	1.43	1.00
2:B:95:VAL:HG22	2:B:101:LYS:HG2	1.44	0.98
4:D:65:GLN:HG3	4:D:93:THR:HG22	1.46	0.95
26:1:828:A:N3	26:1:828:A:H2'	1.80	0.93
26:1:275:A:H62	26:1:296:G:H21	1.18	0.92
18:S:150:LYS:H	18:S:150:LYS:HD2	1.32	0.91
27:2:54:U:H4'	27:2:55:A:H5'	1.54	0.89
2:B:117:GLU:HB2	2:B:130:LEU:HD22	1.55	0.89
26:1:1713:A:N3	26:1:1713:A:H2'	1.87	0.87
26:1:322:A:H2'	26:1:322:A:N3	1.89	0.87
26:1:2821:U:H1'	26:1:2822:C:H5"	1.55	0.86
8:H:73:MET:HB3	8:H:94:ILE:HD11	1.58	0.85
26:1:2534:C:H2'	26:1:2535:G:C8	2.12	0.85
22:X:69:ILE:HD13	26:1:2433:C:H1'	1.59	0.84
26:1:721:A:H8	26:1:2096:G:H21	1.24	0.83
8:H:27:VAL:HG21	8:H:86:ILE:HG13	1.60	0.82
19:U:72:LEU:HD23	19:U:75:MET:HE3	1.61	0.82
26:1:1518:G:H1	26:1:1562:C:H42	1.26	0.82
19:U:17:VAL:HG22	19:U:26:VAL:HG22	1.61	0.82
26:1:1582:U:H5"	26:1:1583:G:H5"	1.62	0.82
26:1:1484:G:H1	26:1:1599:G:H22	1.25	0.81
11:L:123:LYS:HE3	11:L:174:GLY:HA2	1.62	0.81
26:1:64:A:N3	26:1:64:A:H2'	1.94	0.81
18:S:155:VAL:HB	18:S:194:ILE:HG22	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1759:G:H3'	26:1:1760:G:H5"	1.65	0.79
26:1:501:C:H2'	26:1:502:C:H5'	1.63	0.79
26:1:275:A:N6	26:1:296:G:H21	1.79	0.79
26:1:1513:A:H2'	26:1:1514:A:C8	2.19	0.78
26:1:289:U:H5"	26:1:290:U:H5'	1.65	0.78
26:1:1227:U:H2'	26:1:1228:A:H8	1.49	0.78
26:1:2614:A:O2'	26:1:2615:G:H5'	1.84	0.78
26:1:2610:G:H2'	26:1:2611:U:C6	2.19	0.78
26:1:1581:U:H5"	26:1:1583:G:H4'	1.66	0.78
26:1:1488:A:H2'	26:1:1489:A:C8	2.19	0.77
26:1:2479:C:H2'	26:1:2480:A:C8	2.18	0.77
26:1:2615:G:O2'	26:1:2616:A:H5'	1.83	0.77
26:1:903:G:HO2'	26:1:2295:A:HO2'	1.30	0.77
1:A:105:LEU:HB3	1:A:110:ALA:HB2	1.67	0.77
26:1:66:C:H2'	26:1:67:G:H8	1.48	0.77
26:1:2507:C:H2'	26:1:2508:G:H5'	1.67	0.77
26:1:2582:U:O2	26:1:2582:U:H2'	1.86	0.76
26:1:1169:G:OP2	26:1:1170:A:O2'	2.03	0.76
26:1:1722:A:H2'	26:1:1723:A:H8	1.50	0.76
26:1:2083:G:H1	26:1:2639:C:H5	1.30	0.76
26:1:166:A:H2'	26:1:167:U:C6	2.21	0.76
2:B:274:ARG:NH2	26:1:1825:U:OP2	2.20	0.75
5:E:37:LYS:NZ	5:E:48:GLU:OE2	2.19	0.75
26:1:1320:G:N2	26:1:1323:A:OP2	2.16	0.75
19:U:2:SER:OG	19:U:3:ARG:N	2.18	0.75
26:1:1722:A:H2'	26:1:1723:A:C8	2.21	0.75
26:1:659:A:H2'	26:1:659:A:N3	2.02	0.75
7:G:91:VAL:HG11	7:G:100:GLU:HG2	1.67	0.75
26:1:286:U:O2'	26:1:287:G:O4'	2.01	0.75
26:1:28:A:H2'	26:1:29:U:C6	2.22	0.74
27:2:7:G:O6	27:2:106:G:N2	2.20	0.74
26:1:652:A:H2'	26:1:653:G:H8	1.52	0.74
2:B:132:LEU:HD13	2:B:172:VAL:HG21	1.69	0.74
16:Q:8:ARG:NH1	26:1:246:U:OP2	2.21	0.74
26:1:591:A:H4'	26:1:592:A:H5'	1.68	0.74
20:V:22:GLU:HA	20:V:62:LYS:HB2	1.69	0.74
26:1:1577:G:H22	26:1:1589:U:H3	1.35	0.73
11:L:189:ASP:HB3	11:L:194:VAL:HG22	1.70	0.73
17:R:16:VAL:HG22	17:R:25:VAL:HG22	1.70	0.73
26:1:409:G:H2'	26:1:410:G:H1'	1.71	0.73
26:1:275:A:N6	26:1:296:G:N2	2.33	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:2:ALA:HB3	12:M:36:VAL:HG12	1.69	0.73
26:1:1070:A:OP2	26:1:1178:C:O2'	2.07	0.73
5:E:42:ALA:HB2	26:1:2037:G:H5"	1.70	0.73
26:1:2318:U:O2'	26:1:2401:C:O2	2.06	0.72
26:1:651:A:H2'	26:1:652:A:C8	2.24	0.72
26:1:2474:G:N7	26:1:2527:U:H2'	2.04	0.72
26:1:2886:G:H1'	26:1:2888:A:H4'	1.72	0.72
26:1:1540:U:O2	26:1:1624:C:O2'	2.07	0.72
26:1:2534:C:H2'	26:1:2535:G:H8	1.54	0.72
26:1:288:C:H4'	26:1:290:U:H5"	1.71	0.72
26:1:2855:A:H61	26:1:2898:U:H2'	1.55	0.72
26:1:2370:U:HO2'	26:1:2400:U:HO2'	1.36	0.72
6:F:12:ILE:HG13	6:F:89:LEU:HD13	1.70	0.72
12:M:51:LYS:NZ	12:M:51:LYS:HB3	2.03	0.72
2:B:154:ILE:HG21	2:B:176:LEU:HD22	1.72	0.71
26:1:2537:C:H2'	26:1:2538:U:C6	2.25	0.71
26:1:691:A:H2'	26:1:692:G:C8	2.23	0.71
26:1:1651:C:H4'	26:1:1652:A:H5'	1.73	0.71
14:O:2:ARG:NH1	26:1:2312:C:OP2	2.24	0.71
3:C:88:ILE:HA	4:D:50:ALA:HB3	1.72	0.71
26:1:661:U:O2'	26:1:662:G:OP2	2.08	0.71
26:1:282:A:H2'	26:1:283:G:O4'	1.90	0.70
8:H:9:ARG:NH2	27:2:73:G:O2'	2.23	0.70
8:H:9:ARG:HB3	8:H:42:LYS:HE2	1.74	0.70
26:1:2290:C:N4	28:I:23:ASP:OD1	2.24	0.70
10:K:47:ARG:NH1	26:1:74:U:OP2	2.25	0.70
26:1:66:C:H2'	26:1:67:G:C8	2.26	0.70
8:H:61:ILE:HD12	8:H:74:VAL:HB	1.72	0.70
3:C:91:ASN:HD22	3:C:91:ASN:H	1.40	0.70
24:Z:112:ASP:OD2	26:1:1693:G:O2'	2.06	0.70
19:U:28:GLY:HA3	19:U:79:VAL:HB	1.74	0.69
26:1:2606:C:O2'	26:1:2607:U:H5'	1.92	0.69
26:1:2888:A:H2'	26:1:2889:G:C8	2.26	0.69
9:J:19:SER:HB2	26:1:2107:G:H5'	1.75	0.69
14:O:25:ASN:ND2	26:1:2313:A:OP1	2.24	0.69
26:1:481:C:H2'	26:1:482:U:H5'	1.73	0.69
26:1:318:A:N3	26:1:318:A:H2'	2.07	0.69
2:B:65:ILE:HD11	2:B:91:ILE:HG21	1.75	0.69
11:L:138:ARG:HE	26:1:2024:A:H5"	1.57	0.69
26:1:1899:U:H4'	26:1:1900:G:H5"	1.73	0.69
26:1:1506:C:H2'	26:1:1507:A:C8	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:92:G:H2'	26:1:93:U:C6	2.28	0.69
26:1:1946:A:H2'	26:1:1947:C:H5'	1.75	0.69
26:1:656:G:H1'	26:1:659:A:H62	1.58	0.69
7:G:73:PRO:HG3	7:G:101:ILE:HG22	1.75	0.68
9:J:2:GLY:N	26:1:1403:C:OP1	2.26	0.68
19:U:164:TYR:N	19:U:168:TYR:OH	2.20	0.68
26:1:1996:A:H4'	26:1:1996:A:OP1	1.92	0.68
26:1:2294:A:N3	26:1:2294:A:H2'	2.07	0.68
26:1:553:A:N3	26:1:553:A:H2'	2.07	0.68
26:1:2536:G:O2'	26:1:2537:C:H5'	1.92	0.68
28:I:19:LYS:O	28:I:22:ARG:NH2	2.25	0.68
7:G:26:THR:HG23	7:G:33:VAL:HG12	1.75	0.68
26:1:2347:A:H2'	26:1:2347:A:N3	2.09	0.68
26:1:90:A:H4'	26:1:91:A:H5'	1.76	0.68
26:1:160:G:H5"	26:1:167:U:H5	1.58	0.68
11:L:123:LYS:NZ	26:1:2706:A:OP1	2.22	0.68
26:1:509:G:N2	26:1:512:A:OP2	2.23	0.68
26:1:1068:G:H2'	26:1:1069:G:C8	2.28	0.68
26:1:1558:U:H2'	26:1:1559:G:C8	2.29	0.68
26:1:1272:U:H2'	26:1:1273:G:C8	2.28	0.68
4:D:50:ALA:HB1	4:D:51:PRO:HA	1.76	0.67
26:1:332:A:H61	26:1:394:U:H3	1.42	0.67
8:H:21:LEU:HD11	8:H:26:LYS:HB3	1.75	0.67
26:1:2102:U:OP2	26:1:2265:G:O2'	2.13	0.67
26:1:1720:A:H2'	26:1:1721:A:C8	2.30	0.67
19:U:42:THR:OG1	19:U:53:VAL:O	2.12	0.67
26:1:2296:A:H2'	26:1:2297:G:C8	2.30	0.67
26:1:2313:A:H4'	26:1:2314:A:O4'	1.94	0.67
26:1:409:G:H2'	26:1:410:G:C1'	2.25	0.67
26:1:699:U:C4'	26:1:700:A:H5'	2.20	0.67
26:1:2603:G:N3	26:1:2603:G:H2'	2.09	0.67
26:1:2296:A:H2'	26:1:2297:G:H8	1.59	0.66
3:C:78:ARG:HH12	26:1:1195:A:H1'	1.59	0.66
26:1:1463:A:H2	26:1:1625:U:H3	1.44	0.66
26:1:2843:A:H2'	26:1:2844:U:C6	2.31	0.66
3:C:28:LYS:HE2	3:C:38:GLN:HE21	1.60	0.66
26:1:1587:C:H2'	26:1:1588:U:H5'	1.76	0.66
7:G:81:VAL:HG12	7:G:101:ILE:HD11	1.78	0.66
26:1:1575:A:H2	26:1:1591:G:H22	1.42	0.66
26:1:2318:U:OP1	26:1:2407:A:O2'	2.14	0.66
26:1:1431:U:C2'	26:1:1432:A:H5'	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:ASN:HD22	3:C:91:ASN:N	1.91	0.65
10:K:4:LYS:HB2	10:K:52:ARG:HD3	1.78	0.65
26:1:2419:A:H2	26:1:2451:C:H42	1.41	0.65
26:1:692:G:H2'	26:1:693:G:H8	1.61	0.65
26:1:331:G:O6	26:1:395:U:O2	2.14	0.65
26:1:858:U:H2'	26:1:859:C:C6	2.31	0.65
26:1:514:G:O2'	26:1:515:G:H5'	1.97	0.65
26:1:847:A:H2'	26:1:848:U:C6	2.31	0.65
26:1:983:G:C2'	26:1:984:G:H5'	2.26	0.65
26:1:652:A:H2'	26:1:653:G:C8	2.31	0.65
27:2:54:U:H4'	27:2:55:A:C5'	2.25	0.65
26:1:2097:G:H2'	26:1:2098:A:C8	2.32	0.65
6:F:39:LYS:O	6:F:43:GLU:HG3	1.97	0.64
2:B:185:LEU:HD12	2:B:186:SER:H	1.62	0.64
8:H:9:ARG:HH11	8:H:13:GLN:HG3	1.63	0.64
26:1:1063:U:H3	26:1:1186:A:H62	1.45	0.64
22:X:94:ALA:O	22:X:98:GLU:HG2	1.97	0.64
26:1:2567:C:O2'	26:1:2767:A:N3	2.30	0.64
26:1:575:G:O2'	26:1:577:A:N7	2.29	0.64
26:1:755:C:H3'	26:1:756:A:H5"	1.78	0.64
26:1:140:A:H2'	26:1:141:U:C6	2.32	0.64
26:1:1711:G:H1'	26:1:1713:A:H62	1.63	0.64
26:1:2821:U:H4'	26:1:2822:C:OP1	1.97	0.64
8:H:31:VAL:HG22	8:H:91:PHE:HB2	1.78	0.64
26:1:1482:U:H3	26:1:1601:U:H5	1.46	0.64
26:1:889:U:H2'	26:1:890:G:O4'	1.98	0.64
26:1:692:G:H2'	26:1:693:G:C8	2.33	0.64
26:1:1462:G:H8	26:1:1626:A:H62	1.44	0.64
26:1:1565:U:H2'	26:1:1566:G:C8	2.32	0.64
26:1:150:A:H61	26:1:179:A:H2	1.46	0.63
26:1:2605:G:H4'	26:1:2605:G:OP2	1.99	0.63
26:1:896:U:H2'	26:1:897:A:C8	2.32	0.63
27:2:58:C:H2'	27:2:59:U:C6	2.32	0.63
11:L:56:LYS:HE2	11:L:66:ASN:O	1.98	0.63
26:1:1651:C:N4	26:1:1666:A:OP2	2.28	0.63
26:1:1721:A:H2'	26:1:1722:A:C8	2.33	0.63
24:Z:28:GLU:HG2	24:Z:121:LEU:HD12	1.80	0.63
26:1:983:G:H2'	26:1:984:G:H5'	1.80	0.63
26:1:1345:A:H2'	26:1:1346:G:H5'	1.79	0.63
7:G:42:LYS:HG2	7:G:58:GLU:HG3	1.79	0.63
26:1:1510:U:H4'	26:1:1510:U:OP1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2314:A:H62	26:1:2371:U:H3	1.46	0.63
2:B:209:GLY:HA3	26:1:809:A:H5'	1.81	0.62
7:G:77:GLU:OE1	7:G:78:PRO:HD2	1.98	0.62
26:1:1719:C:H2'	26:1:1720:A:C8	2.35	0.62
26:1:2620:U:O2	26:1:2629:A:N6	2.32	0.62
7:G:32:ARG:HB3	7:G:62:ALA:HB1	1.81	0.62
26:1:2609:G:H2'	26:1:2610:G:C8	2.34	0.62
26:1:155:U:O2'	26:1:156:A:H5'	1.99	0.62
26:1:2016:A:H2'	26:1:2017:C:C6	2.35	0.62
26:1:2582:U:O2	26:1:2582:U:C2'	2.47	0.62
26:1:215:G:H2'	26:1:216:A:O4'	2.00	0.62
26:1:748:U:H2'	26:1:749:G:O4'	2.00	0.62
26:1:1216:U:O4	26:1:1219:G:H1'	2.00	0.62
21:W:71:ARG:HH22	21:W:104:ARG:HB2	1.64	0.62
26:1:1512:U:H2'	26:1:1513:A:C8	2.35	0.62
26:1:2609:G:H2'	26:1:2610:G:H8	1.64	0.62
6:F:10:PRO:HD3	10:K:30:PHE:CE1	2.35	0.62
26:1:157:U:H2'	26:1:158:G:H5'	1.80	0.62
26:1:772:A:O2'	26:1:773:G:H5'	2.00	0.62
26:1:516:A:H2'	26:1:517:A:C8	2.34	0.62
26:1:30:G:H2'	26:1:31:C:C6	2.35	0.62
26:1:1891:U:OP1	26:1:2437:G:O2'	2.16	0.62
8:H:16:SER:OG	27:2:89:U:OP1	2.10	0.62
26:1:1479:G:O6	26:1:1605:A:N6	2.33	0.62
26:1:1480:G:H1'	26:1:1520:A:H8	1.65	0.62
26:1:2054:G:H2'	26:1:2055:U:C6	2.35	0.62
2:B:98:ASP:O	26:1:1544:G:N2	2.33	0.61
11:L:52:GLY:O	11:L:85:LYS:HB3	2.00	0.61
24:Z:26:ILE:HD13	24:Z:71:ILE:HD11	1.80	0.61
26:1:964:U:H2'	26:1:965:G:C8	2.35	0.61
23:Y:14:ARG:NH1	26:1:1000:G:N7	2.47	0.61
26:1:1484:G:H1	26:1:1599:G:N2	1.98	0.61
26:1:1601:U:H4'	26:1:1601:U:OP1	1.98	0.61
26:1:92:G:H2'	26:1:93:U:H6	1.65	0.61
4:D:41:VAL:HG12	4:D:48:VAL:CG2	2.30	0.61
26:1:2348:G:H5"	26:1:2349:A:OP2	2.00	0.61
26:1:2537:C:H2'	26:1:2538:U:H6	1.62	0.61
26:1:2579:U:N3	26:1:2581:U:H5"	2.15	0.61
18:S:66:LYS:O	18:S:66:LYS:HG2	2.00	0.61
18:S:37:ILE:HG23	18:S:184:LEU:CD1	2.30	0.61
26:1:281:A:H3'	26:1:282:A:C2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1512:U:H2'	26:1:1513:A:H8	1.66	0.61
26:1:2533:U:HO2'	26:1:2534:C:H6	1.49	0.61
2:B:175:ARG:HG3	2:B:181:VAL:HG22	1.80	0.61
26:1:408:U:H2'	26:1:409:G:H5'	1.82	0.61
12:M:52:HIS:H	12:M:52:HIS:CD2	2.17	0.61
18:S:160:ASP:O	18:S:164:GLU:HG2	2.01	0.61
22:X:68:ASN:OD1	26:1:2431:C:O2'	2.17	0.61
26:1:1881:A:H62	26:1:1915:G:H8	1.48	0.61
26:1:283:G:N2	26:1:287:G:OP1	2.34	0.61
3:C:36:LYS:O	3:C:40:MET:HG3	2.00	0.60
7:G:99:GLU:OE1	7:G:99:GLU:N	2.34	0.60
11:L:6:LEU:HB2	11:L:33:ASN:HD21	1.66	0.60
14:O:22:ASN:HB3	14:O:25:ASN:HB2	1.81	0.60
26:1:9:U:O2'	26:1:10:A:H5'	2.00	0.60
26:1:1920:C:H2'	26:1:1921:C:H5'	1.82	0.60
26:1:1557:C:H2'	26:1:1558:U:C6	2.36	0.60
26:1:1772:G:H2'	26:1:1773:A:H5'	1.82	0.60
26:1:1813:A:O2'	26:1:1965:A:N6	2.35	0.60
26:1:1086:G:HO2'	26:1:1087:C:H6	1.48	0.60
8:H:55:VAL:HG21	8:H:60:VAL:O	2.02	0.60
22:X:51:GLU:HG2	22:X:53:GLY:H	1.67	0.60
26:1:243:U:H2'	26:1:244:A:C8	2.36	0.60
26:1:2858:G:H2'	26:1:2859:G:H8	1.66	0.60
21:W:8:LEU:HD23	21:W:82:ASN:HB3	1.84	0.60
26:1:1489:A:H2'	26:1:1490:G:H8	1.67	0.60
26:1:2822:C:H4'	26:1:2823:G:H2'	1.84	0.60
26:1:200:A:H2'	26:1:201:C:C6	2.37	0.60
18:S:53:ASN:O	18:S:57:VAL:HG23	2.01	0.60
21:W:1:MET:HB2	21:W:2:ILE:HD13	1.84	0.60
26:1:259:A:H2'	26:1:260:A:C8	2.36	0.60
2:B:150:LYS:NZ	26:1:1828:U:OP2	2.35	0.59
10:K:21:SER:HA	10:K:50:ILE:HD13	1.83	0.59
21:W:63:VAL:HG11	21:W:102:VAL:HG22	1.83	0.59
2:B:217:ARG:NH2	26:1:826:A:OP1	2.34	0.59
11:L:5:ILE:HG13	11:L:110:PHE:HE2	1.67	0.59
21:W:2:ILE:HG21	26:1:1709:A:N3	2.17	0.59
26:1:673:G:H2'	26:1:674:C:C6	2.37	0.59
26:1:1072:A:N3	26:1:2513:G:O2'	2.31	0.59
26:1:1431:U:H4'	26:1:1647:A:H4'	1.84	0.59
26:1:1717:G:O2'	26:1:1718:G:H5'	2.03	0.59
26:1:2470:C:O2'	26:1:2471:G:H5'	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2500:U:H2'	26:1:2501:U:H5'	1.83	0.59
8:H:70:ILE:O	8:H:71:LYS:HG2	2.03	0.59
18:S:132:GLU:OE1	18:S:132:GLU:N	2.28	0.59
26:1:261:C:H2'	26:1:262:G:H8	1.66	0.59
18:S:150:LYS:HD2	18:S:150:LYS:N	2.12	0.59
26:1:83:G:H21	26:1:102:A:H2	1.49	0.59
26:1:754:U:H2'	26:1:755:C:C6	2.38	0.59
2:B:221:ARG:O	2:B:224:VAL:HG22	2.01	0.59
5:E:61:ASN:HD21	26:1:540:G:H21	1.50	0.59
7:G:42:LYS:CG	7:G:58:GLU:HG3	2.32	0.59
18:S:46:GLN:NE2	26:1:487:U:O2'	2.36	0.59
10:K:17:GLN:O	10:K:21:SER:CB	2.42	0.59
17:R:23:VAL:HB	17:R:37:GLY:HA3	1.83	0.59
19:U:19:PHE:CZ	19:U:50:ILE:HG21	2.37	0.59
26:1:29:U:H2'	26:1:30:G:C8	2.38	0.59
26:1:691:A:H2'	26:1:692:G:H8	1.67	0.59
19:U:24:VAL:O	19:U:35:ARG:HA	2.02	0.59
26:1:261:C:H2'	26:1:262:G:C8	2.38	0.59
26:1:702:U:H2'	26:1:703:A:C8	2.38	0.59
26:1:2101:U:O2'	26:1:2624:G:O2'	2.21	0.59
8:H:51:VAL:O	8:H:55:VAL:HG12	2.03	0.59
26:1:1304:G:O2'	26:1:2039:G:O6	2.16	0.59
26:1:2468:C:O2'	26:1:2469:C:H5'	2.03	0.59
4:D:41:VAL:HG12	4:D:48:VAL:HG21	1.83	0.58
6:F:9:ARG:NH1	6:F:28:ASP:OD2	2.36	0.58
26:1:1716:C:H2'	26:1:1717:G:C8	2.38	0.58
26:1:2341:A:H2'	26:1:2342:U:C6	2.38	0.58
26:1:2355:A:H2'	26:1:2356:A:C8	2.38	0.58
27:2:5:G:H1	27:2:108:U:H3	1.49	0.58
27:2:78:U:H3	27:2:91:C:H42	1.51	0.58
8:H:49:ILE:HA	8:H:52:ILE:HG22	1.83	0.58
8:H:78:GLN:HB2	8:H:87:THR:HB	1.86	0.58
26:1:622:A:H2'	26:1:623:C:C6	2.38	0.58
26:1:1345:A:C2'	26:1:1346:G:H5'	2.34	0.58
26:1:1873:G:O2'	26:1:1874:A:H5'	2.04	0.58
26:1:896:U:H2'	26:1:897:A:H8	1.68	0.58
26:1:1923:A:H2'	26:1:1924:G:C8	2.38	0.58
1:A:10:VAL:HG11	11:L:196:LEU:HD11	1.85	0.58
1:A:53:ARG:NH2	26:1:2710:C:OP1	2.37	0.58
11:L:116:ILE:HD12	11:L:211:ILE:HG23	1.85	0.58
26:1:178:A:O2'	26:1:179:A:H5'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:MET:HG2	2:B:17:THR:H	1.68	0.58
2:B:180:GLU:HG3	2:B:273:GLY:O	2.03	0.58
11:L:156:MET:HG2	26:1:2598:U:O2	2.04	0.58
26:1:1487:G:H22	26:1:1596:G:H22	1.51	0.58
26:1:1716:C:O2'	26:1:1717:G:H5'	2.03	0.58
