



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 11:36 PM UTC

PDB ID : 8Y39 / pdb_00008y39
EMDB ID : EMD-38876
Title : cryo-EM structure of Staphylococcus aureus(ATCC 29213) 70S ribosome in complex with MCX-190.
Authors : Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on : 2024-01-28
Resolution : 3.60 Å(reported)

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

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A user guide is available at

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

The types of validation reports are described at

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

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

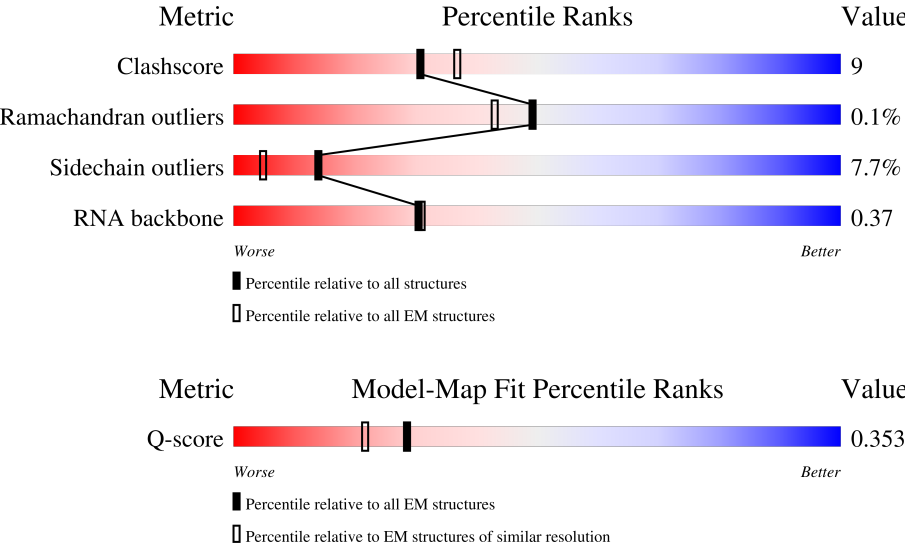
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	2921	
2	B	115	
3	C	274	

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Mol	Chain	Length	Quality of chain
4	D	215	
5	E	206	
6	F	175	
7	G	175	
8	H	145	
9	I	122	
10	J	146	
11	K	137	
12	L	120	
13	M	119	
14	N	114	
15	O	116	
16	P	102	
17	Q	117	
18	R	89	
19	S	103	
20	T	94	
21	U	82	
22	V	58	
23	W	67	
24	X	58	
25	Y	59	
26	Z	48	
27	1	47	
28	2	43	

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Mol	Chain	Length	Quality of chain
29	3	64	
30	4	37	
31	a	1548	
32	b	232	
33	c	217	
34	d	200	
35	e	166	
36	f	98	
37	g	156	
38	h	132	
39	i	130	
40	j	102	
41	k	129	
42	l	149	
43	m	121	
44	n	61	
45	o	89	
46	p	91	
47	q	87	
48	r	80	
49	s	108	
50	t	83	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 138218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2885	Total	C	N	O	P	0	0
			61859	27619	11312	20043	2885		

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

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

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 12 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 14 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 15 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 16 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 19 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 20 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 22 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 23 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 25 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	57	Total	C	N	O	0	0
			353	214	65	74		

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 27 is a protein called Large ribosomal subunit protein bL33B.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1479	Total	C	N	O	P	0	0
			31706	14154	5809	10264	1479		

- Molecule 32 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	224	Total	C	N	O	S	0	0
			1802	1149	314	332	7		

- Molecule 33 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	202	Total	C	N	O	S	0	0
			1596	1005	300	289	2		

- Molecule 34 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	199	Total	C	N	O	S	0	0
			1616	1020	302	292	2		

- Molecule 35 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	156	Total	C	N	O	S	0	0
			1160	731	212	215	2		

- Molecule 36 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	95	Total	C	N	O	S	0	0
			789	498	138	150	3		

- Molecule 37 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	155	Total	C	N	O	S	0	0
			1242	775	239	224	4		

- Molecule 38 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total	C	N	O	S	0	0
			1031	652	183	192	4		

- Molecule 39 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O	S	0	0
			1007	624	201	181	1		

- Molecule 40 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	97	Total	C	N	O	S	0	0
			773	488	141	143	1		

- Molecule 41 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	114	Total	C	N	O	S	0	0
			844	520	160	161	3		

- Molecule 42 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 43 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	116	Total	C	N	O	S	0	0
			922	566	183	172	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 45 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	87	Total	C	N	O	S	0	0
			726	448	149	128	1		

- Molecule 46 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	87	Total	C	N	O	S	0	0
			688	433	127	127	1		

- Molecule 47 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			657	416	117	123	1		

- Molecule 48 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	64	Total	C	N	O	S	0	0
			525	336	98	88	3		

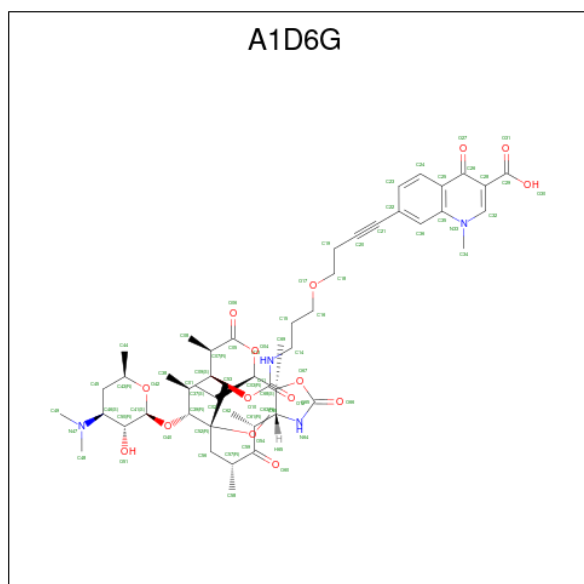
- Molecule 49 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			665	427	121	115	2		

- Molecule 50 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	81	Total	C	N	O	S	0	0
			611	370	120	119	2		

- Molecule 51 is 7-[4-[3-[(1 {S},2 {R},5 {R},6 {S},7 {S},8 {R},9 {R},11 {R},13 {R},14 {R})-8-[(2 {S},3 {R},4 {S},6 {R})-4-(dimethylamino)-6-methyl-3-oxidanyl-oxan-2-yl]oxy-2-ethyl-9-methoxy-1,5,7,9,11,13-hexamethyl-4,12,16-tris(oxidanylidene)-3,17-dioxo-15-azabicyclo[1.2.3.0]heptadecan-6-yl]oxycarbonylamino]propoxy]but-1-ynyl]-1-methyl-4-oxidanylidene-quinoline-3-carboxylic acid (CCD ID: A1D6G) (formula: C₅₀H₇₂N₄O₁₅).



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

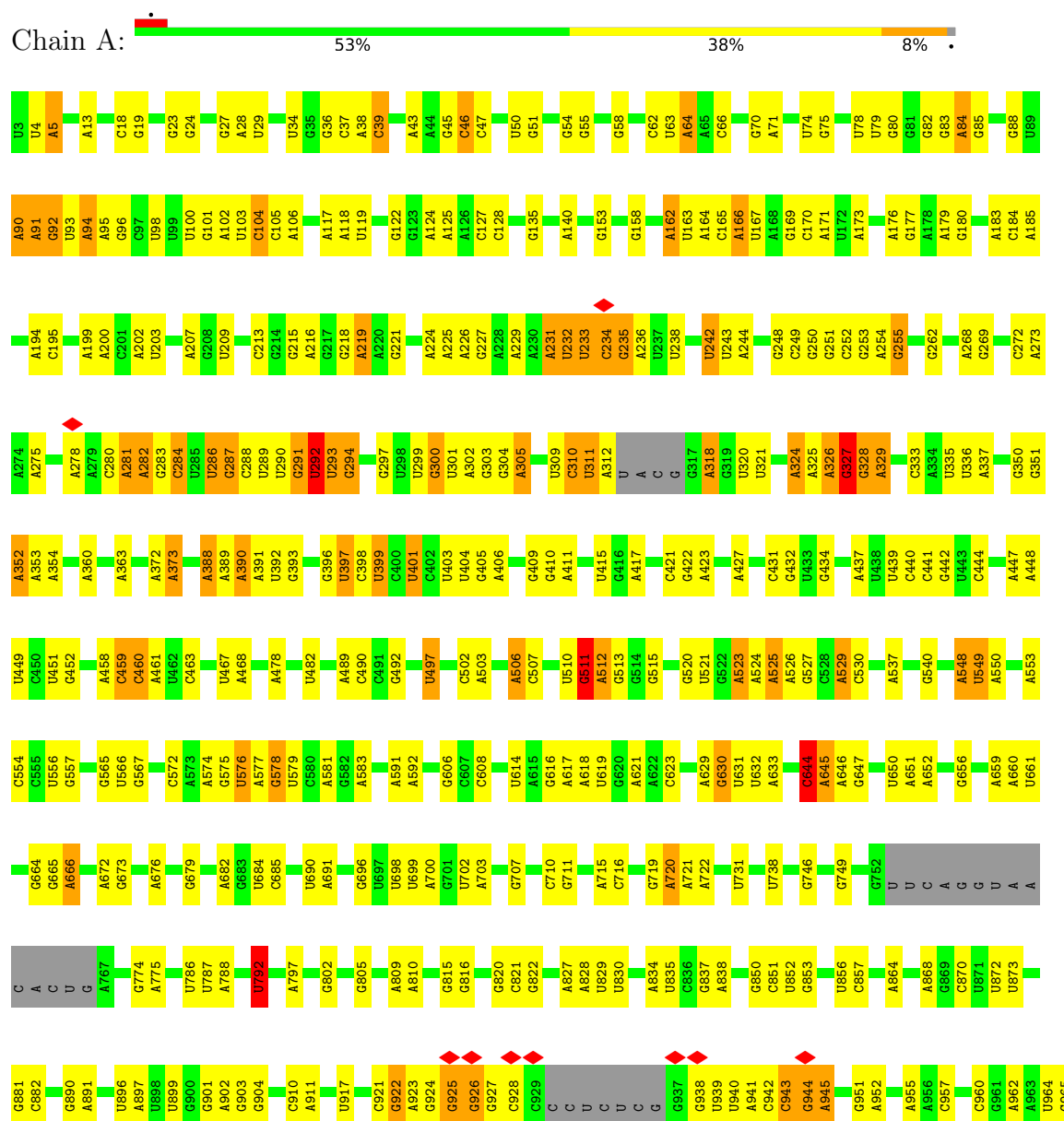
- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

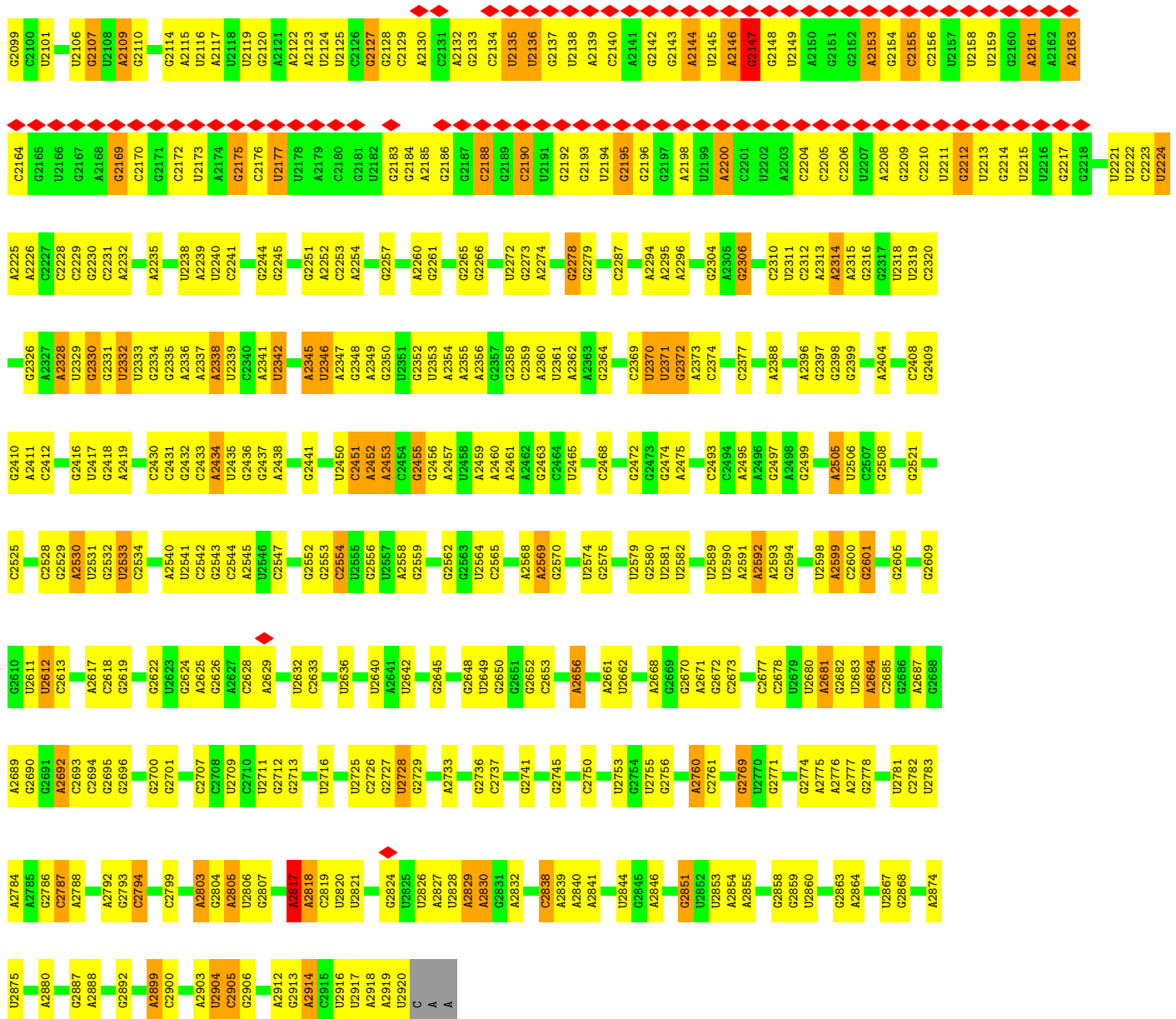
3 Residue-property plots [i](#)

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.

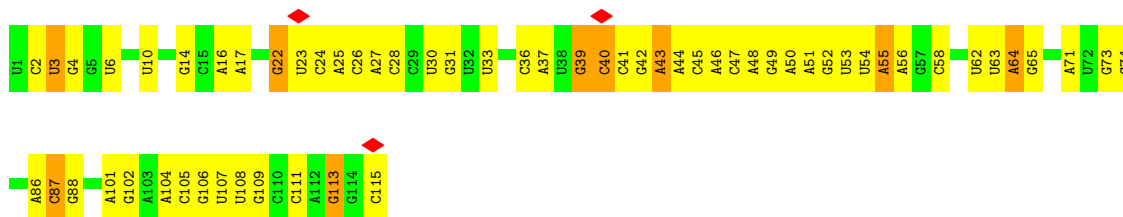
• Molecule 1: 23S ribosomal RNA



A2008	G1915	A1814	A1726	A1634	G1559	G1486	C1387	G1295	A1200	U1127	U1070	U970
U2009	A1916	C1815	C1727	A1635	A1560	G1487	C1387	C1296	G1201	A1128	A1070	U971
	A1917	A1816		A1636	G1561	A1488	A1390	G1297	C1202	A1129	A1071	U972
U2018	G1918	C1817	U1737	A1637	G1562	A1489	A1390	G1300	U1203	A1130	A1072	A973
G2019	C1919	A1818	C1738	G1639	A1567	G1490	A1396	U1301	G1205	A1131	A1065	A974
U2020	C1920	A1819	G1739	U1640	U1568	U1493	G1397	G1302	G1206	A1132	G1066	U975
C2021		G1820	G1740	G1641	U1569	G1494		A1303	G1207	G1133		U976
U2022	A1923	U1821	G1741	G1651	G1571		C1400	A1304	A1208	U1134	A1070	A977
C2023	A1928	C1822	G1742	A1652	G1574	A1497	G1401	U1305		C1135	A1071	
A2024	C1929	A1823	G1743	A1653	A1575	A1498	A1402	U1306	U1215	C1136	A1072	G984
A2025		G1825	A1744	A1654	A1576	A1499		G1307	U1216	G1137	A1073	A985
C2026	C1827	G1826	G1746	G1655	A1577	G1500	G1405	G1308	U1217	U1138		
G2029	G1933	A1828	G1747	C1656	U1504		A1415	G1309	U1218	A1139	U1077	A989
	G1934	A1829		G1657	C1506		U1416	A1310	G1219	U1141		G990
A2032		A1830	G1751	A1658	A1578	A1507		A1311	U1140	A1142		A991
C2035	U1938		G1752	C1659	U1579	A1508	A1421	A1312	A1141	A1143		A992
G2036	A1939	U1835	U1753	A1660	A1580	C1508	A1422		U1142	G1083		C993
G2037	C	A1836	C1754	C1661	U1581	G1509	A1423	C1315	G1144	U1084		G1000
A2040	A	U1843	U1755	A1662	U1582	U1510	A1432	C1316	U1145	U1085		A1001
A2041	U	G1844	U1756		U1583	C1511	U1433	C1326	C1146	C1087		U1002
A2042		U1845	G1757	A1666	U1584	A1512	U1434	C1327	A1147	C1088		A1003
		A1856	G1760		U1585	A1513	C1435	C1328	C1148	A1089		A1004
G2048	A1945		G1761	C1669	U1586		C1436	G1329	U1149	A1090		G1005
U2049	A1946		G1762	A1670	U1587	A1517		U1330	A1150	G1091		
A2050	C1947	G1862	U1763	A1671	U1588	G1522	A1440	C1335	G1151	A1092		G1012
G1948	G1948		U1764	G1672	U1589	G1523	A1443	C1336	U1238	C1093		A1017
A2057	U1949	C1870	A1765	A1678	G1590	C1524		A1337	U1245	U1152		A1018
A2058	U1950	U1871	C1766	A1679	G1591	U1525	A1450	U1338	C1246	A1094		A1019
G2059	C1951	G1872		U1680	G1592	G1526	U1451	U1339	G1247	U1097		
U2061	A1954	G1873	C1769	U1681	U1593	A1527		G1340	U1254	A1098		A1024
A2060	A1955	A1874	C1770	A1684	G1595	G1528	U1454	A1341	G1157	G1099		
G2062	G1956	G1875	A1771		U1596	U1529	U1455	U1342	U1158	G1100		A1027
	G1957		G1783	G1687	U1597	A1530	U1456	U1343	A1159	G1101		G1028
C2070	U1958	A1880		G1688	U1598	U1531	U1457	A1344	C1160	A1102		C1029
		A1881	A1789	A1690	U1602	A	A1458	G1345	U1163	G1103		G1033
C2074	A1964	G1882	G1790	G1691		G		G1346	U1174	U1104		A1034
G2075	A1965	A1883	G1791	G1692	A1605	C	U1460	U1347	G1166	U1105		C1035
A2076	U1966		G1791	G1693	C1606		C1461	U1348		G1106		G1036
C2077	U1967	A1886			G1613	A1537	G1462	U1349	G1169	A1037		A1037
A2078		A1893	A1796	A1699	G1616	A1538	A1463		U1174	C1038		C1038
C2082	U1982	G1894	G1797	U1701	A1617	A1539	U1464	A1359	G1175	C1039		A1040
G2083	G1986	U1800	A1800	U1707	A1618	C1541	G1465	G1360	U1176	G1112		
		U1801	C1801	A1708		C1542	A1471	G1362	A1177	A1113		U1043
A2087	C1989	U1802	U1802	A1709	U1623	U1548	C1472		C1179	G1115		A1044
G2088	C1990	G1803	U1804	U1709	C1624	G1549	G1476	U1366	G1180	A1116		A1045
A2089	G1991	U1805	U1806	A1712	U1625	C1550	U1477		G1181	C1117		G1046
C2091	C1992	U1806	A1713	A1712	U1626	G1551	A1478	C1370	G1182	A1118		G1047
C2092	A1904	A1807	C1714	U1708	U1552	U1551	G1479	G1378	G1183	C1119		C1051
C2093	G1905	U1808	G1717	A1709	A1553	A1553	G1480	A1379	G1184	C1120		A1052
G2094	A1908	C1809	G1718	U1717	U1628	A1554	A1481	G1380	U1185	A1121		A1053
U2095	A1996	U1810	G1719	A1718	U1629	A1555	U1482	U1381	A1186	U1122		A1054
G2096	A1997	A1811	G1719	G1719	G1630	G1556	A1483		A1192	C1123		U1055
C2097	G1998	A1812		C1557	G1631	C1557	G1484	G1384	A1197	A1124		U1056
A2098	U2003	A1813	A1723	U1559	A1632		G1485		G1197	U1125		A1057

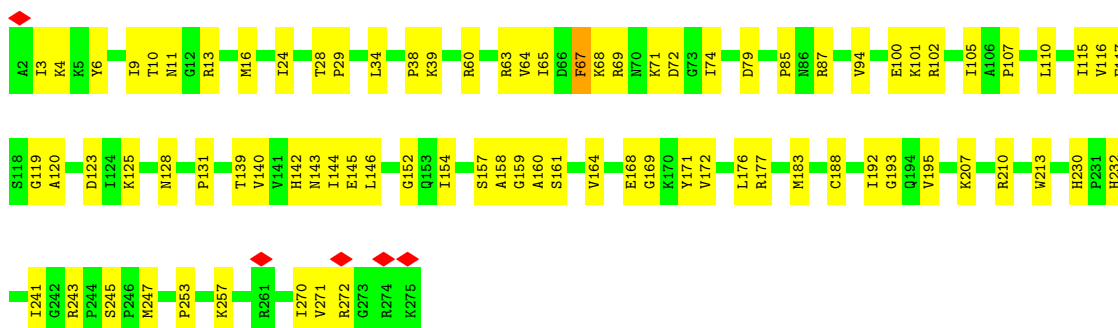


• Molecule 2: 5S ribosomal RNA

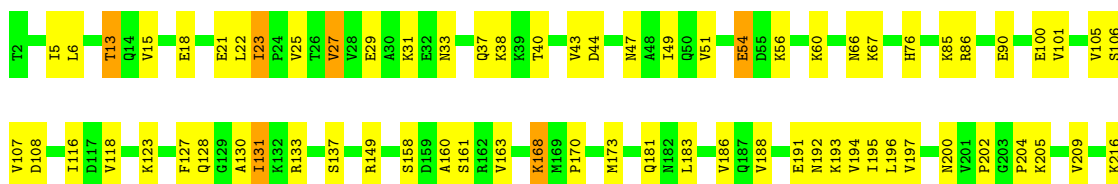


• Molecule 3: Large ribosomal subunit protein uL2

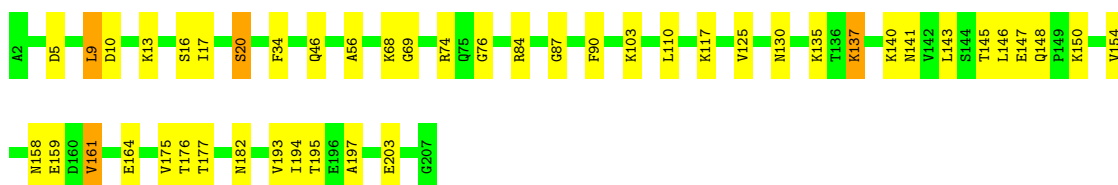
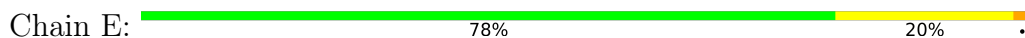




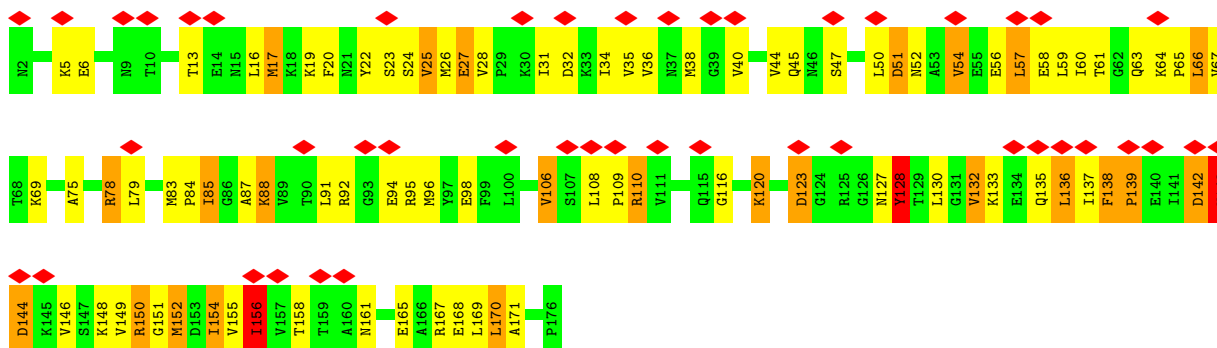
• Molecule 4: Large ribosomal subunit protein uL3



• Molecule 5: Large ribosomal subunit protein uL4

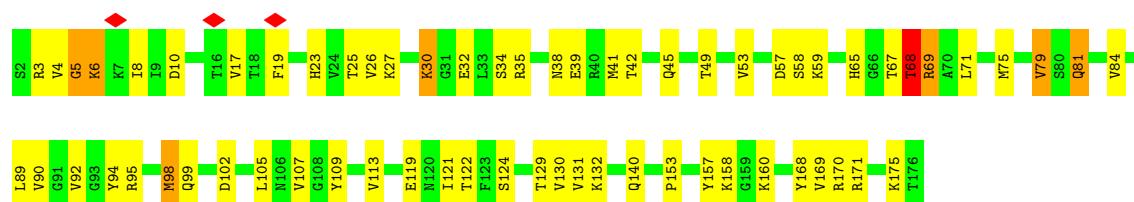


• Molecule 6: Large ribosomal subunit protein uL5



• Molecule 7: Large ribosomal subunit protein uL6





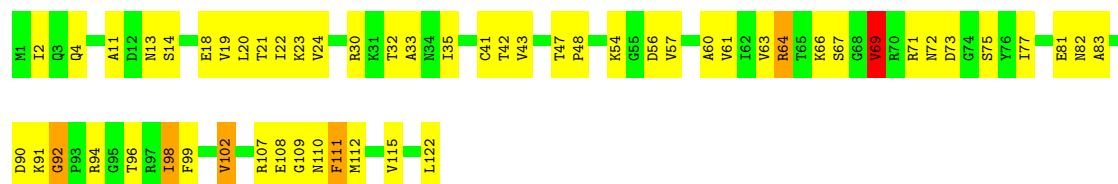
• Molecule 8: Large ribosomal subunit protein uL13

Chain H: 68% 26% 7%



• Molecule 9: Large ribosomal subunit protein uL14

Chain I: 55% 40% . .



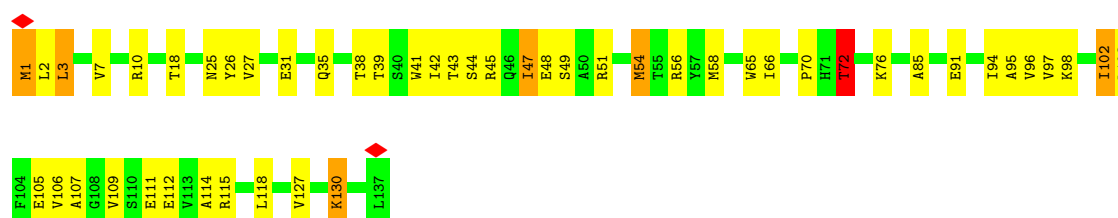
• Molecule 10: Large ribosomal subunit protein uL15

Chain J: 77% 21% .



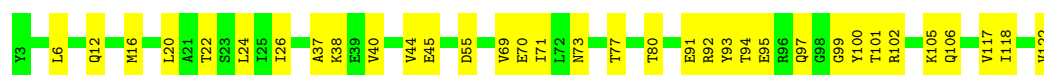
• Molecule 11: Large ribosomal subunit protein uL16

Chain K: 64% 31% . .



• Molecule 12: Large ribosomal subunit protein bL17

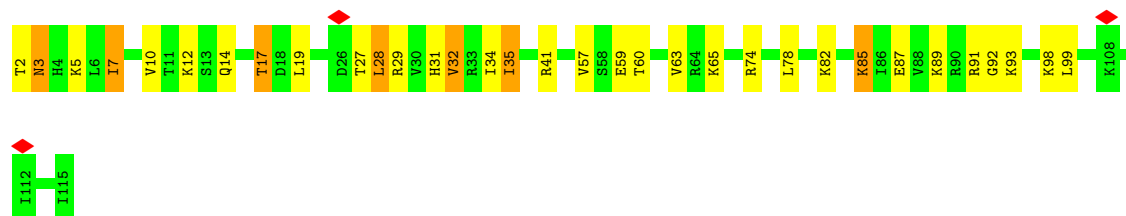
Chain L: 72% 28%



- Molecule 13: Large ribosomal subunit protein uL18



- Molecule 14: Large ribosomal subunit protein bL19



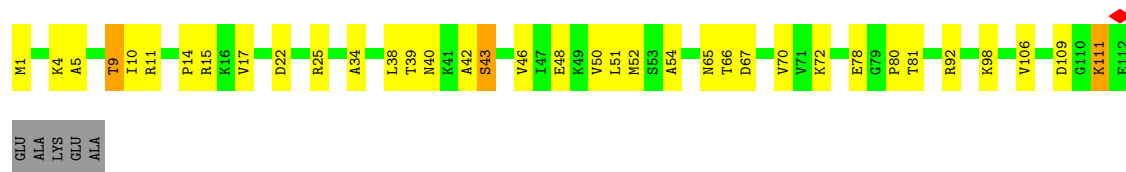
- Molecule 15: Large ribosomal subunit protein bL20



- Molecule 16: Large ribosomal subunit protein bL21



- Molecule 17: Large ribosomal subunit protein uL22



- Molecule 18: Large ribosomal subunit protein uL23

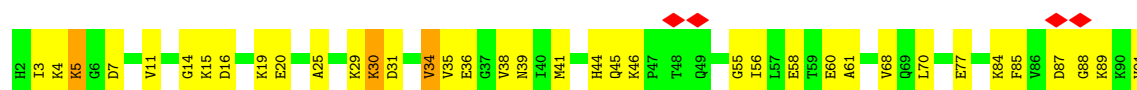
Chain R: 



  F90

- Molecule 19: Large ribosomal subunit protein uL24

Chain S: 



 R92
 I93
 E100
 S103
 R104

- Molecule 20: Large ribosomal subunit protein bL25

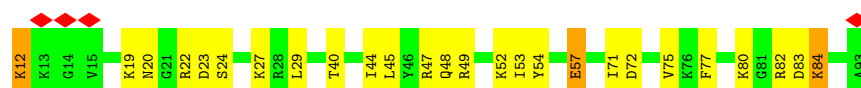
Chain T: 



 I94
 N95

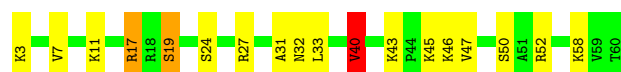
- Molecule 21: Large ribosomal subunit protein bL27

Chain U: 



- Molecule 22: Large ribosomal subunit protein bL28

Chain V: 



- Molecule 23: Large ribosomal subunit protein uL29

Chain W: 



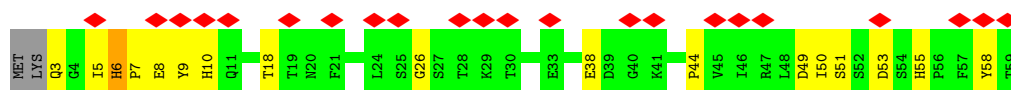
- Molecule 24: Large ribosomal subunit protein uL30

Chain X: 86% 14%



- Molecule 25: Large ribosomal subunit protein bL31B

Chain Y: 37% 68% 27% ..