19:U:19:PHE:HZ	19:U:50:ILE:HD13	1.69	0.58
26:1:659:A:N3	26:1:659:A:C2'	2.67	0.58
26:1:974:U:H2'	26:1:975:U:C6	2.38	0.58
26:1:2745:G:O2'	26:1:2746:G:H5'	2.03	0.58
19:U:71:LEU:O	19:U:75:MET:HG2	2.03	0.58
26:1:1431:U:H2'	26:1:1432:A:H5'	1.85	0.58
26:1:2567:C:C2'	26:1:2568:A:H5'	2.33	0.58
26:1:331:G:O2'	26:1:332:A:OP2	2.16	0.58
26:1:1219:G:HO2'	26:1:1220:A:H8	1.51	0.58
4:D:41:VAL:H	4:D:48:VAL:CG2	2.17	0.57
23:Y:20:ARG:NH1	23:Y:99:PRO:HB2	2.19	0.57
26:1:522:G:N1	26:1:525:A:OP2	2.36	0.57
26:1:1981:G:N3	26:1:2578:C:H5"	2.18	0.57
26:1:1491:C:H2'	26:1:1492:G:C8	2.39	0.57
8:H:16:SER:OG	27:2:89:U:H5"	2.04	0.57
9:J:39:LEU:H	9:J:59:VAL:HG23	1.70	0.57
24:Z:2:GLY:HA2	26:1:2717:A:C8	2.39	0.57
26:1:283:G:H1	26:1:286:U:H5"	1.69	0.57
26:1:2538:U:O2'	26:1:2539:C:H5'	2.03	0.57
9:J:37:ARG:HA	9:J:46:LYS:HA	1.87	0.57
26:1:683:G:H2'	26:1:684:U:C6	2.39	0.57
26:1:2479:C:O2'	26:1:2480:A:H5'	2.04	0.57
5:E:59:GLU:HG2	5:E:66:THR:HG21	1.87	0.57
26:1:1676:A:H2'	26:1:1677:G:C8	2.40	0.57
26:1:2707:C:O2'	26:1:2708:C:H5'	2.03	0.57
7:G:9:VAL:HG12	7:G:70:LEU:HD23	1.85	0.57
26:1:283:G:N1	26:1:286:U:H5"	2.20	0.57
26:1:764:C:H2'	26:1:765:U:C6	2.40	0.57
26:1:2289:U:OP2	28:I:24:SER:OG	2.13	0.57
26:1:2672:G:H4'	26:1:2759:G:O2'	2.04	0.57
26:1:2917:U:H2'	26:1:2918:A:C8	2.40	0.57
18:S:123:LEU:HD11	18:S:194:ILE:CD1	2.35	0.57
19:U:59:LYS:HE3	26:1:1079:U:H5'	1.86	0.57
26:1:694:G:H2'	26:1:695:C:C6	2.40	0.57
26:1:760:A:H2'	26:1:761:A:O4'	2.03	0.57
26:1:763:A:H2'	26:1:764:C:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:O	1:A:42:ILE:HD13	2.04	0.57
2:B:69:ARG:HH21	2:B:116:VAL:HG22	1.70	0.57
8:H:88:HIS:O	8:H:89:ILE:HD13	2.05	0.57
18:S:164:GLU:O	18:S:168:ARG:HB3	2.04	0.57
26:1:43:A:H2'	26:1:44:A:H5'	1.87	0.57
26:1:537:A:H2'	26:1:538:G:O4'	2.05	0.57
26:1:1897:U:H2'	26:1:1898:C:H5'	1.86	0.57
9:J:57:GLY:O	9:J:58:LYS:HE2	2.04	0.57
10:K:28:LEU:HD23	10:K:37:LEU:HD13	1.87	0.57
19:U:44:LYS:HZ2	19:U:46:GLU:HB2	1.68	0.57
19:U:63:THR:HG22	26:1:2776:A:H1'	1.86	0.57
26:1:2052:C:H2'	26:1:2053:U:C6	2.40	0.57
26:1:2844:U:H2'	26:1:2845:G:C8	2.39	0.57
9:J:39:LEU:HD23	9:J:44:PRO:HB3	1.87	0.56
20:V:48:HIS:O	26:1:600:U:O2'	2.20	0.56
26:1:1201:G:H2'	26:1:1202:C:C6	2.40	0.56
26:1:1713:A:N3	26:1:1713:A:C2'	2.65	0.56
1:A:113:GLN:HG2	1:A:114:GLU:H	1.69	0.56
26:1:77:U:H2'	26:1:78:U:C6	2.40	0.56
26:1:396:G:H2'	26:1:397:U:C6	2.40	0.56
1:A:14:GLN:HE22	11:L:15:VAL:HB	1.71	0.56
2:B:140:VAL:HG12	2:B:161:SER:HB2	1.88	0.56
11:L:47:ASN:OD1	11:L:47:ASN:N	2.37	0.56
26:1:207:A:H4'	26:1:208:G:OP1	2.06	0.56
26:1:1487:G:H1	26:1:1596:G:H22	1.51	0.56
26:1:2715:G:OP1	26:1:2740:A:N6	2.35	0.56
1:A:34:ILE:HG22	1:A:36:GLU:H	1.70	0.56
14:O:22:ASN:ND2	26:1:2312:C:OP2	2.38	0.56
26:1:309:U:O2'	26:1:310:C:H5'	2.05	0.56
26:1:688:A:H2'	26:1:689:A:C8	2.41	0.56
26:1:2322:C:O2'	26:1:2323:U:H5'	2.06	0.56
26:1:2472:G:C2'	26:1:2473:G:H5'	2.35	0.56
19:U:48:ASN:O	19:U:49:THR:OG1	2.22	0.56
26:1:966:C:O2'	26:1:967:C:H5'	2.05	0.56
26:1:1588:U:H2'	26:1:1589:U:C6	2.41	0.56
1:A:105:LEU:CB	1:A:110:ALA:HB2	2.35	0.56
13:N:15:LYS:O	13:N:18:THR:OG1	2.13	0.56
26:1:334:A:O2'	26:1:335:U:H5'	2.06	0.56
26:1:738:U:H2'	26:1:739:U:C6	2.41	0.56
26:1:1582:U:H3'	26:1:1584:U:H5"	1.87	0.56
26:1:308:C:H2'	26:1:309:U:C5	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2284:U:O2'	26:1:2285:C:H5'	2.05	0.56
2:B:164:VAL:HG22	2:B:174:ILE:HD13	1.87	0.56
5:E:89:ALA:HB2	26:1:793:G:H5'	1.87	0.56
6:F:23:ASP:N	6:F:23:ASP:OD1	2.39	0.56
26:1:241:C:H2'	26:1:242:U:C6	2.41	0.56
26:1:963:A:H62	26:1:2295:A:H2	1.53	0.56
26:1:1781:C:H2'	26:1:1782:A:C8	2.40	0.56
26:1:1508:C:H2'	26:1:1509:G:C8	2.41	0.56
26:1:1584:U:H2'	26:1:1585:G:H5'	1.88	0.56
26:1:2288:C:O2'	26:1:2289:U:H5'	2.06	0.56
26:1:1159:A:H2'	26:1:1160:C:O4'	2.06	0.55
26:1:1875:A:H2'	26:1:1876:G:O4'	2.06	0.55
26:1:2346:U:O2	26:1:2346:U:O4'	2.24	0.55
1:A:34:ILE:HD11	1:A:43:GLN:OE1	2.06	0.55
22:X:78:ASN:OD1	22:X:114:ASN:HB3	2.05	0.55
26:1:1809:C:O2'	26:1:1810:A:H5'	2.06	0.55
20:V:63:ILE:HD11	20:V:101:LEU:HD23	1.88	0.55
26:1:117:A:H2'	26:1:119:U:O4	2.05	0.55
26:1:2821:U:H1'	26:1:2822:C:C5'	2.32	0.55
21:W:111:PHE:O	21:W:115:VAL:HG22	2.05	0.55
26:1:828:A:N3	26:1:828:A:C2'	2.63	0.55
26:1:2507:C:C2'	26:1:2508:G:H5'	2.36	0.55
5:E:33:ILE:HG13	5:E:51:LEU:HD21	1.88	0.55
10:K:11:THR:O	10:K:15:GLU:HG3	2.07	0.55
23:Y:35:GLN:NE2	23:Y:130:LYS:HE2	2.21	0.55
26:1:527:G:O2'	26:1:552:A:N6	2.40	0.55
26:1:1207:G:O2'	26:1:1208:A:H5'	2.07	0.55
1:A:94:VAL:HG21	1:A:99:LEU:HD21	1.87	0.55
5:E:4:LYS:HG3	5:E:106:VAL:HG22	1.88	0.55
8:H:37:LYS:HG2	8:H:38:ASN:OD1	2.07	0.55
20:V:36:ILE:HD11	20:V:141:TYR:CE2	2.41	0.55
26:1:1869:G:H2'	26:1:1870:C:C6	2.42	0.55
26:1:1926:A:H2	26:1:1929:C:H41	1.52	0.55
26:1:2091:C:H2'	26:1:2092:C:C6	2.42	0.55
27:2:30:U:H2'	27:2:31:G:C8	2.42	0.55
8:H:27:VAL:HG21	8:H:86:ILE:CG1	2.33	0.55
8:H:31:VAL:HG22	8:H:91:PHE:CB	2.37	0.55
22:X:118:ASP:HA	22:X:139:LYS:HE2	1.87	0.55
26:1:446:G:O2'	26:1:447:A:H5"	2.05	0.55
26:1:745:G:H2'	26:1:746:G:C8	2.42	0.55
26:1:787:U:H2'	26:1:788:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2532:G:H2'	26:1:2603:G:H1	1.72	0.55
27:2:28:C:H2'	27:2:29:C:O4'	2.07	0.55
4:D:11:GLN:HE21	4:D:39:LEU:HD11	1.72	0.55
26:1:763:A:H2'	26:1:764:C:C5	2.42	0.55
16:Q:7:HIS:HB2	16:Q:61:LEU:HB3	1.89	0.55
19:U:115:ILE:HG21	19:U:148:ILE:CG1	2.37	0.55
20:V:111:PRO:O	20:V:116:GLY:HA3	2.07	0.55
26:1:1480:G:H1'	26:1:1520:A:C8	2.41	0.55
26:1:2859:G:H2'	26:1:2860:U:C6	2.42	0.55
2:B:40:LYS:HD2	26:1:1840:U:H5"	1.89	0.54
2:B:209:GLY:CA	26:1:809:A:H5'	2.37	0.54
4:D:10:LYS:HD3	20:V:2:ARG:HH12	1.71	0.54
20:V:60:ALA:HB1	20:V:102:ILE:HD12	1.88	0.54
26:1:428:G:H22	26:1:438:U:H3	1.55	0.54
26:1:794:A:H2'	26:1:795:A:H8	1.70	0.54
26:1:2275:C:H2'	26:1:2276:U:H5'	1.89	0.54
11:L:6:LEU:CD1	11:L:53:PHE:HB2	2.38	0.54
26:1:2308:C:C2'	26:1:2309:G:H5'	2.38	0.54
26:1:2841:A:H2'	26:1:2842:G:C8	2.42	0.54
2:B:164:VAL:HG22	2:B:174:ILE:CD1	2.37	0.54
18:S:188:ASN:HD22	22:X:3:LEU:HD12	1.72	0.54
26:1:1897:U:H3	26:1:1899:U:H5'	1.72	0.54
26:1:2270:U:H2'	26:1:2271:U:C6	2.43	0.54
14:O:10:THR:HG21	14:O:44:LEU:HB3	1.89	0.54
18:S:139:PHE:CD1	18:S:167:ALA:HB2	2.43	0.54
26:1:2858:G:H2'	26:1:2859:G:C8	2.42	0.54
26:1:229:A:O2'	26:1:230:A:OP1	2.21	0.54
26:1:674:C:O2'	26:1:675:G:H5'	2.07	0.54
26:1:2604:A:H3'	26:1:2605:G:H5'	1.89	0.54
2:B:184:ILE:HG22	2:B:185:LEU:O	2.08	0.54
4:D:70:LYS:HA	4:D:88:HIS:O	2.07	0.54
16:Q:5:LYS:NZ	26:1:257:G:N7	2.51	0.54
26:1:342:A:N3	26:1:362:C:O2'	2.39	0.54
26:1:1521:A:O2'	26:1:1522:G:H5'	2.07	0.54
26:1:2343:U:O2'	26:1:2344:C:H5'	2.07	0.54
3:C:49:ASP:OD2	26:1:579:U:O2'	2.23	0.54
6:F:15:LYS:HE3	26:1:1430:A:H62	1.72	0.54
26:1:158:G:C6	26:1:159:U:H1'	2.42	0.54
26:1:2516:G:O2'	26:1:2517:G:H5'	2.08	0.54
5:E:90:GLN:HA	26:1:796:A:H5'	1.90	0.54
7:G:10:LYS:HB2	7:G:71:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:121:ILE:CD1	19:U:144:LEU:HG	2.38	0.54
24:Z:42:SER:O	24:Z:46:LYS:HG3	2.08	0.54
26:1:1568:U:H1'	26:1:1570:G:C5	2.42	0.54
26:1:2608:G:N2	26:1:2608:G:OP2	2.40	0.54
18:S:51:VAL:HG11	18:S:91:GLY:HA3	1.89	0.54
26:1:2482:G:H2'	26:1:2483:C:C6	2.43	0.54
26:1:1866:A:H61	26:1:1930:G:H21	1.56	0.53
26:1:2721:G:H2'	26:1:2722:U:C6	2.43	0.53
27:2:29:C:H2'	27:2:30:U:H6	1.73	0.53
12:M:5:GLN:HB3	12:M:57:GLU:HG2	1.89	0.53
19:U:96:ALA:HB1	19:U:103:LEU:HD11	1.90	0.53
22:X:22:GLY:O	22:X:28:GLY:HA3	2.07	0.53
26:1:353:A:O2'	26:1:354:A:OP2	2.20	0.53
26:1:893:G:H2'	26:1:894:A:C8	2.43	0.53
26:1:1478:A:H2'	26:1:1479:G:O4'	2.08	0.53
2:B:16:MET:HG3	2:B:206:GLY:HA3	1.89	0.53
2:B:68:LYS:NZ	2:B:150:LYS:O	2.42	0.53
3:C:106:PHE:O	3:C:110:VAL:HG23	2.08	0.53
8:H:18:LEU:O	8:H:22:ARG:HG3	2.07	0.53
26:1:69:C:H4'	26:1:75:G:N7	2.23	0.53
26:1:350:G:H8	26:1:373:A:H61	1.55	0.53
26:1:1867:G:H2'	26:1:1868:U:C5	2.44	0.53
4:D:20:ILE:HD13	4:D:97:ILE:HD11	1.90	0.53
26:1:1253:G:O2'	26:1:1254:C:H5'	2.07	0.53
26:1:2275:C:C2'	26:1:2276:U:H5'	2.38	0.53
26:1:2226:A:N6	26:1:2251:G:O2'	2.42	0.53
12:M:28:LEU:O	12:M:33:SER:OG	2.23	0.53
19:U:139:GLU:OE2	26:1:2786:G:N2	2.21	0.53
26:1:1222:A:H2'	26:1:1223:A:H8	1.73	0.53
7:G:12:ILE:HB	7:G:67:ASN:O	2.09	0.53
14:O:15:ARG:HG2	14:O:37:SER:OG	2.08	0.53
19:U:2:SER:HB3	26:1:2776:A:OP1	2.09	0.53
19:U:90:VAL:CG2	19:U:163:ARG:HD3	2.38	0.53
26:1:519:G:O2'	26:1:520:G:H5'	2.08	0.53
26:1:1166:G:O2'	26:1:1167:C:H5'	2.09	0.53
26:1:1514:A:H2'	26:1:1515:G:C8	2.43	0.53
27:2:14:G:H8	27:2:14:G:OP2	1.91	0.53
3:C:83:LEU:HD22	3:C:88:ILE:HG12	1.90	0.53
16:Q:53:SER:O	16:Q:56:LYS:HB2	2.09	0.53
26:1:964:U:H2'	26:1:965:G:H8	1.72	0.53
8:H:71:LYS:O	8:H:94:ILE:HD12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1699:A:C2	26:1:2076:A:H5"	2.43	0.53
2:B:3:ILE:HG23	2:B:17:THR:HG23	1.90	0.53
2:B:259:THR:OG1	26:1:1824:C:O2'	2.25	0.53
11:L:123:LYS:CE	11:L:174:GLY:HA2	2.37	0.53
26:1:575:G:N2	26:1:2050:A:OP1	2.42	0.53
26:1:590:U:OP1	26:1:1257:G:O2'	2.24	0.53
26:1:2265:G:N3	26:1:2265:G:H2'	2.24	0.53
20:V:18:VAL:HG12	20:V:139:GLU:O	2.10	0.52
23:Y:27:VAL:HA	23:Y:105:GLU:OE2	2.09	0.52
26:1:1217:U:H1'	26:1:1218:G:N2	2.24	0.52
26:1:2451:C:H5'	26:1:2452:A:H5'	1.91	0.52
26:1:2826:U:H2'	26:1:2827:A:N9	2.24	0.52
19:U:72:LEU:CD2	19:U:75:MET:HE3	2.37	0.52
26:1:1222:A:H2'	26:1:1223:A:C8	2.44	0.52
26:1:1432:A:H4'	26:1:1434:U:C5	2.44	0.52
2:B:75:ASN:OD1	2:B:115:ILE:HG12	2.09	0.52
6:F:10:PRO:HD3	10:K:30:PHE:CD1	2.43	0.52
21:W:91:LYS:HB3	21:W:111:PHE:CD1	2.44	0.52
26:1:52:A:H2'	26:1:53:A:C8	2.44	0.52
26:1:321:U:OP1	26:1:321:U:H6	1.93	0.52
26:1:501:C:C2'	26:1:502:C:H5'	2.36	0.52
18:S:183:VAL:O	18:S:187:THR:HG22	2.10	0.52
26:1:597:U:O2'	26:1:598:G:H5'	2.09	0.52
26:1:848:U:O2'	26:1:849:A:H5'	2.10	0.52
26:1:1645:G:O2'	26:1:1646:U:H5'	2.10	0.52
26:1:2604:A:H3'	26:1:2605:G:C5'	2.40	0.52
3:C:107:ALA:O	3:C:111:THR:HG23	2.10	0.52
4:D:27:VAL:HG11	4:D:33:PHE:HD1	1.74	0.52
20:V:11:ASN:OD1	20:V:11:ASN:N	2.42	0.52
23:Y:68:ILE:HD13	23:Y:103:LEU:HD23	1.91	0.52
26:1:1726:A:H2'	26:1:1727:C:C6	2.45	0.52
26:1:1869:G:H2'	26:1:1870:C:H6	1.75	0.52
2:B:50:THR:HG21	26:1:1840:U:H1'	1.91	0.52
18:S:107:ARG:CD	18:S:206:LEU:HD23	2.40	0.52
26:1:650:U:O2'	26:1:651:A:H5'	2.10	0.52
26:1:1071:A:C2	26:1:2515:A:H5'	2.44	0.52
26:1:1241:A:H2'	26:1:1242:A:C8	2.45	0.52
8:H:41:VAL:HG22	8:H:42:LYS:H	1.74	0.52
18:S:157:GLU:OE1	18:S:157:GLU:N	2.29	0.52
21:W:61:VAL:HG13	21:W:87:ILE:HD13	1.92	0.52
26:1:28:A:H2'	26:1:29:U:H6	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:115:C:H2'	26:1:116:G:C8	2.45	0.52
26:1:591:A:H4'	26:1:592:A:C5'	2.37	0.52
8:H:81:PRO:HB2	23:Y:35:GLN:OE1	2.10	0.52
19:U:175:LYS:HD3	26:1:2558:A:N7	2.25	0.52
26:1:1558:U:H2'	26:1:1559:G:H8	1.71	0.52
26:1:2055:U:O2'	26:1:2056:G:H5'	2.09	0.52
26:1:2427:G:O2'	26:1:2428:U:H5'	2.10	0.52
26:1:2501:U:O2'	26:1:2502:C:OP1	2.24	0.52
27:2:101:A:H5'	27:2:102:G:OP2	2.10	0.52
4:D:38:VAL:HG21	4:D:56:ALA:O	2.09	0.52
5:E:9:THR:H	5:E:102:HIS:HD2	1.56	0.52
7:G:91:VAL:CG1	7:G:100:GLU:HG2	2.38	0.52
18:S:176:THR:OG1	18:S:177:THR:N	2.43	0.52
19:U:44:LYS:HG3	19:U:46:GLU:HG2	1.92	0.52
26:1:948:U:O2'	26:1:949:C:H5'	2.10	0.52
26:1:1598:U:H2'	26:1:1599:G:C8	2.45	0.52
26:1:1598:U:H4'	26:1:1768:C:O2	2.10	0.52
27:2:14:G:OP2	27:2:14:G:C8	2.63	0.52
1:A:28:LEU:HD12	1:A:87:GLU:O	2.11	0.51
26:1:10:A:O2'	26:1:11:U:OP1	2.25	0.51
26:1:1520:A:H2'	26:1:1521:A:O4'	2.09	0.51
11:L:6:LEU:CD2	11:L:210:GLU:HG2	2.40	0.51
26:1:181:G:O2'	26:1:182:C:H5'	2.09	0.51
26:1:306:C:H2'	26:1:307:A:H8	1.74	0.51
2:B:125:LYS:HG3	2:B:128:ASN:OD1	2.10	0.51
14:O:18:ILE:HD13	26:1:2446:U:H5'	1.92	0.51
22:X:27:ASN:O	22:X:31:SER:HA	2.11	0.51
26:1:133:A:H2'	26:1:134:U:O4'	2.10	0.51
26:1:306:C:H2'	26:1:307:A:C8	2.45	0.51
26:1:1585:G:C5	26:1:1586:U:H1'	2.45	0.51
26:1:2845:G:H2'	26:1:2846:A:C8	2.46	0.51
26:1:2875:U:O2'	26:1:2876:G:H5'	2.10	0.51
22:X:54:GLN:OE1	26:1:870:C:O2'	2.25	0.51
26:1:148:U:O2'	26:1:149:U:H5'	2.11	0.51
26:1:269:G:H21	26:1:323:C:H1'	1.74	0.51
26:1:541:G:H2'	26:1:542:A:C8	2.46	0.51
26:1:1353:A:O2'	26:1:1354:G:H5'	2.10	0.51
26:1:1858:G:O2'	26:1:1859:C:H5'	2.11	0.51
26:1:1981:G:O2'	26:1:1983:U:O4	2.13	0.51
26:1:2038:U:H2'	26:1:2039:G:O4'	2.11	0.51
26:1:2846:A:O2'	26:1:2847:U:H5'	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:VAL:HG22	2:B:94:VAL:HG12	1.92	0.51
4:D:24:LYS:HA	4:D:93:THR:HG23	1.92	0.51
11:L:115:VAL:HG12	11:L:214:SER:HB2	1.92	0.51
14:O:5:VAL:HG11	14:O:21:LYS:HG2	1.92	0.51
16:Q:50:VAL:HG23	16:Q:55:MET:HG2	1.93	0.51
26:1:1576:A:H2'	26:1:1577:G:C8	2.46	0.51
26:1:2496:A:H2'	26:1:2497:G:O4'	2.11	0.51
26:1:2674:U:O2'	26:1:2675:G:H5'	2.10	0.51
26:1:2900:C:O4'	26:1:2900:C:O2	2.28	0.51
23:Y:128:LYS:HE3	26:1:1074:G:OP2	2.10	0.51
26:1:434:G:H5"	26:1:435:A:OP2	2.10	0.51
26:1:794:A:H2'	26:1:795:A:C8	2.46	0.51
26:1:2474:G:C8	26:1:2527:U:H2'	2.45	0.51
26:1:2869:G:O2'	26:1:2886:G:N2	2.43	0.51
2:B:117:GLU:HB2	2:B:130:LEU:CD2	2.33	0.51
12:M:11:SER:OG	12:M:13:ILE:HG13	2.10	0.51
20:V:126:TYR:OH	20:V:133:HIS:NE2	2.33	0.51
26:1:318:A:N3	26:1:318:A:C2'	2.74	0.51
26:1:751:A:H2'	26:1:752:G:O4'	2.09	0.51
26:1:1352:C:H2'	26:1:1353:A:C8	2.46	0.51
26:1:1572:G:H2'	26:1:1573:A:C8	2.45	0.51
26:1:1926:A:H2	26:1:1929:C:N4	2.08	0.51
26:1:2543:G:O2'	26:1:2544:C:H5'	2.11	0.51
26:1:2869:G:N2	26:1:2886:G:O2'	2.44	0.51
10:K:14:ILE:O	10:K:18:ILE:HG12	2.11	0.51
18:S:18:GLU:O	18:S:19:LEU:HD23	2.11	0.51
19:U:26:VAL:HG12	19:U:79:VAL:HG21	1.92	0.51
26:1:448:A:O2'	26:1:449:U:H5'	2.11	0.51
26:1:289:U:H5"	26:1:290:U:H3'	1.92	0.51
26:1:2082:C:C2'	26:1:2082:C:O2	2.57	0.51
26:1:2636:U:O2'	26:1:2637:C:H5'	2.11	0.51
26:1:2859:G:O2'	26:1:2860:U:H5'	2.11	0.51
18:S:165:LEU:HD13	26:1:364:A:C8	2.45	0.51
19:U:77:GLN:HA	19:U:80:SER:HB3	1.93	0.51
26:1:37:C:O2'	26:1:38:A:H5'	2.10	0.51
26:1:1745:A:H2'	26:1:1746:G:H5'	1.93	0.51
26:1:2535:G:H2'	26:1:2536:G:H8	1.75	0.51
14:O:15:ARG:HG2	14:O:37:SER:CB	2.41	0.50
26:1:744:A:H62	26:1:1677:G:H21	1.59	0.50
26:1:969:A:O2'	26:1:970:U:H4'	2.11	0.50
26:1:2093:C:O2'	26:1:2094:G:H5'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2537:C:O2'	26:1:2538:U:H5'	2.11	0.50
26:1:2716:U:H5"	26:1:2740:A:C2	2.46	0.50
2:B:77:LYS:NZ	2:B:111:GLU:O	2.34	0.50
2:B:77:LYS:NZ	2:B:112:VAL:O	2.22	0.50
5:E:20:VAL:HG23	5:E:47:ILE:HD12	1.92	0.50
11:L:6:LEU:HD13	11:L:53:PHE:HB2	1.92	0.50
26:1:301:U:O2	26:1:301:U:O4'	2.29	0.50
26:1:762:C:H5"	26:1:763:A:C4	2.47	0.50
26:1:1808:U:O2	26:1:1808:U:C2'	2.59	0.50
8:H:4:LEU:HD13	8:H:47:GLU:OE1	2.11	0.50
8:H:7:ILE:HG13	8:H:42:LYS:HB2	1.94	0.50
26:1:408:U:C2'	26:1:409:G:H5'	2.41	0.50
26:1:622:A:H2'	26:1:623:C:H6	1.76	0.50
26:1:675:G:N2	26:1:678:A:OP2	2.39	0.50
26:1:1226:G:N2	26:1:1227:U:O4	2.44	0.50
26:1:1227:U:H2'	26:1:1228:A:C8	2.38	0.50
26:1:1768:C:O2'	26:1:1769:C:H5'	2.12	0.50
26:1:2919:A:H2'	26:1:2920:U:O4'	2.11	0.50
6:F:6:ILE:HD11	6:F:41:ALA:HB2	1.94	0.50
6:F:55:ILE:HG21	6:F:76:ARG:HE	1.77	0.50
20:V:38:ARG:HH21	26:1:1051:C:H5"	1.76	0.50
23:Y:34:LEU:HD11	23:Y:129:THR:OG1	2.12	0.50
26:1:259:A:H2'	26:1:260:A:H8	1.76	0.50
26:1:1911:A:HO2'	26:1:1912:A:P	2.35	0.50
6:F:14:GLU:OE1	6:F:15:LYS:HB2	2.11	0.50
11:L:116:ILE:HD12	11:L:211:ILE:CG2	2.41	0.50
26:1:830:U:H2'	26:1:831:C:C6	2.46	0.50
26:1:1489:A:H2'	26:1:1490:G:C8	2.47	0.50
26:1:2017:C:H2'	26:1:2018:U:C6	2.46	0.50
26:1:2472:G:H2'	26:1:2473:G:H5'	1.93	0.50
26:1:2533:U:O2'	26:1:2534:C:H6	1.94	0.50
26:1:2535:G:H2'	26:1:2536:G:C8	2.45	0.50
26:1:2827:A:H2'	26:1:2828:U:O4'	2.10	0.50
1:A:26:ASP:HB2	1:A:90:ARG:O	2.12	0.50
26:1:1252:A:H2'	26:1:1253:G:C8	2.47	0.50
26:1:2664:U:O2'	26:1:2665:G:H5'	2.12	0.50
5:E:17:VAL:HG13	5:E:47:ILE:HD11	1.93	0.50
26:1:302:A:H2'	26:1:303:G:C8	2.46	0.50
26:1:392:U:O2'	26:1:393:G:H5'	2.12	0.50
26:1:1480:G:O2'	26:1:1481:A:H5'	2.11	0.50
26:1:1675:G:N2	26:1:1677:G:H2'	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ASP:OD2	2:B:87:ARG:NH1	2.40	0.50
4:D:25:LEU:O	4:D:65:GLN:NE2	2.45	0.50
26:1:1862:G:H1	26:1:1932:C:H5	1.60	0.50
27:2:29:C:H2'	27:2:30:U:C6	2.47	0.50
5:E:48:GLU:O	5:E:52:MET:HG2	2.12	0.50
7:G:16:ASP:HB3	7:G:19:LYS:HE3	1.92	0.50
12:M:51:LYS:HB3	12:M:51:LYS:HZ3	1.75	0.50
19:U:17:VAL:CG2	19:U:26:VAL:HG22	2.38	0.50
19:U:19:PHE:HZ	19:U:50:ILE:HG21	1.76	0.50
21:W:73:ASP:OD2	21:W:73:ASP:N	2.37	0.50
26:1:684:U:H2'	26:1:685:C:C6	2.46	0.50
26:1:1698:A:H1'	26:1:2843:A:H5'	1.93	0.50
26:1:2761:C:H2'	26:1:2762:G:O4'	2.12	0.50
26:1:2885:U:H2'	26:1:2886:G:C8	2.47	0.50
2:B:154:ILE:HG21	2:B:176:LEU:CD2	2.41	0.49
5:E:9:THR:H	5:E:102:HIS:CD2	2.29	0.49
20:V:22:GLU:HG3	20:V:62:LYS:HG3	1.93	0.49
26:1:1932:C:O2	26:1:1932:C:O4'	2.29	0.49
28:I:24:SER:OG	28:I:25:GLU:N	2.45	0.49
3:C:33:LYS:HG2	26:1:1290:G:N3	2.28	0.49
8:H:81:PRO:HG3	23:Y:25:ASN:HB3	1.94	0.49
12:M:47:ILE:HD12	12:M:56:VAL:HG11	1.93	0.49
26:1:221:G:H22	26:1:238:U:H4'	1.77	0.49
26:1:282:A:N6	26:1:288:C:N3	2.61	0.49
26:1:613:G:H2'	26:1:2057:A:N7	2.26	0.49
26:1:672:A:H4'	26:1:673:G:O5'	2.12	0.49
26:1:698:U:O4'	26:1:698:U:O2	2.29	0.49
26:1:1347:G:O2'	26:1:1655:C:H5"	2.12	0.49
26:1:1651:C:C4'	26:1:1652:A:H5'	2.40	0.49
26:1:1756:U:H3	26:1:1773:A:H62	1.60	0.49
28:I:35:ASP:OD1	28:I:76:LYS:HA	2.12	0.49
8:H:21:LEU:CD1	8:H:26:LYS:HB3	2.42	0.49
26:1:2531:U:H2'	29:1:3001:U7Y:O2	2.11	0.49
26:1:2841:A:H2'	26:1:2842:G:H8	1.76	0.49
2:B:69:ARG:O	2:B:189:ARG:NH1	2.45	0.49
11:L:189:ASP:HB3	11:L:194:VAL:CG2	2.41	0.49
21:W:112:MET:HA	21:W:115:VAL:CG2	2.42	0.49
26:1:323:C:O2	26:1:323:C:O4'	2.25	0.49
26:1:1223:A:O2'	26:1:1224:U:H5'	2.12	0.49
26:1:1390:A:H2'	26:1:1391:A:C8	2.47	0.49
26:1:1812:A:H2'	26:1:1814:A:N7	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2614:A:HO2'	26:1:2615:G:H5'	1.78	0.49
26:1:2870:A:H2'	26:1:2871:A:H8	1.75	0.49
18:S:150:LYS:H	18:S:150:LYS:CD	2.16	0.49
26:1:972:A:H2'	26:1:973:A:C8	2.47	0.49
26:1:1013:U:H2'	26:1:1014:U:C6	2.47	0.49
26:1:2494:C:H2'	26:1:2495:A:O4'	2.12	0.49
26:1:2822:C:C4'	26:1:2823:G:H2'	2.42	0.49
27:2:83:C:H2'	27:2:84:U:O4'	2.12	0.49
7:G:31:ASP:HB3	7:G:65:VAL:HG12	1.93	0.49
16:Q:27:ALA:O	16:Q:28:PHE:HB2	2.13	0.49
23:Y:44:SER:HB3	23:Y:70:PRO:HG3	1.95	0.49
26:1:479:C:O2'	26:1:480:U:H5'	2.12	0.49
26:1:754:U:H2'	26:1:755:C:H6	1.76	0.49
26:1:2342:U:H2'	26:1:2343:U:C6	2.48	0.49
26:1:2888:A:H2'	26:1:2889:G:H8	1.74	0.49
3:C:104:LYS:HE2	3:C:104:LYS:HA	1.95	0.49
26:1:156:A:H2'	26:1:157:U:O4'	2.13	0.49
26:1:173:A:O2'	26:1:174:U:H5'	2.13	0.49
26:1:243:U:H5"	26:1:668:C:H5"	1.94	0.49
26:1:541:G:O2'	26:1:542:A:H5'	2.13	0.49
26:1:29:U:H2'	26:1:30:G:H8	1.75	0.49
26:1:161:A:H8	26:1:167:U:H3	1.60	0.49
26:1:404:U:H4'	26:1:405:G:OP1	2.12	0.49
26:1:2856:U:H2'	26:1:2857:A:C8	2.47	0.49
2:B:135:ILE:HD13	2:B:141:VAL:HG11	1.93	0.49
14:O:9:CYS:HB3	14:O:14:ASP:HA	1.95	0.49
19:U:63:THR:HG22	26:1:2776:A:C1'	2.42	0.49
22:X:96:LEU:HD23	22:X:109:ILE:HD12	1.94	0.49
26:1:289:U:H5'	26:1:291:G:C8	2.48	0.49
26:1:545:G:N1	26:1:548:A:OP2	2.44	0.49
26:1:831:C:O2'	26:1:832:C:H5'	2.12	0.49
5:E:82:LEU:HB2	5:E:98:LYS:HB2	1.95	0.49
18:S:120:GLU:O	18:S:120:GLU:HG2	2.11	0.49
26:1:197:G:H2'	26:1:198:A:C8	2.47	0.49
26:1:2818:A:O2'	26:1:2819:C:H5'	2.12	0.49
26:1:2901:U:H2'	26:1:2902:A:H8	1.77	0.49
1:A:36:GLU:O	1:A:36:GLU:HG3	2.13	0.48
4:D:11:GLN:HE21	4:D:39:LEU:CD1	2.25	0.48
10:K:25:LEU:O	10:K:29:ARG:HG2	2.13	0.48
18:S:51:VAL:HG22	18:S:88:ILE:HG13	1.95	0.48
26:1:142:G:H1'	26:1:1640:U:O2'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:293:U:H2'	26:1:294:G:H8	1.78	0.48
26:1:507:C:H2'	26:1:508:C:C6	2.48	0.48
26:1:1253:G:H2'	26:1:1254:C:C6	2.48	0.48
26:1:2326:G:O2'	26:1:2327:A:H5'	2.12	0.48
26:1:2490:C:O2'	26:1:2491:C:H5'	2.13	0.48
14:O:31:GLU:HG2	14:O:46:ARG:CD	2.43	0.48
18:S:107:ARG:HD2	18:S:206:LEU:HD23	1.95	0.48
26:1:746:G:H5'	26:1:1676:A:H1'	1.95	0.48
26:1:898:U:O2'	26:1:899:U:H5'	2.13	0.48
26:1:1710:G:H2'	26:1:1711:G:C8	2.48	0.48
26:1:2271:U:O2'	26:1:2272:U:H5'	2.13	0.48
26:1:2516:G:H21	26:1:2518:U:H3	1.60	0.48
26:1:2532:G:H2'	26:1:2603:G:N1	2.27	0.48
6:F:34:ASN:O	6:F:38:VAL:HG23	2.13	0.48
11:L:6:LEU:HD23	11:L:210:GLU:HG2	1.94	0.48
23:Y:43:THR:HG22	23:Y:45:ARG:H	1.77	0.48
26:1:1403:C:H2'	26:1:1404:A:O4'	2.14	0.48
26:1:2077:C:H2'	26:1:2078:A:O4'	2.13	0.48
2:B:161:SER:HB3	2:B:194:GLN:HG3	1.96	0.48
8:H:79:PHE:CE1	8:H:84:ASN:HA	2.49	0.48
19:U:56:SER:OG	19:U:57:ASP:N	2.46	0.48
26:1:1781:C:O2	26:1:1781:C:O5'	2.32	0.48
26:1:2464:C:C2'	26:1:2465:U:H5'	2.43	0.48
26:1:2607:U:O2'	26:1:2608:G:H5'	2.12	0.48
28:I:27:LYS:HB3	28:I:29:LEU:CD1	2.43	0.48
6:F:50:VAL:HG22	6:F:82:LEU:CD2	2.43	0.48
22:X:83:ASN:O	22:X:119:LYS:NZ	2.46	0.48
26:1:388:A:H1'	26:1:389:A:C2	2.48	0.48
26:1:720:A:O2'	26:1:721:A:H5'	2.13	0.48
26:1:1724:U:N3	26:1:1791:G:OP2	2.45	0.48
26:1:1932:C:H2'	26:1:1957:G:C8	2.49	0.48
2:B:71:LYS:NZ	2:B:98:ASP:OD2	2.46	0.48
4:D:48:VAL:HG21	4:D:53:VAL:HG21	1.96	0.48
16:Q:58:VAL:HG23	16:Q:58:VAL:O	2.13	0.48
18:S:147:GLU:CD	18:S:147:GLU:O	2.51	0.48
26:1:402:C:O4'	26:1:402:C:O2	2.31	0.48
26:1:620:G:O2'	26:1:1292:A:OP1	2.32	0.48
26:1:1350:U:O2'	26:1:1351:C:OP1	2.25	0.48
26:1:1823:U:H2'	26:1:1824:C:C6	2.47	0.48
26:1:1884:G:O2'	26:1:1885:G:H5'	2.13	0.48
26:1:2223:C:O2'	26:1:2224:U:H5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2615:G:HO2'	26:1:2616:A:H5'	1.78	0.48
1:A:18:ASP:OD1	1:A:18:ASP:N	2.47	0.48
18:S:156:THR:C	18:S:198:ALA:HB2	2.34	0.48
21:W:17:ARG:HD2	21:W:47:THR:HG23	1.96	0.48
26:1:1836:A:H2'	26:1:1837:A:C8	2.49	0.48
3:C:61:TRP:CZ2	3:C:93:LYS:HD3	2.49	0.48
7:G:92:ARG:O	7:G:100:GLU:HA	2.14	0.48
9:J:7:VAL:HG21	9:J:58:LYS:NZ	2.29	0.48
11:L:157:ALA:HB2	26:1:2602:C:H5"	1.96	0.48
26:1:672:A:N1	26:1:681:G:O2'	2.46	0.48
26:1:755:C:C3'	26:1:756:A:H5"	2.43	0.48
26:1:1216:U:C4	26:1:1219:G:H1'	2.49	0.48
26:1:1347:G:C3'	26:1:1348:U:H5'	2.44	0.48
11:L:70:ASN:OD1	11:L:70:ASN:N	2.43	0.48
12:M:2:ALA:HB3	12:M:36:VAL:CG1	2.39	0.48
20:V:63:ILE:HD13	20:V:102:ILE:HG12	1.96	0.48
21:W:3:GLN:NE2	26:1:2022:U:O4'	2.47	0.48
21:W:8:LEU:HD23	21:W:82:ASN:CB	2.43	0.48
21:W:108:GLU:HB2	21:W:110:ASN:ND2	2.28	0.48
26:1:787:U:H2'	26:1:788:A:H8	1.79	0.48
26:1:1589:U:O2'	26:1:1590:C:H5'	2.14	0.48
26:1:1886:A:H2'	26:1:1887:G:O4'	2.14	0.48
26:1:2579:U:C2	26:1:2581:U:H5"	2.49	0.48
7:G:40:ILE:CG2	7:G:58:GLU:HG2	2.44	0.47
24:Z:88:GLU:OE1	24:Z:88:GLU:N	2.44	0.47
26:1:555:C:H2'	26:1:556:U:O2	2.14	0.47
26:1:679:G:H2'	26:1:680:C:C6	2.49	0.47
26:1:1323:A:H1'	26:1:1325:U:OP2	2.13	0.47
26:1:1582:U:H3'	26:1:1584:U:C5'	2.43	0.47
26:1:2298:G:OP1	28:I:26:SER:HB3	2.14	0.47
8:H:63:LEU:HD23	8:H:64:GLY:N	2.29	0.47
21:W:108:GLU:HB2	21:W:110:ASN:CG	2.35	0.47
26:1:139:U:H5"	26:1:140:A:OP2	2.13	0.47
26:1:2097:G:H2'	26:1:2098:A:H8	1.79	0.47
26:1:2609:G:O2'	26:1:2610:G:H5'	2.14	0.47
21:W:41:CYS:SG	21:W:58:VAL:HG23	2.54	0.47
23:Y:17:THR:O	23:Y:39:THR:HG21	2.14	0.47
26:1:615:A:H61	26:1:2056:G:H8	1.61	0.47
26:1:1356:G:O2'	26:1:1357:G:H5'	2.14	0.47
26:1:2084:G:O2'	26:1:2085:A:H5'	2.13	0.47
3:C:13:ARG:NH1	26:1:1289:A:H5"	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:LYS:HE2	3:C:38:GLN:NE2	2.29	0.47
3:C:91:ASN:H	3:C:91:ASN:ND2	2.07	0.47
7:G:10:LYS:CB	7:G:71:LEU:HD11	2.44	0.47
11:L:56:LYS:HE3	11:L:86:ARG:HG2	1.96	0.47
18:S:95:ARG:NH2	26:1:1285:A:OP1	2.47	0.47
26:1:984:G:H2'	26:1:985:A:O4'	2.13	0.47
26:1:2237:U:H4'	26:1:2238:U:OP1	2.14	0.47
26:1:2383:C:H2'	26:1:2384:U:O4'	2.14	0.47
26:1:2582:U:O2'	26:1:2583:C:H5'	2.14	0.47
27:2:4:G:O2'	27:2:5:G:H5'	2.14	0.47
4:D:21:PHE:CE2	4:D:94:LYS:HD3	2.49	0.47
26:1:2601:G:H2'	26:1:2602:C:C6	2.50	0.47
26:1:2642:U:H2'	26:1:2643:C:C6	2.49	0.47
18:S:198:ALA:O	18:S:202:VAL:HG13	2.14	0.47
22:X:69:ILE:CD1	26:1:2433:C:H1'	2.39	0.47
23:Y:79:LEU:N	23:Y:79:LEU:HD12	2.29	0.47
26:1:308:C:H2'	26:1:309:U:C6	2.49	0.47
1:A:74:ARG:HG3	1:A:74:ARG:HH11	1.78	0.47
2:B:260:ARG:HB2	26:1:1825:U:OP1	2.14	0.47
6:F:64:ARG:HD2	6:F:72:THR:HG22	1.96	0.47
8:H:22:ARG:NH2	8:H:87:THR:O	2.34	0.47
11:L:5:ILE:HG13	11:L:110:PHE:CE2	2.48	0.47
13:N:40:HIS:ND1	26:1:2835:C:O2'	2.35	0.47
19:U:40:ARG:O	19:U:40:ARG:HG2	2.15	0.47
22:X:103:LYS:NZ	26:1:649:U:O4	2.48	0.47
26:1:279:A:H2'	26:1:280:C:H5'	1.97	0.47
26:1:498:G:N2	26:1:503:A:O2'	2.48	0.47
26:1:788:A:O2'	26:1:1703:U:OP1	2.32	0.47
26:1:797:A:C5	26:1:1808:U:H1'	2.50	0.47
26:1:1596:G:H2'	26:1:1597:U:C6	2.50	0.47
26:1:1979:A:N3	26:1:2587:C:O2'	2.42	0.47
26:1:2041:A:H2'	26:1:2042:A:C8	2.49	0.47
26:1:2308:C:O2'	26:1:2309:G:H5'	2.15	0.47
26:1:2540:A:H2'	26:1:2541:U:C6	2.49	0.47
26:1:2642:U:O2	26:1:2642:U:C2'	2.63	0.47
2:B:16:MET:HG2	2:B:17:THR:N	2.30	0.47
2:B:150:LYS:NZ	2:B:153:GLN:HE22	2.12	0.47
2:B:220:VAL:HG21	26:1:827:A:N7	2.29	0.47
8:H:49:ILE:O	8:H:53:ARG:HG3	2.14	0.47
21:W:63:VAL:CG1	21:W:102:VAL:HG22	2.44	0.47
26:1:696:G:O2'	26:1:697:U:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:ARG:NH1	8:H:13:GLN:HG3	2.29	0.47
26:1:504:G:N2	26:1:515:G:H2'	2.29	0.47
26:1:877:G:H2'	26:1:878:C:C6	2.50	0.47
26:1:1202:C:H2'	26:1:1203:U:C6	2.50	0.47
26:1:2085:A:O2'	26:1:2086:A:H5'	2.14	0.47
10:K:44:ARG:O	10:K:44:ARG:HG2	2.15	0.47
17:R:6:SER:O	17:R:6:SER:OG	2.28	0.47
19:U:90:VAL:HG21	19:U:163:ARG:HD3	1.96	0.47
26:1:363:A:H4'	26:1:365:A:N7	2.30	0.47
26:1:1584:U:C5	26:1:1585:G:H1'	2.50	0.47
26:1:2500:U:C2'	26:1:2501:U:H5'	2.45	0.47
3:C:91:ASN:ND2	3:C:94:MET:HB2	2.30	0.46
6:F:14:GLU:O	6:F:18:GLU:HB2	2.15	0.46
7:G:35:VAL:HB	7:G:38:VAL:HB	1.97	0.46
19:U:25:THR:HG23	19:U:35:ARG:HB2	1.97	0.46
26:1:687:G:N2	26:1:689:A:H2'	2.30	0.46
26:1:901:G:H2'	26:1:902:A:C8	2.50	0.46
26:1:969:A:H3'	26:1:970:U:O4'	2.15	0.46
26:1:1680:U:H2'	26:1:1681:U:C6	2.50	0.46
26:1:2580:G:OP1	26:1:2580:G:N2	2.48	0.46
26:1:2601:G:O2'	26:1:2602:C:H5'	2.15	0.46
1:A:14:GLN:NE2	11:L:16:PHE:H	2.13	0.46
22:X:50:PHE:CZ	26:1:254:A:H5"	2.50	0.46
26:1:2006:C:C2'	26:1:2007:G:H5'	2.46	0.46
6:F:22:GLU:HG2	6:F:23:ASP:N	2.29	0.46
6:F:51:ALA:N	6:F:81:THR:O	2.47	0.46
16:Q:40:GLN:NE2	26:1:2389:G:OP1	2.48	0.46
21:W:101:PRO:HB2	21:W:104:ARG:HH12	1.80	0.46
26:1:451:U:O2'	26:1:452:G:H5'	2.16	0.46
26:1:1721:A:H2'	26:1:1722:A:H8	1.76	0.46
26:1:1737:U:H4'	26:1:1738:C:OP2	2.16	0.46
26:1:1781:C:O2	26:1:1781:C:O4'	2.30	0.46
26:1:2534:C:O2'	26:1:2535:G:H5'	2.16	0.46
26:1:275:A:N6	26:1:296:G:C2	2.82	0.46
26:1:688:A:N1	26:1:2396:A:O2'	2.46	0.46
26:1:962:A:H5"	26:1:2295:A:N6	2.29	0.46
26:1:1751:G:H2'	26:1:1752:C:C6	2.51	0.46
26:1:1864:C:H2'	26:1:1926:A:N6	2.30	0.46
26:1:1942:U:H3'	26:1:1943:A:C2	2.51	0.46
2:B:111:GLU:O	2:B:111:GLU:HG3	2.15	0.46
23:Y:35:GLN:HE22	23:Y:130:LYS:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:409:G:H2'	26:1:410:G:O4'	2.14	0.46
26:1:719:G:H2'	26:1:849:A:H61	1.80	0.46
26:1:1581:U:H5"	26:1:1583:G:C4'	2.40	0.46
26:1:2347:A:N3	26:1:2347:A:C2'	2.77	0.46
26:1:2362:A:H4'	26:1:2362:A:OP1	2.16	0.46
27:2:84:U:O2'	27:2:85:U:O4'	2.33	0.46
11:L:108:ASP:O	11:L:111:VAL:HG23	2.16	0.46
21:W:91:LYS:HD2	21:W:111:PHE:CE1	2.50	0.46
26:1:967:C:O2'	28:I:34:ALA:HB2	2.16	0.46
26:1:1065:A:H2'	26:1:1066:G:H4'	1.97	0.46
26:1:1210:U:H2'	26:1:1211:G:O4'	2.16	0.46
26:1:1595:C:H2'	26:1:1596:G:C8	2.50	0.46
26:1:2580:G:P	26:1:2580:G:H21	2.39	0.46
26:1:2615:G:H2'	26:1:2616:A:C8	2.51	0.46
26:1:2886:G:H1'	26:1:2888:A:C4'	2.45	0.46
8:H:49:ILE:HG13	8:H:50:LYS:N	2.31	0.46
16:Q:52:LYS:O	16:Q:56:LYS:HG2	2.16	0.46
23:Y:79:LEU:HD12	23:Y:79:LEU:H	1.81	0.46
26:1:414:C:O2'	26:1:415:U:H5'	2.16	0.46
26:1:525:A:H4'	26:1:526:A:OP1	2.16	0.46
26:1:632:U:H2'	26:1:633:A:H8	1.80	0.46