- Molecule 26: Large ribosomal subunit protein bL32

Chain Z: 79% 21%



- Molecule 27: Large ribosomal subunit protein bL33B

Chain 1: 66% 28% 6%



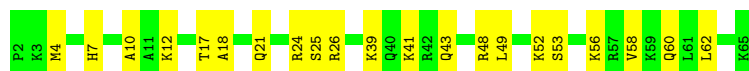
- Molecule 28: Large ribosomal subunit protein bL34

Chain 2: 81% 19%



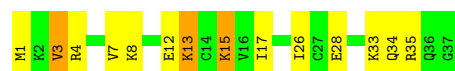
- Molecule 29: Large ribosomal subunit protein bL35

Chain 3: 67% 33%

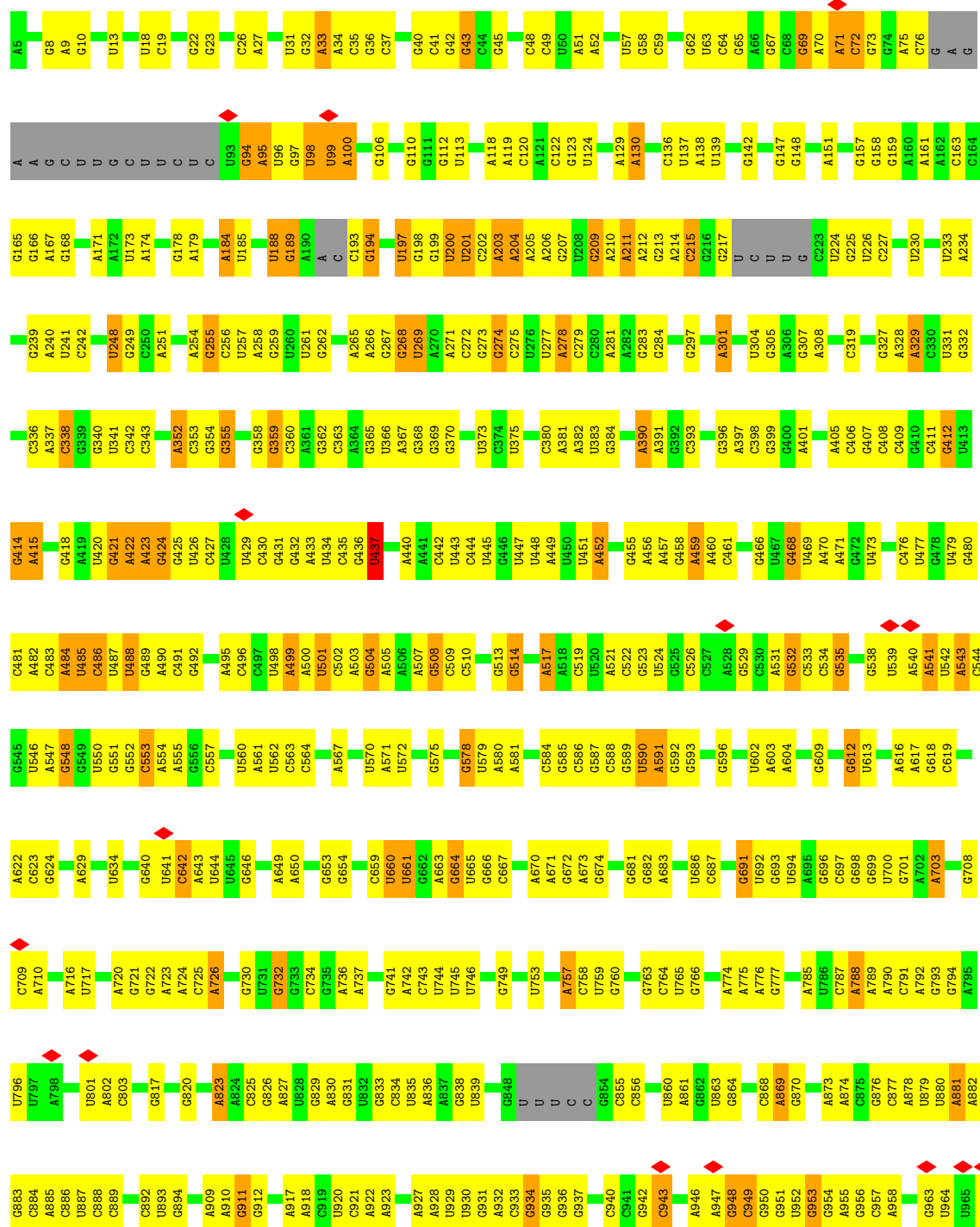


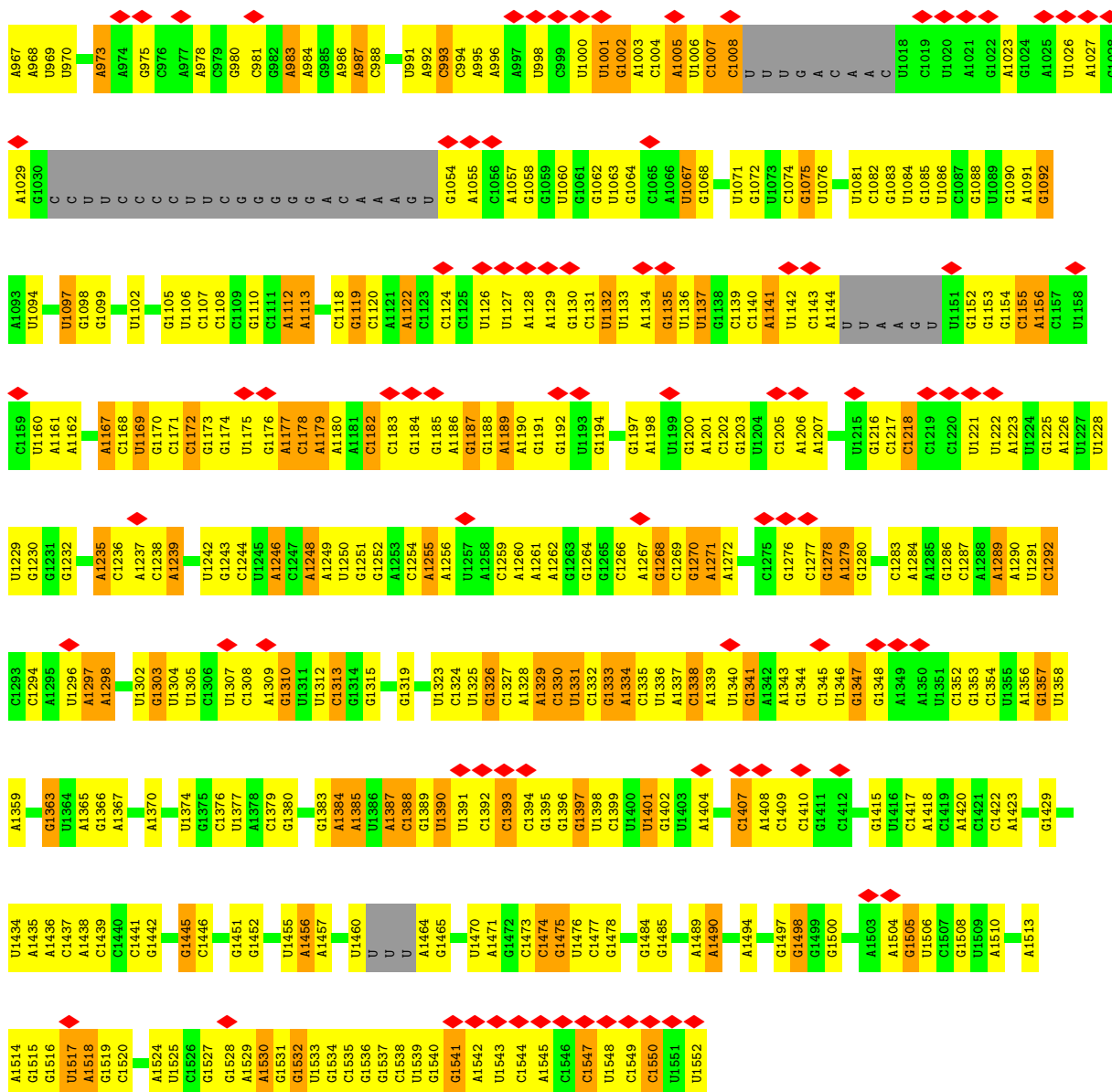
- Molecule 30: Large ribosomal subunit protein bL36

Chain 4: 62% 30% 8%

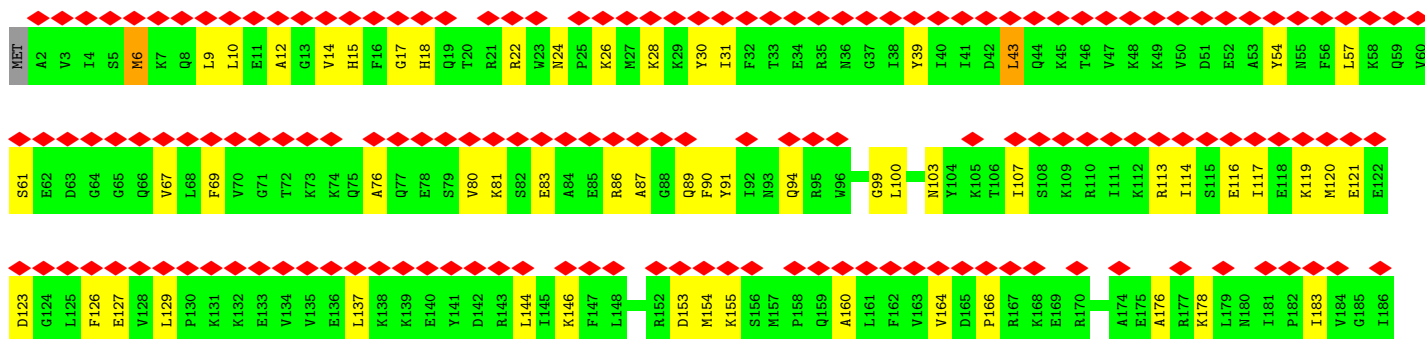
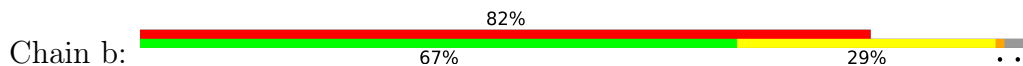


• Molecule 31: 16S ribosomal RNA



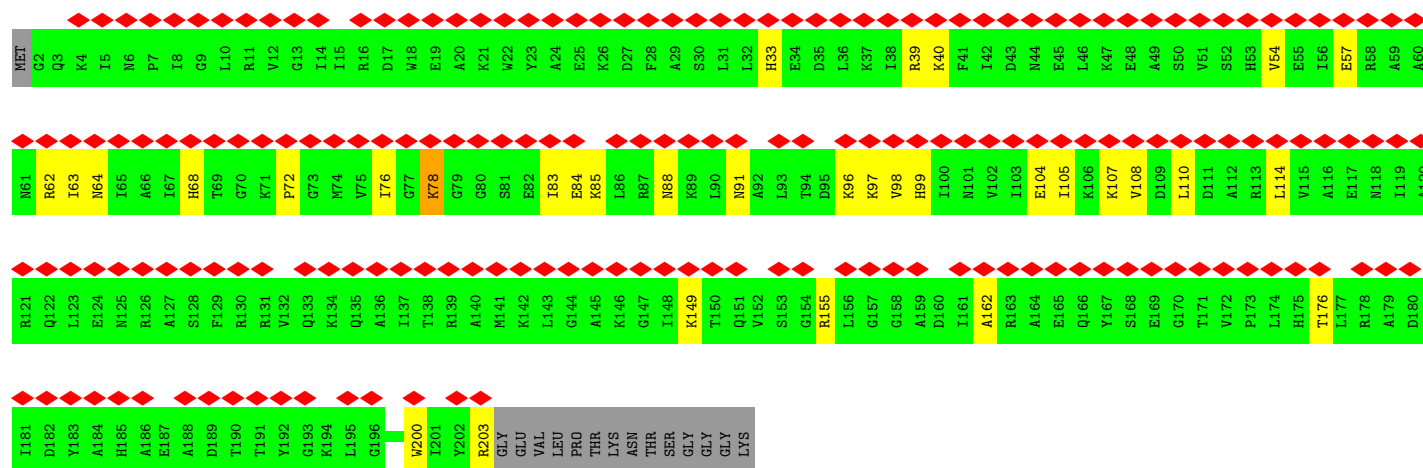
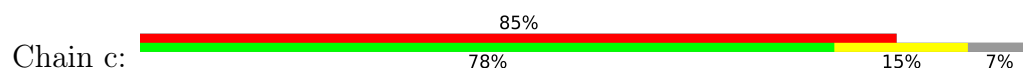


• Molecule 32: Small ribosomal subunit protein uS2

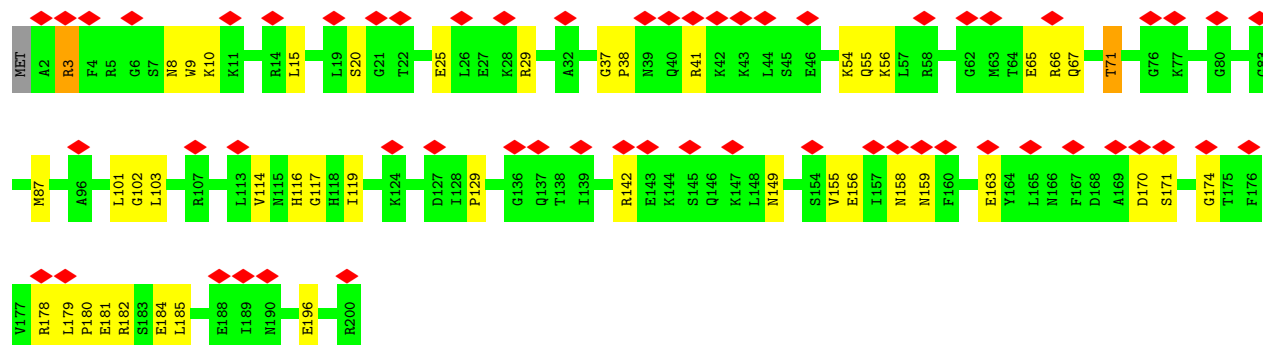
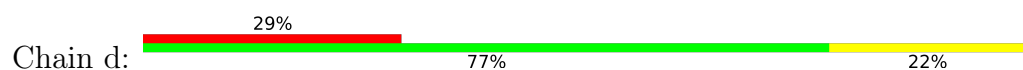




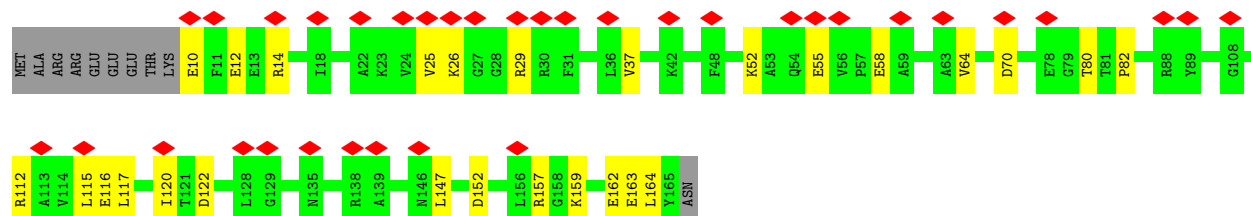
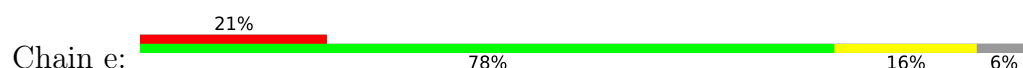
- Molecule 33: Small ribosomal subunit protein uS3



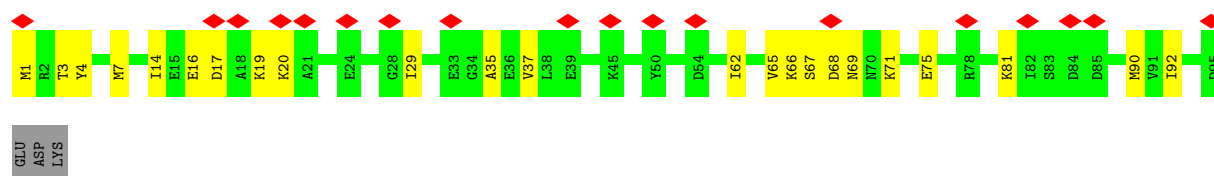
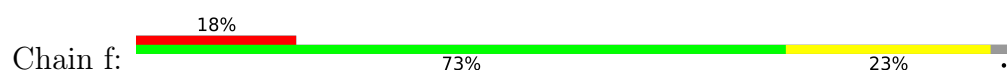
- Molecule 34: Small ribosomal subunit protein uS4



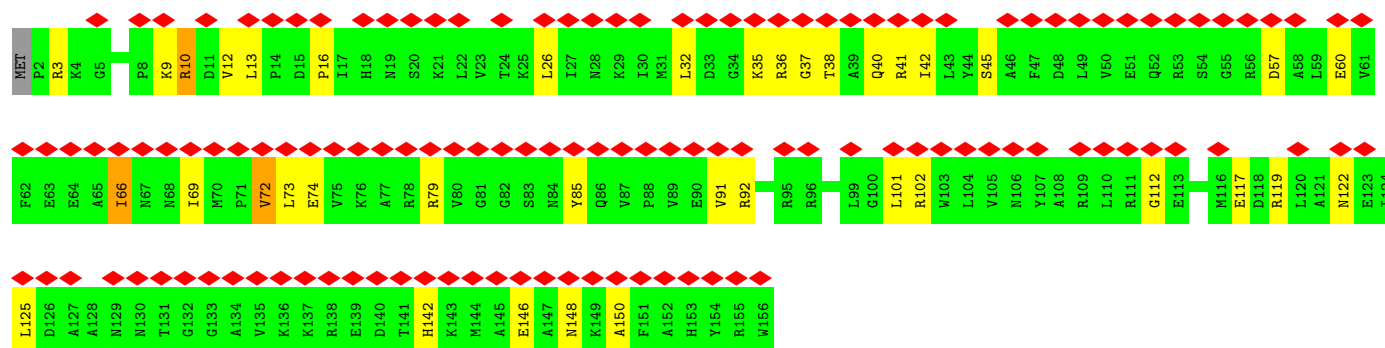
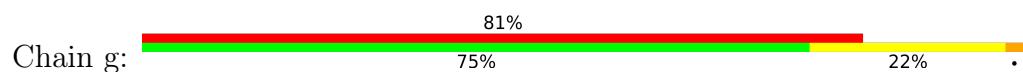
- Molecule 35: Small ribosomal subunit protein uS5



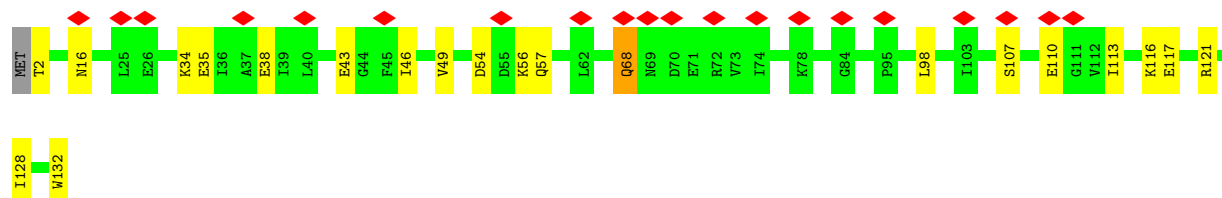
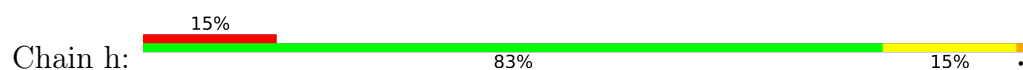
- Molecule 36: Small ribosomal subunit protein bS6



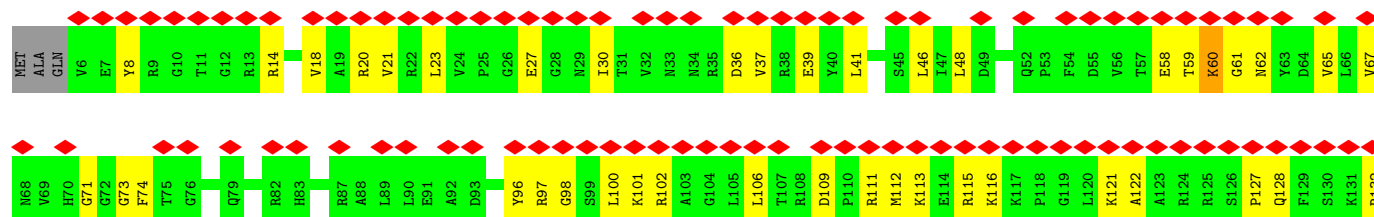
• Molecule 37: Small ribosomal subunit protein uS7



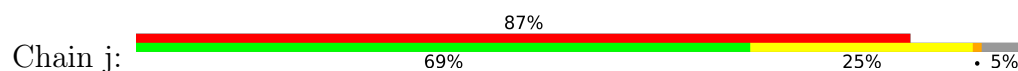
• Molecule 38: Small ribosomal subunit protein uS8

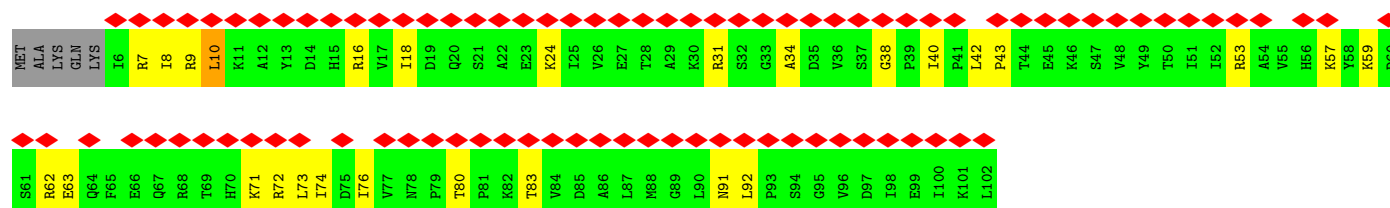


• Molecule 39: Small ribosomal subunit protein uS9

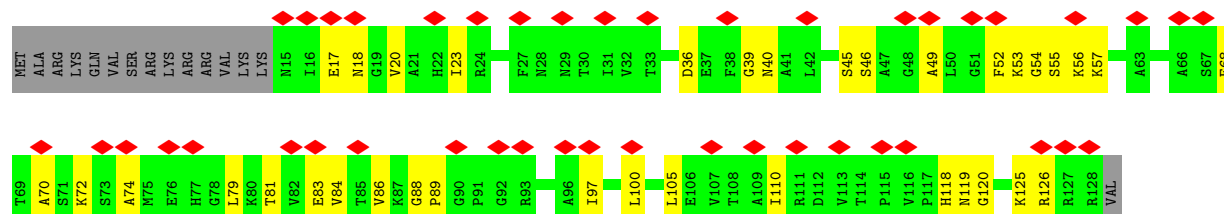


• Molecule 40: Small ribosomal subunit protein uS10

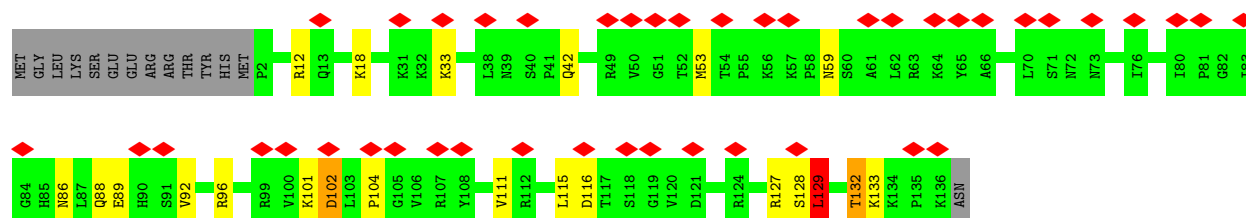
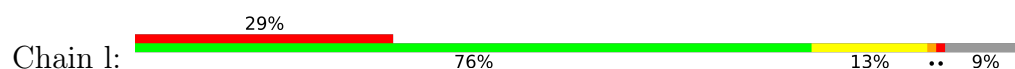




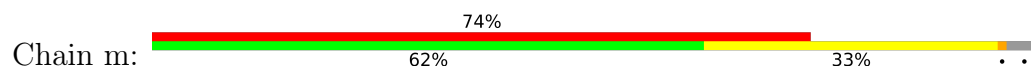
- Molecule 41: Small ribosomal subunit protein uS11



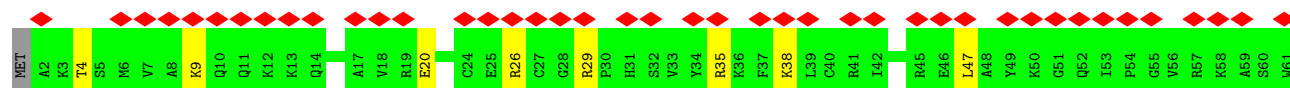
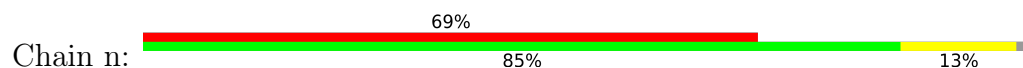
- Molecule 42: Small ribosomal subunit protein uS12



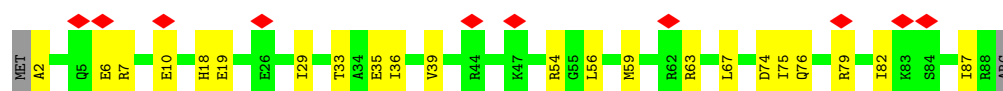
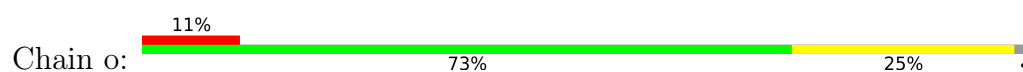
- Molecule 43: Small ribosomal subunit protein uS13



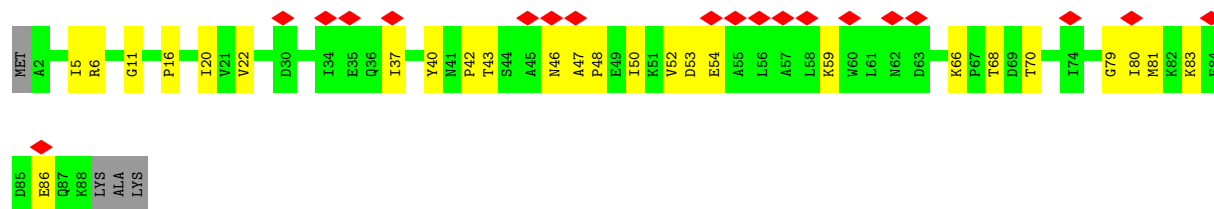
- Molecule 44: Small ribosomal subunit protein uS14B



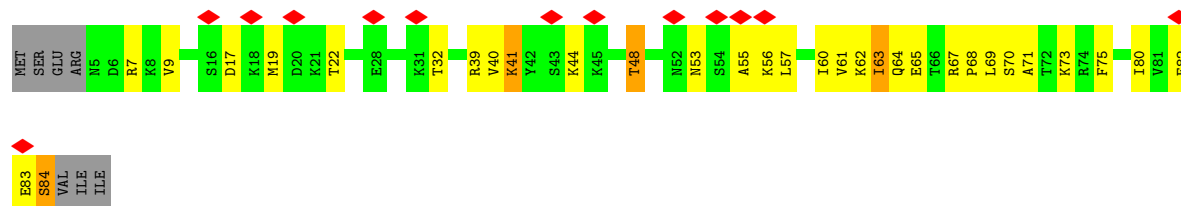
- Molecule 45: Small ribosomal subunit protein uS15



- Molecule 46: Small ribosomal subunit protein bS16



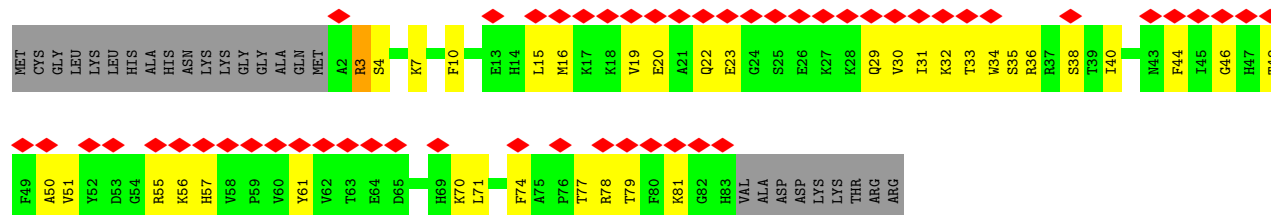
- Molecule 47: Small ribosomal subunit protein uS17



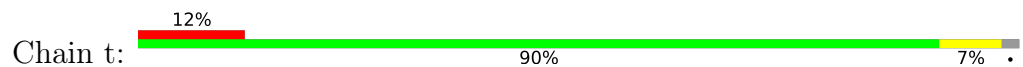
- Molecule 48: Small ribosomal subunit protein bS18

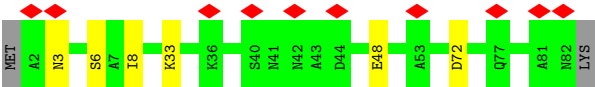


- Molecule 49: Small ribosomal subunit protein uS19



- Molecule 50: Small ribosomal subunit protein bS20





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27177	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.010	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0023	Depositor
Map size ($\text{\AA}$)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.824, 0.824, 0.824	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, OMG, MG, A1D6G, 5MU, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.44	0/69148	0.68	35/107836 (0.0%)
2	B	0.40	0/2733	0.73	1/4257 (0.0%)
3	C	0.96	0/2125	1.23	9/2853 (0.3%)
4	D	1.08	3/1651 (0.2%)	1.18	10/2215 (0.5%)
5	E	0.98	1/1595 (0.1%)	1.21	11/2154 (0.5%)
6	F	0.67	0/1332	1.29	24/1798 (1.3%)
7	G	0.92	1/1277 (0.1%)	1.31	9/1731 (0.5%)
8	H	0.74	0/1165	0.98	5/1570 (0.3%)
9	I	0.93	0/925	1.12	7/1242 (0.6%)
10	J	0.61	0/1100	0.80	3/1467 (0.2%)
11	K	0.96	1/1095 (0.1%)	1.10	10/1472 (0.7%)
12	L	0.63	0/936	0.64	0/1253
13	M	0.90	0/900	1.23	5/1205 (0.4%)
14	N	0.91	1/901 (0.1%)	0.92	3/1209 (0.2%)
15	O	0.54	0/954	0.61	1/1264 (0.1%)
16	P	0.71	0/800	0.96	3/1070 (0.3%)
17	Q	0.97	1/861 (0.1%)	1.02	3/1161 (0.3%)
18	R	0.76	0/723	0.96	2/966 (0.2%)
19	S	0.68	0/779	1.02	4/1043 (0.4%)
20	T	0.68	2/719 (0.3%)	0.89	3/969 (0.3%)
21	U	0.72	0/621	0.89	1/825 (0.1%)
22	V	1.05	1/451 (0.2%)	1.25	4/603 (0.7%)
23	W	0.81	0/542	0.86	1/722 (0.1%)
24	X	0.77	0/451	0.73	2/606 (0.3%)
25	Y	0.48	0/361	0.89	2/500 (0.4%)
26	Z	0.85	0/367	0.99	0/490
27	1	0.90	0/395	1.23	3/530 (0.6%)
28	2	0.51	0/371	0.75	0/484
29	3	0.88	0/526	1.13	5/690 (0.7%)
30	4	1.12	0/299	1.42	6/393 (1.5%)
31	a	0.15	0/35498	0.34	1/55345 (0.0%)
32	b	0.19	0/1829	0.46	0/2455

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.12	0/1618	0.33	0/2173
34	d	0.15	0/1646	0.38	0/2211
35	e	0.25	0/1174	0.47	0/1584
36	f	0.18	0/800	0.45	0/1073
37	g	0.19	0/1262	0.47	1/1698 (0.1%)
38	h	0.22	0/1043	0.41	0/1401
39	i	0.15	0/1023	0.43	0/1374
40	j	0.16	0/785	0.43	0/1060
41	k	0.24	0/859	0.59	0/1161
42	l	0.27	0/1075	0.49	1/1439 (0.1%)
43	m	0.15	0/929	0.40	0/1246
44	n	0.11	0/511	0.33	0/678
45	o	0.12	0/735	0.34	0/982
46	p	0.17	0/699	0.45	0/942
47	q	0.27	0/665	0.48	0/889
48	r	0.25	0/534	0.56	0/715
49	s	0.17	0/683	0.53	1/916 (0.1%)
50	t	0.12	0/611	0.37	0/817
All	All	0.47	11/150082 (0.0%)	0.67	176/224737 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	160	ALA	CA-C	-6.55	1.44	1.52
20	T	76	ASP	CA-C	6.53	1.60	1.52
11	K	97	VAL	C-O	-5.88	1.17	1.24
14	N	59	GLU	CA-C	-5.77	1.45	1.52
4	D	127	PHE	C-O	-5.74	1.17	1.24
7	G	6	LYS	CA-C	-5.23	1.47	1.53
5	E	158	ASN	CA-C	-5.19	1.48	1.53
4	D	13	THR	CA-C	-5.17	1.45	1.52
17	Q	72	LYS	CA-C	-5.10	1.46	1.52
20	T	77	TYR	N-CA	5.09	1.52	1.45
22	V	19	SER	CA-CB	-5.08	1.45	1.53

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	140	GLN	N-CA-C	-10.41	100.32	113.43
6	F	170	LEU	N-CA-C	-10.37	100.63	113.38
6	F	128	TYR	N-CA-C	10.02	121.96	111.14
8	H	58	ILE	N-CA-C	9.44	122.40	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	69	ARG	N-CA-C	-9.04	102.75	113.88
20	T	77	TYR	N-CA-C	8.99	122.81	109.24
7	G	68	THR	CB-CA-C	8.90	124.79	111.17
6	F	45	GLN	N-CA-C	-8.79	102.71	113.97
6	F	19	LYS	N-CA-C	-8.43	102.17	111.36
1	A	1525	U	C4'-C3'-O3'	8.37	121.95	109.40
4	D	23	ILE	CA-C-N	-8.35	110.69	120.13
4	D	23	ILE	C-N-CA	-8.35	110.69	120.13
10	J	84	LYS	N-CA-C	-8.33	102.14	112.88
3	C	146	LEU	N-CA-C	-8.30	103.75	114.04
8	H	3	GLN	N-CA-C	8.25	122.76	111.71
1	A	1918	G	C2'-C3'-O3'	-8.12	101.52	113.70
1	A	1826	G	C3'-C2'-O2'	-8.01	102.59	114.60
9	I	69	VAL	N-CA-C	7.95	120.31	108.46
16	P	50	ALA	CA-C-N	-7.79	110.10	119.84
16	P	50	ALA	C-N-CA	-7.79	110.10	119.84
6	F	52	ASN	N-CA-C	-7.70	102.88	111.28
13	M	19	ARG	N-CA-C	-7.63	103.97	113.20
6	F	142	ASP	N-CA-C	7.56	120.08	110.33
6	F	171	ALA	N-CA-C	-7.56	104.15	113.15
6	F	123	ASP	N-CA-C	-7.42	102.16	113.89
1	A	327	G	C2'-C3'-O3'	7.38	120.57	109.50
1	A	576	U	C2'-C3'-O3'	7.37	120.55	109.50
14	N	28	LEU	N-CA-C	7.36	119.93	108.96
9	I	111	PHE	N-CA-C	-7.34	99.36	109.71
18	R	18	GLU	N-CA-C	-7.33	103.31	111.82
6	F	137	ILE	N-CA-C	7.26	124.44	109.34
29	3	18	ALA	N-CA-C	7.17	119.96	111.71
22	V	40	VAL	N-CA-C	7.16	118.13	108.11
5	E	9	LEU	N-CA-C	-7.11	103.86	112.54
6	F	25	VAL	N-CA-C	-7.09	105.81	112.83
5	E	161	VAL	N-CA-C	7.00	118.60	110.62
30	4	3	VAL	CB-CA-C	6.98	120.07	110.99
25	Y	6	HIS	N-CA-C	6.91	117.55	109.60
1	A	233	U	C4'-C3'-O3'	-6.74	102.88	113.00
4	D	116	ILE	O-C-N	-6.72	115.61	123.00
1	A	511	G	C4'-C3'-O3'	-6.70	102.94	113.00
30	4	4	ARG	CA-C-N	-6.65	112.78	119.56
30	4	4	ARG	C-N-CA	-6.65	112.78	119.56
3	C	67	PHE	N-CA-C	-6.64	105.00	113.23
11	K	56	ARG	N-CA-C	-6.58	103.59	111.69
1	A	1605	A	C2'-C3'-O3'	-6.56	99.66	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1760	G	C4'-C3'-O3'	6.53	119.20	109.40
17	Q	48	GLU	N-CA-C	-6.53	104.25	111.82
6	F	61	THR	N-CA-C	-6.51	100.34	110.17
6	F	26	MET	N-CA-C	-6.45	105.44	113.38
5	E	150	LYS	CA-C-N	-6.44	113.92	123.00
5	E	150	LYS	C-N-CA	-6.44	113.92	123.00
19	S	30	LYS	N-CA-C	-6.43	104.13	114.09
9	I	72	ASN	N-CA-C	6.40	120.19	112.38
3	C	120	ALA	N-CA-C	-6.40	106.69	114.75
19	S	39	ASN	CA-C-N	-6.39	111.94	120.50
19	S	39	ASN	C-N-CA	-6.39	111.94	120.50
37	g	69	ILE	N-CA-C	-6.34	106.80	112.12
7	G	102	ASP	N-CA-C	-6.32	99.80	109.41
2	B	22	G	C4'-C3'-O3'	6.29	118.84	109.40
7	G	30	LYS	N-CA-C	6.27	120.93	113.16
6	F	138	PHE	N-CA-C	6.25	122.81	108.93
4	D	188	VAL	N-CA-C	-6.21	99.42	108.11
13	M	70	VAL	N-CA-C	-6.17	103.38	111.09
13	M	13	LYS	N-CA-C	-6.14	103.19	112.04
29	3	41	LYS	CA-C-O	-6.13	114.38	120.70
6	F	169	LEU	N-CA-C	-6.13	105.39	112.92
6	F	143	TYR	N-CA-C	-6.11	105.67	113.01
49	s	3	ARG	CB-CA-C	-6.10	109.53	116.54
9	I	61	VAL	N-CA-C	6.09	116.69	108.17
18	R	53	VAL	O-C-N	-6.06	116.33	123.00
29	3	25	SER	O-C-N	-6.05	114.70	122.20
1	A	1526	G	C4'-C3'-O3'	6.01	122.02	113.00
11	K	3	LEU	N-CA-C	6.00	119.36	109.58
14	N	32	VAL	N-CA-C	5.99	117.39	108.46
1	A	292	U	C4'-C3'-O3'	-5.96	100.45	109.40
1	A	1556	G	C2'-C3'-O3'	-5.95	104.77	113.70
13	M	95	ASP	CA-CB-CG	-5.93	106.67	112.60
4	D	170	PRO	N-CA-C	5.92	120.52	111.11
17	Q	66	THR	N-CA-C	5.91	120.35	113.20
11	K	72	THR	N-CA-C	5.91	118.16	109.42
9	I	92	GLY	CA-C-N	-5.90	114.53	120.31
9	I	92	GLY	C-N-CA	-5.90	114.53	120.31
1	A	207	A	C2'-C3'-O3'	-5.86	100.72	109.50
1	A	1024	A	C2'-C3'-O3'	-5.85	104.92	113.70
4	D	161	SER	N-CA-C	-5.82	102.60	110.68
4	D	25	VAL	N-CA-C	5.79	118.50	108.95
7	G	153	PRO	CA-C-N	-5.79	113.82	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	153	PRO	C-N-CA	-5.79	113.82	119.78
11	K	96	VAL	N-CA-C	5.77	117.17	109.37
27	1	14	ASP	N-CA-C	5.75	118.69	110.24
1	A	2533	U	C4'-C3'-O3'	5.75	118.02	109.40
30	4	35	ARG	N-CA-C	5.73	123.00	110.80
10	J	95	LEU	N-CA-C	-5.70	105.44	112.90
6	F	50	LEU	N-CA-C	-5.69	105.16	111.36
1	A	2817	A	C4'-C3'-O3'	-5.69	100.86	109.40
1	A	2147	G	C4'-C3'-O3'	-5.69	104.47	113.00
5	E	56	ALA	CA-C-N	5.68	130.24	121.71
5	E	56	ALA	C-N-CA	5.68	130.24	121.71
3	C	72	ASP	N-CA-C	5.68	117.99	108.96
15	O	114	LYS	N-CA-C	-5.67	105.08	112.23
3	C	177	ARG	N-CA-C	5.65	118.98	111.75
22	V	43	LYS	N-CA-C	5.65	117.62	109.48
29	3	58	VAL	N-CA-C	5.63	117.85	111.88
21	U	40	THR	N-CA-C	-5.62	102.44	110.59
4	D	130	ALA	N-CA-C	5.60	119.37	112.54
5	E	158	ASN	N-CA-C	-5.59	98.30	108.65
1	A	232	U	C2'-C3'-O3'	-5.59	105.32	113.70
22	V	24	SER	N-CA-C	5.59	118.92	109.76
1	A	1555	G	C4'-C3'-O3'	-5.58	101.03	109.40
6	F	144	ASP	N-CA-C	5.56	118.10	111.71
29	3	26	ARG	N-CA-C	5.55	119.03	110.42
9	I	60	ALA	N-CA-C	5.55	117.53	108.76
1	A	1348	U	C2'-C3'-O3'	5.53	117.79	109.50
8	H	86	LYS	CA-C-N	-5.51	113.94	122.59
8	H	86	LYS	C-N-CA	-5.51	113.94	122.59
1	A	1826	G	C1'-C2'-O2'	-5.50	103.54	111.80
27	1	36	CYS	CA-C-N	-5.50	114.01	120.12
27	1	36	CYS	C-N-CA	-5.50	114.01	120.12
16	P	51	PRO	N-CA-C	-5.50	101.15	112.47
3	C	193	GLY	CA-C-O	-5.49	118.37	122.37
5	E	87	GLY	N-CA-C	5.49	118.24	111.93
4	D	194	VAL	N-CA-C	5.47	115.86	107.77
1	A	229	A	C4'-C3'-O3'	-5.46	104.81	113.00
8	H	9	GLU	N-CA-C	5.46	119.68	113.19
4	D	60	LYS	N-CA-C	-5.45	100.78	109.23
5	E	103	LYS	N-CA-C	5.45	117.92	111.33
22	V	17	ARG	N-CA-C	-5.45	99.85	108.73
7	G	5	GLY	N-CA-C	5.43	119.06	112.49
1	A	92	G	C4'-C3'-O3'	-5.42	104.87	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	HIS	N-CA-C	-5.42	101.49	109.18
11	K	31	GLU	N-CA-C	-5.40	106.63	113.43
6	F	20	PHE	N-CA-C	-5.39	100.24	109.24
25	Y	44	PRO	N-CA-C	-5.37	101.30	112.36
1	A	2200	A	C2'-C3'-O3'	-5.34	105.69	113.70
11	K	85	ALA	N-CA-C	5.33	118.94	111.74
11	K	48	GLU	N-CA-C	-5.33	105.47	111.28
3	C	28	THR	CB-CA-C	5.32	117.18	109.20
42	l	129	LEU	N-CA-C	-5.32	102.88	110.59
31	a	437	U	C2'-C3'-O3'	-5.30	101.56	109.50
6	F	116	GLY	N-CA-C	-5.26	103.12	110.96
10	J	137	ASP	N-CA-C	5.25	118.15	111.69
20	T	28	PRO	CA-C-O	-5.25	115.45	121.86
5	E	20	SER	N-CA-C	5.25	117.46	110.53
1	A	644	C	O4'-C1'-C2'	-5.25	102.35	107.60
20	T	87	THR	N-CA-C	5.23	119.89	112.93
1	A	2598	U	C2'-C3'-O3'	-5.22	105.87	113.70
1	A	1037	A	C2'-C3'-O3'	-5.20	105.90	113.70
6	F	57	LEU	N-CA-C	5.20	116.95	111.28
11	K	49	SER	N-CA-C	5.19	117.02	111.36
30	4	13	LYS	CA-C-N	-5.19	115.87	122.77
30	4	13	LYS	C-N-CA	-5.19	115.87	122.77
1	A	1027	A	C4'-C3'-O3'	-5.18	105.22	113.00
3	C	38	PRO	CB-CA-C	5.17	116.22	111.87
1	A	444	C	O3'-P-O5'	-5.17	96.24	104.00
1	A	1555	G	C2'-C3'-O3'	-5.17	101.75	109.50
6	F	47	SER	N-CA-C	-5.17	99.80	110.80
17	Q	10	ILE	N-CA-C	-5.16	102.42	109.55
11	K	41	TRP	N-CA-C	-5.16	101.29	109.76
1	A	1555	G	C1'-C2'-O2'	5.15	119.52	111.80
6	F	156	ILE	N-CA-C	5.15	115.47	107.28
1	A	2127	G	C4'-C3'-O3'	-5.14	105.29	113.00
6	F	83	MET	CA-C-N	-5.13	113.92	120.23
6	F	83	MET	C-N-CA	-5.13	113.92	120.23
11	K	10	ARG	N-CA-C	5.13	119.52	113.16
5	E	69	GLY	N-CA-C	5.13	119.79	113.79
1	A	510	U	C4'-C3'-O3'	-5.12	105.32	113.00
1	A	2465	U	C4'-C3'-O3'	-5.09	105.36	113.00
24	X	15	ARG	CA-C-N	-5.08	114.49	119.92
24	X	15	ARG	C-N-CA	-5.08	114.49	119.92
19	S	5	LYS	N-CA-C	5.06	118.72	112.54
14	N	3	ASN	N-CA-C	-5.02	102.05	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	A	C2'-C3'-O3'	-5.02	106.17	113.70
7	G	79	VAL	N-CA-C	-5.01	106.25	113.07
13	M	6	ASP	N-CA-C	-5.00	103.07	110.48
23	W	30	PHE	N-CA-C	-5.00	105.93	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61859	0	31099	435	0
2	B	2445	0	1240	20	0
3	C	2090	0	2201	49	0
4	D	1627	0	1667	35	0
5	E	1572	0	1619	32	0
6	F	1317	0	1323	62	0
7	G	1259	0	1221	41	0
8	H	1143	0	1134	36	0
9	I	918	0	981	51	0
10	J	1086	0	1125	21	0
11	K	1071	0	1123	25	0
12	L	932	0	983	34	0
13	M	891	0	925	28	0
14	N	889	0	937	23	0
15	O	942	0	1014	37	0
16	P	790	0	830	24	0
17	Q	853	0	905	20	0
18	R	715	0	748	28	0
19	S	770	0	809	35	0
20	T	711	0	740	34	0
21	U	615	0	622	18	0
22	V	445	0	466	9	0
23	W	541	0	563	8	0
24	X	449	0	491	2	0
25	Y	353	0	218	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Z	361	0	361	10	0
27	1	390	0	394	4	0
28	2	367	0	415	6	0
29	3	521	0	586	11	0
30	4	296	0	340	7	0
31	a	31706	0	15964	657	0
32	b	1802	0	1866	51	0
33	c	1596	0	1659	24	0
34	d	1616	0	1646	37	0
35	e	1160	0	1223	13	0
36	f	789	0	788	16	0
37	g	1242	0	1276	25	0
38	h	1031	0	1082	15	0
39	i	1007	0	1031	30	0
40	j	773	0	812	19	0
41	k	844	0	851	33	0
42	l	1058	0	1130	15	0
43	m	922	0	970	28	0
44	n	501	0	527	8	0
45	o	726	0	756	16	0
46	p	688	0	713	17	0
47	q	657	0	694	25	0
48	r	525	0	561	11	0
49	s	665	0	668	33	0
50	t	611	0	655	6	0
51	A	69	0	0	0	0
52	A	12	0	0	0	0
All	All	138218	0	91952	2014	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 9.