26:1:893:G:H2'	26:1:894:A:H8	1.80	0.46
26:1:962:A:H2'	26:1:963:A:C8	2.50	0.46
26:1:1290:G:O2'	26:1:1291:A:O4'	2.34	0.46
26:1:1713:A:O2'	26:1:1714:C:H5'	2.15	0.46
26:1:2536:G:O2'	26:1:2537:C:C5'	2.61	0.46
26:1:2608:G:H4'	26:1:2609:G:C8	2.51	0.46
1:A:19:LEU:HD12	1:A:19:LEU:O	2.16	0.46
11:L:138:ARG:CZ	11:L:138:ARG:HB2	2.45	0.46
20:V:113:THR:O	20:V:116:GLY:N	2.49	0.46
24:Z:4:ARG:NH1	26:1:1696:C:OP1	2.49	0.46
26:1:393:G:H2'	26:1:394:U:O4'	2.16	0.46
26:1:432:G:H4'	26:1:433:U:OP2	2.16	0.46
26:1:1463:A:H2'	26:1:1464:U:H5"	1.97	0.46
26:1:2580:G:H8	26:1:2609:G:H21	1.63	0.46
2:B:132:LEU:HG	2:B:188:CYS:O	2.16	0.46
7:G:44:HIS:ND1	7:G:56:ILE:HG12	2.30	0.46
24:Z:25:ILE:HD11	24:Z:81:ALA:HB1	1.98	0.46
26:1:157:U:C2'	26:1:158:G:H5'	2.46	0.46
26:1:888:G:O2'	26:1:889:U:H5'	2.16	0.46
26:1:1245:G:O2'	26:1:1246:C:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1914:C:H2'	26:1:1915:G:H5'	1.97	0.46
26:1:2109:A:H2'	26:1:2110:G:O4'	2.16	0.46
27:2:13:A:H1'	27:2:104:A:C5	2.51	0.46
27:2:15:C:N4	27:2:103:A:H2	2.13	0.46
27:2:96:A:H2'	27:2:97:G:H5'	1.97	0.46
8:H:9:ARG:HB2	8:H:13:GLN:OE1	2.15	0.46
19:U:4:VAL:O	19:U:69:ARG:HD2	2.16	0.46
26:1:37:C:H4'	26:1:497:U:OP1	2.16	0.46
26:1:37:C:C2'	26:1:38:A:H5'	2.45	0.46
26:1:214:G:O2'	26:1:215:G:H5'	2.16	0.46
26:1:617:A:N6	26:1:2061:U:OP2	2.47	0.46
26:1:651:A:H2'	26:1:652:A:H8	1.75	0.46
26:1:1865:C:H4'	26:1:1866:A:H5"	1.98	0.46
26:1:2271:U:H2'	26:1:2272:U:C6	2.51	0.46
27:2:8:A:H61	27:2:105:C:H42	1.63	0.46
19:U:115:ILE:HG21	19:U:148:ILE:HG12	1.96	0.45
23:Y:1:MET:SD	23:Y:45:ARG:HD3	2.56	0.45
26:1:288:C:C4'	26:1:290:U:H5"	2.42	0.45
26:1:409:G:N3	26:1:410:G:H1'	2.32	0.45
26:1:1312:A:H4'	26:1:1313:G:OP1	2.16	0.45
26:1:2234:C:O2'	26:1:2235:A:H5'	2.17	0.45
26:1:2567:C:H2'	26:1:2568:A:H5'	1.98	0.45
26:1:2801:C:H2'	26:1:2802:A:O4'	2.16	0.45
26:1:2845:G:H2'	26:1:2846:A:H8	1.80	0.45
27:2:87:C:O2'	27:2:88:G:H5'	2.16	0.45
2:B:118:SER:HA	2:B:131:PRO:CD	2.46	0.45
4:D:9:GLY:O	26:1:1040:A:H1'	2.16	0.45
7:G:99:GLU:O	7:G:101:ILE:HG23	2.17	0.45
20:V:33:VAL:HG11	20:V:106:ILE:HD13	1.98	0.45
26:1:293:U:H2'	26:1:294:G:C8	2.51	0.45
26:1:704:U:H2'	26:1:705:U:O4'	2.15	0.45
26:1:1582:U:C5'	26:1:1583:G:H5"	2.39	0.45
26:1:1587:C:H2'	26:1:1588:U:C5'	2.42	0.45
26:1:1949:G:H2'	26:1:1950:U:O4'	2.16	0.45
26:1:2650:G:H2'	26:1:2651:G:H8	1.81	0.45
26:1:2725:U:H2'	26:1:2726:C:C6	2.50	0.45
27:2:27:A:H2'	27:2:28:C:H6	1.81	0.45
5:E:59:GLU:H	5:E:59:GLU:HG3	1.60	0.45
7:G:40:ILE:HG22	7:G:58:GLU:HG2	1.98	0.45
21:W:17:ARG:HB2	21:W:45:ASN:HB3	1.98	0.45
26:1:793:G:N3	26:1:793:G:H2'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1027:A:O2'	26:1:1028:G:H5'	2.17	0.45
26:1:1923:A:H2'	26:1:1924:G:H8	1.78	0.45
26:1:2300:A:H2'	26:1:2301:A:C8	2.51	0.45
1:A:41:ARG:C	1:A:42:ILE:HD13	2.37	0.45
2:B:177:ARG:HH21	26:1:1847:U:H5	1.64	0.45
7:G:86:VAL:HG22	7:G:91:VAL:CG2	2.46	0.45
11:L:34:VAL:O	11:L:51:VAL:HA	2.17	0.45
15:P:9:ASN:HD22	15:P:12:LYS:HD2	1.81	0.45
20:V:73:LYS:HG3	20:V:90:ALA:HB2	1.98	0.45
20:V:75:TYR:O	20:V:87:SER:HA	2.17	0.45
26:1:1329:G:H2'	26:1:1330:U:C6	2.51	0.45
26:1:1937:G:H2'	26:1:1938:U:O4'	2.15	0.45
26:1:2101:U:H2'	26:1:2102:U:C6	2.50	0.45
26:1:2715:G:N1	26:1:2747:U:OP2	2.28	0.45
5:E:13:ALA:HA	5:E:99:ARG:HB2	1.98	0.45
26:1:685:C:H2'	26:1:686:U:C6	2.51	0.45
26:1:1251:A:H2'	26:1:1252:A:C8	2.51	0.45
26:1:1426:G:O2'	26:1:1427:U:H5'	2.16	0.45
26:1:1487:G:H22	26:1:1596:G:N2	2.12	0.45
26:1:2857:A:H2'	26:1:2858:G:H8	1.81	0.45
27:2:60:C:H2'	27:2:61:C:H6	1.81	0.45
2:B:50:THR:HG23	2:B:51:VAL:HG23	1.97	0.45
19:U:42:THR:O	19:U:53:VAL:HB	2.16	0.45
26:1:1793:C:O2'	26:1:1794:C:H5'	2.16	0.45
8:H:49:ILE:O	8:H:52:ILE:HG22	2.17	0.45
10:K:46:VAL:O	10:K:50:ILE:HG13	2.16	0.45
15:P:2:VAL:N	26:1:1663:G:HO2'	2.15	0.45
18:S:161:VAL:O	18:S:165:LEU:HG	2.17	0.45
19:U:58:SER:O	19:U:62:ARG:HG3	2.17	0.45
23:Y:39:THR:HG23	23:Y:98:LYS:HG2	1.99	0.45
23:Y:52:ILE:HG22	23:Y:56:ARG:HH11	1.81	0.45
26:1:245:G:N2	26:1:258:A:OP2	2.36	0.45
26:1:2535:G:O3'	26:1:2582:U:H5"	2.17	0.45
5:E:11:ARG:NH2	5:E:98:LYS:HD2	2.31	0.45
20:V:22:GLU:HG3	20:V:62:LYS:CB	2.47	0.45
24:Z:5:LYS:HD2	26:1:2029:G:OP1	2.16	0.45
26:1:156:A:H62	26:1:172:U:H3	1.63	0.45
26:1:427:A:O2'	26:1:428:G:H5'	2.17	0.45
26:1:575:G:N3	26:1:575:G:H2'	2.32	0.45
26:1:1274:G:H8	26:1:1274:G:OP2	1.99	0.45
26:1:1650:G:H5"	26:1:1651:C:OP1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1862:G:H2'	26:1:1863:C:C6	2.52	0.45
2:B:93:LEU:HD12	2:B:102:ARG:O	2.16	0.45
3:C:4:VAL:HG22	26:1:1238:U:H1'	1.99	0.45
3:C:12:ALA:O	3:C:16:LYS:HG3	2.17	0.45
11:L:122:SER:O	11:L:203:GLY:HA2	2.17	0.45
14:O:15:ARG:HG2	14:O:37:SER:HB2	1.99	0.45
24:Z:102:ARG:O	24:Z:102:ARG:HG3	2.17	0.45
26:1:548:A:N3	26:1:550:A:H2'	2.32	0.45
26:1:999:U:H6	26:1:999:U:O5'	1.99	0.45
26:1:1364:C:H2'	26:1:1365:G:O4'	2.17	0.45
26:1:1469:G:O2'	26:1:1470:G:H5'	2.16	0.45
26:1:1501:G:H22	26:1:2729:G:H22	1.65	0.45
26:1:1817:C:H2'	26:1:1818:A:C5	2.51	0.45
26:1:2856:U:H2'	26:1:2857:A:H8	1.82	0.45
2:B:2:ALA:HB3	2:B:20:ASP:CB	2.47	0.45
2:B:154:ILE:CG2	2:B:176:LEU:HD22	2.45	0.45
11:L:50:GLN:HG2	11:L:90:GLU:HG3	1.97	0.45
16:Q:9:GLY:O	16:Q:13:ARG:NH2	2.44	0.45
20:V:22:GLU:HG3	20:V:62:LYS:CG	2.46	0.45
26:1:283:G:H22	26:1:287:G:P	2.40	0.45
26:1:362:C:O2'	26:1:363:A:H5'	2.17	0.45
26:1:402:C:O2'	26:1:403:U:H5'	2.16	0.45
26:1:762:C:H3'	26:1:763:A:O4'	2.17	0.45
26:1:1867:G:H2'	26:1:1868:U:C6	2.51	0.45
26:1:2222:U:O2'	26:1:2223:C:H5'	2.17	0.45
26:1:2838:C:H4'	26:1:2857:A:H4'	1.98	0.45
4:D:14:VAL:HB	4:D:97:ILE:HG13	1.99	0.44
12:M:30:LYS:O	12:M:33:SER:OG	2.35	0.44
13:N:5:LYS:HE2	26:1:2081:A:O2'	2.17	0.44
17:R:2:LYS:HE3	17:R:31:LYS:O	2.17	0.44
21:W:1:MET:HB2	21:W:2:ILE:CD1	2.46	0.44
26:1:1252:A:H2'	26:1:1253:G:H8	1.81	0.44
26:1:1497:A:H2'	26:1:1498:U:H2'	1.98	0.44
26:1:2815:C:C2'	26:1:2816:C:H5'	2.48	0.44
7:G:93:ILE:O	7:G:93:ILE:HG13	2.17	0.44
18:S:51:VAL:CG2	18:S:88:ILE:HG13	2.47	0.44
19:U:125:VAL:HG13	19:U:127:LYS:O	2.17	0.44
21:W:63:VAL:HG13	21:W:102:VAL:HG13	1.98	0.44
26:1:21:A:O2'	26:1:22:C:H5'	2.17	0.44
2:B:115:ILE:HG22	2:B:117:GLU:HG2	1.98	0.44
4:D:50:ALA:HB1	4:D:51:PRO:CA	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:7:LEU:HD21	6:F:38:VAL:HG13	1.99	0.44
7:G:86:VAL:HG22	7:G:91:VAL:HG21	1.99	0.44
22:X:128:PHE:CZ	22:X:143:HIS:HB2	2.53	0.44
24:Z:92:ARG:HD2	24:Z:93:TYR:CZ	2.52	0.44
26:1:82:G:O2'	26:1:83:G:H5'	2.17	0.44
26:1:904:G:H1'	26:1:905:U:H5	1.81	0.44
26:1:1306:A:H2'	26:1:1307:G:O4'	2.17	0.44
26:1:1783:G:H8	26:1:1783:G:H2'	1.70	0.44
26:1:2007:G:O2'	26:1:2009:U:OP2	2.35	0.44
26:1:2239:A:H5"	26:1:2240:U:C4	2.52	0.44
26:1:2613:C:O2'	26:1:2614:A:H5'	2.17	0.44
26:1:2650:G:H2'	26:1:2651:G:C8	2.52	0.44
1:A:68:SER:HB3	21:W:100:GLY:HA2	1.98	0.44
18:S:17:ILE:HD11	18:S:19:LEU:HD11	1.98	0.44
18:S:18:GLU:HG3	18:S:196:GLU:HG2	1.98	0.44
19:U:99:GLN:NE2	19:U:114:GLU:OE1	2.49	0.44
23:Y:110:SER:HB3	23:Y:113:VAL:HG23	1.99	0.44
26:1:183:A:OP2	26:1:183:A:H3'	2.17	0.44
26:1:310:C:H42	26:1:406:A:N6	2.16	0.44
26:1:388:A:H1'	26:1:389:A:H2	1.82	0.44
2:B:123:ASP:OD1	2:B:123:ASP:N	2.49	0.44
6:F:35:LYS:HB2	6:F:53:VAL:HG13	1.98	0.44
8:H:16:SER:CB	27:2:89:U:H5"	2.48	0.44
19:U:155:GLU:OE2	19:U:158:LYS:N	2.35	0.44
26:1:1044:A:H2'	26:1:1045:A:C8	2.52	0.44
26:1:1063:U:H3	26:1:1186:A:N6	2.14	0.44
26:1:1664:G:C2'	26:1:1665:U:H5'	2.47	0.44
26:1:2091:C:H2'	26:1:2092:C:H6	1.82	0.44
10:K:42:ARG:O	10:K:45:THR:HB	2.18	0.44
18:S:139:PHE:HZ	18:S:154:VAL:HG21	1.81	0.44
18:S:167:ALA:HB1	18:S:173:VAL:HG11	1.98	0.44
20:V:40:LYS:HB3	20:V:40:LYS:HE2	1.74	0.44
22:X:110:LYS:HG3	22:X:127:LYS:HB2	2.00	0.44
26:1:100:U:H4'	26:1:101:G:OP2	2.18	0.44
26:1:1190:A:O2'	26:1:1191:U:H5'	2.18	0.44
26:1:1425:G:O2'	26:1:1426:G:H5'	2.18	0.44
26:1:1443:A:H2'	26:1:1444:C:C6	2.52	0.44
26:1:1556:G:O2'	26:1:1557:C:H5'	2.17	0.44
26:1:1567:A:H3'	26:1:1568:U:C5'	2.48	0.44
26:1:2603:G:N3	26:1:2603:G:C2'	2.79	0.44
28:I:31:ALA:O	28:I:32:LYS:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ALA:HB2	26:1:1817:C:O2'	2.17	0.44
5:E:21:LEU:CD2	5:E:47:ILE:HD13	2.47	0.44
8:H:27:VAL:HG12	8:H:28:PRO:O	2.17	0.44
24:Z:4:ARG:HG2	24:Z:39:GLU:CD	2.37	0.44
26:1:242:U:H2'	26:1:243:U:C6	2.52	0.44
26:1:2218:G:H2'	26:1:2219:C:C6	2.53	0.44
26:1:2634:G:H2'	26:1:2635:G:C8	2.53	0.44
9:J:3:LYS:HE2	26:1:1401:G:OP1	2.18	0.44
16:Q:2:PRO:HD2	26:1:712:U:O2	2.18	0.44
18:S:106:ARG:NH2	26:1:661:U:H2'	2.33	0.44
21:W:35:ILE:HG21	21:W:103:ALA:CB	2.47	0.44
26:1:655:A:H2'	26:1:656:G:C8	2.53	0.44
26:1:673:G:H2'	26:1:674:C:H6	1.82	0.44
26:1:796:A:H2'	26:1:834:A:C2	2.52	0.44
26:1:1497:A:N3	26:1:1497:A:H3'	2.33	0.44
26:1:1930:G:H2'	26:1:1931:G:C8	2.53	0.44
26:1:2538:U:H2'	26:1:2539:C:C6	2.52	0.44
26:1:2870:A:H2'	26:1:2871:A:C8	2.52	0.44
26:1:2872:G:O2'	26:1:2873:C:H5'	2.17	0.44
27:2:107:U:O2'	27:2:108:U:H5'	2.16	0.44
2:B:175:ARG:HA	2:B:180:GLU:O	2.18	0.44
18:S:88:ILE:HD12	26:1:1286:G:N2	2.33	0.44
20:V:48:HIS:CD2	20:V:49:VAL:HG13	2.53	0.44
22:X:15:GLU:O	22:X:15:GLU:HG3	2.16	0.44
22:X:126:HIS:O	22:X:145:VAL:HG13	2.18	0.44
26:1:193:A:H2'	26:1:194:A:O4'	2.18	0.44
26:1:756:A:H2'	26:1:757:G:O4'	2.18	0.44
26:1:1521:A:H61	26:1:1559:G:H1	1.66	0.44
26:1:1773:A:H2'	26:1:1774:A:O4'	2.17	0.44
26:1:1821:U:H2'	26:1:1822:C:H6	1.82	0.44
26:1:1897:U:H3	26:1:1899:U:C5'	2.30	0.44
26:1:2439:A:H2'	26:1:2440:G:O4'	2.18	0.44
27:2:5:G:O2'	27:2:6:U:H5'	2.17	0.44
27:2:86:A:O2'	27:2:87:C:O5'	2.34	0.44
6:F:22:GLU:HG2	6:F:23:ASP:OD1	2.17	0.43
7:G:70:LEU:HD12	7:G:81:VAL:HG11	2.00	0.43
18:S:123:LEU:HD11	18:S:194:ILE:HD11	2.00	0.43
26:1:429:C:N4	26:1:431:C:H2'	2.33	0.43
26:1:1772:G:C2'	26:1:1773:A:H5'	2.47	0.43
26:1:2354:A:H2'	26:1:2355:A:C8	2.53	0.43
26:1:2484:U:O2'	26:1:2485:U:H5'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD11	1:A:86:ILE:CG2	2.48	0.43
10:K:38:GLU:OE1	10:K:38:GLU:HA	2.18	0.43
19:U:72:LEU:O	19:U:76:VAL:HG23	2.17	0.43
26:1:126:A:H5"	26:1:127:C:C6	2.53	0.43
26:1:183:A:H3'	26:1:183:A:P	2.58	0.43
26:1:285:U:H2'	26:1:286:U:C5	2.53	0.43
26:1:630:G:H4'	26:1:631:U:H6	1.83	0.43
26:1:1213:C:H2'	26:1:1214:C:H4'	2.00	0.43
26:1:2092:C:H2'	26:1:2093:C:C6	2.52	0.43
26:1:2360:A:OP1	26:1:2361:U:N3	2.51	0.43
26:1:2548:C:O2'	26:1:2549:U:H5'	2.18	0.43
1:A:34:ILE:O	1:A:40:GLU:HA	2.18	0.43
1:A:108:LYS:HB2	1:A:111:ARG:CZ	2.49	0.43
2:B:65:ILE:HG12	2:B:103:TYR:HB3	2.00	0.43
22:X:73:GLU:O	22:X:107:SER:HB2	2.18	0.43
26:1:1749:G:O2'	26:1:1750:U:H5'	2.18	0.43
26:1:2778:G:N3	26:1:2778:G:H2'	2.33	0.43
26:1:2873:C:O2'	26:1:2874:A:H5'	2.18	0.43
3:C:21:ALA:HB1	3:C:24:TYR:CD2	2.53	0.43
14:O:41:LYS:HB2	14:O:41:LYS:HE3	1.68	0.43
19:U:44:LYS:NZ	19:U:49:THR:O	2.51	0.43
26:1:491:C:O2'	26:1:492:G:H5'	2.18	0.43
26:1:667:G:H2'	26:1:668:C:C6	2.53	0.43
26:1:801:A:H2'	26:1:802:G:O4'	2.18	0.43
26:1:1510:U:H3	26:1:1571:G:H1	1.66	0.43
26:1:1545:U:H2'	26:1:1546:A:C8	2.53	0.43
26:1:1668:U:O2'	26:1:1669:C:H5'	2.19	0.43
3:C:31:LEU:HB2	3:C:34:VAL:HG22	1.99	0.43
7:G:12:ILE:HG13	7:G:69:GLN:HB2	2.00	0.43
19:U:164:TYR:O	19:U:165:GLN:HG2	2.19	0.43
26:1:665:G:H4'	26:1:666:A:H5"	1.99	0.43
26:1:1501:G:O2'	26:1:1502:A:H5'	2.19	0.43
26:1:1583:G:H2'	26:1:1585:G:O6	2.18	0.43
26:1:1914:C:C2'	26:1:1915:G:H5'	2.48	0.43
26:1:1937:G:O2'	26:1:1938:U:H5'	2.18	0.43
26:1:2082:C:O2	26:1:2082:C:H2'	2.17	0.43
26:1:2366:G:H2'	26:1:2367:A:O4'	2.19	0.43
26:1:2480:A:H2'	26:1:2481:G:H8	1.84	0.43
26:1:2789:U:O2'	26:1:2790:G:H5'	2.18	0.43
26:1:2897:A:H2'	26:1:2898:U:C6	2.54	0.43
7:G:59:THR:OG1	7:G:60:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:43:PHE:HB3	19:U:52:VAL:HA	2.00	0.43
22:X:51:GLU:N	22:X:51:GLU:OE2	2.52	0.43
2:B:2:ALA:HB3	2:B:20:ASP:HB2	2.00	0.43
5:E:43:SER:O	5:E:47:ILE:HG13	2.18	0.43
15:P:3:LYS:HE2	26:1:732:C:H5"	1.99	0.43
18:S:90:PHE:CE2	26:1:630:G:H5"	2.54	0.43
18:S:157:GLU:HG2	18:S:158:ASN:N	2.34	0.43
20:V:14:ARG:HD3	20:V:52:GLY:O	2.19	0.43
26:1:1517:A:C2'	26:1:1518:G:H5'	2.48	0.43
26:1:1616:A:H2'	26:1:1617:A:C8	2.54	0.43
26:1:1864:C:H2'	26:1:1926:A:H62	1.84	0.43
26:1:2295:A:O2'	26:1:2296:A:H5"	2.18	0.43
26:1:2742:C:H2'	26:1:2743:U:C6	2.53	0.43
24:Z:24:LEU:HD23	24:Z:44:VAL:HG21	2.01	0.43
26:1:160:G:N2	26:1:160:G:OP2	2.51	0.43
26:1:393:G:O2'	26:1:394:U:H5'	2.18	0.43
26:1:1352:C:H2'	26:1:1353:A:H8	1.81	0.43
26:1:1567:A:H3'	26:1:1568:U:H5"	2.00	0.43
8:H:78:GLN:CB	8:H:87:THR:HB	2.48	0.43
13:N:16:ARG:O	13:N:16:ARG:HG2	2.18	0.43
23:Y:2:LEU:HD23	23:Y:2:LEU:HA	1.88	0.43
26:1:367:A:N6	26:1:381:G:O2'	2.43	0.43
26:1:744:A:H2	26:1:778:G:H21	1.66	0.43
26:1:1336:G:O2'	26:1:1684:A:N6	2.51	0.43
26:1:2043:U:H2'	26:1:2044:C:C6	2.54	0.43
26:1:2350:G:O2'	26:1:2351:U:H5'	2.18	0.43
27:2:51:A:H2'	27:2:52:G:C8	2.54	0.43
28:I:73:GLY:HA3	28:I:90:TYR:O	2.19	0.43
3:C:64:ARG:HH22	20:V:4:THR:HG23	1.84	0.43
15:P:25:THR:OG1	15:P:26:LYS:N	2.52	0.43
19:U:3:ARG:O	19:U:7:LYS:HG3	2.18	0.43
20:V:100:ARG:HG3	20:V:100:ARG:HH11	1.83	0.43
23:Y:40:SER:HB2	23:Y:127:VAL:CG1	2.48	0.43
24:Z:26:ILE:CD1	24:Z:71:ILE:HD11	2.46	0.43
26:1:331:G:O6	26:1:395:U:C2	2.72	0.43
26:1:404:U:O2'	26:1:405:G:N7	2.52	0.43
26:1:991:A:H2'	26:1:992:A:C8	2.53	0.43
26:1:2288:C:OP1	28:I:27:LYS:NZ	2.52	0.43
26:1:2615:G:O6	26:1:2634:G:C6	2.72	0.43
26:1:2664:U:C2'	26:1:2665:G:H5'	2.49	0.43
26:1:2676:U:H2'	26:1:2677:C:H6	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LYS:HE3	1:A:12:LYS:HB3	1.90	0.42
1:A:113:GLN:HG2	1:A:114:GLU:N	2.34	0.42
2:B:44:ASN:ND2	26:1:1833:C:O2	2.52	0.42
2:B:124:ILE:O	2:B:124:ILE:HG13	2.19	0.42
4:D:48:VAL:CG2	4:D:53:VAL:HG21	2.48	0.42
8:H:74:VAL:HG23	8:H:89:ILE:CG2	2.49	0.42
19:U:97:GLN:O	19:U:103:LEU:HD12	2.19	0.42
26:1:176:A:H4'	26:1:177:G:OP2	2.18	0.42
26:1:1003:A:HO2'	26:1:2484:U:HO2'	1.60	0.42