All (2014) 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)
20:T:32:TYR:CE1	20:T:92:LEU:HD21	1.62	1.35
20:T:32:TYR:CD1	20:T:92:LEU:HD23	1.74	1.23
20:T:32:TYR:CD1	20:T:92:LEU:CD2	2.21	1.21
20:T:32:TYR:CE1	20:T:92:LEU:CD2	2.22	1.21
1:A:104:C:H5"	1:A:104:C:H6	1.30	0.96
20:T:32:TYR:HE1	20:T:92:LEU:HD21	1.06	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:32:TYR:HD1	20:T:92:LEU:CD2	1.82	0.92
20:T:32:TYR:CD1	20:T:92:LEU:HD21	1.99	0.91
6:F:79:LEU:HD11	6:F:85:ILE:HG12	1.52	0.91
41:k:18:ASN:H	41:k:81:THR:HB	1.41	0.86
1:A:45:G:H5''	1:A:46:C:H5'	1.56	0.85
31:a:214:A:H2	31:a:225:G:H1	1.25	0.84
1:A:104:C:H5''	1:A:104:C:C6	2.13	0.84
6:F:31:ILE:HG23	6:F:96:MET:SD	2.22	0.80
3:C:230:HIS:HD2	3:C:232:HIS:H	1.25	0.79
30:4:7:VAL:HG22	30:4:34:GLN:HB3	1.64	0.79
1:A:162:A:H8	1:A:2244:G:H21	1.28	0.79
1:A:656:G:H21	1:A:660:A:H2	1.31	0.78
3:C:140:VAL:HG13	3:C:161:SER:HB2	1.65	0.78
31:a:672:G:H22	31:a:749:G:H1	1.31	0.77
31:a:950:G:H21	31:a:1353:G:H1	1.32	0.77
32:b:100:LEU:HA	32:b:107:ILE:HG13	1.67	0.77
31:a:481:C:H2'	31:a:482:A:H8	1.50	0.76
31:a:214:A:C2	31:a:225:G:N1	2.51	0.76
37:g:112:GLY:HA2	37:g:119:ARG:HD3	1.66	0.76
3:C:79:ASP:C	3:C:79:ASP:OD1	2.28	0.76
31:a:75:A:H8	31:a:94:G:H21	1.32	0.76
17:Q:40:ASN:CG	17:Q:40:ASN:O	2.28	0.76
31:a:1136:U:H4'	40:j:7:ARG:HH12	1.49	0.76
6:F:127:ASN:HB3	6:F:155:VAL:HB	1.67	0.76
31:a:721:G:H2'	31:a:722:G:C8	2.21	0.76
31:a:934:G:H1	31:a:1401:U:H3	1.34	0.75
31:a:725:C:H4'	41:k:119:ASN:HD22	1.50	0.75
7:G:69:ARG:C	7:G:69:ARG:HD3	2.11	0.75
31:a:1484:G:H2'	31:a:1485:G:C8	2.22	0.75
1:A:2684:A:H1'	1:A:2692:A:N6	2.02	0.74
11:K:25:ASN:C	11:K:26:TYR:HD1	1.94	0.74
31:a:1134:A:H4'	40:j:38:GLY:HA3	1.70	0.74
33:c:88:ASN:HA	33:c:91:ASN:HB2	1.70	0.74
27:1:5:VAL:HG11	27:1:30:ILE:HD11	1.70	0.73
1:A:2575:G:H1'	9:I:23:LYS:NZ	2.03	0.73
31:a:1082:C:H2'	31:a:1083:G:H8	1.53	0.73
13:M:92:ILE:C	13:M:92:ILE:HD12	2.14	0.73
31:a:215:C:H42	31:a:224:U:H3	1.36	0.73
31:a:831:G:HO2'	38:h:2:THR:N	1.86	0.73
1:A:292:U:H1'	1:A:293:U:H5'	1.69	0.73
1:A:1478:A:H61	1:A:1605:A:H61	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2419:A:H2	1:A:2451:C:H42	1.35	0.72
11:K:65:TRP:HH2	11:K:107:ALA:HB3	1.54	0.72
9:I:90:ASP:C	9:I:90:ASP:OD1	2.31	0.72
1:A:506:A:H2	1:A:515:G:H21	1.35	0.72
6:F:65:PRO:HB2	6:F:87:ALA:HB1	1.72	0.72
10:J:84:LYS:HG3	10:J:84:LYS:O	1.87	0.72
43:m:34:LEU:HD12	43:m:39:VAL:HB	1.72	0.72
7:G:119:GLU:N	7:G:119:GLU:OE2	2.23	0.72
12:L:26:ILE:HD12	12:L:71:ILE:HD11	1.72	0.71
5:E:154:VAL:HG22	5:E:193:VAL:CG2	2.19	0.71
19:S:4:LYS:HE2	19:S:92:ARG:NH1	2.05	0.71
32:b:69:PHE:HB3	32:b:80:VAL:HG13	1.72	0.71
1:A:721:A:H8	1:A:2096:G:H21	1.38	0.71
13:M:63:ILE:O	13:M:72:LEU:HD21	1.91	0.71
11:K:112:GLU:OE1	11:K:112:GLU:N	2.23	0.71
3:C:16:MET:HE1	3:C:207:LYS:HG3	1.72	0.71
12:L:26:ILE:CD1	12:L:71:ILE:HD11	2.21	0.70
32:b:114:ILE:HD11	32:b:144:LEU:HB3	1.72	0.70
2:B:2:C:H41	2:B:113:G:H1	1.37	0.70
10:J:80:ASP:C	10:J:80:ASP:OD1	2.33	0.70
31:a:1277:C:N3	31:a:1337:A:O2'	2.23	0.70
1:A:1578:A:H1'	1:A:1588:U:H3	1.56	0.70
31:a:424:G:H2'	31:a:425:G:H8	1.55	0.70
31:a:522:C:H2'	31:a:523:G:H8	1.57	0.70
37:g:72:VAL:H	37:g:142:HIS:HE1	1.40	0.70
9:I:32:THR:CG2	9:I:33:ALA:N	2.55	0.70
13:M:46:ASP:OD1	13:M:48:ASN:N	2.25	0.70
1:A:1483:A:H62	1:A:1599:G:H8	1.40	0.70
19:S:3:ILE:HD12	19:S:4:LYS:N	2.06	0.69
31:a:722:G:H2'	31:a:723:A:C8	2.27	0.69
11:K:114:ALA:O	11:K:118:LEU:HG	1.92	0.69
46:p:5:ILE:HG12	46:p:22:VAL:HG22	1.74	0.69
3:C:34:LEU:HD21	3:C:63:ARG:HG3	1.73	0.69
31:a:1248:A:N1	31:a:1309:A:N6	2.40	0.69
1:A:1881:A:H62	1:A:1915:G:H8	1.40	0.69
1:A:2859:G:H4'	12:L:45:GLU:OE2	1.91	0.69
31:a:1544:C:H2'	31:a:1545:A:C8	2.27	0.69
13:M:100:LEU:H	13:M:100:LEU:HD12	1.55	0.69
31:a:1407:C:OP2	35:e:29:ARG:NH2	2.26	0.69
1:A:2306:G:N7	21:U:22:ARG:NH2	2.37	0.69
4:D:27:VAL:HG11	14:N:7:ILE:HG13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1290:G:N2	15:O:33:LYS:HG2	2.08	0.69
3:C:74:ILE:HD12	3:C:74:ILE:H	1.58	0.69
31:a:1359:A:H1'	31:a:1384:A:H61	1.58	0.69
39:i:36:ASP:HB3	39:i:39:GLU:HG2	1.75	0.69
39:i:14:ARG:NH1	39:i:109:ASP:OD2	2.26	0.69
26:Z:29:GLU:HG2	26:Z:36:TYR:CE1	2.28	0.69
31:a:1002:G:H2'	31:a:1004:C:H41	1.57	0.69
11:K:70:PRO:HA	11:K:95:ALA:HB2	1.74	0.68
10:J:83:ASN:ND2	10:J:117:LEU:HA	2.07	0.68
31:a:22:G:H2'	31:a:23:G:C8	2.29	0.68
31:a:517:A:H8	31:a:551:G:O2'	1.77	0.68
31:a:921:C:H2'	31:a:922:A:C8	2.28	0.68
20:T:32:TYR:CE1	20:T:92:LEU:HD23	2.09	0.68
4:D:37:GLN:OE1	4:D:76:HIS:HE1	1.77	0.68
31:a:459:A:N6	31:a:488:U:O2'	2.27	0.68
3:C:164:VAL:HG13	3:C:172:VAL:HG11	1.74	0.68
8:H:9:GLU:HG3	8:H:9:GLU:O	1.93	0.68
31:a:791:C:H2'	31:a:792:A:H8	1.59	0.68
8:H:68:ASN:O	8:H:68:ASN:OD1	2.12	0.68
31:a:1249:A:H62	31:a:1309:A:H61	1.41	0.68
36:f:37:VAL:HG22	36:f:65:VAL:HG12	1.75	0.68
1:A:2314:A:H62	1:A:2371:U:H3	1.41	0.68
3:C:145:GLU:HB2	3:C:188:CYS:HB3	1.76	0.68
5:E:193:VAL:O	5:E:193:VAL:HG23	1.93	0.68
32:b:61:SER:HB3	32:b:221:ILE:HG13	1.75	0.68
3:C:60:ARG:HD3	3:C:85:PRO:HB2	1.75	0.67
9:I:32:THR:HG22	9:I:33:ALA:N	2.10	0.67
15:O:105:ALA:HB1	16:P:40:PHE:HZ	1.59	0.67
12:L:92:ARG:HG2	12:L:93:TYR:CE1	2.29	0.67
31:a:224:U:H2'	31:a:225:G:H8	1.59	0.67
31:a:73:G:H22	31:a:96:U:H3	1.43	0.67
31:a:1366:G:H2'	31:a:1367:A:C8	2.30	0.67
1:A:578:G:N2	15:O:48:ARG:HH22	1.92	0.67
1:A:1084:U:H3	1:A:1159:A:H61	1.43	0.67
19:S:100:GLU:C	19:S:100:GLU:CD	2.63	0.67
1:A:2341:A:H5'	6:F:35:VAL:HG11	1.77	0.67
31:a:983:A:OP1	44:n:29:ARG:NH2	2.27	0.67
1:A:2037:G:H5''	17:Q:42:ALA:HB2	1.77	0.67
5:E:125:VAL:HG13	5:E:194:ILE:HG23	1.77	0.67
31:a:681:G:H2'	31:a:682:G:C8	2.30	0.67
6:F:161:ASN:HB2	6:F:165:GLU:OE1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:411:C:H5''	34:d:129:PRO:HD2	1.77	0.67
49:s:79:THR:OG1	49:s:81:LYS:NZ	2.28	0.66
9:I:112:MET:HA	9:I:112:MET:HE3	1.76	0.66
31:a:532:G:H2'	31:a:533:C:C6	2.30	0.66
3:C:74:ILE:HD12	3:C:74:ILE:N	2.11	0.66
49:s:50:ALA:HB1	49:s:57:HIS:HB3	1.76	0.66
31:a:955:A:H2'	31:a:956:G:C8	2.31	0.66
6:F:69:LYS:HG3	6:F:84:PRO:HA	1.78	0.66
46:p:54:GLU:HG2	46:p:80:ILE:HD11	1.78	0.66
29:3:7:HIS:HD2	29:3:10:ALA:H	1.42	0.66
31:a:531:A:N6	42:l:102:ASP:OD2	2.28	0.66
1:A:1304:G:H5''	17:Q:15:ARG:HH22	1.61	0.66
1:A:1556:G:H2'	1:A:1557:C:H5'	1.77	0.66
15:O:104:LYS:H	15:O:104:LYS:CE	2.08	0.66
48:r:39:SER:OG	48:r:40:GLU:N	2.28	0.66
9:I:47:THR:HG23	9:I:48:PRO:HD2	1.78	0.66
17:Q:109:ASP:HB3	17:Q:111:LYS:HG2	1.78	0.65
32:b:129:LEU:HD21	32:b:137:LEU:HD12	1.79	0.65
13:M:33:VAL:HG11	13:M:105:VAL:HG22	1.77	0.65
31:a:1026:U:H2'	31:a:1027:A:H8	1.61	0.65
6:F:63:GLN:HA	25:Y:7:PRO:HD2	1.78	0.65
6:F:127:ASN:HA	6:F:156:ILE:HG13	1.79	0.65
10:J:83:ASN:HD21	10:J:117:LEU:HA	1.58	0.65
29:3:7:HIS:HD2	29:3:10:ALA:N	1.94	0.65
31:a:214:A:H2	31:a:225:G:N1	1.92	0.65
31:a:777:G:H4'	31:a:1524:A:H4'	1.77	0.65
31:a:1067:U:H2'	31:a:1068:G:H8	1.62	0.65
48:r:17:TYR:O	48:r:17:TYR:HD1	1.80	0.65
1:A:1290:G:N2	15:O:33:LYS:CG	2.60	0.65
31:a:444:C:H5''	34:d:149:ASN:HD21	1.60	0.65
17:Q:14:PRO:HA	17:Q:17:VAL:HG22	1.79	0.65
1:A:78:U:H2'	1:A:79:U:C6	2.32	0.64
1:A:1478:A:H61	1:A:1605:A:N6	1.95	0.64
21:U:49:ARG:HG2	21:U:49:ARG:HH11	1.62	0.64
31:a:1092:G:N7	35:e:52:LYS:NZ	2.45	0.64
31:a:1533:U:H2'	31:a:1534:G:H8	1.62	0.64
7:G:5:GLY:HA2	7:G:69:ARG:HG3	1.78	0.64
31:a:106:G:H1	50:t:6:SER:HG	1.43	0.64
31:a:130:A:H5'	47:q:67:ARG:HD3	1.80	0.64
31:a:470:A:H2'	31:a:471:A:C8	2.33	0.64
31:a:1003:A:C8	31:a:1226:A:H4'	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1437:C:H2'	31:a:1438:A:H8	1.62	0.64
1:A:2575:G:H1'	9:I:23:LYS:HZ2	1.63	0.64
7:G:8:ILE:C	7:G:69:ARG:HH21	2.05	0.64
31:a:948:G:OP1	37:g:102:ARG:NH1	2.30	0.64
31:a:1422:C:H2'	31:a:1423:A:C8	2.31	0.64
11:K:118:LEU:HD23	11:K:118:LEU:N	2.11	0.64
40:j:40:ILE:HB	40:j:73:LEU:HB2	1.80	0.64
5:E:159:GLU:OE1	5:E:177:THR:HG21	1.98	0.64
1:A:1575:A:O2'	1:A:1576:A:O5'	2.16	0.64
8:H:70:GLU:OE1	8:H:70:GLU:HA	1.97	0.64
31:a:18:U:H2'	31:a:19:C:C6	2.33	0.64
31:a:1387:A:OP1	37:g:92:ARG:NH1	2.25	0.64
8:H:22:GLU:HA	8:H:62:LYS:HB2	1.79	0.64
31:a:1552:U:O5'	32:b:22:ARG:NH2	2.31	0.64
49:s:46:GLY:HA2	49:s:61:TYR:HE1	1.62	0.64
3:C:34:LEU:CD2	3:C:63:ARG:HG3	2.27	0.64
31:a:98:U:O2	31:a:99:U:N3	2.31	0.64
31:a:507:A:H1'	31:a:508:G:C8	2.32	0.64
31:a:1260:A:H2'	31:a:1261:A:C8	2.32	0.64
6:F:91:LEU:HD12	6:F:95:ARG:HB2	1.80	0.64
16:P:62:VAL:HG22	16:P:95:LEU:CD2	2.28	0.64
19:S:3:ILE:HD12	19:S:3:ILE:C	2.23	0.64
19:S:55:GLY:C	19:S:56:ILE:HD12	2.23	0.64
1:A:162:A:H8	1:A:2244:G:N2	1.96	0.64
1:A:2332:U:H1'	6:F:151:GLY:HA3	1.78	0.64
43:m:3:ARG:HA	43:m:8:ASP:HA	1.80	0.64
31:a:682:G:H2'	31:a:683:A:H8	1.63	0.63
31:a:691:G:N2	41:k:39:GLY:O	2.31	0.63
13:M:55:GLN:OE1	13:M:56:ALA:CA	2.45	0.63
31:a:485:U:H2'	31:a:486:C:C6	2.33	0.63
31:a:699:G:O6	41:k:57:LYS:NZ	2.28	0.63
31:a:1383:G:OP2	31:a:1383:G:N2	2.26	0.63
1:A:2859:G:C4'	12:L:45:GLU:OE2	2.46	0.63
6:F:51:ASP:HA	6:F:54:VAL:HB	1.79	0.63
31:a:382:A:H5'	31:a:459:A:H2	1.63	0.63
31:a:436:G:H5''	34:d:10:LYS:HG3	1.79	0.63
33:c:107:LYS:HD2	33:c:110:LEU:HD12	1.79	0.63
3:C:253:PRO:HB2	3:C:257:LYS:HG3	1.81	0.63
31:a:513:G:H2'	31:a:514:G:C8	2.34	0.63
18:R:8:LYS:HE3	18:R:30:ASP:HA	1.80	0.63
31:a:214:A:N1	31:a:225:G:O6	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:546:U:H2'	31:a:547:A:H8	1.63	0.63
31:a:943:C:H42	31:a:948:G:H1	1.47	0.63
31:a:1170:G:N2	31:a:1192:G:H22	1.96	0.63
36:f:3:THR:OG1	36:f:66:LYS:NZ	2.32	0.63
11:K:58:MET:HE2	11:K:109:VAL:HG11	1.80	0.63
31:a:147:G:H2'	31:a:148:G:C8	2.34	0.63
31:a:670:A:H2'	31:a:671:A:C8	2.34	0.63
32:b:6:MET:SD	32:b:6:MET:N	2.70	0.63
15:O:104:LYS:H	15:O:104:LYS:CD	2.10	0.63
18:R:19:ALA:HB1	18:R:24:LYS:HB2	1.81	0.63
31:a:455:G:H21	31:a:495:A:H2	1.44	0.63
31:a:736:A:H2'	31:a:737:A:C8	2.34	0.63
33:c:63:ILE:HB	33:c:97:LYS:HB3	1.80	0.63
31:a:1276:G:N2	31:a:1279:A:OP2	2.31	0.62
32:b:117:ILE:HA	32:b:120:MET:SD	2.39	0.62
1:A:1216:U:H2'	1:A:1218:G:H8	1.62	0.62
1:A:2432:G:H2'	1:A:2438:A:H61	1.63	0.62
7:G:69:ARG:HD3	7:G:69:ARG:O	1.98	0.62
31:a:534:C:OP2	42:l:101:LYS:NZ	2.27	0.62
50:t:48:GLU:OE2	50:t:48:GLU:N	2.29	0.62
5:E:193:VAL:CG2	5:E:193:VAL:O	2.47	0.62
13:M:46:ASP:OD1	13:M:46:ASP:C	2.42	0.62
18:R:22:GLU:OE1	18:R:24:LYS:HG3	2.00	0.62
31:a:1129:A:H1'	31:a:1189:A:C4	2.34	0.62
39:i:121:LYS:HG3	39:i:127:PRO:HB3	1.80	0.62
5:E:164:GLU:HG3	5:E:175:VAL:HG11	1.80	0.62
11:K:25:ASN:C	11:K:26:TYR:CD1	2.75	0.62
19:S:100:GLU:CD	19:S:100:GLU:O	2.42	0.62
29:3:39:LYS:HG2	29:3:43:GLN:HE21	1.65	0.62
31:a:9:A:N6	34:d:196:GLU:O	2.31	0.62
31:a:1392:C:H4'	37:g:79:ARG:HH21	1.63	0.62
48:r:42:GLY:O	48:r:68:ARG:NH2	2.31	0.62
1:A:1986:G:N3	31:a:1494:A:H2	1.97	0.62
1:A:2575:G:N3	9:I:23:LYS:NZ	2.47	0.62
7:G:169:VAL:O	7:G:171:ARG:HG2	2.00	0.62
15:O:104:LYS:H	15:O:104:LYS:HE2	1.64	0.62
26:Z:24:VAL:HG13	26:Z:25:PRO:HD2	1.81	0.62
31:a:560:U:H2'	31:a:561:A:H8	1.64	0.62
36:f:69:ASN:OD1	36:f:71:LYS:NZ	2.22	0.62
1:A:2328:A:H61	1:A:2342:U:H3	1.48	0.62
12:L:92:ARG:HG2	12:L:93:TYR:CD1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:64:ARG:HG3	9:I:83:ALA:HB3	1.81	0.61
9:I:91:LYS:HE3	9:I:111:PHE:CZ	2.35	0.61
31:a:423:A:HO2'	31:a:424:G:H8	1.48	0.61
3:C:9:ILE:HD12	3:C:10:THR:OG1	2.00	0.61
6:F:31:ILE:HD12	6:F:158:THR:CG2	2.29	0.61
32:b:83:GLU:HG3	32:b:214:THR:HG23	1.80	0.61
41:k:97:ILE:HA	41:k:100:LEU:HD12	1.80	0.61
31:a:1088:G:N2	31:a:1091:A:OP2	2.27	0.61
33:c:149:LYS:HB3	33:c:200:TRP:HB2	1.82	0.61
5:E:20:SER:N	5:E:203:GLU:OE2	2.29	0.61
5:E:154:VAL:HG22	5:E:193:VAL:HG21	1.82	0.61
49:s:3:ARG:HH11	49:s:10:PHE:HB2	1.66	0.61
1:A:351:G:O2'	19:S:15:LYS:NZ	2.33	0.61
7:G:41:MET:SD	7:G:65:HIS:HA	2.40	0.61
11:K:27:VAL:HG13	11:K:105:GLU:HG2	1.82	0.61
31:a:722:G:H2'	31:a:723:A:H8	1.64	0.61
1:A:262:G:H21	1:A:666:A:H8	1.49	0.61
31:a:469:U:H2'	31:a:470:A:C8	2.35	0.61
7:G:27:LYS:HG2	7:G:32:GLU:CB	2.30	0.61
31:a:1170:G:H22	31:a:1192:G:H22	1.49	0.61
31:a:1535:C:H2'	31:a:1536:G:H8	1.65	0.61
1:A:1917:A:C5	1:A:1918:G:H1'	2.35	0.61
18:R:48:VAL:HG12	18:R:85:GLY:HA3	1.82	0.61
31:a:1238:C:H2'	31:a:1239:A:C8	2.36	0.61
31:a:1251:G:H2'	31:a:1252:G:H8	1.66	0.61
1:A:2499:G:H21	1:A:2505:A:H62	1.48	0.61
32:b:15:HIS:HB3	32:b:43:LEU:HD21	1.82	0.60
31:a:301:A:H5'	31:a:617:A:H61	1.66	0.60
31:a:398:C:H2'	31:a:399:G:H8	1.65	0.60
6:F:108:LEU:HB2	25:Y:51:SER:HA	1.84	0.60
31:a:495:A:H5''	31:a:496:C:H5	1.66	0.60
31:a:1527:G:N1	31:a:1530:A:OP2	2.32	0.60
6:F:143:TYR:CD1	43:m:3:ARG:NH2	2.68	0.60
31:a:744:U:H2'	31:a:745:U:H6	1.66	0.60
33:c:78:LYS:H	33:c:78:LYS:HD2	1.65	0.60
34:d:9:TRP:CD1	34:d:25:GLU:HG2	2.36	0.60
41:k:20:VAL:HG12	41:k:83:GLU:HB2	1.83	0.60
16:P:62:VAL:HG22	16:P:95:LEU:HD21	1.83	0.60
31:a:1336:U:H2'	31:a:1337:A:H8	1.65	0.60
1:A:221:G:H22	1:A:238:U:H4'	1.66	0.60
9:I:90:ASP:OD1	9:I:90:ASP:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:205:A:H2'	31:a:206:A:C8	2.37	0.60
31:a:918:A:OP1	42:l:18:LYS:NZ	2.31	0.60
1:A:2863:G:HO2'	14:N:2:THR:N	1.99	0.60
10:J:84:LYS:O	10:J:84:LYS:CG	2.50	0.60
4:D:38:LYS:HE2	4:D:101:VAL:HG23	1.82	0.60
6:F:106:VAL:HG21	6:F:139:PRO:HG3	1.83	0.60
34:d:163:GLU:OE1	34:d:178:ARG:NH1	2.34	0.60
5:E:154:VAL:HA	5:E:193:VAL:HG22	1.84	0.60
31:a:483:C:H2'	31:a:484:A:C8	2.37	0.60
6:F:38:MET:HE2	6:F:150:ARG:HG3	1.84	0.60
34:d:158:ASN:OD1	34:d:159:ASN:N	2.34	0.60
1:A:1378:U:C6	18:R:79:ILE:HD13	2.37	0.59
31:a:469:U:H2'	31:a:470:A:H8	1.67	0.59
31:a:498:U:H2'	31:a:499:A:H8	1.67	0.59
28:2:22:ARG:HD2	28:2:31:VAL:HG21	1.84	0.59
31:a:590:U:H2'	31:a:591:A:H8	1.67	0.59
1:A:1218:G:H2'	1:A:1219:G:C8	2.37	0.59
31:a:726:A:H5'	41:k:119:ASN:HD21	1.66	0.59
34:d:102:GLY:HA3	34:d:158:ASN:HD22	1.67	0.59
47:q:60:ILE:HD13	47:q:82:GLU:HG3	1.84	0.59
3:C:164:VAL:HG13	3:C:172:VAL:CG1	2.32	0.59
31:a:384:G:H5''	46:p:6:ARG:HB2	1.84	0.59
31:a:765:U:OP1	31:a:830:A:O2'	2.20	0.59
31:a:1238:C:H2'	31:a:1239:A:H8	1.68	0.59
1:A:1254:C:OP1	15:O:11:ARG:HD2	2.03	0.59
5:E:154:VAL:HG22	5:E:193:VAL:HG22	1.84	0.59
31:a:1187:G:H3'	31:a:1188:G:H8	1.67	0.59
31:a:1261:A:N3	31:a:1379:C:O2'	2.34	0.59
31:a:1002:G:O2'	31:a:1003:A:N7	2.35	0.59
34:d:117:GLY:O	34:d:142:ARG:NH1	2.36	0.59
6:F:95:ARG:HH22	25:Y:9:TYR:HB3	1.68	0.59
18:R:6:ILE:HD11	18:R:41:ALA:HB2	1.83	0.59
29:3:17:THR:OG1	29:3:21:GLN:HB2	2.01	0.59
31:a:563:C:H2'	31:a:564:C:C6	2.38	0.59
1:A:1934:G:H1	1:A:1950:U:H3	1.51	0.59
13:M:72:LEU:O	13:M:76:VAL:HG23	2.03	0.59
31:a:451:U:HO2'	31:a:452:A:H8	1.50	0.59
39:i:100:LEU:HD13	39:i:106:LEU:HD21	1.84	0.59
47:q:56:LYS:HZ2	47:q:84:SER:HB2	1.67	0.59
6:F:31:ILE:HD12	6:F:158:THR:HG23	1.85	0.58
11:K:39:THR:HB	11:K:98:LYS:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:535:G:O2'	31:a:543:A:N1	2.34	0.58
31:a:723:A:H2'	31:a:724:A:C8	2.37	0.58
47:q:60:ILE:HB	47:q:82:GLU:HG2	1.83	0.58
9:I:73:ASP:OD1	9:I:75:SER:HB3	2.03	0.58
31:a:513:G:H2'	31:a:514:G:H8	1.66	0.58
31:a:981:C:OP2	40:j:59:LYS:NZ	2.32	0.58
31:a:1297:A:H2'	31:a:1298:A:C8	2.39	0.58
1:A:437:A:H4'	1:A:459:C:OP1	2.03	0.58
15:O:36:LYS:O	15:O:40:MET:HG3	2.03	0.58
28:2:22:ARG:HD2	28:2:31:VAL:CG2	2.34	0.58
31:a:1201:A:H2'	31:a:1202:C:C6	2.38	0.58
48:r:74:PRO:HG3	48:r:77:LYS:HD3	1.84	0.58
1:A:1039:C:C5	8:H:1:MET:HA	2.39	0.58
3:C:13:ARG:O	3:C:13:ARG:HG3	2.04	0.58
6:F:32:ASP:C	6:F:32:ASP:OD1	2.46	0.58
6:F:58:GLU:HB2	25:Y:7:PRO:HG2	1.86	0.58
31:a:744:U:H2'	31:a:745:U:C6	2.39	0.58
31:a:1338:C:C2	31:a:1339:A:C8	2.91	0.58
31:a:1365:A:H2'	31:a:1366:G:H8	1.68	0.58
1:A:1401:G:OP1	22:V:3:LYS:HE3	2.03	0.58
3:C:160:ALA:H	3:C:195:VAL:HG22	1.68	0.58
6:F:75:ALA:HA	6:F:78:ARG:HH12	1.67	0.58
19:S:87:ASP:HB3	19:S:89:LYS:NZ	2.18	0.58
21:U:27:LYS:O	21:U:29:LEU:HG	2.04	0.58
26:Z:8:THR:HG23	26:Z:12:ARG:HB3	1.86	0.58
31:a:517:A:H8	31:a:551:G:HO2'	1.52	0.58
31:a:1160:U:H4'	40:j:43:PRO:HG3	1.85	0.58
31:a:1329:A:OP1	49:s:70:LYS:NZ	2.36	0.58
1:A:227:G:H1	1:A:233:U:H3	1.51	0.58
1:A:630:G:N7	10:J:33:ARG:NH1	2.51	0.58
31:a:721:G:H2'	31:a:722:G:H8	1.66	0.58
4:D:56:LYS:HE3	4:D:66:ASN:O	2.04	0.57
31:a:1084:U:O2	32:b:103:ASN:ND2	2.37	0.57
31:a:1133:U:O4	31:a:1134:A:N6	2.37	0.57
33:c:96:LYS:HG2	33:c:98:VAL:HG13	1.86	0.57
8:H:117:GLU:O	8:H:121:LYS:HG3	2.03	0.57
31:a:682:G:H2'	31:a:683:A:C8	2.39	0.57
31:a:1434:U:H2'	31:a:1435:A:C8	2.39	0.57
1:A:1051:C:OP1	8:H:38:ARG:NH1	2.37	0.57
3:C:140:VAL:CG1	3:C:161:SER:HB2	2.33	0.57
16:P:23:GLU:OE2	16:P:23:GLU:HA	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:72:THR:HG23	16:P:72:THR:O	2.04	0.57
17:Q:34:ALA:HB3	26:Z:27:MET:HE1	1.84	0.57
19:S:56:ILE:HD12	19:S:56:ILE:N	2.18	0.57
25:Y:38:GLU:OE1	25:Y:38:GLU:N	2.37	0.57
31:a:547:A:H2'	31:a:548:G:C8	2.38	0.57
31:a:949:C:H3'	31:a:950:G:H8	1.68	0.57
31:a:1260:A:H2'	31:a:1261:A:H8	1.69	0.57
1:A:650:U:H3	1:A:666:A:H2	1.51	0.57
1:A:1115:G:N1	1:A:1136:C:OP2	2.36	0.57
4:D:191:GLU:OE1	4:D:191:GLU:N	2.30	0.57
11:K:65:TRP:HZ3	11:K:106:VAL:C	2.12	0.57
1:A:925:G:H3'	1:A:926:G:C8	2.39	0.57
21:U:49:ARG:HG2	21:U:49:ARG:NH1	2.18	0.57
31:a:765:U:H2'	31:a:766:G:O4'	2.04	0.57
31:a:1330:C:H2'	31:a:1331:U:C6	2.40	0.57
40:j:24:LYS:HD2	40:j:91:ASN:HB2	1.85	0.57
3:C:154:ILE:HG21	3:C:176:LEU:HD22	1.87	0.57
31:a:22:G:H2'	31:a:23:G:H8	1.70	0.57
31:a:1366:G:H2'	31:a:1367:A:H8	1.68	0.57
34:d:178:ARG:NH2	34:d:184:GLU:OE2	2.37	0.57
37:g:72:VAL:H	37:g:142:HIS:CE1	2.22	0.57
6:F:94:GLU:O	6:F:98:GLU:OE1	2.23	0.57
27:1:5:VAL:HG13	27:1:47:GLU:HG3	1.86	0.57
31:a:1170:G:H22	31:a:1192:G:H1	1.51	0.57
1:A:1065:A:H62	1:A:1185:U:H3	1.53	0.57
19:S:7:ASP:OD1	19:S:7:ASP:N	2.36	0.57
20:T:31:VAL:HG12	20:T:91:PHE:HB2	1.86	0.57
31:a:193:C:HO2'	31:a:194:G:P	2.27	0.57
31:a:563:C:H2'	31:a:564:C:H6	1.70	0.57
31:a:570:U:H1'	42:l:12:ARG:HD2	1.86	0.57
31:a:996:A:H61	31:a:1228:U:H3	1.53	0.57
31:a:206:A:H2'	31:a:207:G:C8	2.40	0.57
31:a:398:C:H2'	31:a:399:G:C8	2.39	0.57
46:p:40:TYR:HD1	46:p:50:ILE:HG22	1.69	0.57
31:a:422:A:H3'	31:a:423:A:H8	1.70	0.57
31:a:1323:U:H2'	31:a:1324:C:H6	1.70	0.57