26:1:1360:G:C2'	26:1:1361:G:H5'	2.49	0.42
26:1:1821:U:H2'	26:1:1822:C:C6	2.53	0.42
26:1:2306:G:N7	28:I:22:ARG:NH1	2.67	0.42
26:1:2769:G:O2'	26:1:2770:U:H5'	2.19	0.42
1:A:35:ILE:O	1:A:35:ILE:HG22	2.20	0.42
1:A:74:ARG:HG2	1:A:76:PHE:CZ	2.54	0.42
6:F:49:LYS:HE3	6:F:49:LYS:HB3	1.87	0.42
7:G:4:LYS:H	7:G:4:LYS:HG2	1.65	0.42
21:W:5:GLU:HG3	26:1:1713:A:C8	2.54	0.42
26:1:542:A:H2'	26:1:543:G:H8	1.85	0.42
26:1:848:U:H2'	26:1:849:A:H8	1.82	0.42
26:1:2869:G:H1'	26:1:2888:A:C5	2.54	0.42
8:H:80:ASP:OD1	8:H:81:PRO:HD2	2.20	0.42
14:O:34:LYS:HE3	26:1:2372:G:OP2	2.20	0.42
19:U:77:GLN:HB3	19:U:83:TYR:OH	2.18	0.42
26:1:632:U:H2'	26:1:633:A:C8	2.54	0.42
26:1:909:G:H2'	26:1:910:C:C6	2.54	0.42
26:1:2244:G:O2'	26:1:2245:G:H5'	2.18	0.42
2:B:205:VAL:O	2:B:210:ARG:HD3	2.19	0.42
12:M:44:ARG:O	12:M:47:ILE:HG12	2.20	0.42
16:Q:8:ARG:O	16:Q:12:LYS:HG3	2.20	0.42
19:U:24:VAL:HG11	19:U:72:LEU:HD21	2.01	0.42
21:W:1:MET:CB	21:W:2:ILE:HD13	2.50	0.42
24:Z:27:SER:O	24:Z:28:GLU:HB2	2.19	0.42
26:1:2775:A:O2'	26:1:2776:A:H5'	2.19	0.42
26:1:2847:U:H2'	26:1:2848:G:H8	1.84	0.42
27:2:39:G:P	27:2:41:C:H41	2.43	0.42
2:B:140:VAL:CG1	2:B:161:SER:HB2	2.49	0.42
5:E:11:ARG:O	5:E:11:ARG:HG3	2.20	0.42
11:L:144:GLY:O	26:1:2607:U:H5"	2.19	0.42
14:O:32:MET:O	14:O:44:LEU:HD23	2.20	0.42
20:V:26:LEU:HD22	20:V:65:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:79:SER:O	20:V:80:ASN:HB2	2.19	0.42
26:1:660:A:O2'	26:1:661:U:H2'	2.20	0.42
26:1:920:A:H2'	26:1:921:C:O4'	2.20	0.42
26:1:1514:A:N6	26:1:1566:G:H22	2.17	0.42
26:1:1598:U:H2'	26:1:1599:G:H8	1.84	0.42
26:1:1645:G:H2'	26:1:1646:U:O4'	2.20	0.42
26:1:1664:G:O2'	26:1:1665:U:H5'	2.20	0.42
26:1:1829:A:H2'	26:1:1830:A:C8	2.55	0.42
26:1:2318:U:O2'	26:1:2401:C:H1'	2.19	0.42
27:2:11:A:H2'	27:2:11:A:N3	2.33	0.42
7:G:70:LEU:O	7:G:78:PRO:HA	2.20	0.42
11:L:51:VAL:HG21	11:L:91:PHE:HE2	1.84	0.42
18:S:184:LEU:HA	18:S:187:THR:HG22	2.01	0.42
23:Y:68:ILE:HG22	23:Y:101:ARG:HD3	2.01	0.42
23:Y:124:LYS:O	26:1:2511:G:O2'	2.28	0.42
26:1:805:G:H2'	26:1:806:A:O4'	2.18	0.42
26:1:1481:A:O2'	26:1:1562:C:H4'	2.20	0.42
26:1:2421:C:H2'	26:1:2422:C:O4'	2.20	0.42
26:1:2607:U:H2'	26:1:2608:G:C4	2.54	0.42
26:1:2846:A:H2'	26:1:2847:U:C6	2.54	0.42
2:B:56:GLY:O	2:B:215:GLY:HA2	2.18	0.42
3:C:35:ALA:O	3:C:39:VAL:HG23	2.19	0.42
6:F:55:ILE:CG2	6:F:76:ARG:HE	2.32	0.42
9:J:17:ARG:HB2	9:J:27:ARG:HD2	2.01	0.42
14:O:10:THR:HG22	14:O:46:ARG:HB2	2.02	0.42
15:P:12:LYS:O	15:P:16:VAL:HG23	2.20	0.42
22:X:79:LEU:HD11	22:X:135:ALA:HB3	2.01	0.42
26:1:10:A:HO2'	26:1:11:U:P	2.39	0.42
26:1:302:A:H2'	26:1:303:G:H8	1.84	0.42
26:1:474:A:H2'	26:1:475:A:C8	2.55	0.42
26:1:539:G:H2'	26:1:540:G:C8	2.55	0.42
26:1:1219:G:O2'	26:1:1220:A:H8	2.02	0.42
26:1:1303:A:H4'	26:1:1304:G:OP1	2.19	0.42
26:1:1521:A:H61	26:1:1559:G:H22	1.67	0.42
27:2:28:C:H1'	27:2:55:A:H61	1.85	0.42
27:2:76:A:H62	27:2:93:G:H21	1.68	0.42
2:B:181:VAL:HB	2:B:272:ARG:HG2	2.02	0.42
6:F:15:LYS:HE2	26:1:1428:U:O2'	2.19	0.42
11:L:83:ALA:O	11:L:85:LYS:HG2	2.19	0.42
20:V:19:ILE:HG12	20:V:57:VAL:HG22	2.02	0.42
21:W:63:VAL:HG21	21:W:85:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1575:A:O2'	26:1:1576:A:H5'	2.20	0.42
26:1:1612:C:O2'	26:1:1613:G:OP2	2.33	0.42
26:1:2312:C:C2'	26:1:2313:A:H5'	2.49	0.42
7:G:44:HIS:HB3	26:1:529:A:O4'	2.20	0.42
8:H:31:VAL:HA	8:H:91:PHE:O	2.20	0.42
14:O:6:THR:HG22	14:O:18:ILE:HG22	2.02	0.42
14:O:9:CYS:CB	14:O:14:ASP:HA	2.49	0.42
26:1:64:A:N3	26:1:64:A:C2'	2.73	0.42
26:1:116:G:H2'	26:1:118:A:C8	2.54	0.42
26:1:587:C:O2'	26:1:588:G:H5'	2.20	0.42
26:1:847:A:H2'	26:1:848:U:H6	1.81	0.42
26:1:962:A:H2'	26:1:963:A:H8	1.84	0.42
26:1:1343:U:O4	26:1:1650:G:H2'	2.19	0.42
26:1:2527:U:O2'	26:1:2528:C:H5'	2.20	0.42
27:2:12:U:O2	27:2:12:U:O4'	2.37	0.42
11:L:8:ARG:HA	11:L:207:GLY:O	2.19	0.42
22:X:92:THR:O	22:X:96:LEU:HB2	2.20	0.42
24:Z:29:ARG:HH22	24:Z:118:ILE:HD13	1.83	0.42
26:1:723:C:H2'	26:1:724:C:C6	2.55	0.42
26:1:963:A:H5"	27:2:92:C:O2'	2.19	0.42
26:1:1488:A:H2'	26:1:1489:A:H8	1.78	0.42
26:1:1612:C:O2	26:1:1613:G:O2'	2.28	0.42
26:1:2061:U:O2'	26:1:2062:G:H5'	2.20	0.42
26:1:2811:U:H2'	26:1:2812:U:C6	2.55	0.42
2:B:185:LEU:HD12	2:B:186:SER:N	2.32	0.41
6:F:13:THR:OG1	6:F:17:SER:HB3	2.20	0.41
8:H:79:PHE:HE1	8:H:84:ASN:HA	1.84	0.41
21:W:31:LYS:O	21:W:32:THR:OG1	2.30	0.41
22:X:91:VAL:CG1	22:X:96:LEU:HD13	2.50	0.41
26:1:115:C:O2'	26:1:116:G:H5'	2.20	0.41
26:1:491:C:C2'	26:1:492:G:H5'	2.50	0.41
26:1:744:A:H2'	26:1:745:G:O4'	2.19	0.41
26:1:890:G:HO2'	26:1:891:A:H8	1.66	0.41
26:1:1170:A:H4'	26:1:1171:A:O5'	2.19	0.41
26:1:1583:G:H2'	26:1:1585:G:C6	2.55	0.41
26:1:1924:G:H2'	26:1:1925:U:C6	2.55	0.41
26:1:2855:A:N6	26:1:2898:U:H2'	2.31	0.41
27:2:96:A:C2'	27:2:97:G:H5'	2.50	0.41
2:B:100:GLU:OE2	2:B:102:ARG:NE	2.28	0.41
3:C:94:MET:CE	3:C:94:MET:HA	2.50	0.41
16:Q:10:ALA:O	16:Q:14:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:182:ASN:ND2	26:1:661:U:OP2	2.53	0.41
19:U:107:VAL:HG22	19:U:107:VAL:O	2.19	0.41
26:1:27:G:N2	26:1:557:G:O2'	2.36	0.41
26:1:252:C:H5"	26:1:2421:C:O2'	2.19	0.41
26:1:963:A:H2'	26:1:964:U:O4'	2.19	0.41
26:1:2058:A:C6	26:1:2525:C:H1'	2.56	0.41
26:1:2231:C:H2'	26:1:2232:A:H8	1.85	0.41
26:1:2583:C:H2'	26:1:2584:G:O4'	2.20	0.41
7:G:27:LEU:HD22	7:G:30:LYS:CE	2.50	0.41
13:N:41:ARG:NE	24:Z:115:GLU:OE1	2.45	0.41
16:Q:24:ARG:O	16:Q:47:ALA:HB1	2.20	0.41
21:W:28:SER:HB3	26:1:2590:U:H4'	2.02	0.41
22:X:96:LEU:HD23	22:X:109:ILE:CD1	2.50	0.41
24:Z:39:GLU:OE1	26:1:2717:A:N6	2.51	0.41
26:1:288:C:H5'	26:1:290:U:H5"	2.02	0.41
26:1:1719:C:O2	26:1:1719:C:C2'	2.68	0.41
11:L:191:GLU:O	11:L:191:GLU:HG2	2.20	0.41
19:U:125:VAL:O	19:U:125:VAL:HG12	2.19	0.41
26:1:52:A:N6	26:1:116:G:O2'	2.54	0.41
26:1:1510:U:H2'	26:1:1511:C:C6	2.55	0.41
26:1:1513:A:H2'	26:1:1514:A:H8	1.76	0.41
26:1:2745:G:HO2'	26:1:2746:G:H5'	1.83	0.41
2:B:78:VAL:HA	2:B:94:VAL:HG12	2.02	0.41
18:S:67:GLN:HB3	18:S:68:LYS:H	1.64	0.41
21:W:8:LEU:CD2	21:W:82:ASN:HB3	2.50	0.41
22:X:2:LYS:HD3	22:X:2:LYS:HA	1.66	0.41
23:Y:135:GLU:OE1	23:Y:135:GLU:N	2.53	0.41
26:1:629:A:O2'	26:1:630:G:N2	2.53	0.41
26:1:772:A:HO2'	26:1:773:G:H5'	1.85	0.41
26:1:819:A:H4'	26:1:822:G:O2'	2.20	0.41
26:1:1560:A:O2'	26:1:1561:G:C8	2.73	0.41
26:1:1901:C:C2'	26:1:1902:G:H5'	2.51	0.41
1:A:31:HIS:CD2	1:A:44:VAL:HG22	2.56	0.41
8:H:37:LYS:HG2	8:H:38:ASN:CG	2.41	0.41
19:U:149:ARG:HD2	19:U:149:ARG:O	2.19	0.41
21:W:12:ASP:HB3	21:W:14:SER:OG	2.21	0.41
22:X:14:LYS:NZ	26:1:1232:G:OP1	2.53	0.41
24:Z:13:ARG:NH2	26:1:2717:A:OP2	2.53	0.41
26:1:31:C:O2'	26:1:32:C:H5'	2.21	0.41
26:1:504:G:H1'	26:1:505:U:H5	1.86	0.41
26:1:541:G:H2'	26:1:542:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:837:G:N3	26:1:2099:G:O2'	2.44	0.41
26:1:1863:C:H2'	26:1:1864:C:C6	2.56	0.41
26:1:2606:C:H2'	26:1:2607:U:O2	2.20	0.41
2:B:146:LEU:HD23	2:B:146:LEU:HA	1.93	0.41
21:W:43:VAL:CG1	21:W:54:LYS:HA	2.50	0.41
24:Z:4:ARG:HG2	24:Z:39:GLU:OE2	2.21	0.41
26:1:319:G:N3	26:1:319:G:H2'	2.36	0.41
26:1:748:U:O2'	26:1:749:G:H5'	2.19	0.41
26:1:1481:A:H2'	26:1:1482:U:O4'	2.21	0.41
26:1:1483:A:H2'	26:1:1484:G:O4'	2.20	0.41
26:1:2020:U:O2	26:1:2020:U:C2'	2.68	0.41
26:1:2346:U:H1'	26:1:2347:A:C5	2.56	0.41
26:1:2612:U:O2	26:1:2612:U:O5'	2.39	0.41
26:1:2889:G:H2'	26:1:2890:C:C6	2.56	0.41
2:B:180:GLU:HA	2:B:273:GLY:O	2.21	0.41
13:N:24:VAL:HG13	13:N:25:PRO:HD2	2.02	0.41
15:P:30:LYS:HB3	15:P:30:LYS:HE2	1.76	0.41
21:W:24:VAL:HG13	21:W:33:ALA:HB2	2.03	0.41
26:1:405:G:N2	26:1:406:A:H1'	2.36	0.41
26:1:955:A:N3	26:1:2291:C:O2'	2.43	0.41
27:2:47:C:H2'	27:2:48:A:C8	2.56	0.41
27:2:97:G:H2'	27:2:98:A:C8	2.56	0.41
2:B:98:ASP:OD1	2:B:99:GLY:N	2.54	0.41
2:B:167:LYS:HG2	2:B:172:VAL:HG12	2.02	0.41
5:E:109:ASP:OD2	5:E:111:LYS:HE3	2.21	0.41
7:G:20:GLU:OE1	7:G:71:LEU:HD21	2.21	0.41
8:H:8:ILE:HG13	8:H:40:SER:O	2.21	0.41
8:H:48:PHE:O	8:H:51:VAL:HG12	2.21	0.41
9:J:12:ALA:HB2	9:J:30:ASN:HD22	1.85	0.41
14:O:21:LYS:O	14:O:21:LYS:HG3	2.21	0.41
17:R:17:ILE:HD13	17:R:26:ILE:HD13	2.02	0.41
18:S:37:ILE:HG23	18:S:184:LEU:HD12	2.01	0.41
18:S:179:GLN:HE22	18:S:201:LYS:NZ	2.18	0.41
19:U:165:GLN:H	19:U:168:TYR:HE2	1.69	0.41
20:V:8:ASN:OD1	20:V:9:GLU:N	2.54	0.41
20:V:60:ALA:O	20:V:63:ILE:HG12	2.20	0.41
21:W:68:GLY:HA3	21:W:77:ILE:O	2.21	0.41
23:Y:23:GLY:O	23:Y:101:ARG:NH2	2.54	0.41
24:Z:102:ARG:NH2	24:Z:122:VAL:HG23	2.35	0.41
26:1:206:U:OP2	26:1:207:A:O2'	2.25	0.41
26:1:289:U:H5'	26:1:291:G:N7	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:556:U:O2'	26:1:557:G:H5'	2.21	0.41
26:1:1751:G:H2'	26:1:1752:C:H6	1.85	0.41
26:1:1962:G:H1'	26:1:1991:G:N2	2.36	0.41
26:1:2538:U:HO2'	26:1:2539:C:H5'	1.85	0.41
26:1:2612:U:O2	26:1:2612:U:O4'	2.38	0.41
26:1:2857:A:H2'	26:1:2858:G:C8	2.55	0.41
27:2:76:A:C2'	27:2:77:G:H5'	2.51	0.41
18:S:199:ALA:O	18:S:202:VAL:HG22	2.21	0.41
19:U:9:ILE:HD12	19:U:50:ILE:HG13	2.03	0.41
20:V:99:GLU:O	20:V:103:GLU:HG3	2.21	0.41
21:W:97:ARG:O	21:W:98:ILE:HD13	2.20	0.41
22:X:60:ARG:NH1	26:1:2455:G:H21	2.19	0.41
22:X:96:LEU:HA	22:X:96:LEU:HD12	1.79	0.41
26:1:153:G:H2'	26:1:154:A:C8	2.56	0.41
26:1:1503:U:H5'	26:1:1504:U:C6	2.56	0.41
7:G:42:LYS:HG3	7:G:58:GLU:HG3	2.04	0.40
7:G:64:HIS:ND1	7:G:66:SER:HB3	2.36	0.40
26:1:2341:A:H2'	26:1:2342:U:H6	1.81	0.40
1:A:8:GLU:O	1:A:9:ALA:HB3	2.20	0.40
2:B:13:ARG:NH2	26:1:773:G:H5"	2.37	0.40
2:B:78:VAL:HG22	2:B:94:VAL:CG1	2.51	0.40
9:J:17:ARG:HB2	9:J:27:ARG:CD	2.51	0.40
26:1:268:A:O2'	26:1:269:G:O4'	2.31	0.40
26:1:1058:U:O2'	26:1:1059:A:H5'	2.20	0.40
26:1:2901:U:H2'	26:1:2902:A:C8	2.55	0.40
2:B:31:LYS:O	2:B:32:SER:OG	2.35	0.40
11:L:119:THR:HG23	11:L:179:THR:HG22	2.04	0.40
19:U:17:VAL:HG13	19:U:26:VAL:HG22	2.02	0.40
21:W:28:SER:HB3	26:1:2590:U:O2'	2.22	0.40
24:Z:6:LEU:HD21	24:Z:39:GLU:HG3	2.02	0.40
26:1:661:U:HO2'	26:1:662:G:P	2.41	0.40
26:1:848:U:H2'	26:1:849:A:C8	2.56	0.40
26:1:2229:C:H5"	26:1:2230:G:OP1	2.22	0.40
26:1:2547:C:O2'	26:1:2548:C:H5'	2.21	0.40
1:A:26:ASP:HB3	1:A:91:ARG:HA	2.03	0.40
1:A:31:HIS:HB3	1:A:42:ILE:CG2	2.51	0.40
11:L:172:ARG:HD3	26:1:2842:G:H5"	2.03	0.40
18:S:74:ARG:H	18:S:74:ARG:HG2	1.61	0.40
18:S:89:VAL:HG21	26:1:629:A:H5'	2.04	0.40
18:S:90:PHE:HE2	26:1:630:G:H5"	1.87	0.40
21:W:65:THR:HG22	21:W:67:SER:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1024:A:N3	26:1:2064:A:O2'	2.43	0.40
26:1:1083:G:H2'	26:1:1084:U:C6	2.57	0.40
26:1:1218:G:H2'	26:1:1219:G:C8	2.56	0.40
26:1:1720:A:H2'	26:1:1721:A:H8	1.82	0.40
26:1:2054:G:H2'	26:1:2055:U:H6	1.84	0.40
26:1:2263:C:H2'	26:1:2264:G:O4'	2.22	0.40
2:B:148:PRO:HD3	2:B:185:LEU:HD23	2.04	0.40
7:G:79:THR:HG22	7:G:96:LYS:HG3	2.02	0.40
8:H:4:LEU:HD13	8:H:47:GLU:CD	2.42	0.40
13:N:39:SER:O	13:N:40:HIS:HB2	2.20	0.40
19:U:19:PHE:CZ	19:U:50:ILE:HD13	2.53	0.40
21:W:2:ILE:HG21	26:1:1709:A:C2	2.56	0.40
26:1:230:A:H5'	26:1:231:A:C2	2.56	0.40
26:1:481:C:C2'	26:1:482:U:H5'	2.46	0.40
26:1:1196:C:O2'	26:1:1197:C:H5'	2.21	0.40
26:1:1758:A:N3	26:1:1758:A:H5"	2.37	0.40
26:1:1912:A:H2'	26:1:1913:U:O4'	2.22	0.40
26:1:1945:A:O2'	26:1:1947:C:N4	2.55	0.40
26:1:1954:A:O2'	26:1:1955:A:H5'	2.21	0.40
26:1:2474:G:N7	26:1:2528:C:H5'	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	111/116 (96%)	101 (91%)	10 (9%)	0	100	100
2	B	273/277 (99%)	247 (90%)	26 (10%)	0	100	100
3	C	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
4	D	98/105 (93%)	87 (89%)	11 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	109/117 (93%)	103 (94%)	6 (6%)	0	100	100
6	F	85/91 (93%)	73 (86%)	12 (14%)	0	100	100
7	G	85/105 (81%)	79 (93%)	6 (7%)	0	100	100
8	H	91/107 (85%)	88 (97%)	3 (3%)	0	100	100
9	J	57/62 (92%)	52 (91%)	5 (9%)	0	100	100
10	K	56/72 (78%)	52 (93%)	4 (7%)	0	100	100
11	L	213/217 (98%)	199 (93%)	14 (7%)	0	100	100
12	M	54/58 (93%)	50 (93%)	4 (7%)	0	100	100
13	N	48/57 (84%)	41 (85%)	7 (15%)	0	100	100
14	O	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
15	P	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
16	Q	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
17	R	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
18	S	190/207 (92%)	177 (93%)	13 (7%)	0	100	100
19	U	172/175 (98%)	152 (88%)	20 (12%)	0	100	100
20	V	141/145 (97%)	134 (95%)	7 (5%)	0	100	100
21	W	119/122 (98%)	107 (90%)	12 (10%)	0	100	100
22	X	142/146 (97%)	124 (87%)	18 (13%)	0	100	100
23	Y	134/144 (93%)	130 (97%)	4 (3%)	0	100	100
24	Z	110/122 (90%)	104 (94%)	6 (6%)	0	100	100
25	a	114/119 (96%)	98 (86%)	16 (14%)	0	100	100
28	I	76/85 (89%)	69 (91%)	7 (9%)	0	100	100
All	All	2776/2968 (94%)	2551 (92%)	225 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	99/102 (97%)	96 (97%)	3 (3%)	41	71
2	B	222/224 (99%)	221 (100%)	1 (0%)	88	94
3	C	96/98 (98%)	92 (96%)	4 (4%)	30	62
4	D	85/89 (96%)	85 (100%)	0	100	100
5	E	90/94 (96%)	87 (97%)	3 (3%)	38	69
6	F	79/82 (96%)	77 (98%)	2 (2%)	47	75
7	G	76/91 (84%)	75 (99%)	1 (1%)	69	87
8	H	81/95 (85%)	81 (100%)	0	100	100
9	J	49/51 (96%)	49 (100%)	0	100	100
10	K	53/65 (82%)	52 (98%)	1 (2%)	57	81
11	L	173/175 (99%)	168 (97%)	5 (3%)	42	72
12	M	50/52 (96%)	49 (98%)	1 (2%)	55	80
13	N	45/49 (92%)	45 (100%)	0	100	100
14	O	45/47 (96%)	45 (100%)	0	100	100
15	P	39/45 (87%)	39 (100%)	0	100	100
16	Q	55/56 (98%)	55 (100%)	0	100	100
17	R	35/35 (100%)	35 (100%)	0	100	100
18	S	158/170 (93%)	155 (98%)	3 (2%)	57	81
19	U	152/153 (99%)	150 (99%)	2 (1%)	69	87
20	V	122/123 (99%)	120 (98%)	2 (2%)	62	84
21	W	99/100 (99%)	98 (99%)	1 (1%)	76	90
22	X	110/112 (98%)	108 (98%)	2 (2%)	59	82
23	Y	113/119 (95%)	113 (100%)	0	100	100
24	Z	94/102 (92%)	94 (100%)	0	100	100
25	a	92/95 (97%)	91 (99%)	1 (1%)	73	89
28	I	61/66 (92%)	60 (98%)	1 (2%)	62	84
All	All	2373/2490 (95%)	2340 (99%)	33 (1%)	68	86

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	18	ASP
1	A	94	VAL

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Mol	Chain	Res	Type
2	B	260	ARG
3	C	9	VAL
3	C	88	ILE
3	C	91	ASN
3	C	94	MET
5	E	59	GLU
5	E	62	TYR
5	E	64	MET
6	F	65	MET
6	F	68	TYR
7	G	80	ARG
10	K	7	ARG
11	L	42	GLU
11	L	47	ASN
11	L	54	GLU
11	L	64	LYS
11	L	178	VAL
12	M	51	LYS
18	S	77	THR
18	S	148	GLN
18	S	152	VAL
19	U	40	ARG
19	U	97	GLN
20	V	11	ASN
20	V	112	SER
21	W	73	ASP
22	X	29	LYS
22	X	33	ARG
25	a	28	LYS
28	I	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	HIS
2	B	128	ASN
2	B	142	HIS
2	B	153	GLN
2	B	226	ASN
3	C	38	GLN
3	C	91	ASN
4	D	28	ASN

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Mol	Chain	Res	Type
5	E	61	ASN
5	E	102	HIS
6	F	69	GLN
8	H	88	HIS
9	J	30	ASN
10	K	27	ASN
11	L	33	ASN
11	L	146	HIS
11	L	176	ASN
11	L	200	ASN
12	M	19	GLN
12	M	46	GLN
12	M	52	HIS
14	O	45	HIS
15	P	7	GLN
15	P	9	ASN
15	P	13	HIS
16	Q	31	HIS
16	Q	35	ASN
18	S	40	GLN
18	S	46	GLN
18	S	119	GLN
18	S	121	ASN
18	S	148	GLN
18	S	179	GLN
18	S	188	ASN
19	U	45	GLN
19	U	77	GLN
19	U	97	GLN
20	V	48	HIS
20	V	104	ASN
20	V	136	GLN
22	X	27	ASN
23	Y	25	ASN
23	Y	35	GLN
24	Z	79	GLN
25	a	102	HIS

5.3.3 RNA (i)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	1	2654/2923 (90%)	749 (28%)	236 (8%)
27	2	111/115 (96%)	36 (32%)	17 (15%)
All	All	2765/3038 (91%)	785 (28%)	253 (9%)

All (785) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	1	11	U
26	1	18	C
26	1	20	C
26	1	27	G
26	1	28	A
26	1	33	U
26	1	34	U
26	1	35	G
26	1	38	A
26	1	51	G
26	1	55	G
26	1	58	G
26	1	60	U
26	1	61	A
26	1	62	C
26	1	63	U
26	1	64	A
26	1	65	A
26	1	66	C
26	1	71	A
26	1	72	U
26	1	74	U
26	1	75	G
26	1	79	U
26	1	90	A
26	1	91	A
26	1	96	G
26	1	99	U
26	1	115	C
26	1	117	A
26	1	118	A
26	1	119	U
26	1	124	A
26	1	125	A

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Mol	Chain	Res	Type
26	1	126	A
26	1	139	U
26	1	150	A
26	1	158	G
26	1	159	U
26	1	160	G
26	1	161	A
26	1	162	A
26	1	163	U
26	1	164	A
26	1	165	C
26	1	166	A
26	1	169	G
26	1	176	A
26	1	177	G
26	1	180	G
26	1	183	A
26	1	184	C
26	1	191	A
26	1	199	A
26	1	200	A
26	1	201	C
26	1	202	A
26	1	203	U
26	1	205	U
26	1	208	G
26	1	216	A
26	1	218	G
26	1	219	A
26	1	224	A
26	1	225	A
26	1	227	G
26	1	230	A
26	1	233	U
26	1	244	A
26	1	247	A
26	1	248	G
26	1	251	G
26	1	252	C
26	1	253	G
26	1	255	G
26	1	258	A

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Mol	Chain	Res	Type
26	1	263	G
26	1	264	G
26	1	267	G
26	1	268	A
26	1	269	G
26	1	270	C
26	1	284	C
26	1	286	U
26	1	290	U
26	1	291	G
26	1	298	U
26	1	300	G
26	1	301	U
26	1	302	A
26	1	303	G
26	1	304	G
26	1	310	C
26	1	311	U
26	1	319	G
26	1	320	U
26	1	321	U
26	1	322	A
26	1	323	C
26	1	324	A
26	1	325	A
26	1	326	A
26	1	327	G
26	1	331	G
26	1	332	A
26	1	338	G
26	1	354	A
26	1	359	A
26	1	366	G
26	1	372	A
26	1	373	A
26	1	377	U
26	1	381	G
26	1	399	U
26	1	400	C
26	1	401	U
26	1	402	C
26	1	403	U

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Mol	Chain	Res	Type
26	1	404	U
26	1	405	G
26	1	410	G
26	1	432	G
26	1	434	G
26	1	435	A
26	1	446	G
26	1	447	A
26	1	450	C
26	1	451	U
26	1	452	G
26	1	457	G
26	1	458	A
26	1	463	C
26	1	466	C
26	1	472	C
26	1	473	U
26	1	474	A
26	1	489	A
26	1	493	A
26	1	498	G
26	1	500	A
26	1	501	C
26	1	502	C
26	1	503	A
26	1	504	G
26	1	505	U
26	1	506	A
26	1	507	C
26	1	508	C
26	1	515	G
26	1	517	A
26	1	523	A
26	1	526	A
26	1	527	G
26	1	536	A
26	1	540	G
26	1	541	G
26	1	546	A
26	1	547	A
26	1	550	A
26	1	551	G

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Mol	Chain	Res	Type
26	1	552	A
26	1	553	A
26	1	554	C
26	1	555	C
26	1	557	G
26	1	558	A
26	1	565	G
26	1	566	U
26	1	567	G
26	1	574	A
26	1	575	G
26	1	576	U
26	1	577	A
26	1	578	G
26	1	583	A
26	1	590	U
26	1	592	A
26	1	593	U
26	1	594	G
26	1	600	U
26	1	604	G
26	1	606	G
26	1	614	U
26	1	615	A
26	1	616	G
26	1	617	A
26	1	618	A
26	1	629	A
26	1	630	G
26	1	631	U
26	1	646	A
26	1	647	G
26	1	650	U
26	1	651	A
26	1	656	G
26	1	657	U
26	1	658	A
26	1	659	A
26	1	660	A
26	1	661	U
26	1	662	G
26	1	665	G

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Mol	Chain	Res	Type
26	1	666	A
26	1	667	G
26	1	668	C
26	1	672	A
26	1	673	G
26	1	675	G
26	1	682	A
26	1	683	G
26	1	688	A
26	1	689	A
26	1	690	U
26	1	691	A
26	1	694	G
26	1	696	G
26	1	697	U
26	1	698	U
26	1	699	U
26	1	700	A
26	1	721	A
26	1	722	A
26	1	723	C
26	1	730	A
26	1	731	U
26	1	744	A
26	1	745	G
26	1	756	A
26	1	761	A
26	1	762	C
26	1	763	A
26	1	768	A
26	1	775	A
26	1	781	C
26	1	791	U
26	1	792	U
26	1	793	G
26	1	794	A
26	1	796	A
26	1	802	G
26	1	808	G
26	1	809	A
26	1	819	A
26	1	820	G

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Mol	Chain	Res	Type
26	1	822	G
26	1	824	A
26	1	827	A
26	1	828	A
26	1	829	U
26	1	830	U
26	1	831	C
26	1	836	C
26	1	837	G
26	1	839	A
26	1	846	G
26	1	847	A
26	1	849	A
26	1	850	G
26	1	855	U
26	1	856	U
26	1	857	C
26	1	858	U
26	1	872	U
26	1	873	U
26	1	883	C
26	1	892	U
26	1	894	A
26	1	895	U
26	1	903	G
26	1	904	G
26	1	905	U
26	1	911	A
26	1	951	G
26	1	955	A
26	1	964	U
26	1	970	U
26	1	971	U
26	1	972	A
26	1	973	A
26	1	974	U
26	1	977	A
26	1	982	G
26	1	984	G
26	1	985	A
26	1	989	A
26	1	990	G

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Mol	Chain	Res	Type
26	1	991	A
26	1	1002	U
26	1	1005	G
26	1	1018	A
26	1	1026	C
26	1	1027	A
26	1	1029	C
26	1	1040	A
26	1	1045	A
26	1	1055	A
26	1	1056	U
26	1	1057	A
26	1	1063	U
26	1	1064	A
26	1	1065	A
26	1	1066	G
26	1	1067	U
26	1	1069	G
26	1	1070	A
26	1	1077	U
26	1	1087	C
26	1	1160	C
26	1	1173	A
26	1	1176	U
26	1	1177	A
26	1	1178	C
26	1	1179	C
26	1	1185	U
26	1	1186	A
26	1	1187	A
26	1	1188	A
26	1	1202	C
26	1	1209	U
26	1	1211	G
26	1	1214	C
26	1	1216	U
26	1	1217	U
26	1	1218	G
26	1	1219	G
26	1	1220	A
26	1	1224	U
26	1	1230	G

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Mol	Chain	Res	Type
26	1	1258	A
26	1	1263	A
26	1	1274	G
26	1	1275	A
26	1	1276	G
26	1	1278	G
26	1	1288	G
26	1	1289	A
26	1	1290	G
26	1	1291	A
26	1	1293	U
26	1	1294	G
26	1	1295	C
26	1	1300	G
26	1	1309	G
26	1	1310	A
26	1	1311	A
26	1	1312	A
26	1	1313	G
26	1	1323	A
26	1	1337	A
26	1	1338	U
26	1	1339	U
26	1	1345	A
26	1	1346	G
26	1	1348	U
26	1	1350	U
26	1	1351	C
26	1	1358	A
26	1	1366	U
26	1	1375	G
26	1	1378	U
26	1	1380	G
26	1	1389	U
26	1	1390	A
26	1	1402	A
26	1	1405	G
26	1	1415	A
26	1	1416	U
26	1	1421	A
26	1	1423	C
26	1	1424	A

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Mol	Chain	Res	Type
26	1	1432	A
26	1	1433	U
26	1	1447	A
26	1	1448	U
26	1	1462	G
26	1	1463	A
26	1	1464	U
26	1	1471	A
26	1	1472	C
26	1	1476	G
26	1	1477	U
26	1	1482	U
26	1	1487	G
26	1	1488	A
26	1	1489	A
26	1	1490	G
26	1	1491	C
26	1	1492	G
26	1	1493	U
26	1	1497	A
26	1	1499	U
26	1	1500	G
26	1	1503	U
26	1	1504	U
26	1	1507	A
26	1	1508	C
26	1	1509	G
26	1	1510	U
26	1	1511	C
26	1	1514	A
26	1	1515	G
26	1	1516	C
26	1	1519	U
26	1	1521	A
26	1	1522	G
26	1	1546	A
26	1	1547	C
26	1	1557	C
26	1	1559	G
26	1	1561	G
26	1	1565	U
26	1	1566	G

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Mol	Chain	Res	Type
26	1	1567	A
26	1	1568	U
26	1	1569	G
26	1	1570	G
26	1	1573	A
26	1	1574	G
26	1	1575	A
26	1	1576	A
26	1	1579	C
26	1	1580	A
26	1	1581	U
26	1	1583	G
26	1	1585	G
26	1	1586	U
26	1	1588	U
26	1	1591	G
26	1	1592	A
26	1	1593	G
26	1	1594	U
26	1	1595	C
26	1	1596	G
26	1	1597	U
26	1	1598	U
26	1	1599	G
26	1	1600	A
26	1	1601	U
26	1	1605	A
26	1	1606	C
26	1	1613	G
26	1	1614	A
26	1	1616	A
26	1	1618	A
26	1	1625	U
26	1	1627	G
26	1	1639	G
26	1	1650	G
26	1	1652	A
26	1	1653	A
26	1	1654	A
26	1	1660	A
26	1	1663	G
26	1	1675	G

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Mol	Chain	Res	Type
26	1	1676	A
26	1	1677	G
26	1	1678	A
26	1	1683	U
26	1	1686	G
26	1	1690	A
26	1	1691	G
26	1	1692	C
26	1	1693	G
26	1	1711	G
26	1	1712	A
26	1	1713	A
26	1	1716	C
26	1	1717	G
26	1	1718	G
26	1	1719	C
26	1	1721	A
26	1	1730	C
26	1	1737	U
26	1	1740	G
26	1	1742	A
26	1	1756	U
26	1	1758	A
26	1	1759	G
26	1	1760	G
26	1	1772	G
26	1	1773	A
26	1	1780	G
26	1	1781	C
26	1	1782	A
26	1	1783	G
26	1	1789	A
26	1	1790	G
26	1	1791	G
26	1	1800	A
26	1	1805	U
26	1	1806	U
26	1	1807	A
26	1	1808	U
26	1	1809	C
26	1	1810	A
26	1	1811	A

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Mol	Chain	Res	Type
26	1	1812	A
26	1	1813	A
26	1	1814	A
26	1	1826	G
26	1	1827	C
26	1	1828	U
26	1	1829	A
26	1	1835	U
26	1	1836	A
26	1	1843	U
26	1	1853	C
26	1	1856	A
26	1	1862	G
26	1	1863	C
26	1	1865	C
26	1	1866	A
26	1	1875	A
26	1	1881	A
26	1	1893	A
26	1	1898	C
26	1	1909	C
26	1	1910	G
26	1	1912	A
26	1	1924	G
26	1	1925	U
26	1	1926	A
26	1	1927	A
26	1	1929	C
26	1	1930	G
26	1	1931	G
26	1	1932	C
26	1	1933	G
26	1	1934	G
26	1	1940	A
26	1	1941	C
26	1	1942	U
26	1	1943	A
26	1	1944	U
26	1	1945	A
26	1	1946	A
26	1	1953	U
26	1	1954	A

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Mol	Chain	Res	Type
26	1	1955	A
26	1	1956	G
26	1	1957	G
26	1	1958	U
26	1	1960	G
26	1	1963	A
26	1	1964	A
26	1	1965	A
26	1	1967	U
26	1	1982	U
26	1	1993	A
26	1	1994	C
26	1	1996	A
26	1	1997	A
26	1	1998	A
26	1	1999	G
26	1	2009	U
26	1	2017	C
26	1	2018	U
26	1	2019	G
26	1	2020	U
26	1	2023	C
26	1	2048	G
26	1	2050	A
26	1	2056	G
26	1	2057	A
26	1	2058	A
26	1	2059	G
26	1	2060	A
26	1	2061	U
26	1	2063	C
26	1	2068	U
26	1	2070	C
26	1	2073	G
26	1	2078	A
26	1	2079	G
26	1	2082	C
26	1	2083	G
26	1	2085	A
26	1	2086	A
26	1	2087	A
26	1	2088	G

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Mol	Chain	Res	Type
26	1	2089	A
26	1	2096	G
26	1	2097	G
26	1	2098	A
26	1	2104	A
26	1	2107	G
26	1	2120	G
26	1	2226	A
26	1	2231	C
26	1	2237	U
26	1	2239	A
26	1	2240	U
26	1	2241	C
26	1	2252	A
26	1	2265	G
26	1	2270	U
26	1	2286	G
26	1	2294	A
26	1	2295	A
26	1	2296	A
26	1	2309	G
26	1	2310	C
26	1	2313	A
26	1	2315	A
26	1	2316	G
26	1	2346	U
26	1	2347	A
26	1	2348	G
26	1	2349	A
26	1	2361	U
26	1	2362	A
26	1	2374	C
26	1	2410	G
26	1	2412	C
26	1	2426	G
26	1	2433	C
26	1	2446	U
26	1	2452	A
26	1	2455	G
26	1	2456	G
26	1	2457	A
26	1	2459	A

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Mol	Chain	Res	Type
26	1	2461	A
26	1	2462	A
26	1	2465	U
26	1	2466	A
26	1	2467	C
26	1	2468	C
26	1	2469	C
26	1	2471	G
26	1	2473	G
26	1	2474	G
26	1	2475	A
26	1	2479	C
26	1	2480	A
26	1	2486	A
26	1	2492	C
26	1	2496	A
26	1	2501	U
26	1	2502	C
26	1	2514	G
26	1	2521	G
26	1	2523	C
26	1	2528	C
26	1	2529	G
26	1	2530	A
26	1	2531	U
26	1	2532	G
26	1	2533	U
26	1	2534	C
26	1	2535	G
26	1	2536	G
26	1	2537	C
26	1	2545	A
26	1	2556	G
26	1	2561	C
26	1	2562	G
26	1	2568	A
26	1	2578	C
26	1	2580	G
26	1	2581	U
26	1	2582	U
26	1	2593	A
26	1	2594	G

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Mol	Chain	Res	Type
26	1	2599	A
26	1	2600	C
26	1	2601	G
26	1	2602	C
26	1	2603	G
26	1	2604	A
26	1	2605	G
26	1	2607	U
26	1	2608	G
26	1	2609	G
26	1	2610	G
26	1	2611	U
26	1	2612	U
26	1	2613	C
26	1	2614	A
26	1	2615	G
26	1	2616	A
26	1	2630	G
26	1	2635	G
26	1	2636	U
26	1	2637	C
26	1	2638	C
26	1	2639	C
26	1	2640	U
26	1	2641	A
26	1	2642	U
26	1	2643	C
26	1	2648	G
26	1	2649	U
26	1	2650	G
26	1	2657	G
26	1	2661	A
26	1	2673	C
26	1	2675	G
26	1	2677	C
26	1	2688	G
26	1	2690	G
26	1	2695	G
26	1	2708	C
26	1	2716	U
26	1	2718	C
26	1	2732	A

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Mol	Chain	Res	Type
26	1	2740	A
26	1	2741	G
26	1	2744	G
26	1	2745	G
26	1	2749	G
26	1	2753	U
26	1	2754	G
26	1	2760	A
26	1	2762	G
26	1	2771	G
26	1	2773	U
26	1	2775	A
26	1	2792	A
26	1	2793	G
26	1	2805	A
26	1	2817	A
26	1	2818	A
26	1	2822	C
26	1	2823	G
26	1	2824	G
26	1	2827	A
26	1	2828	U
26	1	2840	A
26	1	2843	A
26	1	2844	U
26	1	2845	G
26	1	2848	G
26	1	2855	A
26	1	2856	U
26	1	2868	G
26	1	2869	G
26	1	2870	A
26	1	2886	G
26	1	2887	G
26	1	2888	A
26	1	2890	C
26	1	2892	G
26	1	2898	U
26	1	2899	A
26	1	2900	C
26	1	2901	U
26	1	2908	U