48:r:38:ILE:HD12	48:r:42:GLY:HA2	1.86	0.57
1:A:2049:U:OP2	26:Z:12:ARG:NH2	2.37	0.56
31:a:736:A:H2'	31:a:737:A:H8	1.70	0.56
31:a:1357:G:N7	39:i:14:ARG:NH2	2.52	0.56
31:a:1531:G:H2'	31:a:1532:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:ASP:OD1	4:D:44:ASP:O	2.23	0.56
31:a:588:C:H2'	31:a:589:G:O4'	2.04	0.56
33:c:62:ARG:HD2	33:c:98:VAL:HG22	1.86	0.56
34:d:178:ARG:NH2	34:d:181:GLU:OE1	2.37	0.56
38:h:113:ILE:HB	38:h:117:GLU:OE1	2.05	0.56
1:A:320:U:H5	1:A:326:A:N7	2.04	0.56
1:A:1044:A:H2'	1:A:1045:A:C8	2.40	0.56
1:A:2361:U:H5'	13:M:17:ARG:HG2	1.87	0.56
8:H:21:ALA:HB3	8:H:60:ALA:H	1.71	0.56
11:K:38:THR:OG1	11:K:127:VAL:HG23	2.04	0.56
13:M:55:GLN:OE1	13:M:56:ALA:N	2.38	0.56
16:P:50:ALA:HB3	16:P:51:PRO:HD3	1.86	0.56
18:R:27:PHE:HZ	18:R:87:ILE:HG21	1.70	0.56
29:3:21:GLN:HB3	29:3:49:LEU:HD22	1.87	0.56
31:a:547:A:H2'	31:a:548:G:H8	1.70	0.56
31:a:653:G:C2	31:a:654:G:C8	2.94	0.56
31:a:994:C:H2'	31:a:995:A:H8	1.68	0.56
31:a:1329:A:C8	31:a:1333:G:C5	2.93	0.56
31:a:1261:A:H2'	31:a:1262:A:C8	2.41	0.56
1:A:1259:U:OP1	16:P:69:LYS:NZ	2.38	0.56
1:A:2222:U:H2'	1:A:2223:C:C6	2.41	0.56
6:F:130:LEU:HB2	6:F:154:ILE:CD1	2.35	0.56
37:g:26:LEU:HD13	37:g:101:LEU:HD22	1.87	0.56
1:A:1183:G:OP2	8:H:73:LYS:NZ	2.36	0.56
3:C:29:PRO:HB2	3:C:34:LEU:HD11	1.87	0.56
31:a:1074:C:OP2	31:a:1075:G:O2'	2.23	0.56
46:p:83:LYS:HA	46:p:86:GLU:HG2	1.88	0.56
1:A:926:G:H21	1:A:941:A:H62	1.53	0.56
1:A:1479:G:H2'	1:A:1480:G:C8	2.41	0.56
31:a:331:U:H2'	31:a:332:G:O4'	2.06	0.56
31:a:508:G:H2'	31:a:509:C:C6	2.41	0.56
31:a:1082:C:H2'	31:a:1083:G:C8	2.39	0.56
38:h:107:SER:HB2	38:h:128:ILE:HD11	1.88	0.56
31:a:546:U:H2'	31:a:547:A:C8	2.41	0.56
31:a:787:C:H2'	31:a:788:A:O4'	2.06	0.56
31:a:1071:U:H2'	31:a:1072:G:H8	1.71	0.56
31:a:1304:U:H2'	31:a:1305:U:C6	2.41	0.56
20:T:84:ASN:O	20:T:85:GLN:HG3	2.06	0.56
31:a:106:G:N1	50:t:6:SER:OG	2.32	0.56
43:m:64:LYS:HD2	43:m:68:ASP:HB2	1.88	0.56
1:A:2618:C:N4	1:A:2619:G:O6	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:28:LYS:HG2	13:M:93:VAL:HG22	1.88	0.55
31:a:495:A:H5''	31:a:496:C:C5	2.41	0.55
31:a:1541:G:H2'	31:a:1542:A:C2	2.40	0.55
47:q:17:ASP:OD2	47:q:57:LEU:N	2.38	0.55
31:a:1437:C:H2'	31:a:1438:A:C8	2.41	0.55
47:q:9:VAL:HG22	47:q:64:GLN:HG3	1.87	0.55
4:D:186:VAL:HG22	4:D:196:LEU:HB3	1.87	0.55
21:U:19:LYS:NZ	21:U:19:LYS:HB3	2.20	0.55
43:m:11:ARG:O	43:m:13:LYS:HG2	2.06	0.55
1:A:2048:G:OP1	26:Z:9:SER:OG	2.24	0.55
7:G:6:LYS:N	7:G:65:HIS:HE1	2.04	0.55
13:M:55:GLN:CD	13:M:55:GLN:C	2.75	0.55
31:a:328:A:HO2'	31:a:1445:G:HO2'	1.55	0.55
31:a:397:A:H3'	31:a:398:C:H6	1.71	0.55
18:R:25:TYR:CE2	18:R:82:LEU:HD21	2.40	0.55
31:a:352:A:H5''	31:a:353:C:H5	1.71	0.55
1:A:1574:G:H1	1:A:1590:C:H5	1.54	0.55
31:a:720:A:H2'	31:a:721:G:C8	2.42	0.55
31:a:1141:A:O2'	31:a:1142:U:O5'	2.25	0.55
37:g:45:SER:HB3	37:g:117:GLU:HG2	1.88	0.55
31:a:590:U:H2'	31:a:591:A:C8	2.41	0.55
49:s:31:ILE:H	49:s:31:ILE:HD12	1.70	0.55
8:H:3:GLN:HE21	15:O:94:MET:HE1	1.71	0.55
9:I:71:ARG:HH11	14:N:74:ARG:CZ	2.18	0.55
12:L:106:GLN:NE2	12:L:118:ILE:HD12	2.22	0.55
31:a:42:G:H2'	31:a:43:G:C8	2.41	0.55
8:H:70:GLU:OE1	8:H:70:GLU:CA	2.53	0.55
31:a:448:U:C2	31:a:449:A:C8	2.94	0.55
31:a:1324:C:H2'	31:a:1325:U:O2	2.07	0.55
32:b:219:ASP:HA	32:b:222:LEU:HD12	1.89	0.55
1:A:901:G:H2'	1:A:902:A:C8	2.42	0.55
14:N:60:THR:CG2	14:N:60:THR:O	2.55	0.55
23:W:44:ARG:HD2	23:W:48:LYS:NZ	2.22	0.55
31:a:35:C:H2'	31:a:36:G:H8	1.73	0.55
34:d:65:GLU:C	34:d:67:GLN:H	2.15	0.55
1:A:2098:A:H2'	1:A:2099:G:C8	2.42	0.54
31:a:509:C:H2'	31:a:510:C:C6	2.43	0.54
1:A:1003:A:H2'	1:A:1004:A:C8	2.42	0.54
2:B:40:C:C6	6:F:66:LEU:HD13	2.43	0.54
12:L:95:GLU:O	12:L:97:GLN:NE2	2.40	0.54
18:R:9:ARG:HG2	18:R:28:ASP:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:89:LYS:N	19:S:89:LYS:HD2	2.22	0.54
31:a:1026:U:H2'	31:a:1027:A:C8	2.42	0.54
31:a:1167:A:N6	31:a:1187:G:N7	2.55	0.54
35:e:159:LYS:HE3	35:e:163:GLU:HB3	1.87	0.54
36:f:20:LYS:H	36:f:20:LYS:HD2	1.72	0.54
36:f:35:ALA:HA	36:f:67:SER:HB3	1.88	0.54
1:A:1378:U:C6	18:R:79:ILE:CD1	2.91	0.54
7:G:69:ARG:C	7:G:69:ARG:CD	2.81	0.54
31:a:661:U:C2	38:h:56:LYS:HD2	2.42	0.54
31:a:458:G:OP2	31:a:459:A:O2'	2.26	0.54
31:a:723:A:H2'	31:a:724:A:H8	1.73	0.54
37:g:85:TYR:HH	41:k:55:SER:HG	1.53	0.54
1:A:1478:A:N6	1:A:1605:A:H61	2.06	0.54
1:A:2838:C:OP2	12:L:38:LYS:NZ	2.40	0.54
22:V:17:ARG:HB2	22:V:27:ARG:HG3	1.89	0.54
31:a:433:A:H2'	31:a:434:U:C6	2.43	0.54
31:a:753:U:OP1	31:a:860:U:O2'	2.26	0.54
35:e:80:THR:HG22	35:e:122:ASP:HB2	1.88	0.54
46:p:42:PRO:HA	46:p:48:PRO:HB3	1.89	0.54
19:S:41:MET:O	19:S:58:GLU:HA	2.07	0.54
31:a:521:A:H2'	31:a:522:C:C6	2.42	0.54
37:g:57:ASP:HB3	37:g:60:GLU:HB2	1.89	0.54
41:k:45:SER:HB3	41:k:70:ALA:HB2	1.87	0.54
1:A:1290:G:H21	15:O:33:LYS:HG2	1.71	0.54
18:R:49:LYS:HB3	18:R:84:GLU:HB3	1.90	0.54
18:R:55:ILE:HD12	18:R:78:ALA:HB2	1.89	0.54
20:T:94:ILE:HD12	20:T:94:ILE:N	2.23	0.54
31:a:277:U:H2'	31:a:278:A:H8	1.73	0.54
31:a:1235:A:H1'	49:s:78:ARG:HD3	1.89	0.54
38:h:110:GLU:OE1	38:h:110:GLU:N	2.40	0.54
9:I:91:LYS:HD2	9:I:111:PHE:CE1	2.43	0.54
31:a:873:A:H2'	31:a:874:A:C8	2.43	0.54
31:a:1365:A:H2'	31:a:1366:G:C8	2.42	0.54
31:a:1398:U:H2'	31:a:1399:C:C6	2.42	0.54
33:c:155:ARG:H	33:c:162:ALA:HA	1.72	0.54
41:k:52:PHE:HD1	41:k:56:LYS:HB3	1.73	0.54
43:m:90:ARG:HB2	43:m:97:VAL:HG12	1.90	0.54
46:p:79:GLY:O	46:p:83:LYS:HG3	2.08	0.54
31:a:508:G:H2'	31:a:509:C:H6	1.73	0.54
31:a:876:G:O2'	31:a:882:A:N1	2.40	0.54
40:j:53:ARG:HG2	40:j:63:GLU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:C:H4'	1:A:1090:A:H5''	1.90	0.53
20:T:49:ILE:HG22	20:T:53:ARG:NH1	2.23	0.53
31:a:214:A:N1	31:a:225:G:C6	2.76	0.53
31:a:823:A:N7	31:a:1520:C:O2'	2.30	0.53
5:E:34:PHE:CE1	10:J:6:LEU:HD13	2.43	0.53
9:I:71:ARG:HH11	14:N:74:ARG:NH2	2.06	0.53
9:I:71:ARG:HD2	14:N:74:ARG:HH21	1.73	0.53
13:M:18:VAL:C	13:M:20:THR:H	2.16	0.53
31:a:33:A:H2'	31:a:34:A:C8	2.43	0.53
31:a:34:A:N3	42:l:42:GLN:NE2	2.55	0.53
31:a:57:U:H2'	31:a:58:G:H8	1.72	0.53
1:A:293:U:H2'	1:A:294:G:O4'	2.08	0.53
8:H:24:GLN:HG2	8:H:29:LEU:HD12	1.88	0.53
31:a:63:U:OP1	31:a:393:C:O2'	2.26	0.53
1:A:1290:G:H21	15:O:33:LYS:CG	2.20	0.53
8:H:37:LEU:HD11	8:H:110:LEU:HD11	1.91	0.53
15:O:104:LYS:H	15:O:104:LYS:HD3	1.72	0.53
18:R:49:LYS:HG2	18:R:83:LYS:HE2	1.90	0.53
31:a:423:A:O2'	31:a:424:G:H8	1.92	0.53
31:a:445:U:O2'	34:d:116:HIS:ND1	2.35	0.53
31:a:1402:G:O2'	31:a:1513:A:O5'	2.26	0.53
1:A:1484:G:H3'	1:A:1485:G:H8	1.73	0.53
12:L:6:LEU:HD13	12:L:16:MET:HE1	1.89	0.53
31:a:1167:A:N6	31:a:1188:G:H1'	2.23	0.53
32:b:54:TYR:HE2	32:b:216:LYS:HG3	1.73	0.53
42:l:59:ASN:ND2	42:l:102:ASP:OD1	2.42	0.53
46:p:53:ASP:OD1	46:p:54:GLU:N	2.42	0.53
31:a:205:A:H2'	31:a:206:A:H8	1.72	0.53
31:a:860:U:H2'	31:a:861:A:H8	1.74	0.53
37:g:85:TYR:OH	41:k:55:SER:OG	2.25	0.53
23:W:58:ARG:NH1	23:W:61:GLU:OE2	2.39	0.53
31:a:424:G:H2'	31:a:425:G:C8	2.39	0.53
31:a:1543:U:H2'	31:a:1544:C:O4'	2.09	0.53
34:d:9:TRP:CG	34:d:25:GLU:HG2	2.44	0.53
1:A:252:C:O2	29:3:12:LYS:NZ	2.40	0.53
5:E:141:ASN:O	5:E:145:THR:HG23	2.09	0.53
8:H:54:TYR:CE1	8:H:122:LYS:HD2	2.43	0.53
9:I:32:THR:CG2	9:I:33:ALA:H	2.20	0.53
31:a:272:C:H2'	31:a:273:G:O4'	2.09	0.53
31:a:1131:C:C2	31:a:1132:U:C5	2.96	0.53
33:c:84:GLU:O	33:c:88:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:A:C5	1:A:459:C:H1'	2.44	0.53
1:A:665:G:H4'	1:A:666:A:H5''	1.91	0.53
2:B:73:G:H21	20:T:88:HIS:HD2	1.56	0.53
8:H:36:ILE:HD11	8:H:141:TYR:CE1	2.43	0.53
31:a:1075:G:H1'	31:a:1200:G:H21	1.74	0.53
32:b:127:GLU:N	32:b:127:GLU:OE2	2.42	0.53
39:i:8:TYR:HB2	39:i:23:LEU:HB2	1.91	0.53
1:A:1463:A:H2	1:A:1625:U:H3	1.57	0.53
1:A:2122:A:H2'	1:A:2123:A:O4'	2.08	0.53
1:A:2372:G:H4'	1:A:2373:A:H5''	1.91	0.53
1:A:2452:A:H4'	1:A:2453:A:H5''	1.90	0.53
1:A:2774:G:O2'	7:G:67:THR:HG23	2.09	0.53
17:Q:4:LYS:HD2	17:Q:106:VAL:HG22	1.90	0.53
1:A:512:A:H5''	1:A:512:A:H8	1.72	0.52
1:A:684:U:H2'	1:A:685:C:C6	2.43	0.52
1:A:2575:G:H1'	9:I:23:LYS:HZ1	1.74	0.52
15:O:102:ASP:OD1	15:O:104:LYS:HE2	2.08	0.52
15:O:116:ALA:O	15:O:117:LEU:C	2.49	0.52
31:a:1542:A:H2'	31:a:1543:U:C6	2.44	0.52
36:f:1:MET:SD	36:f:68:ASP:HB3	2.49	0.52
1:A:1080:G:H1	1:A:1163:U:H3	1.57	0.52
1:A:2146:A:H62	1:A:2195:G:H22	1.58	0.52
31:a:500:A:H2'	31:a:501:U:C6	2.44	0.52
15:O:107:ALA:O	15:O:111:THR:HG23	2.08	0.52
31:a:1153:G:H2'	31:a:1154:G:C8	2.44	0.52
37:g:16:PRO:HA	39:i:48:LEU:HD22	1.91	0.52
1:A:1150:A:H3'	1:A:1151:G:H8	1.74	0.52
1:A:1741:G:OP2	1:A:1742:A:O2'	2.23	0.52
3:C:210:ARG:HA	3:C:213:TRP:CE3	2.44	0.52
12:L:102:ARG:HH22	12:L:122:VAL:HG23	1.74	0.52
31:a:213:G:H2'	31:a:214:A:C8	2.45	0.52
31:a:381:A:C2	31:a:382:A:C8	2.98	0.52
31:a:934:G:H1'	31:a:1513:A:C4	2.45	0.52
1:A:792:5MU:H4'	17:Q:92:ARG:HH12	1.74	0.52
3:C:29:PRO:CB	3:C:34:LEU:HD11	2.39	0.52
5:E:164:GLU:HA	5:E:175:VAL:HG21	1.92	0.52
16:P:6:GLU:HB2	16:P:39:LEU:HD11	1.90	0.52
18:R:56:MET:HE1	18:R:79:ILE:HD11	1.90	0.52
20:T:52:ILE:O	20:T:56:GLY:N	2.38	0.52
31:a:42:G:H2'	31:a:43:G:H8	1.75	0.52
31:a:366:U:C2	31:a:367:A:C8	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:8:ILE:HB	40:j:74:ILE:HG13	1.90	0.52
41:k:17:GLU:N	41:k:17:GLU:OE2	2.42	0.52
1:A:84:A:H1'	1:A:85:G:O4'	2.09	0.52
1:A:548:A:H4'	1:A:549:U:H5'	1.92	0.52
3:C:94:VAL:HG22	3:C:102:ARG:O	2.10	0.52
6:F:130:LEU:HB2	6:F:154:ILE:HD12	1.91	0.52
20:T:37:LYS:HG3	20:T:38:ASN:N	2.23	0.52
36:f:29:ILE:HD12	36:f:29:ILE:H	1.73	0.52
49:s:35:SER:HG	49:s:38:SER:HG	1.56	0.52
1:A:1758:A:H61	1:A:1771:A:H62	1.57	0.52
1:A:2136:U:H3'	1:A:2147:G:OP1	2.09	0.52
1:A:2540:A:H2'	1:A:2541:U:C6	2.45	0.52
1:A:2854:A:H2'	1:A:2899:A:H61	1.75	0.52
6:F:132:VAL:O	6:F:151:GLY:HA2	2.10	0.52
9:I:22:ILE:HD11	9:I:42:THR:HG23	1.90	0.52
16:P:27:VAL:CG2	16:P:31:ASP:HB2	2.40	0.52
31:a:1286:G:N3	31:a:1292:C:O2'	2.40	0.52
31:a:1289:A:O2'	31:a:1291:U:OP2	2.20	0.52
1:A:1699:A:H4'	4:D:128:GLN:HA	1.91	0.52
1:A:2581:U:H2'	1:A:2582:U:C6	2.45	0.52
1:A:2760:A:C5	4:D:216:LYS:HE2	2.45	0.52
20:T:8:ILE:HG13	20:T:41:VAL:HG12	1.91	0.52
31:a:950:G:N2	31:a:1353:G:H1	2.04	0.52
43:m:49:THR:HB	43:m:52:GLU:HG3	1.92	0.52
1:A:352:A:H4'	19:S:14:GLY:HA2	1.92	0.52
1:A:896:U:H2'	1:A:897:A:C8	2.44	0.52
1:A:1669:C:H2'	1:A:1670:A:O4'	2.10	0.52
1:A:2316:G:O6	1:A:2370:U:H5	1.93	0.52
4:D:47:ASN:OD1	4:D:47:ASN:O	2.28	0.52
4:D:191:GLU:HG2	4:D:192:ASN:N	2.24	0.52
31:a:368:G:H2'	31:a:369:G:C8	2.45	0.52
31:a:523:G:H2'	31:a:524:U:H6	1.75	0.52
31:a:541:A:O2'	31:a:543:A:OP1	2.28	0.52
31:a:1167:A:N7	31:a:1190:A:N6	2.57	0.52
31:a:1260:A:C8	31:a:1297:A:C2	2.98	0.52
3:C:67:PHE:HE1	3:C:105:ILE:HD11	1.75	0.52
19:S:87:ASP:HB3	19:S:89:LYS:HZ2	1.75	0.52
28:2:31:VAL:HG12	28:2:34:ARG:NH2	2.25	0.52
31:a:18:U:H2'	31:a:19:C:H6	1.71	0.52
31:a:257:U:H2'	31:a:258:A:C8	2.45	0.51
31:a:420:U:H1'	34:d:29:ARG:CZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:612:G:H2'	31:a:613:U:C6	2.45	0.51
31:a:870:G:HO2'	31:a:883:G:HO2'	1.58	0.51
31:a:1062:G:H2'	31:a:1063:U:C6	2.45	0.51
31:a:1141:A:C2'	31:a:1142:U:O5'	2.58	0.51
36:f:16:GLU:HG3	36:f:20:LYS:NZ	2.25	0.51
49:s:22:GLN:HE22	49:s:31:ILE:HD11	1.75	0.51
1:A:388:A:H2'	1:A:389:A:H2	1.74	0.51
1:A:2711:U:OP1	14:N:60:THR:HG21	2.09	0.51
13:M:83:LYS:O	13:M:87:LYS:HG2	2.11	0.51
20:T:39:VAL:HG12	20:T:41:VAL:HG13	1.93	0.51
31:a:407:G:H2'	31:a:408:C:C6	2.45	0.51
31:a:724:A:H1'	41:k:120:GLY:HA2	1.92	0.51
31:a:1394:C:H2'	31:a:1395:G:H8	1.75	0.51
31:a:384:G:OP1	46:p:68:THR:HG21	2.10	0.51
31:a:617:A:C2	31:a:618:G:H1'	2.45	0.51
31:a:1333:G:H2'	31:a:1334:A:C8	2.46	0.51
32:b:67:VAL:HG22	32:b:160:ALA:HB3	1.91	0.51
32:b:89:GLN:HE21	32:b:221:ILE:HG12	1.75	0.51
38:h:54:ASP:OD1	38:h:56:LYS:N	2.43	0.51
1:A:738:U:O2'	1:A:1390:A:N3	2.44	0.51
1:A:1485:G:O2'	1:A:1672:G:OP1	2.24	0.51
1:A:2435:U:H2'	1:A:2436:G:C8	2.46	0.51
6:F:120:LYS:HD3	6:F:167:ARG:HH21	1.76	0.51
9:I:112:MET:HE3	9:I:112:MET:CA	2.37	0.51
13:M:30:ARG:HH21	13:M:45:ILE:HG12	1.74	0.51
14:N:29:ARG:HD3	14:N:89:LYS:HD3	1.92	0.51
20:T:60:VAL:C	20:T:61:ILE:HD13	2.35	0.51
31:a:521:A:H2'	31:a:522:C:H6	1.75	0.51
31:a:1169:U:O4'	31:a:1192:G:N2	2.44	0.51
33:c:39:ARG:NH1	33:c:54:VAL:O	2.44	0.51
1:A:1261:G:N7	16:P:70:LYS:NZ	2.56	0.51
1:A:2760:A:C6	4:D:216:LYS:HG2	2.44	0.51
6:F:143:TYR:O	6:F:146:VAL:HG22	2.11	0.51
8:H:29:LEU:HA	8:H:143:LEU:HD11	1.93	0.51
9:I:2:ILE:HD11	9:I:82:ASN:OD1	2.10	0.51
31:a:370:G:N2	31:a:373:U:OP2	2.42	0.51
31:a:709:C:H5''	31:a:710:A:H3'	1.93	0.51
31:a:1532:G:H2'	31:a:1533:U:C2	2.46	0.51
1:A:702:U:H2'	1:A:703:A:C8	2.46	0.51
1:A:921:C:H2'	1:A:922:G:C8	2.45	0.51
1:A:2599:A:OP1	1:A:2601:G:H4'	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:87:ASP:O	19:S:89:LYS:HD2	2.11	0.51
31:a:776:A:H4'	31:a:1534:G:H21	1.75	0.51
32:b:80:VAL:HG12	32:b:91:TYR:HB2	1.93	0.51
41:k:68:GLU:O	41:k:72:LYS:HG2	2.10	0.51
1:A:297:G:H4'	1:A:304:G:O3'	2.11	0.51
1:A:1055:A:OP1	15:O:75:SER:OG	2.28	0.51
1:A:1315:C:H2'	1:A:1316:G:H8	1.75	0.51
4:D:118:VAL:HG12	4:D:183:LEU:HD12	1.93	0.51
7:G:23:HIS:NE2	7:G:34:SER:HB3	2.26	0.51
9:I:111:PHE:O	9:I:115:VAL:HG23	2.10	0.51
20:T:61:ILE:HD13	20:T:61:ILE:N	2.25	0.51
32:b:94:GLN:HG3	32:b:146:LYS:HG2	1.91	0.51
1:A:2144:A:C8	1:A:2176:C:H5'	2.46	0.51
6:F:31:ILE:HA	6:F:158:THR:HG22	1.93	0.51
19:S:11:VAL:HG12	19:S:68:VAL:HG12	1.92	0.51
31:a:911:G:H2'	31:a:912:G:H8	1.75	0.51
1:A:162:A:H2	1:A:166:A:H61	1.58	0.51
1:A:644:C:O2'	1:A:645:A:H8	1.94	0.51
1:A:943:C:H2'	1:A:944:G:C8	2.46	0.51
31:a:199:G:H2'	31:a:200:U:C6	2.46	0.51
31:a:987:A:C2	31:a:1329:A:C4	2.98	0.51
1:A:396:G:H2'	1:A:397:U:O4'	2.11	0.51
1:A:2163:A:H62	1:A:2183:G:H21	1.57	0.51
1:A:2867:U:OP1	14:N:98:LYS:NZ	2.37	0.51
4:D:67:LYS:HA	4:D:86:ARG:HH22	1.76	0.51
15:O:104:LYS:CD	15:O:104:LYS:N	2.74	0.51
31:a:96:U:H2'	31:a:97:G:H8	1.75	0.51
31:a:1535:C:H2'	31:a:1536:G:C8	2.46	0.51
45:o:29:ILE:HD13	45:o:67:LEU:HG	1.92	0.51
47:q:55:ALA:HB2	47:q:80:ILE:HD11	1.93	0.51
1:A:631:U:H1'	5:E:90:PHE:HB3	1.93	0.50
1:A:2036:G:C2	1:A:2037:G:C8	3.00	0.50
31:a:1106:U:H2'	31:a:1107:C:C6	2.46	0.50
1:A:1265:G:N7	15:O:16:LYS:NZ	2.59	0.50
1:A:2622:G:N2	1:A:2625:A:OP2	2.38	0.50
5:E:195:THR:HG22	5:E:197:ALA:H	1.76	0.50
13:M:18:VAL:C	13:M:20:THR:N	2.69	0.50
15:O:104:LYS:HD3	15:O:104:LYS:N	2.26	0.50
18:R:89:LEU:O	18:R:90:PHE:C	2.54	0.50
31:a:1232:G:OP1	31:a:1331:U:O2'	2.22	0.50
7:G:90:VAL:O	7:G:94:TYR:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:55:GLN:OE1	13:M:56:ALA:HA	2.10	0.50
30:4:17:ILE:HD13	30:4:26:ILE:HG12	1.93	0.50
31:a:468:G:O6	31:a:482:A:N6	2.44	0.50
31:a:791:C:H2'	31:a:792:A:C8	2.44	0.50
31:a:834:C:O2	38:h:16:ASN:ND2	2.44	0.50
31:a:955:A:H2'	31:a:956:G:H8	1.74	0.50
34:d:66:ARG:O	34:d:66:ARG:HG2	2.10	0.50
1:A:2328:A:N6	1:A:2342:U:H3	2.09	0.50
3:C:11:ASN:C	3:C:13:ARG:H	2.19	0.50
4:D:5:ILE:HG21	4:D:195:ILE:CD1	2.41	0.50
6:F:32:ASP:OD2	13:M:2:ILE:HD11	2.10	0.50
14:N:60:THR:O	14:N:60:THR:HG23	2.11	0.50
39:i:116:LYS:HG3	39:i:122:ALA:HA	1.93	0.50
1:A:283:G:H3'	1:A:284:C:C6	2.47	0.50
8:H:74:VAL:CG2	8:H:87:SER:HB2	2.42	0.50
31:a:948:G:H2'	31:a:949:C:C6	2.46	0.50
49:s:30:VAL:O	49:s:30:VAL:HG12	2.11	0.50
1:A:1707:U:O2'	1:A:2713:G:H4'	2.12	0.50
1:A:1992:C:H2'	1:A:1993:A:C8	2.46	0.50
7:G:89:LEU:HD22	7:G:95:ARG:O	2.11	0.50
31:a:504:G:H21	31:a:505:A:H3'	1.75	0.50
31:a:966:U:H4'	49:s:79:THR:HG23	1.94	0.50
39:i:30:ILE:HG13	39:i:65:VAL:CG2	2.42	0.50
40:j:18:ILE:HG13	40:j:72:ARG:HG2	1.92	0.50
1:A:94:A:H2'	1:A:95:A:C8	2.47	0.50
1:A:194:A:H2'	1:A:195:C:C6	2.47	0.50
1:A:1401:G:OP1	22:V:3:LYS:CE	2.59	0.50
2:B:44:A:H5''	13:M:7:LYS:HE3	1.94	0.50
9:I:32:THR:HG23	9:I:33:ALA:H	1.77	0.50
19:S:100:GLU:C	19:S:100:GLU:OE2	2.55	0.50
27:1:22:ASN:HD22	27:1:23:LYS:H	1.59	0.50
31:a:592:G:H2'	31:a:593:G:H8	1.76	0.50
31:a:1323:U:H2'	31:a:1324:C:C6	2.46	0.50
31:a:1441:C:H2'	31:a:1442:G:O4'	2.12	0.50
1:A:1806:U:H5	1:A:1811:A:N7	2.10	0.50
1:A:2123:A:C2	1:A:2124:U:C5	3.00	0.50
3:C:79:ASP:OD1	3:C:79:ASP:O	2.29	0.50
31:a:123:G:H2'	31:a:124:U:C6	2.47	0.50
31:a:366:U:H2'	31:a:367:A:H8	1.77	0.50
31:a:1477:C:H2'	31:a:1478:G:O4'	2.12	0.50
1:A:1400:C:O2'	1:A:1836:A:N3	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2775:A:H5''	7:G:4:VAL:HG21	1.94	0.50
9:I:42:THR:HG22	9:I:57:VAL:HG22	1.93	0.50
10:J:2:LYS:HB2	10:J:5:GLU:HG3	1.94	0.50
12:L:24:LEU:HD23	12:L:44:VAL:HG21	1.94	0.50
31:a:383:U:OP1	46:p:70:THR:HG21	2.12	0.50
31:a:483:C:O2'	31:a:484:A:H5'	2.12	0.50
31:a:1142:U:H6	31:a:1142:U:H5''	1.77	0.50
31:a:1524:A:H2'	31:a:1525:U:C6	2.47	0.50
1:A:324:A:H2'	1:A:325:A:O4'	2.11	0.49
1:A:2024:A:H5''	4:D:131:ILE:HD11	1.94	0.49
5:E:159:GLU:OE1	5:E:177:THR:CG2	2.59	0.49
13:M:6:ASP:OD1	13:M:7:LYS:N	2.45	0.49
31:a:699:G:H22	31:a:703:A:H5''	1.77	0.49
31:a:726:A:H5'	41:k:119:ASN:ND2	2.25	0.49
31:a:1376:C:O2'	40:j:62:ARG:NH2	2.44	0.49
33:c:57:GLU:HB2	33:c:64:ASN:HB3	1.93	0.49
1:A:1182:G:N3	8:H:109:MET:HE2	2.26	0.49
7:G:23:HIS:C	7:G:23:HIS:ND1	2.70	0.49
12:L:91:GLU:OE1	12:L:91:GLU:N	2.44	0.49
25:Y:55:HIS:ND1	25:Y:58:TYR:O	2.43	0.49
31:a:41:C:H2'	31:a:42:G:H8	1.77	0.49
31:a:860:U:H2'	31:a:861:A:C8	2.48	0.49
31:a:1394:C:C2	31:a:1395:G:C8	3.00	0.49
31:a:1398:U:H2'	31:a:1399:C:H6	1.77	0.49
34:d:41:ARG:NE	34:d:41:ARG:HA	2.27	0.49
41:k:74:ALA:HB1	41:k:79:LEU:HG	1.94	0.49
1:A:1097:U:H4'	1:A:1098:A:OP2	2.12	0.49
1:A:2142:G:N2	1:A:2188:C:OP1	2.45	0.49
3:C:119:GLY:O	3:C:131:PRO:HD3	2.12	0.49
23:W:2:LYS:O	23:W:2:LYS:HD2	2.12	0.49
31:a:1172:C:C2	31:a:1173:G:C8	3.00	0.49
33:c:68:HIS:HB3	33:c:105:ILE:HD11	1.93	0.49
37:g:142:HIS:O	37:g:146:GLU:HG2	2.13	0.49
1:A:2858:G:C4	1:A:2859:G:C8	3.01	0.49
3:C:157:SER:O	3:C:195:VAL:HG21	2.12	0.49
31:a:509:C:OP1	42:l:127:ARG:NH2	2.46	0.49
31:a:920:U:H2'	31:a:921:C:C6	2.47	0.49
31:a:1001:U:N3	31:a:1054:G:O2'	2.42	0.49
31:a:1353:G:H2'	31:a:1354:C:C6	2.47	0.49
11:K:72:THR:HB	11:K:94:ILE:HG12	1.95	0.49