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Mol	Chain	Res	Type
26	1	2911	A
27	2	9	C
27	2	10	U
27	2	11	A
27	2	12	U
27	2	13	A
27	2	14	G
27	2	23	U
27	2	24	C
27	2	27	A
27	2	28	C
27	2	29	C
27	2	30	U
27	2	32	U
27	2	42	G
27	2	47	C
27	2	48	A
27	2	49	G
27	2	50	A
27	2	51	A
27	2	52	G
27	2	53	U
27	2	63	U
27	2	64	A
27	2	71	A
27	2	82	A
27	2	83	C
27	2	84	U
27	2	85	U
27	2	86	A
27	2	87	C
27	2	88	G
27	2	94	C
27	2	100	U
27	2	101	A
27	2	104	A
27	2	113	G

All (253) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1	10	A

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Mol	Chain	Res	Type
26	1	27	G
26	1	33	U
26	1	34	U
26	1	60	U
26	1	62	C
26	1	63	U
26	1	64	A
26	1	65	A
26	1	90	A
26	1	123	G
26	1	124	A
26	1	125	A
26	1	161	A
26	1	162	A
26	1	163	U
26	1	164	A
26	1	165	C
26	1	199	A
26	1	201	C
26	1	202	A
26	1	224	A
26	1	229	A
26	1	250	G
26	1	251	G
26	1	252	C
26	1	267	G
26	1	268	A
26	1	269	G
26	1	299	U
26	1	300	G
26	1	301	U
26	1	318	A
26	1	319	G
26	1	320	U
26	1	321	U
26	1	322	A
26	1	324	A
26	1	325	A
26	1	326	A
26	1	401	U
26	1	433	U
26	1	450	C

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Mol	Chain	Res	Type
26	1	473	U
26	1	493	A
26	1	500	A
26	1	503	A
26	1	504	G
26	1	505	U
26	1	525	A
26	1	549	U
26	1	551	G
26	1	553	A
26	1	554	C
26	1	556	U
26	1	557	G
26	1	614	U
26	1	615	A
26	1	616	G
26	1	617	A
26	1	629	A
26	1	630	G
26	1	655	A
26	1	656	G
26	1	657	U
26	1	658	A
26	1	659	A
26	1	660	A
26	1	664	G
26	1	665	G
26	1	672	A
26	1	681	G
26	1	682	A
26	1	688	A
26	1	689	A
26	1	690	U
26	1	696	G
26	1	721	A
26	1	744	A
26	1	791	U
26	1	792	U
26	1	793	G
26	1	796	A
26	1	827	A
26	1	829	U

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Mol	Chain	Res	Type
26	1	846	G
26	1	854	G
26	1	856	U
26	1	903	G
26	1	904	G
26	1	972	A
26	1	973	A
26	1	1025	A
26	1	1026	C
26	1	1063	U
26	1	1064	A
26	1	1065	A
26	1	1066	G
26	1	1185	U
26	1	1186	A
26	1	1187	A
26	1	1274	G
26	1	1275	A
26	1	1288	G
26	1	1289	A
26	1	1290	G
26	1	1291	A
26	1	1350	U
26	1	1414	G
26	1	1415	A
26	1	1486	C
26	1	1487	G
26	1	1488	A
26	1	1489	A
26	1	1490	G
26	1	1491	C
26	1	1507	A
26	1	1508	C
26	1	1509	G
26	1	1514	A
26	1	1515	G
26	1	1521	A
26	1	1546	A
26	1	1558	U
26	1	1559	G
26	1	1564	G
26	1	1566	G

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Mol	Chain	Res	Type
26	1	1568	U
26	1	1572	G
26	1	1573	A
26	1	1574	G
26	1	1575	A
26	1	1591	G
26	1	1593	G
26	1	1594	U
26	1	1595	C
26	1	1596	G
26	1	1599	G
26	1	1674	U
26	1	1675	G
26	1	1677	G
26	1	1678	A
26	1	1711	G
26	1	1712	A
26	1	1713	A
26	1	1715	U
26	1	1716	C
26	1	1717	G
26	1	1718	G
26	1	1788	U
26	1	1789	A
26	1	1806	U
26	1	1807	A
26	1	1808	U
26	1	1809	C
26	1	1810	A
26	1	1811	A
26	1	1812	A
26	1	1813	A
26	1	1865	C
26	1	1923	A
26	1	1926	A
26	1	1927	A
26	1	1931	G
26	1	1932	C
26	1	1933	G
26	1	1953	U
26	1	1954	A
26	1	1956	G

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Mol	Chain	Res	Type
26	1	1957	G
26	1	1997	A
26	1	2019	G
26	1	2057	A
26	1	2058	A
26	1	2059	G
26	1	2060	A
26	1	2078	A
26	1	2082	C
26	1	2085	A
26	1	2096	G
26	1	2269	G
26	1	2294	A
26	1	2295	A
26	1	2345	A
26	1	2346	U
26	1	2347	A
26	1	2460	A
26	1	2461	A
26	1	2465	U
26	1	2466	A
26	1	2469	C
26	1	2474	G
26	1	2479	C
26	1	2501	U
26	1	2527	U
26	1	2528	C
26	1	2530	A
26	1	2531	U
26	1	2532	G
26	1	2533	U
26	1	2535	G
26	1	2536	G
26	1	2579	U
26	1	2580	G
26	1	2581	U
26	1	2582	U
26	1	2599	A
26	1	2600	C
26	1	2603	G
26	1	2604	A
26	1	2607	U

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Mol	Chain	Res	Type
26	1	2608	G
26	1	2611	U
26	1	2612	U
26	1	2613	C
26	1	2614	A
26	1	2634	G
26	1	2635	G
26	1	2636	U
26	1	2637	C
26	1	2638	C
26	1	2639	C
26	1	2640	U
26	1	2641	A
26	1	2648	G
26	1	2821	U
26	1	2827	A
26	1	2843	A
26	1	2854	A
26	1	2855	A
26	1	2868	G
26	1	2869	G
26	1	2885	U
26	1	2886	G
26	1	2887	G
26	1	2899	A
27	2	8	A
27	2	9	C
27	2	10	U
27	2	11	A
27	2	12	U
27	2	13	A
27	2	27	A
27	2	29	C
27	2	30	U
27	2	48	A
27	2	49	G
27	2	51	A
27	2	52	G
27	2	82	A
27	2	84	U
27	2	85	U
27	2	86	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	U7Y	1	3001	-	28,30,30	5.58	19 (67%)	38,43,43	2.48	15 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	U7Y	1	3001	-	-	7/14/26/26	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	3001	U7Y	N4-N3	13.53	1.55	1.34
29	1	3001	U7Y	C13-N6	12.23	1.48	1.36
29	1	3001	U7Y	C12-C7	8.82	1.52	1.37
29	1	3001	U7Y	C9-C8	8.00	1.52	1.40
29	1	3001	U7Y	C6-C5	7.44	1.52	1.39
29	1	3001	U7Y	C10-C11	6.53	1.52	1.39
29	1	3001	U7Y	C2-N5	6.45	1.48	1.35
29	1	3001	U7Y	C4-C3	5.76	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	3001	U7Y	O3-C16	-5.53	1.19	1.42
29	1	3001	U7Y	C8-C7	-5.27	1.31	1.39
29	1	3001	U7Y	C4-C5	-5.10	1.28	1.39
29	1	3001	U7Y	O2-C15	-5.07	1.39	1.46
29	1	3001	U7Y	O2-C13	5.03	1.42	1.35
29	1	3001	U7Y	C12-C11	-4.62	1.31	1.39
29	1	3001	U7Y	C10-C9	-4.18	1.31	1.38
29	1	3001	U7Y	C3-C2	-3.14	1.31	1.38
29	1	3001	U7Y	C6-N5	-2.95	1.28	1.34
29	1	3001	U7Y	C1-N4	-2.93	1.26	1.33
29	1	3001	U7Y	C2-C1	2.33	1.52	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	3001	U7Y	C14-N6-C13	-6.90	107.28	111.28
29	1	3001	U7Y	C17-N1-C1	-6.50	121.60	129.38
29	1	3001	U7Y	O2-C13-N6	-5.18	106.26	109.83
29	1	3001	U7Y	O2-C13-O1	3.92	126.71	122.37
29	1	3001	U7Y	C14-N6-C11	3.59	127.53	121.45
29	1	3001	U7Y	N4-N3-N2	-3.23	106.45	110.09
29	1	3001	U7Y	C15-C14-N6	3.17	105.00	101.81
29	1	3001	U7Y	O2-C15-C14	2.79	107.38	104.57
29	1	3001	U7Y	C15-O2-C13	-2.68	108.03	110.15
29	1	3001	U7Y	C9-C8-C7	2.63	119.89	116.10
29	1	3001	U7Y	C1-N1-N2	2.53	116.77	112.08
29	1	3001	U7Y	C17-N1-N2	2.51	121.63	117.81
29	1	3001	U7Y	O1-C13-N6	-2.37	127.03	128.91
29	1	3001	U7Y	C12-C7-C8	-2.34	119.95	123.64
29	1	3001	U7Y	C5-C6-N5	-2.28	120.56	124.32

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	1	3001	U7Y	N1-C1-C2-C3
29	1	3001	U7Y	N1-C1-C2-N5
29	1	3001	U7Y	N4-C1-C2-C3
29	1	3001	U7Y	N4-C1-C2-N5
29	1	3001	U7Y	C14-C15-C16-O3
29	1	3001	U7Y	O2-C15-C16-O3
29	1	3001	U7Y	C12-C11-N6-C13

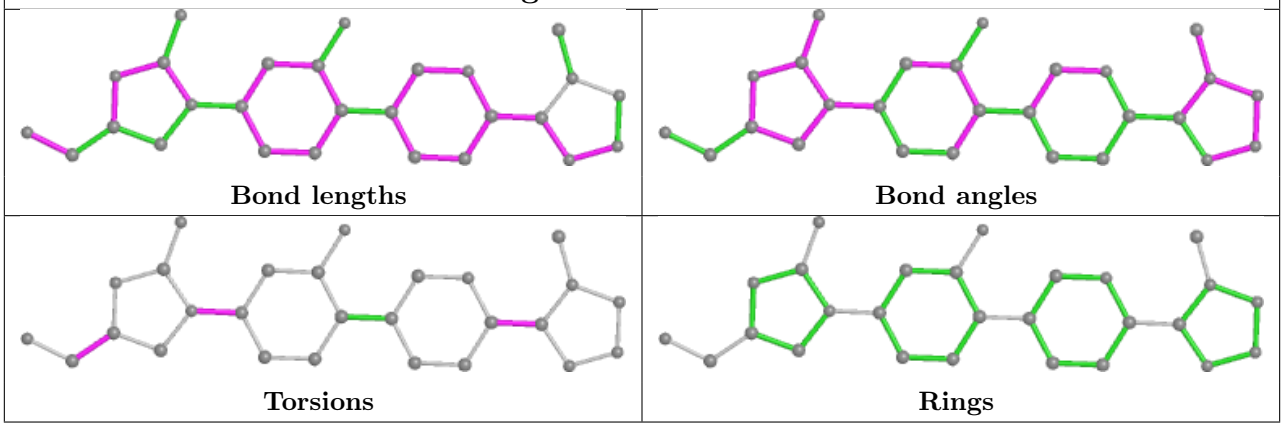
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1	3001	U7Y	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand U7Y 1 3001



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.

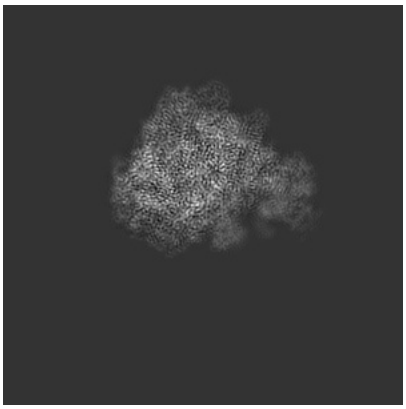
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21888. These allow visual inspection of the internal detail of the map and identification of artifacts.

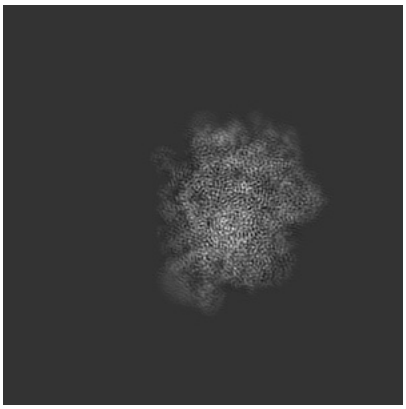
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

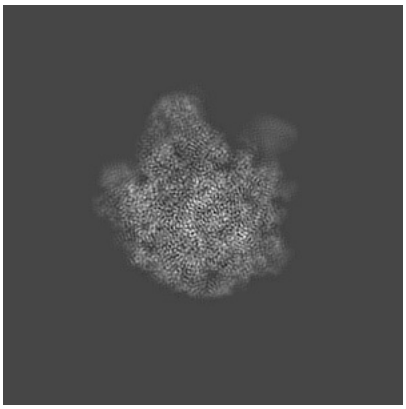
6.1.1 Primary map



X

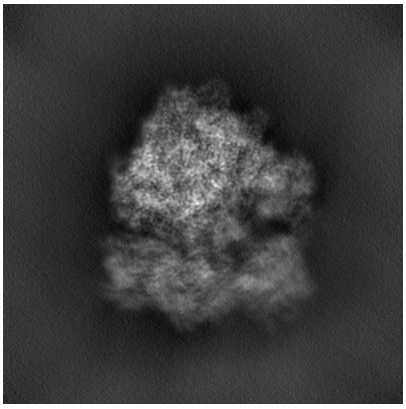


Y

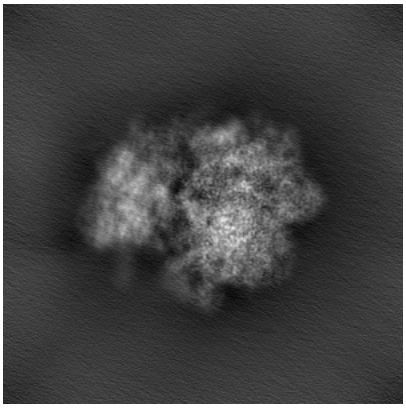


Z

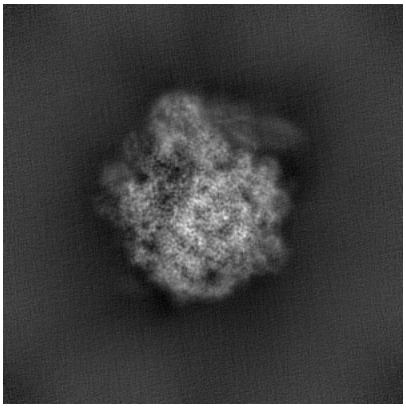
6.1.2 Raw map



X



Y

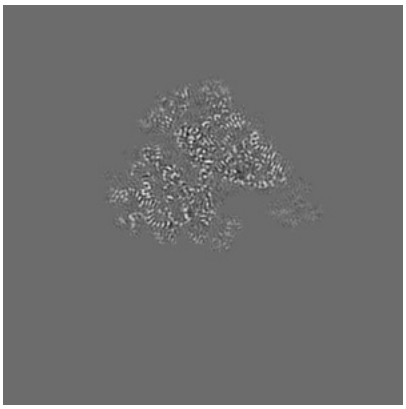


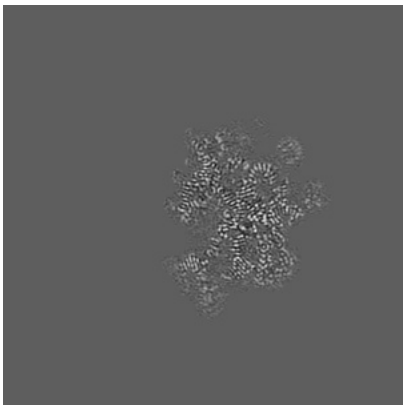
Z

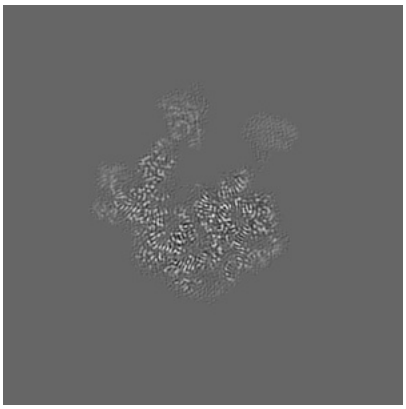
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

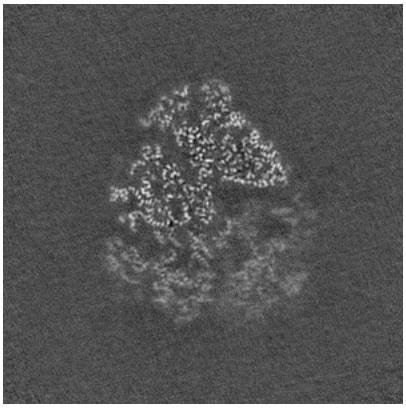
6.2.1 Primary map

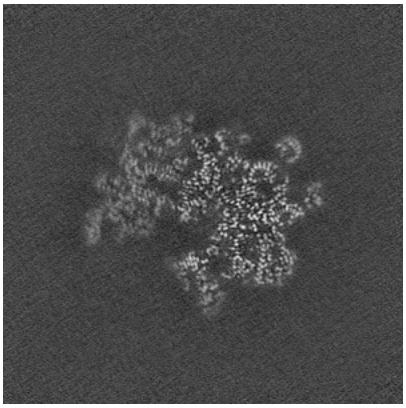

X Index: 216

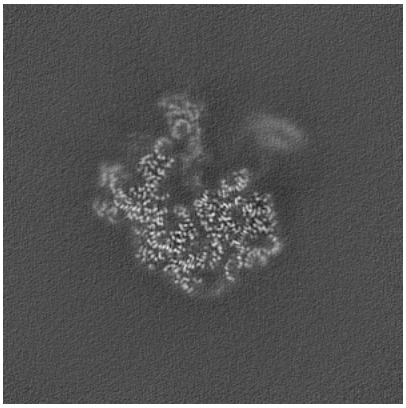

Y Index: 216


Z Index: 216

6.2.2 Raw map


X Index: 216


Y Index: 216


Z Index: 216

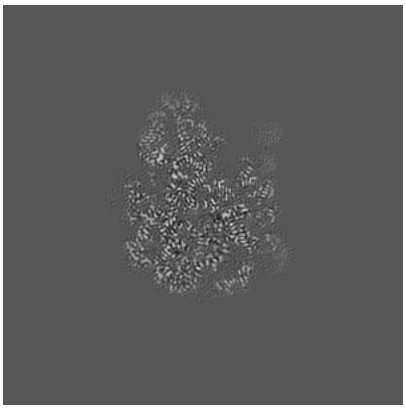
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

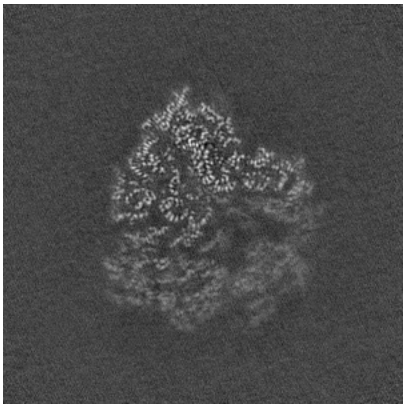
X Index: 206

Y Index: 195

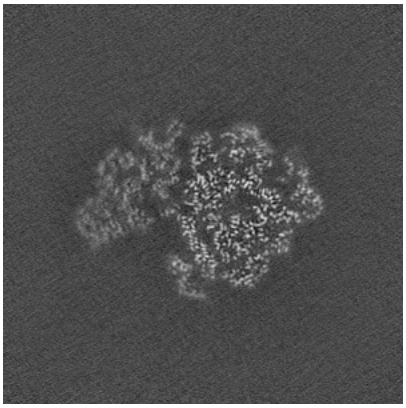


Z Index: 242

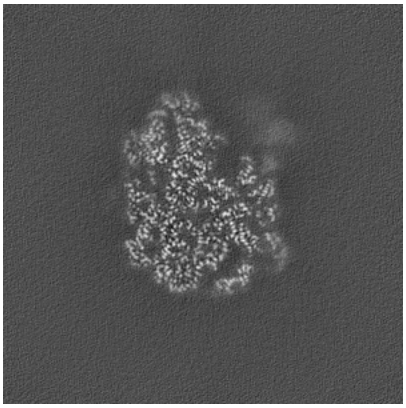
6.3.2 Raw map



X Index: 205



Y Index: 199

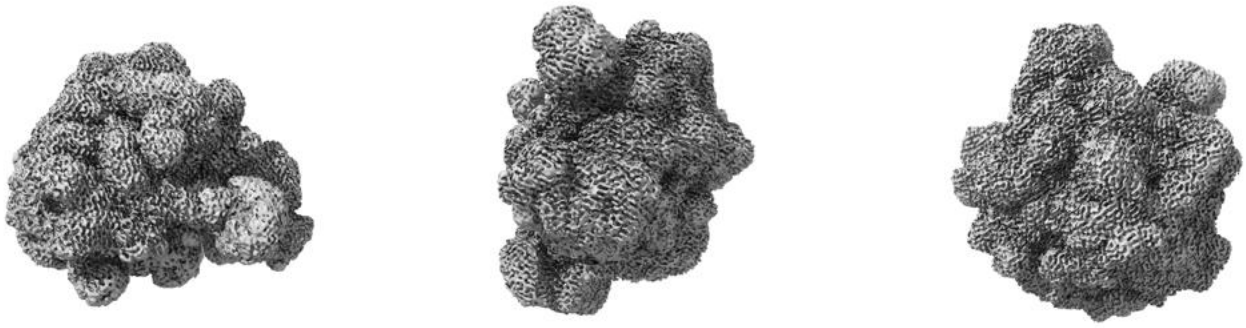


Z Index: 242

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

6.4 Orthogonal surface views (i)

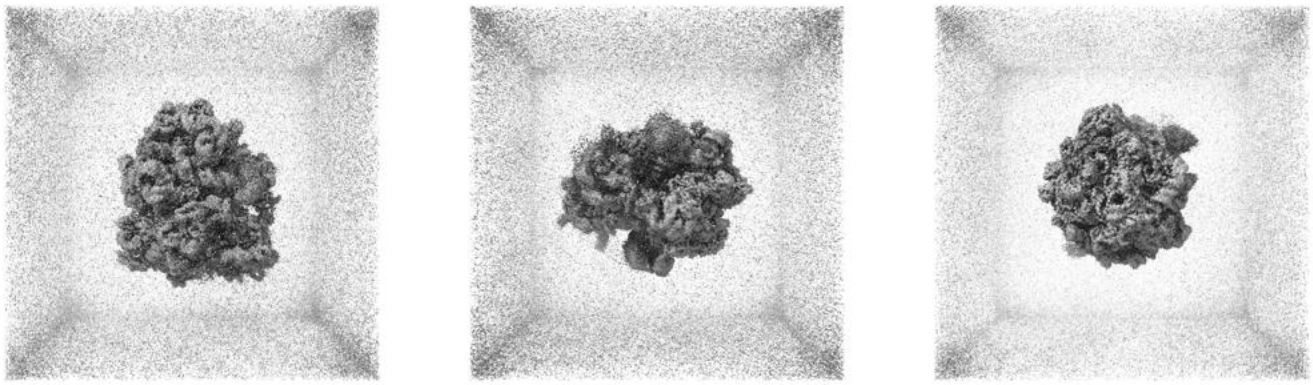
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

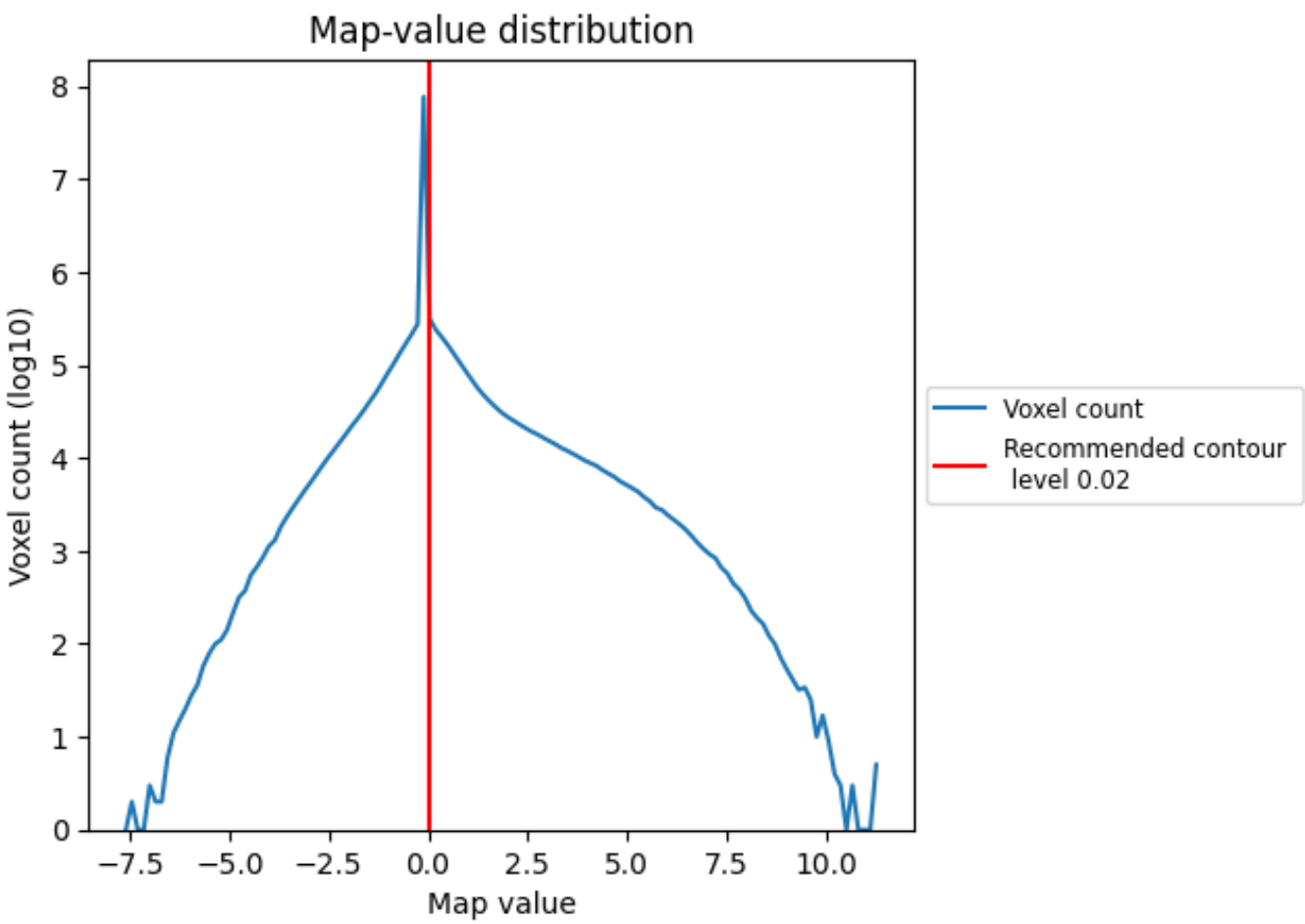
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

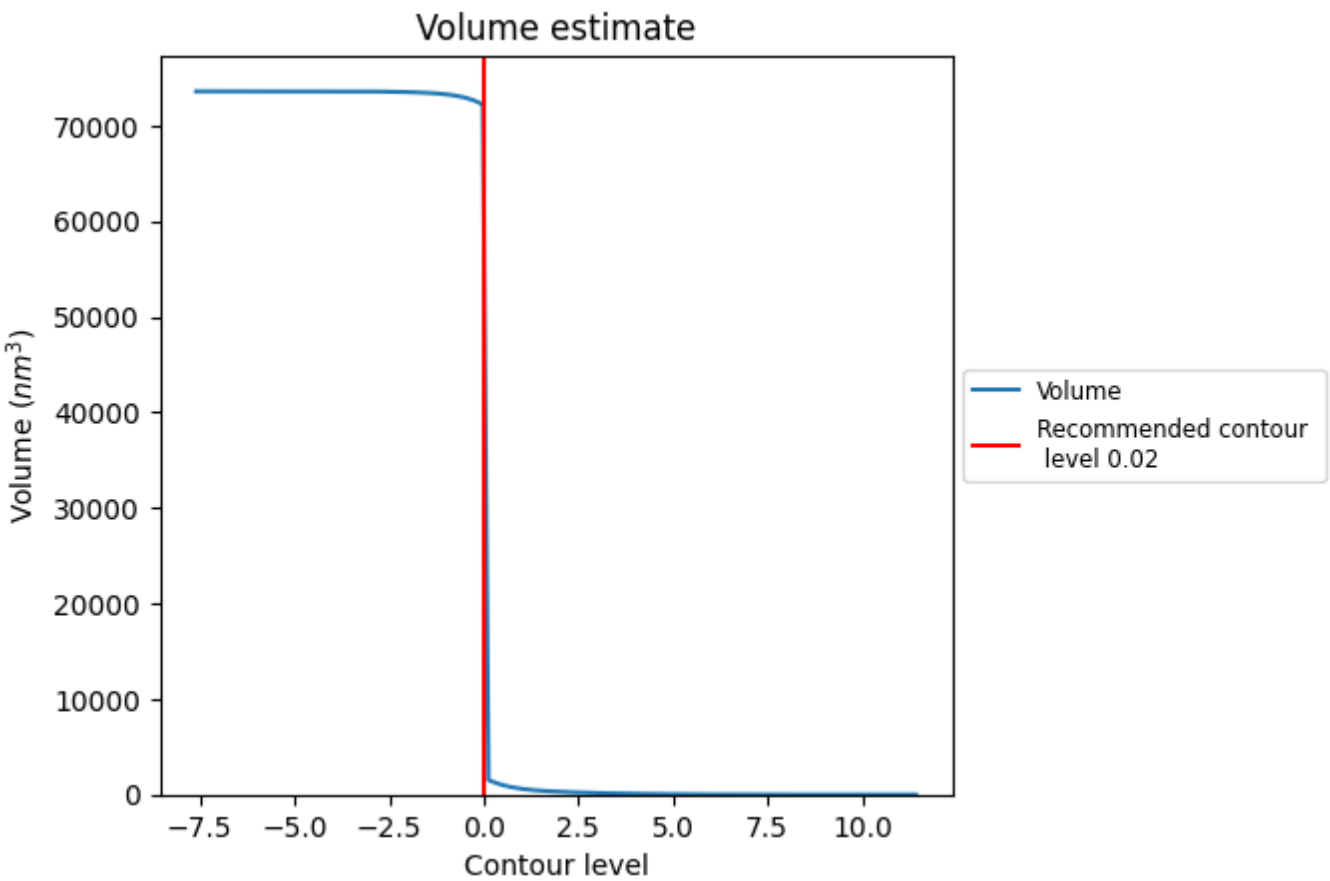
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

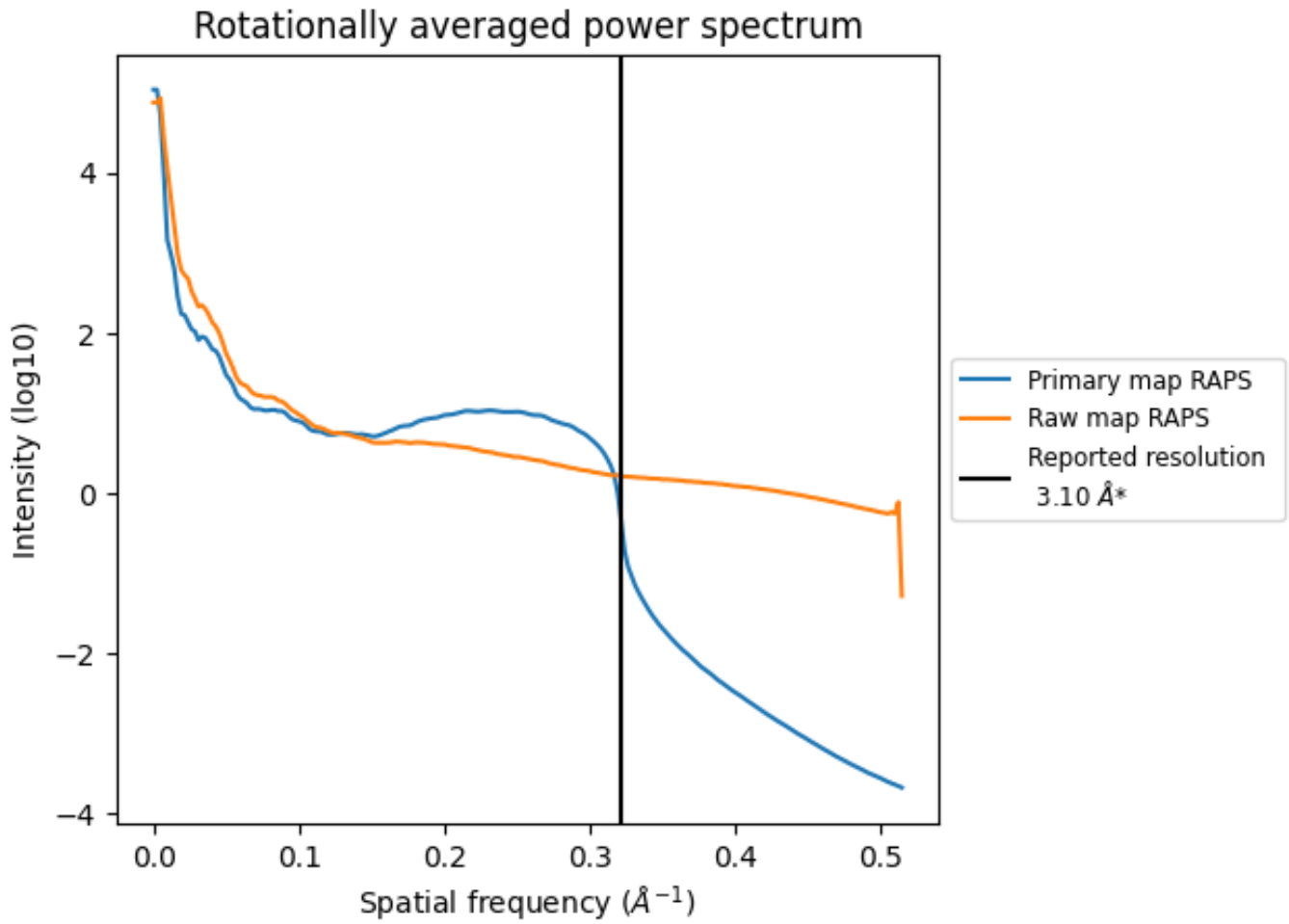
7.2 Volume estimate (i)



The volume at the recommended contour level is 51111 nm^3; this corresponds to an approximate mass of 46170 kDa.

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

7.3 Rotationally averaged power spectrum (i)

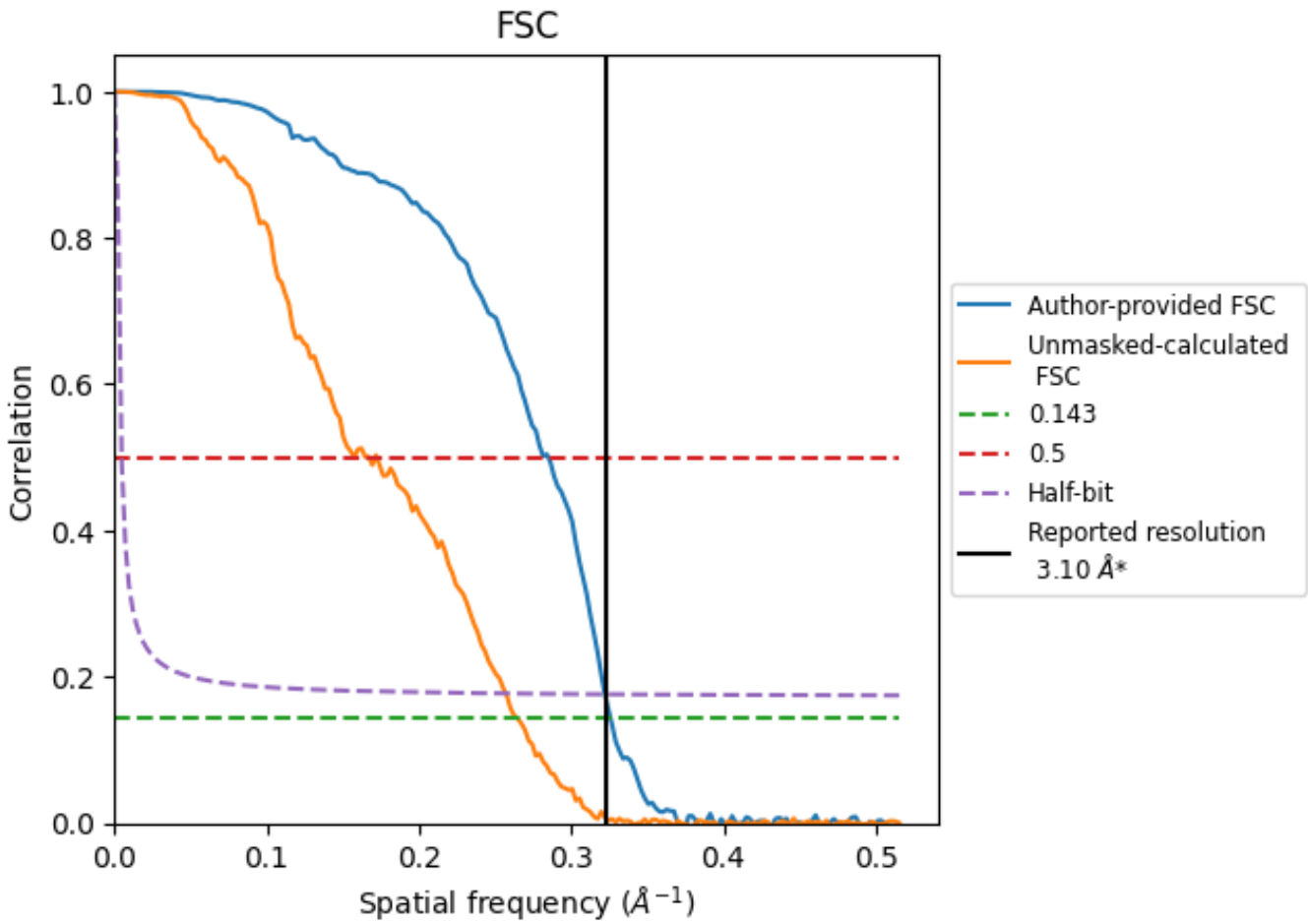


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

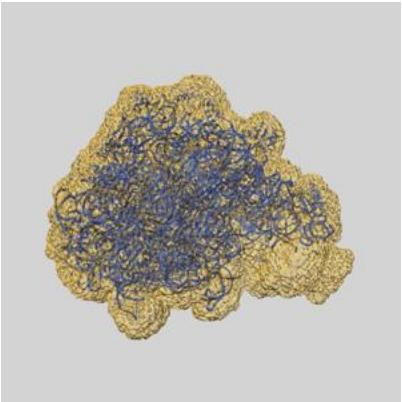
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.51	3.10
Unmasked-calculated*	3.78	5.98	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 3.1 by more than 10 %

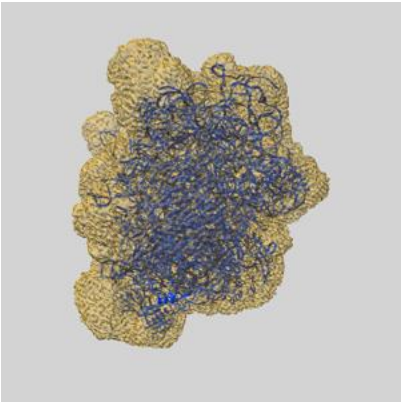
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21888 and PDB model 6WRU. Per-residue inclusion information can be found in section 3 on page 10.

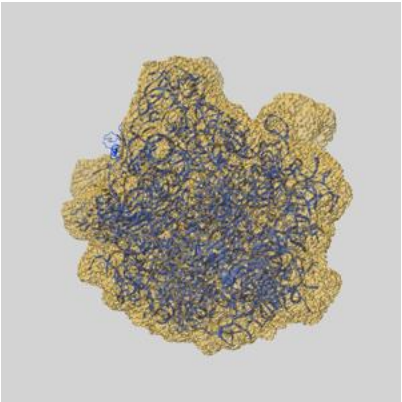
9.1 Map-model overlay (i)



X



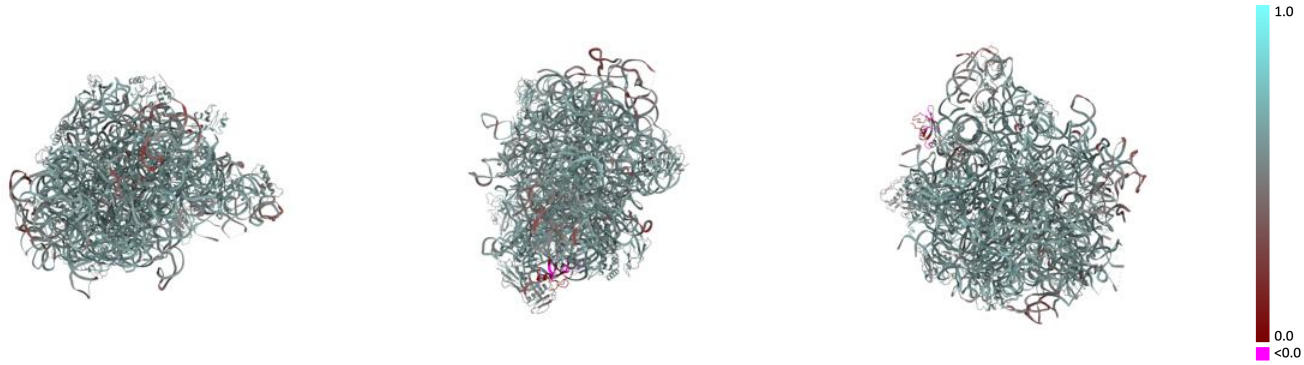
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

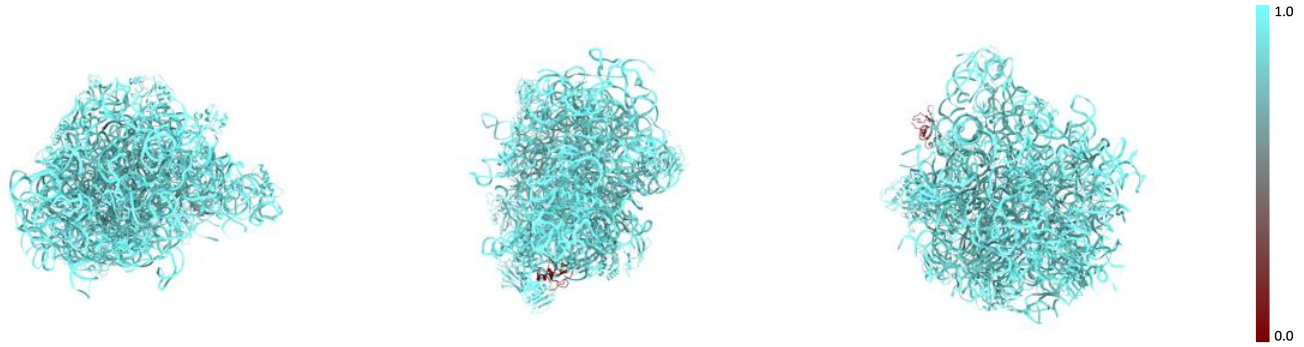
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

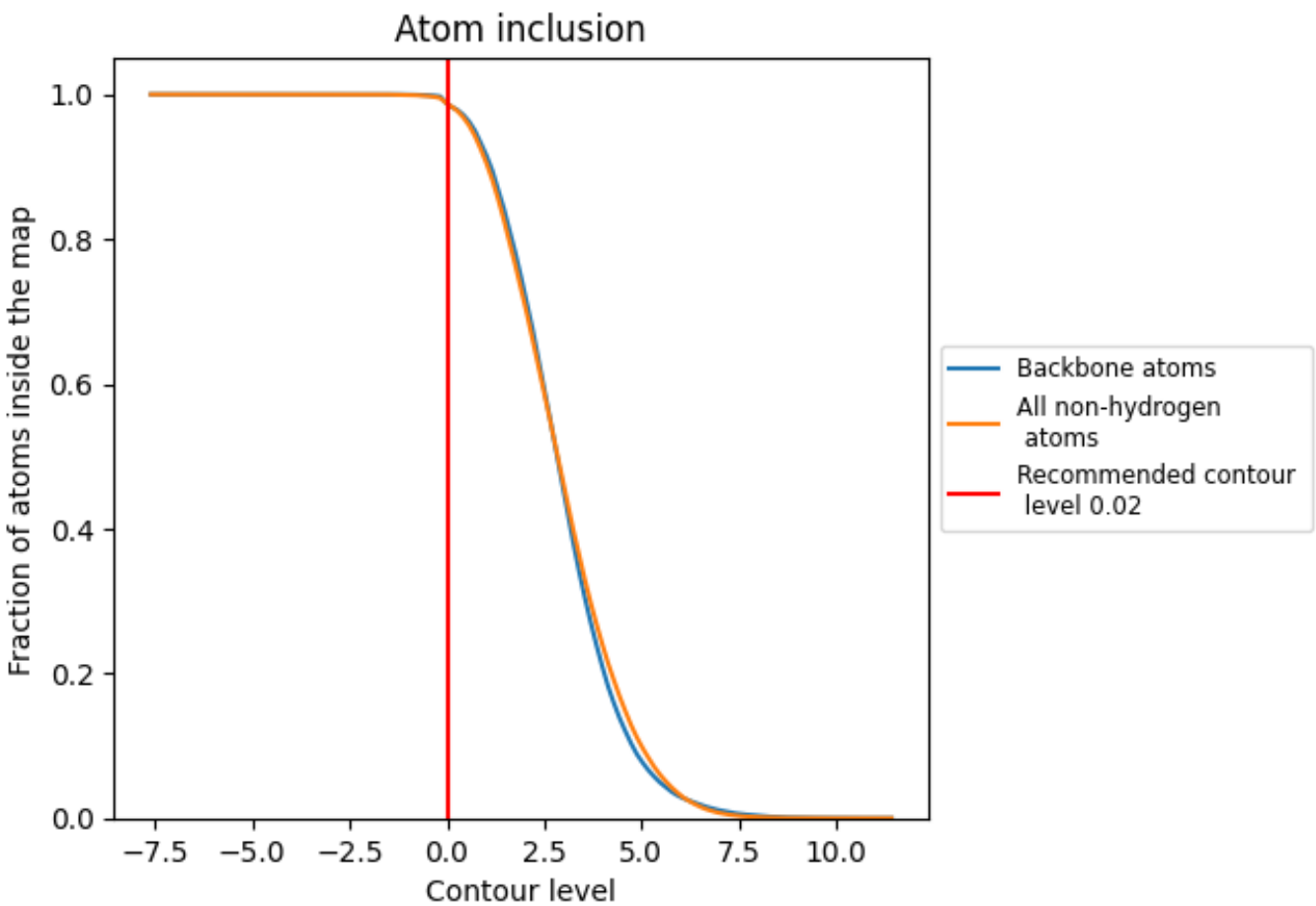
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9861	0.5670
1	0.9922	0.5730
2	0.9903	0.4860
A	0.9943	0.5800
B	0.9888	0.5890
C	0.9912	0.5910
D	0.9974	0.5820
E	0.9940	0.5940
F	0.9841	0.5540
G	0.9941	0.5620
H	0.3796	0.1680
I	0.9879	0.5810
J	0.9911	0.5570
K	0.9871	0.5310
L	0.9819	0.5700
M	0.9835	0.5730
N	0.9948	0.5930
O	0.9788	0.5610
P	0.9886	0.6100
Q	0.9980	0.6180
R	1.0000	0.5920
S	0.9868	0.5690
U	0.9850	0.4980
V	0.9928	0.5920
W	0.9876	0.5730
X	0.9896	0.5760
Y	0.9953	0.5910
Z	0.9919	0.5870
a	0.9886	0.5220