14:N:19:LEU:H	14:N:19:LEU:CD2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:9:TYR:CE1	25:Y:26:GLY:HA2	2.47	0.49
31:a:499:A:C2	31:a:500:A:C5	3.00	0.49
31:a:1260:A:H4'	39:i:71:GLY:HA2	1.94	0.49
31:a:1438:A:H2'	31:a:1439:C:H6	1.78	0.49
38:h:46:ILE:HD11	38:h:49:VAL:HG22	1.94	0.49
38:h:117:GLU:O	38:h:121:ARG:HG2	2.13	0.49
1:A:897:A:H5'	24:X:45:GLY:HA3	1.94	0.49
1:A:2154:G:H2'	1:A:2155:C:C6	2.47	0.49
5:E:164:GLU:HG3	5:E:175:VAL:CG1	2.42	0.49
15:O:76:TYR:CZ	15:O:80:MET:HG3	2.48	0.49
31:a:202:C:H2'	31:a:203:A:C8	2.48	0.49
31:a:341:U:C2	31:a:342:C:C5	3.00	0.49
31:a:954:G:C2	31:a:955:A:C8	3.01	0.49
31:a:1106:U:H2'	31:a:1107:C:H6	1.78	0.49
32:b:87:ALA:HB1	32:b:221:ILE:HG21	1.93	0.49
39:i:59:THR:HG22	39:i:62:ASN:HB2	1.93	0.49
1:A:327:G:H1	1:A:399:U:H3	1.60	0.49
1:A:579:U:H5'	15:O:42:SER:OG	2.13	0.49
1:A:787:U:H2'	1:A:788:A:C8	2.47	0.49
1:A:1699:A:N6	1:A:2032:A:O2'	2.46	0.49
15:O:78:ARG:CD	15:O:78:ARG:N	2.75	0.49
16:P:1:MET:O	16:P:15:GLU:HB3	2.13	0.49
31:a:161:A:N6	31:a:355:G:O2'	2.46	0.49
1:A:578:G:H21	15:O:48:ARG:HH22	1.58	0.49
1:A:707:G:H5''	10:J:16:ARG:HB3	1.94	0.49
1:A:2786:G:H1'	1:A:2787:C:H5'	1.95	0.49
1:A:2867:U:H2'	1:A:2868:G:O4'	2.13	0.49
31:a:36:G:N2	42:l:128:SER:OG	2.46	0.49
31:a:274:G:H3'	47:q:71:ALA:HB2	1.94	0.49
31:a:917:A:H2'	31:a:918:A:H8	1.77	0.49
31:a:946:A:H2'	31:a:947:A:C8	2.47	0.49
34:d:114:VAL:HG22	34:d:119:ILE:HG13	1.93	0.49
5:E:5:ASP:HA	5:E:13:LYS:NZ	2.28	0.49
7:G:38:ASN:HD22	7:G:41:MET:HG3	1.78	0.49
11:K:35:GLN:HA	11:K:102:ILE:HA	1.95	0.49
11:K:111:GLU:OE2	11:K:115:ARG:NH2	2.45	0.49
12:L:73:ASN:HB2	12:L:77:THR:OG1	2.13	0.49
12:L:100:TYR:O	12:L:101:THR:HG23	2.13	0.49
31:a:266:A:H2'	31:a:267:G:H8	1.78	0.49
31:a:502:C:O2'	31:a:504:G:H1'	2.13	0.49
31:a:774:A:C2	31:a:775:A:H1'	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:963:G:H2'	31:a:964:U:C6	2.48	0.49
31:a:1544:C:H2'	31:a:1545:A:H8	1.74	0.49
42:l:88:GLN:N	42:l:88:GLN:OE1	2.45	0.49
47:q:63:ILE:HG23	47:q:75:PHE:HB3	1.95	0.49
1:A:1530:A:H2'	1:A:1531:U:C6	2.47	0.49
1:A:2338:A:O2'	6:F:79:LEU:HD22	2.12	0.49
16:P:27:VAL:HG22	16:P:28:ASN:N	2.26	0.49
31:a:953:G:N1	31:a:1348:G:OP2	2.27	0.49
31:a:975:G:H4'	39:i:132:ARG:HB3	1.94	0.49
31:a:1006:U:H2'	31:a:1007:C:C6	2.48	0.49
31:a:1340:U:H2'	31:a:1341:G:O4'	2.13	0.49
31:a:1513:A:H2	31:a:1516:G:H22	1.59	0.49
34:d:87:MET:HE1	34:d:182:ARG:CZ	2.43	0.49
47:q:56:LYS:NZ	47:q:84:SER:HB2	2.27	0.49
1:A:427:A:N1	1:A:439:U:H5	2.10	0.48
1:A:852:U:C2	1:A:853:G:C8	3.01	0.48
12:L:70:GLU:OE2	12:L:80:THR:HG22	2.13	0.48
31:a:209:G:H2'	31:a:210:A:C8	2.48	0.48
31:a:618:G:C2	31:a:619:C:C6	3.01	0.48
35:e:157:ARG:HH21	38:h:43:GLU:HB3	1.78	0.48
1:A:90:A:H4'	1:A:91:A:H5'	1.94	0.48
1:A:1754:C:H2'	1:A:1755:U:C6	2.48	0.48
7:G:168:TYR:CE2	7:G:170:ARG:HG2	2.48	0.48
8:H:103:GLU:HB2	8:H:125:VAL:HG11	1.95	0.48
18:R:22:GLU:OE1	18:R:23:ASP:N	2.47	0.48
31:a:63:U:H2'	31:a:64:C:C6	2.48	0.48
1:A:281:A:H2'	1:A:282:A:C8	2.48	0.48
1:A:1701:U:OP1	4:D:149:ARG:N	2.47	0.48
1:A:1753:U:H1'	1:A:2880:A:H1'	1.94	0.48
1:A:1821:U:H2'	1:A:1822:C:C6	2.48	0.48
1:A:2338:A:O2'	6:F:79:LEU:CD2	2.62	0.48
31:a:994:C:H2'	31:a:995:A:C8	2.47	0.48
31:a:1129:A:C2	31:a:1130:G:C8	3.01	0.48
1:A:1072:A:N6	1:A:1169:G:H2'	2.27	0.48
8:H:17:TYR:HA	8:H:139:GLU:O	2.13	0.48
12:L:55:ASP:C	12:L:55:ASP:OD1	2.55	0.48
31:a:1518:A:H2'	31:a:1519:G:C8	2.49	0.48
46:p:11:GLY:HA3	46:p:16:PRO:HA	1.95	0.48
1:A:104:C:C6	1:A:104:C:C5'	2.92	0.48
3:C:232:HIS:CE1	3:C:247:MET:H	2.32	0.48
13:M:77:GLY:O	13:M:80:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1135:G:O2'	31:a:1155:C:N3	2.46	0.48
31:a:1538:C:H2'	31:a:1539:U:C6	2.49	0.48
31:a:1473:C:O2'	31:a:1474:C:H5'	2.14	0.48
32:b:76:ALA:HB2	32:b:164:VAL:HG11	1.96	0.48
47:q:70:SER:OG	47:q:73:LYS:HG3	2.13	0.48
49:s:32:LYS:HA	49:s:50:ALA:HB3	1.96	0.48
1:A:529:A:C8	19:S:44:HIS:HD2	2.31	0.48
9:I:19:VAL:HG22	9:I:20:LEU:N	2.28	0.48
9:I:63:VAL:HB	9:I:102:VAL:HG22	1.94	0.48
15:O:76:TYR:O	15:O:80:MET:HG2	2.13	0.48
17:Q:5:ALA:HB3	17:Q:54:ALA:HB2	1.96	0.48
31:a:592:G:H2'	31:a:593:G:C8	2.49	0.48
31:a:1136:U:H1'	31:a:1137:U:H2'	1.95	0.48
31:a:1326:G:N2	31:a:1328:A:H3'	2.28	0.48
42:l:92:VAL:O	42:l:116:ASP:HB3	2.13	0.48
45:o:36:ILE:HG23	45:o:56:LEU:HD11	1.96	0.48
1:A:1315:C:H5'	12:L:20:LEU:CD2	2.43	0.48
1:A:2022:U:O2'	1:A:2023:C:OP1	2.29	0.48
14:N:3:ASN:HD22	14:N:7:ILE:HG21	1.79	0.48
15:O:111:THR:O	15:O:115:ASP:OD2	2.31	0.48
19:S:87:ASP:O	19:S:89:LYS:CE	2.62	0.48
21:U:48:GLN:OE1	21:U:52:LYS:N	2.46	0.48
25:Y:18:THR:HG21	25:Y:49:ASP:O	2.14	0.48
31:a:271:A:H2'	31:a:272:C:C6	2.49	0.48
31:a:1470:U:H2'	31:a:1471:A:H8	1.78	0.48
31:a:1473:C:C2'	31:a:1474:C:H5'	2.44	0.48
40:j:9:ARG:HB3	40:j:73:LEU:HD23	1.96	0.48
41:k:53:LYS:HD3	41:k:54:GLY:O	2.14	0.48
43:m:14:ARG:HH21	43:m:17:ILE:HD11	1.79	0.48
1:A:78:U:H2'	1:A:79:U:H6	1.78	0.48
1:A:1279:C:C2	1:A:1280:U:C5	3.02	0.48
1:A:1290:G:N2	15:O:33:LYS:HG3	2.28	0.48
1:A:2632:U:H2'	1:A:2633:C:C6	2.48	0.48
1:A:2903:A:H5'	1:A:2904:U:H5''	1.96	0.48
21:U:71:ILE:HD12	21:U:72:ASP:O	2.13	0.48
31:a:59:C:O2	31:a:59:C:H2'	2.14	0.48
31:a:886:C:C2	31:a:887:U:C5	3.02	0.48
31:a:1191:G:H1'	31:a:1192:G:C8	2.49	0.48
33:c:33:HIS:HE1	44:n:38:LYS:HB3	1.79	0.48
34:d:101:LEU:HD11	34:d:174:GLY:HA3	1.96	0.48
39:i:21:VAL:HA	39:i:67:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:15:LEU:HD11	49:s:33:THR:HG23	1.94	0.48
1:A:881:G:C6	1:A:882:C:C5	3.02	0.48
1:A:1712:A:O2'	1:A:1718:G:N7	2.37	0.48
1:A:1805:U:H3'	1:A:1811:A:N6	2.29	0.48
8:H:15:LYS:HD2	8:H:17:TYR:OH	2.14	0.48
12:L:94:THR:HG23	12:L:95:GLU:HG3	1.95	0.48
31:a:855:C:H2'	31:a:856:C:H6	1.79	0.48
32:b:121:GLU:HG3	32:b:126:PHE:CD2	2.49	0.48
2:B:55:A:H4'	6:F:27:GLU:HG2	1.95	0.47
19:S:3:ILE:HD12	19:S:4:LYS:O	2.14	0.47
20:T:32:TYR:HE1	20:T:92:LEU:CD2	1.86	0.47
31:a:586:C:O2'	31:a:736:A:N3	2.41	0.47
31:a:1255:A:N6	31:a:1303:G:O6	2.47	0.47
31:a:1326:G:N1	31:a:1329:A:OP2	2.42	0.47
31:a:1392:C:H2'	31:a:1393:C:H6	1.78	0.47
31:a:1438:A:H2'	31:a:1439:C:C6	2.49	0.47
1:A:38:A:H2'	1:A:39:C:O4'	2.14	0.47
1:A:1206:G:N2	16:P:90:GLN:OE1	2.47	0.47
1:A:1300:G:C6	1:A:1301:U:C4	3.02	0.47
7:G:8:ILE:CB	7:G:69:ARG:NH2	2.77	0.47
31:a:509:C:H2'	31:a:510:C:H6	1.78	0.47
31:a:1083:G:H2'	31:a:1084:U:C6	2.49	0.47
1:A:944:G:H2'	1:A:945:A:O4'	2.14	0.47
1:A:2272:U:H5''	1:A:2273:G:H5'	1.96	0.47
1:A:2727:G:H2'	1:A:2728:U:C6	2.49	0.47
2:B:47:C:H2'	2:B:48:A:C8	2.49	0.47
31:a:434:U:OP1	34:d:29:ARG:HD2	2.14	0.47
31:a:553:C:OP1	34:d:54:LYS:NZ	2.47	0.47
32:b:99:GLY:O	32:b:103:ASN:HB3	2.14	0.47
50:t:72:ASP:OD1	50:t:72:ASP:N	2.47	0.47
1:A:388:A:H8	1:A:389:A:C2	2.33	0.47
1:A:1575:A:HO2'	1:A:1576:A:P	2.38	0.47
1:A:2662:U:O2'	4:D:90:GLU:OE1	2.31	0.47
6:F:13:THR:O	6:F:17:MET:HB2	2.13	0.47
31:a:1217:C:C2'	31:a:1218:C:H5'	2.44	0.47
32:b:12:ALA:HA	32:b:208:ARG:HG3	1.95	0.47
33:c:72:PRO:HG3	33:c:104:GLU:HG3	1.96	0.47
40:j:42:LEU:HB3	40:j:71:LYS:HB2	1.97	0.47
9:I:81:GLU:OE1	9:I:82:ASN:O	2.33	0.47
31:a:34:A:H2'	31:a:35:C:C6	2.50	0.47
31:a:266:A:H2'	31:a:267:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:498:U:H2'	31:a:499:A:C8	2.47	0.47
39:i:58:GLU:N	39:i:58:GLU:OE2	2.47	0.47
1:A:1494:G:H5''	1:A:1574:G:O3'	2.14	0.47
1:A:1633:A:H1'	1:A:1634:A:H5'	1.96	0.47
1:A:2224:U:H2'	1:A:2251:G:H1	1.80	0.47
1:A:2432:G:H2'	1:A:2438:A:N6	2.28	0.47
19:S:85:PHE:HD1	19:S:88:GLY:C	2.23	0.47
31:a:305:G:N2	31:a:308:A:OP2	2.37	0.47
31:a:1325:U:H2'	31:a:1326:G:O4'	2.14	0.47
39:i:58:GLU:HB3	39:i:60:LYS:HZ3	1.79	0.47
41:k:54:GLY:C	41:k:56:LYS:H	2.22	0.47
43:m:72:GLU:OE2	43:m:76:ASN:ND2	2.47	0.47
1:A:1084:U:H2'	1:A:1085:U:O4'	2.15	0.47
1:A:1512:U:H2'	1:A:1567:A:N6	2.29	0.47
1:A:1726:A:OP2	1:A:1743:G:N2	2.47	0.47
1:A:1929:C:H5''	3:C:241:ILE:HB	1.96	0.47
1:A:2318:U:H2'	1:A:2319:U:C6	2.50	0.47
3:C:157:SER:O	3:C:195:VAL:CG2	2.63	0.47
4:D:54:GLU:O	4:D:85:LYS:HD3	2.15	0.47
7:G:45:GLN:O	7:G:45:GLN:HG2	2.13	0.47
9:I:73:ASP:OD1	9:I:75:SER:CB	2.62	0.47
31:a:612:G:H2'	31:a:613:U:H6	1.80	0.47
31:a:643:A:H2'	31:a:644:U:C6	2.50	0.47
31:a:698:G:H2'	31:a:699:G:C8	2.50	0.47
31:a:745:U:H2'	31:a:746:U:H6	1.78	0.47
31:a:749:G:OP1	45:o:2:ALA:HB2	2.15	0.47
31:a:884:C:C4	31:a:885:A:N7	2.83	0.47
31:a:1197:G:H4'	39:i:115:ARG:NH2	2.29	0.47
31:a:1541:G:H2'	31:a:1542:A:N3	2.29	0.47
41:k:17:GLU:HG2	41:k:18:ASN:OD1	2.14	0.47
45:o:6:GLU:OE1	45:o:6:GLU:N	2.40	0.47
49:s:71:LEU:HD23	49:s:71:LEU:H	1.79	0.47
1:A:1315:C:H5'	12:L:20:LEU:HD21	1.96	0.47
10:J:6:LEU:C	10:J:6:LEU:HD12	2.40	0.47
10:J:70:ASN:OD1	10:J:70:ASN:O	2.33	0.47
14:N:19:LEU:H	14:N:19:LEU:HD23	1.80	0.47
16:P:62:VAL:HG22	16:P:95:LEU:HD23	1.96	0.47
31:a:328:A:O2'	31:a:1445:G:O2'	2.25	0.47
32:b:83:GLU:OE1	32:b:86:ARG:NH1	2.46	0.47
1:A:2839:A:O2'	1:A:2841:A:N7	2.47	0.47
9:I:42:THR:HA	9:I:56:ASP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:4:ARG:HD2	23:W:23:GLU:HA	1.97	0.47
20:T:78:GLN:HB2	20:T:88:HIS:H	1.80	0.47
21:U:80:LYS:HE3	21:U:80:LYS:HB3	1.77	0.47
22:V:46:LYS:C	22:V:47:VAL:HG13	2.40	0.47
31:a:920:U:C2	31:a:921:C:C5	3.02	0.47
31:a:1007:C:H2'	31:a:1008:C:O4'	2.14	0.47
41:k:84:VAL:HB	41:k:110:ILE:HD13	1.97	0.47
1:A:896:U:H2'	1:A:897:A:H8	1.80	0.47
1:A:1876:G:H1	1:A:1920:C:H42	1.63	0.47
2:B:40:C:O4'	6:F:66:LEU:HD22	2.15	0.47
3:C:100:GLU:OE2	3:C:102:ARG:HD3	2.15	0.47
22:V:40:VAL:HG23	22:V:45:LYS:HB3	1.96	0.47
31:a:932:A:H2'	31:a:933:C:C6	2.50	0.47
31:a:1090:G:H2'	31:a:1091:A:C8	2.50	0.47
31:a:1333:G:H2'	31:a:1334:A:H8	1.80	0.47
32:b:9:LEU:HB3	32:b:14:VAL:HB	1.97	0.47
1:A:962:A:H5''	1:A:2295:A:H61	1.80	0.46
1:A:1290:G:C2	15:O:33:LYS:HG3	2.51	0.46
6:F:69:LYS:HE2	6:F:69:LYS:HB2	1.70	0.46
6:F:88:LYS:HB2	6:F:88:LYS:HE3	1.75	0.46
8:H:3:GLN:HE22	16:P:13:LYS:H	1.63	0.46
31:a:468:G:C6	31:a:482:A:C6	3.03	0.46
31:a:1339:A:C5	31:a:1340:U:C5	3.03	0.46
31:a:1464:A:H2'	31:a:1465:G:C8	2.51	0.46
35:e:112:ARG:NH1	35:e:116:GLU:OE2	2.43	0.46
36:f:29:ILE:HG21	36:f:75:GLU:HB3	1.97	0.46
1:A:441:C:H2'	1:A:442:G:C8	2.51	0.46
1:A:1693:G:C6	1:A:2036:G:O6	2.68	0.46
19:S:25:ALA:HB3	19:S:34:VAL:CG1	2.45	0.46
21:U:23:ASP:OD1	21:U:24:SER:N	2.43	0.46
31:a:776:A:H4'	31:a:1534:G:N2	2.29	0.46
32:b:86:ARG:NE	32:b:222:LEU:HD11	2.29	0.46
43:m:46:LYS:HG3	43:m:47:ASP:OD1	2.15	0.46
48:r:25:HIS:ND1	48:r:25:HIS:C	2.73	0.46
1:A:350:G:H8	1:A:373:A:N6	2.14	0.46
1:A:363:A:OP1	5:E:135:LYS:NZ	2.48	0.46
1:A:901:G:H2'	1:A:902:A:H8	1.80	0.46
1:A:1072:A:H2'	1:A:1073:A:C8	2.50	0.46
1:A:1737:U:H5''	1:A:1738:C:H5	1.80	0.46
1:A:1823:U:H2'	1:A:1824:C:C6	2.50	0.46
1:A:2817:A:H1'	1:A:2818:A:H5'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:93:LEU:HA	8:H:93:LEU:HD23	1.76	0.46
30:4:15:LYS:HB3	30:4:15:LYS:HE3	1.66	0.46
31:a:1229:U:H2'	31:a:1230:G:C8	2.50	0.46
32:b:166:PRO:HG2	32:b:187:VAL:HG12	1.97	0.46
33:c:57:GLU:O	33:c:64:ASN:N	2.36	0.46
35:e:25:VAL:HG22	35:e:26:LYS:H	1.81	0.46
47:q:61:VAL:HG12	47:q:80:ILE:HG12	1.97	0.46
1:A:1578:A:H1'	1:A:1588:U:N3	2.28	0.46
1:A:2459:A:H2'	1:A:2460:A:C8	2.50	0.46
2:B:71:A:C2	20:T:38:ASN:ND2	2.84	0.46
2:B:86:A:H8	2:B:87:C:H5''	1.80	0.46
3:C:168:GLU:HB3	3:C:169:GLY:H	1.65	0.46
31:a:732:G:OP2	31:a:863:U:O2'	2.23	0.46
31:a:745:U:C2	31:a:746:U:C5	3.03	0.46
31:a:1142:U:H6	31:a:1142:U:C5'	2.28	0.46
31:a:1170:G:C5	31:a:1171:C:C6	3.04	0.46
31:a:1278:G:H2'	31:a:1279:A:C8	2.51	0.46
33:c:96:LYS:HB2	33:c:96:LYS:HE3	1.66	0.46
34:d:67:GLN:O	34:d:71:THR:OG1	2.32	0.46
36:f:1:MET:SD	36:f:1:MET:N	2.76	0.46
1:A:924:G:H2'	1:A:925:G:C8	2.51	0.46
1:A:1829:A:H2'	1:A:1830:A:C8	2.50	0.46
1:A:2359:C:OP1	21:U:54:TYR:OH	2.29	0.46
5:E:5:ASP:HB2	5:E:13:LYS:HE2	1.97	0.46
6:F:92:ARG:O	6:F:96:MET:CE	2.64	0.46
11:K:65:TRP:CH2	11:K:107:ALA:HB3	2.42	0.46
16:P:16:GLU:HA	16:P:97:ILE:HB	1.96	0.46
31:a:203:A:O2'	31:a:204:A:O5'	2.30	0.46
31:a:390:A:H2'	31:a:391:A:C8	2.50	0.46
31:a:425:G:H2'	31:a:426:U:C6	2.51	0.46
31:a:561:A:H2'	31:a:562:U:C6	2.50	0.46
31:a:1197:G:H2'	31:a:1198:A:C8	2.50	0.46
31:a:1388:C:O4'	37:g:92:ARG:NH1	2.48	0.46
31:a:1445:G:H2'	31:a:1446:C:C6	2.51	0.46
34:d:149:ASN:N	34:d:149:ASN:OD1	2.46	0.46
35:e:115:LEU:HD22	35:e:120:ILE:HG21	1.98	0.46
1:A:2144:A:H1'	1:A:2175:G:H4'	1.97	0.46
1:A:2146:A:N6	1:A:2195:G:H22	2.13	0.46
31:a:552:G:OP1	34:d:55:GLN:NE2	2.46	0.46
31:a:716:A:H2'	31:a:717:U:C6	2.50	0.46
32:b:154:MET:HE3	32:b:155:LYS:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:40:ILE:HD11	49:s:71:LEU:HB3	1.98	0.46
1:A:1422:A:H1'	1:A:1423:C:C6	2.51	0.46
1:A:1899:U:H1'	1:A:1900:G:C8	2.50	0.46
1:A:2124:U:C4	1:A:2125:U:C4	3.04	0.46
1:A:2645:G:H21	4:D:163:VAL:HG21	1.81	0.46
12:L:106:GLN:NE2	12:L:118:ILE:CD1	2.79	0.46
31:a:41:C:H2'	31:a:42:G:C8	2.51	0.46
41:k:74:ALA:O	41:k:79:LEU:HD23	2.16	0.46
1:A:84:A:H1'	1:A:85:G:C1'	2.46	0.46
1:A:720:A:OP1	5:E:76:GLY:HA3	2.16	0.46
1:A:2854:A:H2'	1:A:2899:A:N6	2.31	0.46
6:F:120:LYS:HD3	6:F:120:LYS:HA	1.66	0.46
9:I:71:ARG:HH11	14:N:74:ARG:NE	2.14	0.46
31:a:137:U:OP1	46:p:66:LYS:NZ	2.48	0.46
31:a:927:A:H2'	31:a:928:A:C8	2.51	0.46
31:a:1154:G:N2	31:a:1156:A:H62	2.14	0.46
43:m:65:VAL:HG13	43:m:66:GLU:H	1.80	0.46
1:A:1336:G:N1	1:A:1684:A:OP2	2.42	0.46
3:C:139:THR:HG21	3:C:192:ILE:HD12	1.97	0.46
25:Y:9:TYR:CZ	25:Y:26:GLY:HA2	2.51	0.46
31:a:272:C:O2'	47:q:68:PRO:O	2.28	0.46
31:a:887:U:H2'	31:a:888:C:H6	1.81	0.46
31:a:1185:G:C2	31:a:1186:A:C8	3.04	0.46
37:g:10:ARG:H	37:g:10:ARG:HG2	1.49	0.46
39:i:98:GLY:O	39:i:102:ARG:NH2	2.48	0.46
1:A:2153:A:C4'	1:A:2190:C:H42	2.29	0.46
4:D:33:ASN:HB2	4:D:105:VAL:HB	1.98	0.46
23:W:7:ARG:O	23:W:60:ARG:NH2	2.49	0.46
31:a:501:U:H2'	31:a:502:C:C2	2.51	0.46
31:a:692:U:H2'	31:a:693:G:O4'	2.15	0.46
46:p:20:ILE:HG22	46:p:37:ILE:HB	1.98	0.46
47:q:53:ASN:O	47:q:53:ASN:ND2	2.49	0.46
50:t:33:LYS:HE3	50:t:33:LYS:HB3	1.78	0.46
1:A:64:A:H1'	18:R:65:MET:HB2	1.98	0.45
1:A:632:U:H2'	1:A:633:A:H8	1.82	0.45
7:G:92:VAL:O	7:G:92:VAL:HG23	2.16	0.45
7:G:98:MET:HE3	7:G:98:MET:HB3	1.81	0.45
8:H:68:ASN:O	8:H:68:ASN:CG	2.58	0.45
14:N:91:ARG:HG3	14:N:92:GLY:H	1.81	0.45
15:O:45:TYR:CD1	15:O:48:ARG:NH2	2.84	0.45
15:O:78:ARG:N	15:O:78:ARG:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:36:GLU:HA	19:S:60:GLU:OE2	2.16	0.45
31:a:412:G:O6	31:a:507:A:N1	2.49	0.45
31:a:435:C:H5''	34:d:10:LYS:HD3	1.97	0.45
31:a:1097:U:H2'	31:a:1098:G:H8	1.80	0.45
31:a:1336:U:H2'	31:a:1337:A:C8	2.48	0.45
31:a:1417:C:C2	31:a:1418:A:C8	3.04	0.45
34:d:3:ARG:HD2	34:d:3:ARG:HA	1.47	0.45
1:A:1128:A:C8	1:A:1129:A:C8	3.04	0.45
3:C:230:HIS:CD2	3:C:232:HIS:H	2.16	0.45
8:H:73:LYS:O	8:H:73:LYS:HG3	2.17	0.45
20:T:55:VAL:HG21	20:T:59:GLY:HA3	1.98	0.45
30:4:1:MET:HE2	30:4:1:MET:HB2	1.80	0.45
31:a:622:A:H2'	31:a:623:C:C6	2.51	0.45
31:a:1310:G:P	31:a:1345:C:H42	2.38	0.45
31:a:1435:A:H2'	31:a:1436:A:O4'	2.16	0.45
9:I:18:GLU:OE2	9:I:19:VAL:N	2.49	0.45
21:U:57:GLU:CD	21:U:57:GLU:N	2.73	0.45
31:a:36:G:H2'	31:a:37:C:C6	2.51	0.45
31:a:470:A:H2'	31:a:471:A:H8	1.79	0.45
31:a:562:U:C2	31:a:563:C:C5	3.03	0.45
31:a:1278:G:N2	31:a:1337:A:H1'	2.32	0.45
34:d:179:LEU:HD12	34:d:180:PRO:HD2	1.98	0.45
38:h:68:GLN:HE21	38:h:68:GLN:HB3	1.61	0.45
45:o:75:ILE:H	45:o:75:ILE:HD12	1.81	0.45
49:s:33:THR:HB	49:s:51:VAL:HA	1.98	0.45
1:A:1198:G:OP2	15:O:58:ARG:NH2	2.40	0.45
1:A:1278:G:C8	1:A:1279:C:C6	3.05	0.45
1:A:2431:C:H2'	1:A:2432:G:O4'	2.15	0.45
4:D:128:GLN:HG3	4:D:173:MET:HE3	1.98	0.45
5:E:137:LYS:HB3	5:E:137:LYS:HE2	1.42	0.45
5:E:146:LEU:O	5:E:148:GLN:OE1	2.34	0.45
16:P:100:ILE:HG22	16:P:101:ASN:N	2.32	0.45
31:a:1390:U:C4	37:g:3:ARG:HG2	2.52	0.45
31:a:1505:G:C2	31:a:1506:U:C5	3.04	0.45
39:i:27:GLU:HA	39:i:61:GLY:O	2.17	0.45
41:k:36:ASP:OD1	41:k:40:ASN:N	2.48	0.45
1:A:631:U:H2'	1:A:632:U:C6	2.52	0.45
1:A:1880:A:H2'	1:A:1881:A:C8	2.51	0.45
1:A:2253:C:C2	1:A:2254:A:C8	3.05	0.45
1:A:2294:A:H5''	1:A:2295:A:H5'	1.97	0.45
6:F:17:MET:HE3	6:F:17:MET:HB3	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:11:ARG:C	17:Q:11:ARG:HH11	2.23	0.45
27:1:9:CYS:SG	27:1:12:CYS:N	2.88	0.45
31:a:561:A:H2'	31:a:562:U:H6	1.81	0.45
31:a:659:C:H2'	31:a:660:U:C6	2.51	0.45
31:a:954:G:H1	31:a:1246:A:H61	1.65	0.45
31:a:1001:U:H4'	31:a:1002:G:O5'	2.15	0.45
31:a:1394:C:H2'	31:a:1395:G:C8	2.52	0.45
42:l:86:ASN:OD1	42:l:86:ASN:N	2.48	0.45
48:r:44:ILE:HD13	48:r:61:THR:HG23	1.99	0.45
1:A:511:G:H4'	28:2:17:HIS:CD2	2.51	0.45
1:A:523:A:H2'	1:A:524:A:C8	2.52	0.45
1:A:925:G:H3'	1:A:926:G:H8	1.82	0.45
1:A:1758:A:H5''	1:A:1759:G:H21	1.80	0.45
4:D:118:VAL:HG23	4:D:209:VAL:HB	1.99	0.45
5:E:146:LEU:C	5:E:147:GLU:HG3	2.41	0.45
6:F:110:ARG:HD3	6:F:136:LEU:HA	1.99	0.45
9:I:35:ILE:HD13	9:I:69:VAL:HG22	1.98	0.45
10:J:15:GLU:OE2	10:J:16:ARG:O	2.34	0.45
10:J:61:LEU:HD21	29:3:24:ARG:HD2	1.98	0.45
12:L:55:ASP:OD1	12:L:55:ASP:O	2.35	0.45
18:R:9:ARG:HG2	18:R:28:ASP:CB	2.46	0.45
31:a:197:U:C2	31:a:198:G:C8	3.05	0.45
31:a:382:A:C6	31:a:383:U:C4	3.04	0.45
31:a:987:A:C8	31:a:988:C:H5	2.34	0.45
31:a:1243:G:H2'	31:a:1244:C:C6	2.51	0.45
31:a:1259:C:O2'	39:i:73:GLY:O	2.29	0.45
32:b:17:GLY:HA2	32:b:188:ASP:OD1	2.16	0.45
43:m:51:ASP:OD1	43:m:52:GLU:N	2.49	0.45
1:A:273:A:N1	1:A:415:U:H4'	2.32	0.45
1:A:651:A:H2'	1:A:652:A:C8	2.50	0.45
1:A:719:G:H5''	5:E:76:GLY:N	2.32	0.45
1:A:1225:G:H3'	1:A:1226:G:H8	1.81	0.45
1:A:1932:C:H4'	1:A:1956:G:H8	1.82	0.45
1:A:2122:A:C4	1:A:2123:A:C8	3.04	0.45
5:E:5:ASP:HA	5:E:13:LYS:HZ1	1.81	0.45
9:I:91:LYS:HE3	9:I:111:PHE:CE1	2.51	0.45
31:a:775:A:C4	31:a:776:A:C8	3.04	0.45
32:b:113:ARG:O	32:b:117:ILE:HG13	2.17	0.45
40:j:10:LEU:HB2	40:j:18:ILE:HD11	1.98	0.45
1:A:1801:C:O2	1:A:1801:C:H2'	2.16	0.45
4:D:29:GLU:OE1	4:D:31:LYS:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:51:ARG:HA	11:K:54:MET:HE2	1.97	0.45
16:P:27:VAL:CG2	16:P:28:ASN:N	2.79	0.45
17:Q:40:ASN:O	17:Q:40:ASN:ND2	2.50	0.45
18:R:57:ASN:OD1	18:R:76:ARG:NH1	2.48	0.45
31:a:409:C:O2'	31:a:629:A:N3	2.49	0.45
31:a:451:U:O2'	31:a:452:A:O5'	2.35	0.45
31:a:967:A:H2'	31:a:968:A:C8	2.52	0.45
31:a:1132:U:C2	31:a:1133:U:C5	3.04	0.45
31:a:1187:G:H3'	31:a:1188:G:C8	2.49	0.45
31:a:1516:G:H5''	31:a:1517:U:H2'	1.99	0.45
1:A:1000:G:N2	1:A:1003:A:H3'	2.32	0.45
1:A:1315:C:H2'	1:A:1316:G:C8	2.52	0.45
1:A:1680:U:H2'	1:A:1681:U:C6	2.51	0.45
1:A:1818:A:C2'	1:A:1819:G:H5'	2.47	0.45
1:A:2279:G:C8	21:U:12:LYS:HD2	2.51	0.45
1:A:2369:C:H3'	1:A:2370:U:O2	2.17	0.45
31:a:205:A:C2	31:a:206:A:C5	3.04	0.45
31:a:328:A:H2'	31:a:329:A:C8	2.52	0.45
31:a:444:C:H2'	31:a:445:U:C6	2.52	0.45
31:a:452:A:N6	31:a:499:A:N6	2.64	0.45
31:a:674:G:H5'	31:a:734:C:H1'	1.99	0.45
31:a:1197:G:H2'	31:a:1198:A:H8	1.82	0.45
34:d:8:ASN:OD1	34:d:20:SER:OG	2.29	0.45
37:g:36:ARG:HG3	37:g:40:GLN:HG3	1.99	0.45
49:s:32:LYS:HG3	49:s:34:TRP:HZ3	1.81	0.45
1:A:90:A:H1'	1:A:91:A:C8	2.52	0.45
1:A:249:C:O2'	1:A:431:C:H4'	2.16	0.45
1:A:1308:C:H5''	1:A:1309:G:C5'	2.47	0.45
7:G:23:HIS:CE1	7:G:34:SER:HB3	2.52	0.45
9:I:71:ARG:NH1	14:N:74:ARG:CZ	2.80	0.45
16:P:27:VAL:CG2	16:P:31:ASP:CB	2.94	0.45
19:S:16:ASP:OD1	19:S:19:LYS:NZ	2.46	0.45
22:V:40:VAL:CG2	22:V:45:LYS:HB3	2.47	0.45
23:W:62:ILE:HD12	23:W:62:ILE:HA	1.68	0.45
31:a:34:A:H2'	31:a:35:C:H6	1.82	0.45
31:a:110:G:H1	31:a:338:C:H41	1.65	0.45
31:a:666:G:C6	31:a:667:C:C4	3.05	0.45
32:b:18:HIS:HB2	32:b:189:THR:HB	1.98	0.45
33:c:76:ILE:HA	33:c:83:ILE:HB	1.99	0.45
41:k:53:LYS:HD3	41:k:54:GLY:N	2.32	0.45
45:o:56:LEU:HA	45:o:59:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2917:U:H2'	1:A:2918:A:C8	2.52	0.44
16:P:20:ILE:HG13	16:P:95:LEU:HB2	1.98	0.44
17:Q:46:VAL:O	17:Q:50:VAL:HG23	2.17	0.44
31:a:271:A:H2'	31:a:272:C:C5	2.52	0.44
31:a:341:U:H2'	31:a:342:C:H6	1.82	0.44
31:a:911:G:C2	31:a:912:G:C8	3.05	0.44
44:n:20:GLU:OE2	44:n:20:GLU:N	2.45	0.44
47:q:19:MET:HE3	47:q:22:THR:HG22	1.99	0.44
1:A:1379:A:HO2'	1:A:1381:U:P	2.38	0.44
1:A:2022:U:H3'	1:A:2023:C:H2'	1.98	0.44
1:A:2564:U:H2'	1:A:2565:C:C6	2.53	0.44
9:I:107:ARG:HD3	9:I:115:VAL:HG11	1.98	0.44
31:a:423:A:O2'	31:a:424:G:O5'	2.36	0.44
32:b:28:LYS:HE3	32:b:28:LYS:HB3	1.72	0.44
46:p:59:LYS:HE3	46:p:59:LYS:HB3	1.86	0.44
1:A:1115:G:N2	1:A:1136:C:OP2	2.50	0.44
1:A:2212:G:H2'	1:A:2213:U:C6	2.52	0.44
1:A:2260:A:H2'	1:A:2261:G:C8	2.51	0.44
31:a:550:U:H2'	31:a:551:G:C8	2.52	0.44
31:a:683:A:H1'	41:k:118:HIS:CG	2.53	0.44
31:a:839:U:O2'	31:a:1550:C:OP1	2.31	0.44
31:a:920:U:H2'	31:a:921:C:H6	1.82	0.44
31:a:1102:U:C2	31:a:1106:U:C4	3.06	0.44
31:a:1118:C:C4	31:a:1119:G:C8	3.04	0.44
32:b:120:MET:HA	32:b:123:ASP:CG	2.42	0.44
37:g:150:ALA:HB3	41:k:56:LYS:NZ	2.32	0.44
48:r:31:THR:O	48:r:35:LYS:HG3	2.17	0.44
1:A:2278:OMG:HM23	1:A:2278:OMG:H1'	1.49	0.44
1:A:2670:G:H2'	1:A:2671:A:C8	2.52	0.44
3:C:74:ILE:N	3:C:74:ILE:CD1	2.80	0.44
18:R:46:PHE:CE2	18:R:87:ILE:HG23	2.52	0.44
31:a:277:U:H2'	31:a:278:A:C8	2.51	0.44
31:a:957:C:OP2	43:m:107:ARG:HG2	2.18	0.44
31:a:1359:A:H1'	31:a:1384:A:N6	2.28	0.44
31:a:1395:G:C4	31:a:1396:G:C8	3.06	0.44
31:a:1396:G:N3	31:a:1397:G:C8	2.86	0.44
31:a:1550:C:OP2	31:a:1550:C:H6	2.01	0.44
33:c:33:HIS:CE1	44:n:38:LYS:HB3	2.51	0.44
33:c:85:LYS:HA	33:c:88:ASN:HD21	1.83	0.44
33:c:110:LEU:HD13	33:c:203:ARG:HD3	1.98	0.44
1:A:923:A:H2'	1:A:924:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2874:A:H2'	1:A:2875:U:C6	2.53	0.44
2:B:28:C:H1'	2:B:55:A:H61	1.82	0.44
6:F:34:ILE:HG13	6:F:91:LEU:HB2	1.99	0.44
6:F:35:VAL:HG12	6:F:155:VAL:HG22	1.98	0.44
11:K:43:THR:O	11:K:47:ILE:HG13	2.17	0.44
30:4:13:LYS:HD2	30:4:28:GLU:CD	2.42	0.44
31:a:63:U:H2'	31:a:64:C:H6	1.82	0.44
31:a:490:A:H2'	31:a:491:C:O4'	2.18	0.44
31:a:1094:U:O2'	31:a:1113:A:OP2	2.35	0.44
31:a:1325:U:H2'	31:a:1326:G:C8	2.53	0.44
31:a:1552:U:H3'	32:b:22:ARG:HH12	1.83	0.44
34:d:179:LEU:HD12	34:d:179:LEU:HA	1.88	0.44
34:d:182:ARG:HA	34:d:185:LEU:HD12	1.99	0.44
40:j:34:ALA:HB1	40:j:76:ILE:HD11	1.99	0.44
43:m:107:ARG:NH2	43:m:113:VAL:HG22	2.33	0.44
1:A:1312:A:N7	12:L:12:GLN:HG2	2.33	0.44
1:A:1806:U:H5'	1:A:1807:A:O5'	2.18	0.44
2:B:64:A:N6	2:B:104:A:H2'	2.33	0.44
7:G:90:VAL:O	7:G:94:TYR:CD2	2.71	0.44
12:L:69:VAL:HG12	12:L:70:GLU:N	2.32	0.44
20:T:84:ASN:C	20:T:85:GLN:HG3	2.42	0.44
26:Z:29:GLU:OE1	26:Z:34:GLY:O	2.34	0.44
31:a:660:U:C5	31:a:760:G:C4	3.06	0.44
31:a:929:U:H2'	31:a:930:U:C6	2.52	0.44
31:a:951:G:C2	31:a:1352:C:C2	3.06	0.44
31:a:1297:A:H8	31:a:1363:G:O2'	2.00	0.44
39:i:46:LEU:HD11	39:i:74:PHE:HD1	1.81	0.44
40:j:16:ARG:HD3	40:j:16:ARG:HA	1.64	0.44
1:A:529:A:H5'	19:S:44:HIS:HB3	2.00	0.44
1:A:1617:A:H2'	1:A:1618:A:C8	2.53	0.44
1:A:2793:G:C2	1:A:2794:C:C6	3.06	0.44
7:G:17:VAL:HG13	7:G:26:VAL:HG22	1.99	0.44
20:T:72:VAL:HG21	20:T:91:PHE:HB3	2.00	0.44
31:a:421:G:H5''	31:a:436:G:N2	2.32	0.44
31:a:697:C:OP1	41:k:46:SER:OG	2.31	0.44
31:a:1107:C:H2'	31:a:1108:C:H6	1.82	0.44
31:a:1228:U:OP1	44:n:9:LYS:HE3	2.17	0.44
31:a:1330:C:H42	49:s:36:ARG:HB2	1.82	0.44
35:e:162:GLU:OE1	35:e:162:GLU:N	2.49	0.44
45:o:29:ILE:HG23	45:o:63:ARG:HG3	1.99	0.44
1:A:2035:C:H2'	1:A:2036:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:92:ARG:HD2	12:L:93:TYR:CZ	2.52	0.44
31:a:189:G:N2	31:a:202:C:H1'	2.32	0.44
31:a:563:C:C2	31:a:564:C:C5	3.06	0.44
31:a:758:C:C2	31:a:759:U:C5	3.06	0.44
31:a:855:C:C2	31:a:856:C:C5	3.06	0.44
31:a:987:A:N7	31:a:1328:A:N6	2.65	0.44
31:a:1287:C:H1'	31:a:1292:C:O2	2.18	0.44
31:a:1541:G:C2	31:a:1542:A:C6	3.06	0.44
1:A:1328:C:C2	1:A:1329:G:C8	3.05	0.44
1:A:1745:A:H2	31:a:1485:G:O2'	2.01	0.44
1:A:2123:A:C4	1:A:2124:U:C5	3.06	0.44
1:A:2591:A:O2'	1:A:2592:A:O5'	2.26	0.44
1:A:2725:U:H2'	1:A:2726:C:C6	2.53	0.44
19:S:45:GLN:OE1	19:S:46:LYS:N	2.51	0.44
19:S:91:VAL:HG22	19:S:92:ARG:N	2.31	0.44
31:a:434:U:H2'	31:a:435:C:C6	2.53	0.44
31:a:479:U:H2'	31:a:480:G:H8	1.82	0.44
31:a:618:G:C6	31:a:619:C:C5	3.05	0.44
31:a:1005:A:C5	31:a:1006:U:C4	3.05	0.44
36:f:90:MET:HG2	36:f:92:ILE:HD13	1.99	0.44
45:o:75:ILE:HD12	45:o:75:ILE:N	2.33	0.44
47:q:19:MET:HG3	47:q:22:THR:HB	2.00	0.44
47:q:32:THR:HG22	47:q:39:ARG:HG2	2.00	0.44
49:s:15:LEU:HD12	49:s:15:LEU:HA	1.75	0.44
49:s:19:VAL:HG21	49:s:44:PHE:CE1	2.53	0.44
1:A:1712:A:N3	1:A:1714:C:N4	2.65	0.43
4:D:168:LYS:HB2	4:D:168:LYS:HE3	1.36	0.43
13:M:41:TYR:CD2	13:M:57:SER:OG	2.65	0.43
31:a:342:C:C2	31:a:343:C:C5	3.06	0.43
31:a:365:G:C2	31:a:366:U:C5	3.06	0.43
31:a:485:U:O2'	31:a:486:C:H5'	2.17	0.43
31:a:616:A:H2'	31:a:617:A:O4'	2.17	0.43
31:a:725:C:H4'	41:k:119:ASN:ND2	2.27	0.43
31:a:764:C:H2'	31:a:765:U:C6	2.53	0.43
31:a:909:A:H2'	31:a:910:A:C8	2.53	0.43
31:a:1201:A:H2'	31:a:1202:C:H6	1.81	0.43
32:b:81:LYS:HG3	32:b:91:TYR:CZ	2.52	0.43
36:f:90:MET:HE1	48:r:66:ARG:HB3	1.99	0.43
39:i:112:MET:SD	39:i:113:LYS:N	2.91	0.43
1:A:300:G:N1	1:A:467:U:O2'	2.50	0.43
2:B:73:G:H21	20:T:88:HIS:CD2	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:19:ILE:HG13	8:H:55:VAL:HG13	2.00	0.43
14:N:17:THR:C	14:N:19:LEU:H	2.26	0.43
14:N:35:ILE:H	14:N:35:ILE:HG12	1.50	0.43
19:S:7:ASP:HB2	19:S:70:LEU:HD21	2.00	0.43
21:U:54:TYR:HE2	21:U:84:LYS:HG2	1.83	0.43
31:a:262:G:O6	31:a:281:A:N6	2.50	0.43
31:a:742:A:H2'	31:a:743:C:H6	1.83	0.43
31:a:1182:C:H2'	31:a:1183:C:H6	1.83	0.43
31:a:1229:U:H2'	31:a:1230:G:H8	1.83	0.43
43:m:114:LYS:O	43:m:114:LYS:HG2	2.18	0.43
49:s:71:LEU:HA	49:s:74:PHE:HD1	1.83	0.43
1:A:305:A:H62	1:A:410:G:H21	1.67	0.43
1:A:1103:G:O6	1:A:1124:A:N6	2.51	0.43
1:A:2273:G:H2'	1:A:2274:A:H8	1.83	0.43
1:A:2611:U:H2'	1:A:2612:U:H2'	2.00	0.43
8:H:37:LEU:C	8:H:37:LEU:HD12	2.42	0.43
9:I:43:VAL:HG23	9:I:54:LYS:HA	2.00	0.43
9:I:77:ILE:O	9:I:77:ILE:HG23	2.18	0.43
9:I:91:LYS:CE	9:I:109:GLY:O	2.66	0.43
10:J:143:HIS:ND1	10:J:143:HIS:O	2.51	0.43
15:O:33:LYS:HB2	15:O:33:LYS:HE3	1.75	0.43
19:S:84:LYS:CE	19:S:93:ILE:HD12	2.48	0.43
20:T:94:ILE:HD12	20:T:94:ILE:H	1.82	0.43
22:V:31:ALA:HB3	22:V:33:LEU:HG	1.99	0.43
31:a:1131:C:H2'	31:a:1132:U:H6	1.83	0.43
31:a:1302:U:H2'	31:a:1303:G:C8	2.53	0.43
32:b:6:MET:O	32:b:10:LEU:HD23	2.18	0.43
37:g:150:ALA:HB3	41:k:56:LYS:HZ2	1.83	0.43
50:t:3:ASN:HB3	50:t:8:ILE:HD11	1.99	0.43
1:A:2769:G:H5''	30:4:1:MET:HE3	2.01	0.43
1:A:2793:G:H2'	1:A:2793:G:N3	2.34	0.43
4:D:123:LYS:HE3	4:D:204:PRO:HA	2.00	0.43
6:F:69:LYS:HG3	6:F:84:PRO:CA	2.47	0.43
13:M:95:ASP:OD1	13:M:95:ASP:C	2.60	0.43
14:N:98:LYS:C	14:N:99:LEU:HD22	2.43	0.43
31:a:122:C:OP1	31:a:319:C:O2'	2.35	0.43
31:a:383:U:C2	31:a:384:G:C8	3.07	0.43
31:a:932:A:H2'	31:a:933:C:H6	1.82	0.43
43:m:19:LEU:HD22	43:m:25:ILE:HG21	1.99	0.43
1:A:409:G:H3'	1:A:410:G:C8	2.54	0.43
1:A:786:U:H2'	1:A:787:U:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:U:H4'	1:A:1186:A:O5'	2.18	0.43
1:A:2829:A:H3'	1:A:2830:A:H8	1.84	0.43
18:R:52:SER:OG	18:R:81:THR:CG2	2.66	0.43
31:a:184:A:C8	31:a:207:G:N2	2.85	0.43
31:a:304:U:O2'	31:a:564:C:O2	2.36	0.43
31:a:1171:C:C2	31:a:1172:C:C5	3.06	0.43
31:a:1216:G:C4	31:a:1217:C:C6	3.06	0.43
39:i:30:ILE:HG22	39:i:37:VAL:HB	2.01	0.43
3:C:74:ILE:H	3:C:74:ILE:CD1	2.28	0.43
8:H:36:ILE:HG22	8:H:37:LEU:N	2.32	0.43
9:I:24:VAL:HG23	9:I:24:VAL:O	2.18	0.43
30:4:33:LYS:HB2	30:4:33:LYS:HE2	1.86	0.43
31:a:57:U:H2'	31:a:58:G:C8	2.54	0.43
31:a:358:G:H2'	31:a:359:G:C8	2.54	0.43
31:a:877:C:H2'	31:a:878:A:O4'	2.19	0.43
31:a:956:G:H2'	31:a:957:C:C6	2.54	0.43
31:a:1137:U:C4	40:j:73:LEU:HD11	2.53	0.43
31:a:1536:G:H2'	31:a:1537:G:H8	1.83	0.43
47:q:41:LYS:HB2	47:q:41:LYS:HE2	1.71	0.43
49:s:29:GLN:HA	49:s:29:GLN:OE1	2.17	0.43
1:A:1141:U:H2'	1:A:1142:A:C4	2.53	0.43
1:A:1804:U:O2	1:A:1804:U:O4'	2.37	0.43
7:G:23:HIS:C	7:G:23:HIS:HD1	2.26	0.43
7:G:92:VAL:O	7:G:92:VAL:CG2	2.67	0.43
11:K:111:GLU:HG2	11:K:112:GLU:OE1	2.19	0.43
19:S:3:ILE:CD1	19:S:4:LYS:O	2.66	0.43
31:a:13:U:H4'	31:a:534:C:H4'	2.01	0.43
31:a:204:A:C2	31:a:205:A:C5	3.06	0.43
31:a:340:G:C2	31:a:341:U:C6	3.06	0.43
31:a:414:G:C2	31:a:415:A:C8	3.06	0.43
31:a:422:A:C8	31:a:423:A:C8	3.07	0.43
31:a:483:C:H2'	31:a:484:A:H8	1.81	0.43
31:a:484:A:C4	31:a:485:U:C5	3.06	0.43
31:a:1170:G:C6	31:a:1171:C:C5	3.07	0.43
31:a:1182:C:H2'	31:a:1183:C:C6	2.53	0.43
39:i:41:LEU:HD13	39:i:46:LEU:HB3	2.01	0.43
47:q:62:LYS:HE2	47:q:62:LYS:HB2	1.75	0.43
49:s:23:GLU:OE1	49:s:23:GLU:N	2.51	0.43
1:A:1152:U:C5	1:A:1153:C:C2	3.07	0.43
1:A:2355:A:H2'	1:A:2356:A:C8	2.53	0.43
1:A:2656:A:C6	1:A:2914:A:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2799:C:H5'	4:D:181:GLN:NE2	2.34	0.43
1:A:2859:G:C4	1:A:2860:U:C5	3.07	0.43
7:G:105:LEU:HD23	7:G:105:LEU:HA	1.91	0.43
9:I:35:ILE:H	9:I:35:ILE:HD12	1.84	0.43
10:J:80:ASP:OD1	10:J:81:GLN:N	2.52	0.43
18:R:23:ASP:OD2	18:R:82:LEU:HD12	2.18	0.43
31:a:617:A:C5	31:a:618:G:C8	3.07	0.43
31:a:835:U:H5	31:a:881:A:N1	2.17	0.43
31:a:888:C:H2'	31:a:889:C:H6	1.83	0.43
31:a:921:C:H2'	31:a:922:A:H8	1.82	0.43
31:a:956:G:H5''	43:m:107:ARG:HB2	2.00	0.43
31:a:1176:G:H3'	31:a:1177:A:C5'	2.49	0.43
32:b:90:PHE:HE1	32:b:153:ASP:HB2	1.84	0.43
34:d:15:LEU:HD13	34:d:56:LYS:HA	2.00	0.43
34:d:155:VAL:HG13	34:d:156:GLU:HG3	2.01	0.43
42:l:96:ARG:HG2	42:l:111:VAL:HG22	2.01	0.43
43:m:85:SER:OG	43:m:87:ARG:O	2.37	0.43
1:A:441:C:H2'	1:A:442:G:H8	1.83	0.43
1:A:2106:U:H2'	1:A:2107:G:O4'	2.19	0.43
1:A:2142:G:O2'	1:A:2192:G:N1	2.45	0.43
1:A:2332:U:H1'	6:F:151:GLY:CA	2.48	0.43
3:C:67:PHE:CE1	3:C:105:ILE:HD11	2.54	0.43
10:J:88:GLY:N	10:J:120:LYS:O	2.50	0.43
13:M:11:ARG:HE	13:M:11:ARG:HB3	1.63	0.43
13:M:55:GLN:CD	13:M:56:ALA:N	2.77	0.43
31:a:71:A:H3'	31:a:72:C:C5'	2.49	0.43
31:a:479:U:H2'	31:a:480:G:C8	2.54	0.43
31:a:742:A:H2'	31:a:743:C:C6	2.54	0.43
31:a:1161:A:O2'	31:a:1162:A:H5''	2.19	0.43
1:A:1435:C:H2'	1:A:1436:C:C6	2.53	0.43
1:A:2707:C:H5'	4:D:202:PRO:HA	2.01	0.43
5:E:146:LEU:O	5:E:147:GLU:CD	2.61	0.43
16:P:36:ASP:OD1	16:P:36:ASP:N	2.44	0.43
17:Q:11:ARG:HH21	17:Q:98:LYS:HB3	1.83	0.43
31:a:203:A:C2	31:a:204:A:C5	3.07	0.43
31:a:261:U:H2'	31:a:262:G:H8	1.83	0.43
31:a:1085:G:O2'	31:a:1112:A:N1	2.48	0.43
31:a:1242:U:P	39:i:128:GLN:HE21	2.42	0.43
31:a:1455:U:O2'	31:a:1456:A:OP1	2.29	0.43
1:A:556:U:H4'	1:A:1273:G:H4'	2.01	0.42
1:A:1094:A:C6	1:A:2778:G:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1583:G:H4'	1:A:1584:U:O4'	2.19	0.42
1:A:2701:G:H4'	9:I:30:ARG:HD3	2.00	0.42
20:T:31:VAL:HG12	20:T:91:PHE:CB	2.47	0.42
23:W:28:LEU:HD21	23:W:42:ARG:NH1	2.34	0.42
31:a:522:C:H2'	31:a:523:G:C8	2.46	0.42
31:a:560:U:N3	31:a:561:A:N7	2.67	0.42
31:a:617:A:C6	31:a:618:G:C8	3.07	0.42
31:a:946:A:H2'	31:a:947:A:H8	1.84	0.42
31:a:952:U:O2'	39:i:128:GLN:OE1	2.29	0.42
31:a:1126:U:H2'	31:a:1127:U:C6	2.54	0.42
31:a:1171:C:C2'	31:a:1172:C:H5'	2.49	0.42
31:a:1228:U:H2'	31:a:1229:U:C6	2.54	0.42
31:a:1271:A:N6	31:a:1284:A:O2'	2.52	0.42
46:p:46:ASN:HB3	46:p:47:ALA:H	1.65	0.42
1:A:460:C:N4	1:A:2435:U:O4	2.52	0.42
1:A:1000:G:H2'	1:A:1001:A:H2'	2.01	0.42
1:A:1630:A:H1'	1:A:1631:G:C8	2.54	0.42
1:A:2135:U:H4'	1:A:2177:U:H1'	2.00	0.42
15:O:76:TYR:CE1	15:O:80:MET:HG3	2.53	0.42
15:O:102:ASP:OD1	15:O:104:LYS:CE	2.67	0.42
16:P:65:GLN:HG2	16:P:93:THR:HG22	2.01	0.42
24:X:40:ASN:OD1	24:X:40:ASN:C	2.62	0.42
31:a:165:G:C2	31:a:166:G:C8	3.07	0.42
31:a:267:G:O2'	31:a:268:G:H5'	2.20	0.42
31:a:612:G:C6	31:a:643:A:C6	3.07	0.42
31:a:1133:U:H2'	31:a:1134:A:C8	2.55	0.42
32:b:117:ILE:HG23	32:b:120:MET:HE1	2.01	0.42
35:e:55:GLU:HB2	35:e:58:GLU:OE2	2.19	0.42
37:g:37:GLY:O	37:g:41:ARG:HD2	2.19	0.42
38:h:98:LEU:HD22	38:h:132:TRP:HB2	2.00	0.42
42:l:129:LEU:H	42:l:129:LEU:HG	1.49	0.42
43:m:91:HIS:ND1	43:m:97:VAL:HG11	2.34	0.42
45:o:7:ARG:HA	45:o:10:GLU:OE2	2.19	0.42
45:o:76:GLN:OE1	45:o:76:GLN:HA	2.19	0.42
1:A:300:G:H1	1:A:467:U:HO2'	1.65	0.42
1:A:1197:C:H2'	1:A:1198:G:O4'	2.19	0.42
2:B:43:A:H2'	2:B:44:A:O4'	2.19	0.42
8:H:15:LYS:CD	8:H:17:TYR:CZ	3.02	0.42
11:K:76:LYS:HB3	11:K:91:GLU:OE1	2.19	0.42
21:U:44:ILE:HG21	21:U:47:ARG:HG2	2.01	0.42
31:a:699:G:H2'	31:a:700:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1167:A:C2	31:a:1191:G:C5	3.07	0.42
32:b:121:GLU:HG3	32:b:126:PHE:HD2	1.83	0.42
34:d:103:LEU:HD13	34:d:103:LEU:HA	1.92	0.42
43:m:86:TYR:CZ	43:m:90:ARG:HD2	2.54	0.42
49:s:30:VAL:HG22	49:s:48:THR:HG21	2.01	0.42
1:A:27:G:N2	1:A:557:G:H1'	2.34	0.42
1:A:37:C:H4'	1:A:497:U:OP1	2.20	0.42
1:A:1726:A:H2'	1:A:1727:C:C6	2.55	0.42
1:A:1917:A:H3'	1:A:1918:G:O4'	2.20	0.42
1:A:2304:G:OP2	21:U:20:ASN:OD1	2.37	0.42
8:H:15:LYS:HD2	8:H:17:TYR:CZ	2.54	0.42
9:I:20:LEU:O	9:I:41:CYS:HB2	2.19	0.42
21:U:54:TYR:HD2	21:U:80:LYS:HD3	1.85	0.42
31:a:123:G:H2'	31:a:124:U:H6	1.84	0.42
31:a:211:A:H1'	31:a:212:A:O4'	2.20	0.42
31:a:432:G:H2'	31:a:433:A:C8	2.54	0.42
31:a:468:G:H2'	31:a:469:U:C6	2.54	0.42
31:a:571:A:H2'	31:a:575:G:C8	2.54	0.42
31:a:745:U:H2'	31:a:746:U:C6	2.54	0.42
31:a:911:G:N3	31:a:912:G:C8	2.87	0.42
31:a:1327:C:H2'	31:a:1328:A:O4'	2.20	0.42
32:b:57:LEU:HD23	32:b:57:LEU:HA	1.82	0.42
37:g:66:ILE:HA	37:g:66:ILE:HD13	1.69	0.42
49:s:55:ARG:HG2	49:s:56:LYS:N	2.34	0.42
1:A:231:A:H3'	1:A:231:A:N3	2.35	0.42
1:A:286:U:H4'	1:A:287:G:C8	2.54	0.42
3:C:117:GLU:O	3:C:128:ASN:HB2	2.19	0.42
12:L:22:THR:O	12:L:26:ILE:HG12	2.20	0.42
13:M:40:ILE:HG23	13:M:76:VAL:HG21	2.01	0.42
19:S:45:GLN:OE1	19:S:45:GLN:CA	2.67	0.42
31:a:992:A:H5'	31:a:993:C:OP2	2.19	0.42
37:g:148:ASN:HD22	37:g:148:ASN:N	2.16	0.42
47:q:7:ARG:HB3	47:q:65:GLU:HG3	2.01	0.42
1:A:283:G:H3'	1:A:284:C:H6	1.83	0.42
1:A:1238:U:O4'	15:O:4:VAL:HG23	2.20	0.42
1:A:1296:C:O2'	1:A:1297:G:H5'	2.19	0.42
1:A:1378:U:H3'	1:A:1434:U:O2	2.20	0.42
1:A:1844:G:H2'	1:A:1845:U:H5'	2.00	0.42
3:C:100:GLU:OE2	3:C:102:ARG:CD	2.68	0.42
21:U:77:PHE:CD1	21:U:77:PHE:N	2.88	0.42
31:a:661:U:H5	38:h:57:GLN:OE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:973:A:H4'	40:j:57:LYS:HE3	2.00	0.42
31:a:1271:A:C5	31:a:1272:A:C8	3.07	0.42
32:b:114:ILE:CD1	32:b:144:LEU:HB3	2.44	0.42
33:c:40:LYS:NZ	33:c:40:LYS:HB3	2.35	0.42
35:e:82:PRO:HG2	35:e:147:LEU:HD22	2.02	0.42
37:g:74:GLU:HB2	37:g:91:VAL:HG22	2.01	0.42
44:n:26:ARG:HD2	44:n:47:LEU:HD11	2.00	0.42
1:A:328:G:H1'	1:A:329:A:H5'	2.00	0.42
1:A:1873:G:H2'	1:A:1874:A:C8	2.54	0.42
1:A:2273:G:H2'	1:A:2274:A:C8	2.55	0.42
1:A:2346:U:OP2	1:A:2346:U:C6	2.73	0.42
3:C:171:TYR:HB3	3:C:183:MET:HB3	2.02	0.42
6:F:22:TYR:HB3	6:F:27:GLU:HB3	2.01	0.42
9:I:90:ASP:OD1	9:I:92:GLY:N	2.53	0.42
10:J:121:LEU:C	10:J:121:LEU:HD12	2.44	0.42
12:L:105:LYS:HA	12:L:117:VAL:HG12	2.02	0.42
16:P:34:THR:HG23	16:P:34:THR:O	2.18	0.42
19:S:41:MET:CE	19:S:61:ALA:HB2	2.50	0.42
31:a:248:U:H2'	31:a:249:G:C8	2.55	0.42
31:a:500:A:O2'	31:a:501:U:H5'	2.19	0.42
31:a:562:U:H2'	31:a:563:C:H6	1.84	0.42
31:a:1058:G:H5''	44:n:4:THR:HG21	2.01	0.42
31:a:1310:G:H1'	31:a:1313:C:N4	2.35	0.42
31:a:1434:U:H2'	31:a:1435:A:H8	1.82	0.42
32:b:54:TYR:CE2	32:b:216:LYS:HG3	2.53	0.42
34:d:37:GLY:N	34:d:38:PRO:HD2	2.35	0.42
36:f:14:ILE:HG21	36:f:19:LYS:HG3	2.02	0.42
41:k:53:LYS:O	41:k:56:LYS:HB2	2.19	0.42
41:k:88:GLY:HA2	41:k:89:PRO:HD3	1.93	0.42
43:m:90:ARG:HD3	43:m:97:VAL:HA	2.01	0.42
43:m:94:GLY:HA2	43:m:109:ARG:HH21	1.85	0.42
1:A:1306:A:H1'	1:A:2040:A:N6	2.35	0.42
6:F:78:ARG:HD3	6:F:78:ARG:HA	1.57	0.42
7:G:35:ARG:HB2	7:G:75:MET:HE1	2.01	0.42
9:I:4:GLN:HA	9:I:21:THR:HG23	2.00	0.42
9:I:20:LEU:HD12	9:I:21:THR:N	2.35	0.42
18:R:65:MET:HE2	18:R:65:MET:HB3	1.90	0.42
31:a:26:C:H2'	31:a:27:A:H8	1.85	0.42
31:a:94:G:H5'	31:a:95:A:OP1	2.20	0.42
31:a:421:G:H3'	31:a:436:G:H22	1.83	0.42
31:a:609:G:C6	31:a:646:G:C6	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:892:C:H2'	31:a:893:U:C6	2.54	0.42
31:a:910:A:C5	31:a:911:G:H1'	2.55	0.42
35:e:37:VAL:HG11	35:e:64:VAL:HG22	2.02	0.42
43:m:16:VAL:HG13	43:m:17:ILE:HG12	2.01	0.42
46:p:20:ILE:HD13	46:p:52:VAL:HG22	2.02	0.42
46:p:52:VAL:HG12	46:p:53:ASP:O	2.19	0.42
1:A:390:A:H2'	1:A:391:A:C8	2.55	0.42
1:A:1203:U:C2	1:A:1204:G:C8	3.08	0.42
1:A:1816:A:H2'	1:A:1817:C:O4'	2.20	0.42
1:A:2228:C:H2'	1:A:2229:C:C6	2.55	0.42
1:A:2253:C:H2'	1:A:2254:A:O4'	2.19	0.42
3:C:69:ARG:HE	3:C:69:ARG:HB3	1.57	0.42
7:G:3:ARG:O	7:G:4:VAL:C	2.62	0.42
7:G:68:THR:HA	7:G:71:LEU:HB2	2.01	0.42
7:G:89:LEU:H	7:G:129:THR:HG23	1.84	0.42
9:I:108:GLU:C	9:I:110:ASN:H	2.28	0.42
11:K:130:LYS:HE2	11:K:130:LYS:HB3	1.95	0.42
12:L:37:ALA:HA	12:L:40:VAL:HG12	2.00	0.42
18:R:63:LYS:HB3	18:R:63:LYS:HE2	1.81	0.42
19:S:20:GLU:N	19:S:20:GLU:OE2	2.52	0.42
20:T:84:ASN:O	20:T:85:GLN:CG	2.68	0.42
31:a:51:A:O2'	31:a:368:G:N2	2.53	0.42
31:a:265:A:H2'	31:a:266:A:C8	2.55	0.42
31:a:342:C:H2'	31:a:343:C:H6	1.85	0.42
31:a:470:A:C6	31:a:480:G:C6	3.08	0.42
31:a:1099:G:O2'	31:a:1178:C:N4	2.48	0.42
31:a:1267:A:O2'	31:a:1268:G:N7	2.53	0.42
37:g:38:THR:O	37:g:42:ILE:HG12	2.20	0.42
38:h:116:LYS:HE2	38:h:116:LYS:HB2	1.83	0.42
41:k:23:ILE:HB	41:k:86:VAL:HG12	2.02	0.42
43:m:61:ASP:OD1	43:m:61:ASP:N	2.49	0.42
1:A:1476:G:H5''	1:A:1476:G:H8	1.85	0.42
1:A:2161:A:H61	1:A:2184:G:C2'	2.33	0.42
3:C:157:SER:O	3:C:158:ALA:C	2.63	0.42
4:D:6:LEU:HD23	4:D:6:LEU:HA	1.89	0.42
7:G:131:VAL:HG12	7:G:132:LYS:N	2.34	0.42
8:H:60:ALA:HB3	8:H:127:GLY:HA2	2.02	0.42
9:I:63:VAL:HG23	9:I:64:ARG:HG2	2.02	0.42
10:J:47:ARG:NH2	10:J:50:PHE:HD1	2.18	0.42
18:R:56:MET:CE	18:R:79:ILE:HD11	2.50	0.42
31:a:112:G:H2'	31:a:113:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:262:G:OP1	47:q:70:SER:OG	2.28	0.42
31:a:432:G:H2'	31:a:433:A:H8	1.85	0.42
31:a:1357:G:H8	39:i:111:ARG:O	2.02	0.42
31:a:1370:A:OP2	44:n:35:ARG:NH2	2.53	0.42
31:a:1489:A:H2'	31:a:1490:A:H8	1.83	0.42
41:k:105:LEU:HD23	41:k:105:LEU:HA	1.91	0.42
1:A:242:U:H2'	1:A:243:U:O4'	2.20	0.41
1:A:318:A:H62	1:A:401:U:H3	1.66	0.41
1:A:870:C:H4'	1:A:2455:G:C5	2.55	0.41
1:A:1303:A:O4'	1:A:1305:U:C6	2.73	0.41
1:A:1692:C:O2	1:A:1692:C:O4'	2.38	0.41
1:A:1751:G:H1'	1:A:1783:G:C4	2.55	0.41
1:A:2101:U:O2'	1:A:2624:G:H1'	2.20	0.41
2:B:108:U:H2'	2:B:109:G:C8	2.55	0.41
4:D:49:ILE:HD12	4:D:51:VAL:HG23	2.02	0.41
6:F:152:MET:HB2	6:F:152:MET:HE2	1.62	0.41
12:L:16:MET:HE2	12:L:16:MET:HB3	1.84	0.41
17:Q:22:ASP:OD1	17:Q:25:ARG:NH1	2.47	0.41
21:U:19:LYS:HB3	21:U:19:LYS:HZ3	1.84	0.41
31:a:69:G:H22	31:a:100:A:H2	1.68	0.41
31:a:352:A:O2'	31:a:354:G:N1	2.48	0.41
31:a:1248:A:H8	31:a:1251:G:O2'	2.04	0.41
42:l:53:MET:HE1	42:l:104:PRO:HD2	2.01	0.41
49:s:3:ARG:HB3	49:s:4:SER:H	1.61	0.41
49:s:32:LYS:HG3	49:s:34:TRP:CZ3	2.55	0.41
1:A:291:G:H2'	1:A:292:U:C2	2.55	0.41
1:A:1235:C:C2	1:A:1236:G:C8	3.08	0.41
1:A:2338:A:H1'	6:F:79:LEU:HD22	2.02	0.41
3:C:107:PRO:HD2	3:C:110:LEU:HD22	2.01	0.41
6:F:128:TYR:HB2	6:F:156:ILE:HG12	2.02	0.41
11:K:38:THR:OG1	11:K:127:VAL:CG2	2.69	0.41
25:Y:18:THR:HG22	25:Y:53:ASP:OD2	2.20	0.41
31:a:26:C:H2'	31:a:27:A:C8	2.54	0.41
31:a:203:A:N3	31:a:204:A:C8	2.88	0.41
31:a:248:U:H2'	31:a:249:G:H8	1.84	0.41
31:a:1176:G:H3'	31:a:1177:A:H5''	2.01	0.41
31:a:1338:C:N3	31:a:1339:A:N7	2.68	0.41
31:a:1347:G:H5''	31:a:1348:G:OP1	2.20	0.41
31:a:1422:C:H2'	31:a:1423:A:H8	1.79	0.41
47:q:56:LYS:NZ	47:q:83:GLU:O	2.46	0.41
47:q:56:LYS:HE3	47:q:56:LYS:HB3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:16:MET:O	49:s:20:GLU:HG2	2.21	0.41
49:s:33:THR:HG21	49:s:71:LEU:HD11	2.02	0.41
1:A:351:G:H2'	1:A:352:A:C8	2.55	0.41
1:A:1335:C:H2'	1:A:1336:G:O4'	2.20	0.41
1:A:1415:A:H1'	1:A:1416:U:C5	2.55	0.41
1:A:1692:C:H5	1:A:2036:G:H1	1.68	0.41
1:A:2332:U:O4	6:F:40:VAL:HG12	2.19	0.41
1:A:2803:A:C2	1:A:2805:A:C2	3.08	0.41
1:A:2859:G:O4'	12:L:45:GLU:OE2	2.38	0.41
14:N:19:LEU:HD23	14:N:19:LEU:O	2.20	0.41
16:P:24:LYS:NZ	16:P:24:LYS:HB3	2.35	0.41
17:Q:34:ALA:HB3	26:Z:27:MET:CE	2.50	0.41
31:a:188:U:H5'	31:a:189:G:OP2	2.19	0.41
31:a:224:U:H2'	31:a:225:G:C8	2.48	0.41
31:a:254:A:H1'	31:a:255:G:H4'	2.03	0.41
31:a:507:A:H62	31:a:554:A:H2'	1.85	0.41
31:a:744:U:C2	31:a:745:U:C5	3.08	0.41
31:a:931:G:H2'	31:a:932:A:C8	2.55	0.41
31:a:956:G:H2'	31:a:957:C:H6	1.84	0.41
31:a:1533:U:H2'	31:a:1534:G:C8	2.50	0.41
32:b:120:MET:HA	32:b:123:ASP:OD1	2.20	0.41
38:h:34:LYS:O	38:h:38:GLU:HG3	2.20	0.41
1:A:253:G:H2'	1:A:254:A:C8	2.55	0.41
1:A:458:A:H61	1:A:2438:A:H1'	1.85	0.41
1:A:579:U:O2'	15:O:49:ASP:OD2	2.30	0.41
1:A:710:C:H2'	1:A:711:G:H8	1.86	0.41
1:A:902:A:O2'	1:A:903:G:H5'	2.20	0.41
1:A:1346:G:OP2	28:2:10:LYS:NZ	2.48	0.41
1:A:1804:U:H5	1:A:1814:A:N1	2.18	0.41
1:A:1862:G:H1	1:A:1932:C:H5	1.68	0.41
1:A:1928:A:H2'	1:A:1929:C:C6	2.55	0.41
1:A:2541:U:H2'	1:A:2542:C:C6	2.55	0.41
5:E:110:LEU:HD23	5:E:110:LEU:HA	1.95	0.41
6:F:31:ILE:CG2	6:F:96:MET:SD	3.03	0.41
7:G:158:LYS:HA	7:G:171:ARG:NH2	2.35	0.41
11:K:1:MET:HG2	11:K:66:ILE:HG21	2.01	0.41
15:O:104:LYS:HE2	15:O:104:LYS:N	2.33	0.41
23:W:19:LYS:HB3	23:W:19:LYS:HE3	1.24	0.41
31:a:98:U:H4'	31:a:99:U:H5'	2.02	0.41
31:a:261:U:H2'	31:a:262:G:C8	2.55	0.41
31:a:307:G:H2'	31:a:308:A:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:561:A:C4	31:a:562:U:C5	3.08	0.41
31:a:957:C:H2'	31:a:958:A:H8	1.85	0.41
31:a:1337:A:C4	31:a:1338:C:C5	3.09	0.41
33:c:64:ASN:HA	33:c:99:HIS:HB2	2.01	0.41
39:i:23:LEU:HD23	39:i:65:VAL:HG12	2.02	0.41
45:o:18:HIS:ND1	45:o:19:GLU:O	2.53	0.41
1:A:127:C:H2'	1:A:128:C:C6	2.56	0.41
1:A:234:C:H3'	1:A:235:G:H4'	2.01	0.41
1:A:250:G:C2	1:A:255:G:C6	3.08	0.41
1:A:1053:A:C8	1:A:1197:C:O2'	2.72	0.41
1:A:1751:G:H1'	1:A:1783:G:N3	2.35	0.41
1:A:1800:A:C8	1:A:1856:A:C8	3.08	0.41
1:A:2345:A:H5'	1:A:2346:U:OP2	2.20	0.41
2:B:3:U:H2'	2:B:4:G:C8	2.56	0.41
2:B:47:C:H2'	2:B:48:A:H8	1.85	0.41
4:D:197:VAL:O	4:D:197:VAL:HG23	2.21	0.41
8:H:38:ARG:HH11	8:H:38:ARG:HG3	1.85	0.41
20:T:13:GLN:HB3	20:T:18:LEU:CD2	2.50	0.41
31:a:686:U:H2'	31:a:687:C:H6	1.86	0.41
31:a:757:A:C2	31:a:758:C:C5	3.09	0.41
31:a:855:C:H2'	31:a:856:C:C6	2.54	0.41
31:a:1343:A:H2'	31:a:1344:G:O4'	2.20	0.41
31:a:1376:C:H2'	31:a:1377:U:C6	2.56	0.41
32:b:129:LEU:HD12	32:b:129:LEU:HA	1.90	0.41
35:e:14:ARG:HB2	35:e:117:LEU:HD11	2.02	0.41
39:i:97:ARG:HG3	39:i:101:LYS:HG3	2.03	0.41
1:A:864:A:N7	1:A:1227:U:C5	2.88	0.41
1:A:2680:U:H2'	1:A:2681:A:C2	2.56	0.41
1:A:2905:C:N4	26:Z:39:SER:OG	2.47	0.41
7:G:5:GLY:HA2	7:G:69:ARG:CG	2.45	0.41
7:G:130:VAL:O	7:G:130:VAL:HG12	2.20	0.41
11:K:26:TYR:CD1	11:K:26:TYR:N	2.88	0.41
28:2:4:ARG:O	28:2:7:GLN:OE1	2.39	0.41
29:3:7:HIS:CD2	29:3:10:ALA:H	2.31	0.41
31:a:241:U:H2'	31:a:242:C:C6	2.55	0.41
31:a:509:C:H1'	31:a:557:C:H1'	2.03	0.41
31:a:1057:A:N6	31:a:1221:U:O2'	2.52	0.41
31:a:1179:A:H2'	31:a:1180:A:C8	2.56	0.41
45:o:35:GLU:O	45:o:39:VAL:HG23	2.20	0.41
1:A:219:A:C8	1:A:478:A:N6	2.88	0.41
1:A:1247:G:O2'	1:A:1275:A:N1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2109:A:H3'	1:A:2110:G:H8	1.86	0.41
1:A:2863:G:C2	1:A:2864:A:C8	3.08	0.41
2:B:64:A:H61	2:B:104:A:H2'	1.86	0.41
5:E:68:LYS:HB3	5:E:68:LYS:HE3	1.76	0.41
6:F:95:ARG:HH22	25:Y:9:TYR:CB	2.34	0.41
7:G:157:TYR:O	7:G:171:ARG:NH2	2.53	0.41
20:T:3:SER:O	20:T:3:SER:OG	2.31	0.41
20:T:22:ARG:HE	20:T:22:ARG:HB2	1.67	0.41
31:a:138:A:H2'	31:a:139:U:C6	2.55	0.41
31:a:987:A:C4	31:a:1329:A:C2	3.08	0.41
31:a:1086:U:H5''	32:b:178:LYS:HE3	2.02	0.41
31:a:1340:U:C4	31:a:1341:G:C6	3.09	0.41
34:d:41:ARG:HA	34:d:41:ARG:HE	1.85	0.41
34:d:170:ASP:O	34:d:171:SER:OG	2.33	0.41
39:i:102:ARG:CZ	39:i:102:ARG:HB2	2.50	0.41
43:m:15:VAL:HG22	43:m:48:LEU:HD11	2.02	0.41
45:o:82:ILE:HG12	45:o:87:ILE:O	2.20	0.41
1:A:525:A:H1'	1:A:526:A:H5''	2.01	0.41
1:A:1229:G:OP1	10:J:30:THR:OG1	2.39	0.41
1:A:1329:G:H2'	1:A:1330:U:C6	2.55	0.41
1:A:2026:C:H5''	1:A:2750:C:O2'	2.20	0.41
1:A:2107:G:H5'	22:V:19:SER:CB	2.51	0.41
1:A:2786:G:HO2'	1:A:2787:C:H6	1.69	0.41
6:F:57:LEU:HD23	6:F:57:LEU:HA	1.82	0.41
6:F:130:LEU:HB2	6:F:154:ILE:HD11	2.01	0.41
9:I:11:ALA:HB1	9:I:99:PHE:O	2.21	0.41
29:3:48:ARG:HG2	29:3:48:ARG:HH11	1.85	0.41
31:a:69:G:C2	31:a:70:A:H1'	2.56	0.41
31:a:418:G:H2'	31:a:437:U:C4	2.56	0.41
31:a:484:A:O2'	31:a:485:U:H6	2.04	0.41
31:a:602:U:H2'	31:a:603:A:C8	2.55	0.41
31:a:612:G:O6	31:a:643:A:N6	2.54	0.41
31:a:887:U:H2'	31:a:888:C:C6	2.55	0.41
31:a:1183:C:H2'	31:a:1184:G:C8	2.56	0.41
31:a:1270:G:OP1	31:a:1294:C:H4'	2.21	0.41
31:a:1319:G:OP2	43:m:98:ARG:NH2	2.54	0.41
31:a:1489:A:H2'	31:a:1490:A:C8	2.56	0.41
31:a:1527:G:C6	31:a:1531:G:C6	3.08	0.41
42:l:33:LYS:HD3	42:l:33:LYS:HA	1.77	0.41
1:A:27:G:H22	1:A:557:G:H1'	1.84	0.41
1:A:310:C:O2'	1:A:311:U:H2'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:C:H2'	1:A:399:U:O4'	2.20	0.41
1:A:422:G:H2'	1:A:423:A:H8	1.86	0.41
1:A:774:G:O4'	3:C:207:LYS:NZ	2.53	0.41
1:A:1326:C:H2'	1:A:1327:C:H6	1.86	0.41
1:A:1712:A:N3	1:A:1714:C:C4	2.89	0.41
1:A:1747:G:O2'	31:a:1439:C:H4'	2.21	0.41
1:A:1989:C:H4'	1:A:1990:C:C5	2.56	0.41
1:A:2330:G:H4'	6:F:123:ASP:HA	2.02	0.41
1:A:2553:G:C2	1:A:2554:C:H1'	2.56	0.41
1:A:2617:A:H2'	1:A:2618:C:C6	2.56	0.41
1:A:2677:C:H2'	1:A:2678:C:C6	2.56	0.41
1:A:2727:G:H2'	1:A:2728:U:H6	1.86	0.41
1:A:2851:G:H1'	1:A:2903:A:H2'	2.02	0.41
3:C:6:TYR:CD2	3:C:16:MET:HG2	2.56	0.41
3:C:39:LYS:HB2	3:C:39:LYS:HE2	1.67	0.41
4:D:15:VAL:HG23	4:D:23:ILE:HB	2.03	0.41
4:D:40:THR:OG1	4:D:43:VAL:HB	2.21	0.41
7:G:10:ASP:OD1	7:G:69:ARG:CZ	2.68	0.41
7:G:30:LYS:HE3	7:G:81:GLN:C	2.46	0.41
8:H:69:LYS:HE2	8:H:69:LYS:HB3	1.83	0.41
9:I:71:ARG:NH1	14:N:74:ARG:NE	2.69	0.41
13:M:92:ILE:HD12	13:M:93:VAL:N	2.36	0.41
14:N:93:LYS:O	14:N:93:LYS:HG2	2.20	0.41
29:3:39:LYS:NZ	29:3:43:GLN:HE22	2.19	0.41
31:a:178:G:C2	31:a:179:A:C8	3.08	0.41
31:a:432:G:C2	31:a:433:A:C5	3.09	0.41
31:a:476:C:H2'	31:a:477:U:H6	1.86	0.41
31:a:642:C:H2'	31:a:643:A:H8	1.86	0.41
31:a:642:C:H2'	31:a:643:A:C8	2.56	0.41
31:a:663:A:H2'	31:a:664:G:O4'	2.21	0.41
31:a:665:U:C2	31:a:666:G:C8	3.09	0.41
31:a:736:A:N7	45:o:54:ARG:HD2	2.36	0.41
31:a:1081:U:H2'	31:a:1082:C:H6	1.85	0.41
31:a:1084:U:C2	31:a:1085:G:C8	3.09	0.41
31:a:1122:A:N1	33:c:176:THR:HG22	2.36	0.41
31:a:1235:A:OP1	43:m:101:LYS:HA	2.21	0.41
31:a:1497:G:H2'	31:a:1498:G:C8	2.55	0.41
36:f:62:ILE:HG12	48:r:29:LYS:NZ	2.35	0.41
47:q:19:MET:H	47:q:19:MET:HG2	1.72	0.41
47:q:48:THR:HG21	47:q:63:ILE:HG13	2.02	0.41
49:s:3:ARG:HH21	49:s:7:LYS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:4:SER:HB2	49:s:7:LYS:HE3	2.03	0.41
1:A:409:G:H3'	1:A:410:G:H8	1.85	0.41
1:A:1088:C:H5'	1:A:1092:A:H1'	2.02	0.41
1:A:1358:A:H3'	1:A:1359:A:H8	1.86	0.41
1:A:1539:A:H2'	1:A:1541:C:C5	2.56	0.41
1:A:1708:A:N3	1:A:1709:A:C8	2.88	0.41
1:A:2074:C:H2'	1:A:2075:G:H8	1.86	0.41
1:A:2115:A:H2'	1:A:2116:U:O4'	2.21	0.41
1:A:2544:C:C2	1:A:2569:A:N6	2.89	0.41
2:B:39:G:H8	2:B:40:C:H3'	1.86	0.41
3:C:100:GLU:HG3	3:C:101:LYS:N	2.35	0.41
3:C:143:ASN:ND2	3:C:152:GLY:HA3	2.36	0.41
3:C:159:GLY:H	3:C:195:VAL:HG23	1.86	0.41
4:D:133:ARG:HG3	4:D:173:MET:HG3	2.03	0.41
6:F:63:GLN:HG3	25:Y:6:HIS:HB2	2.03	0.41
7:G:19:PHE:CD1	7:G:45:GLN:NE2	2.89	0.41
8:H:95:ARG:CG	8:H:96:THR:HG23	2.51	0.41
12:L:102:ARG:NH2	12:L:122:VAL:HG23	2.35	0.41
20:T:49:ILE:O	20:T:53:ARG:HG2	2.21	0.41
31:a:203:A:C4	31:a:204:A:C8	3.08	0.41
31:a:283:G:C2	31:a:284:G:C8	3.09	0.41
31:a:623:C:H2'	31:a:624:G:H8	1.86	0.41
31:a:833:G:O6	31:a:885:A:N6	2.54	0.41
31:a:885:A:H2'	31:a:886:C:C6	2.56	0.41
31:a:1384:A:H2'	31:a:1384:A:N3	2.36	0.41
32:b:30:TYR:HE2	32:b:199:VAL:HG11	1.84	0.41
36:f:7:MET:HG2	48:r:70:MET:HE2	2.01	0.41
49:s:56:LYS:HD2	49:s:56:LYS:HA	1.82	0.41
1:A:512:A:H5''	1:A:512:A:C8	2.55	0.40
1:A:2041:A:H2'	1:A:2042:A:C8	2.56	0.40
1:A:2590:U:C2	1:A:2592:A:OP2	2.74	0.40
1:A:2725:U:C2	1:A:2726:C:C5	3.09	0.40
6:F:142:ASP:HB3	6:F:144:ASP:H	1.86	0.40
8:H:107:LYS:NZ	8:H:120:GLY:O	2.55	0.40
9:I:13:ASN:HD21	9:I:96:THR:H	1.69	0.40
17:Q:39:THR:OG1	26:Z:25:PRO:HG3	2.21	0.40
31:a:369:G:H2'	31:a:370:G:O4'	2.20	0.40
31:a:776:A:C4	31:a:777:G:C8	3.09	0.40
31:a:992:A:H2	31:a:993:C:C6	2.40	0.40
31:a:1185:G:N3	31:a:1186:A:C8	2.89	0.40
31:a:1216:G:C5	31:a:1217:C:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1535:C:C2	31:a:1536:G:C8	3.09	0.40
31:a:1535:C:C2	31:a:1536:G:N7	2.89	0.40
31:a:1547:C:H6	31:a:1547:C:H2'	1.66	0.40
32:b:54:TYR:CE1	32:b:220:ALA:HA	2.56	0.40
32:b:176:ALA:HB3	32:b:183:ILE:HD11	2.02	0.40
45:o:75:ILE:HG22	45:o:79:ARG:HE	1.85	0.40
1:A:4:U:H2'	1:A:5:A:C8	2.56	0.40
1:A:660:A:H8	5:E:182:ASN:HB3	1.85	0.40
1:A:2652:G:H2'	1:A:2653:C:O4'	2.20	0.40
1:A:2736:G:C6	1:A:2737:C:C4	3.09	0.40
5:E:34:PHE:CD1	10:J:6:LEU:HD13	2.56	0.40
5:E:146:LEU:O	5:E:147:GLU:HG3	2.21	0.40
6:F:152:MET:H	6:F:152:MET:HG3	1.63	0.40
14:N:31:HIS:CD2	14:N:85:LYS:HG2	2.56	0.40
17:Q:9:THR:HG23	17:Q:80:PRO:HD2	2.03	0.40
31:a:75:A:N6	31:a:94:G:O2'	2.34	0.40
31:a:869:A:H3'	31:a:870:G:H8	1.87	0.40
32:b:116:GLU:O	32:b:119:LYS:HB3	2.21	0.40
40:j:18:ILE:HD12	40:j:18:ILE:HA	1.82	0.40
1:A:851:C:C2	1:A:852:U:C5	3.09	0.40
1:A:2091:C:H2'	1:A:2092:C:C6	2.56	0.40
1:A:2319:U:O2'	1:A:2320:C:H5'	2.21	0.40
2:B:46:A:H2'	2:B:47:C:O4'	2.21	0.40
7:G:160:LYS:HB3	7:G:160:LYS:HE2	1.70	0.40
8:H:92:GLU:OE2	8:H:95:ARG:NH1	2.54	0.40
10:J:93:PRO:HD3	10:J:124:LYS:O	2.22	0.40
11:K:54:MET:HE2	11:K:54:MET:HB2	1.82	0.40
12:L:92:ARG:CG	12:L:93:TYR:CE1	3.01	0.40
18:R:6:ILE:HD11	18:R:41:ALA:CB	2.51	0.40
19:S:5:LYS:O	19:S:5:LYS:HG3	2.15	0.40
31:a:269:U:H2'	31:a:271:A:OP2	2.21	0.40
31:a:1131:C:H2'	31:a:1132:U:C6	2.57	0.40
31:a:1261:A:H2'	31:a:1262:A:H8	1.84	0.40
31:a:1384:A:O2'	31:a:1385:A:H5'	2.22	0.40
43:m:79:ARG:O	43:m:83:ILE:HG13	2.20	0.40
1:A:421:C:H2'	1:A:422:G:H8	1.86	0.40
1:A:650:U:H5	1:A:664:G:C5	2.39	0.40
1:A:1723:A:H2	1:A:1791:G:O4'	2.04	0.40
1:A:2136:U:H5'	1:A:2169:G:H21	1.87	0.40
1:A:2257:G:H1'	22:V:32:ASN:HA	2.04	0.40
1:A:2564:U:H2'	1:A:2565:C:H6	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2689:A:C4	1:A:2690:G:H1'	2.57	0.40
2:B:74:G:H5''	20:T:18:LEU:HD11	2.03	0.40
6:F:36:VAL:HG12	6:F:36:VAL:O	2.21	0.40
13:M:72:LEU:HD23	13:M:75:LYS:HG3	2.04	0.40
17:Q:111:LYS:HB3	17:Q:111:LYS:HE3	1.66	0.40
31:a:200:U:O2'	31:a:201:U:O5'	2.34	0.40
31:a:240:A:H2'	31:a:241:U:C6	2.57	0.40
31:a:457:A:H2'	31:a:458:G:O4'	2.22	0.40
31:a:838:G:H2'	31:a:839:U:O4'	2.21	0.40
31:a:1067:U:H2'	31:a:1068:G:C8	2.50	0.40
31:a:1185:G:H2'	31:a:1186:A:H8	1.87	0.40
31:a:1474:C:O2'	31:a:1475:G:H8	2.04	0.40
33:c:108:VAL:HG13	33:c:114:LEU:HD13	2.04	0.40
36:f:4:TYR:HB2	36:f:65:VAL:HG22	2.02	0.40
39:i:20:ARG:O	39:i:67:VAL:HA	2.22	0.40
45:o:29:ILE:O	45:o:33:THR:OG1	2.38	0.40
1:A:984:G:H2'	1:A:985:A:O4'	2.21	0.40
1:A:2434:A:N3	1:A:2434:A:H2'	2.37	0.40
4:D:37:GLN:OE1	4:D:76:HIS:CE1	2.66	0.40
6:F:109:PRO:HA	25:Y:50:ILE:HG12	2.02	0.40
9:I:19:VAL:HG23	9:I:42:THR:C	2.46	0.40
12:L:99:GLY:O	12:L:100:TYR:HB2	2.21	0.40
12:L:100:TYR:C	12:L:122:VAL:HG12	2.47	0.40
17:Q:14:PRO:HG3	17:Q:78:GLU:HG3	2.03	0.40
17:Q:17:VAL:HG12	17:Q:43:SER:HB3	2.03	0.40
18:R:52:SER:OG	18:R:81:THR:HG21	2.21	0.40
19:S:87:ASP:C	19:S:89:LYS:HD2	2.46	0.40
29:3:4:MET:HE1	29:3:60:GLN:OE1	2.22	0.40
31:a:578:G:H2'	31:a:579:U:C6	2.57	0.40
31:a:618:G:C5	31:a:619:C:C5	3.10	0.40
31:a:623:C:H2'	31:a:624:G:C8	2.57	0.40
31:a:696:G:O5'	41:k:49:ALA:HA	2.22	0.40
31:a:1004:C:N3	31:a:1005:A:C2	2.90	0.40
31:a:1023:A:C8	31:a:1229:U:H1'	2.56	0.40
31:a:1141:A:H2'	31:a:1142:U:C6	2.56	0.40
32:b:24:ASN:HD21	32:b:26:LYS:HD3	1.86	0.40
32:b:31:ILE:HD12	32:b:39:TYR:HB3	2.04	0.40
37:g:122:ASN:O	37:g:125:LEU:HG	2.21	0.40
40:j:80:THR:O	40:j:83:THR:OG1	2.35	0.40
49:s:3:ARG:HH21	49:s:7:LYS:CD	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	272/274 (99%)	245 (90%)	26 (10%)	1 (0%)	30	61
4	D	213/215 (99%)	200 (94%)	13 (6%)	0	100	100
5	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
6	F	173/175 (99%)	144 (83%)	28 (16%)	1 (1%)	21	54
7	G	173/175 (99%)	157 (91%)	16 (9%)	0	100	100
8	H	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
9	I	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	49
10	J	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
11	K	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
12	L	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
13	M	117/119 (98%)	107 (92%)	10 (8%)	0	100	100
14	N	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
15	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
16	P	100/102 (98%)	93 (93%)	5 (5%)	2 (2%)	6	32
17	Q	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
18	R	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
19	S	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
20	T	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
21	U	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
22	V	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
23	W	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
24	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
25	Y	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
26	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
27	1	45/47 (96%)	41 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
30	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
32	b	222/232 (96%)	211 (95%)	11 (5%)	0	100	100
33	c	200/217 (92%)	190 (95%)	10 (5%)	0	100	100
34	d	197/200 (98%)	187 (95%)	10 (5%)	0	100	100
35	e	154/166 (93%)	150 (97%)	4 (3%)	0	100	100
36	f	93/98 (95%)	87 (94%)	6 (6%)	0	100	100
37	g	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	h	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
39	i	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
40	j	95/102 (93%)	89 (94%)	6 (6%)	0	100	100
41	k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
42	l	133/149 (89%)	122 (92%)	10 (8%)	1 (1%)	16	49
43	m	114/121 (94%)	105 (92%)	9 (8%)	0	100	100
44	n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
45	o	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
46	p	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
47	q	78/87 (90%)	74 (95%)	4 (5%)	0	100	100
48	r	62/80 (78%)	60 (97%)	2 (3%)	0	100	100
49	s	80/108 (74%)	73 (91%)	7 (9%)	0	100	100
50	t	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
All	All	5323/5563 (96%)	4978 (94%)	339 (6%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	51	PRO
9	I	98	ILE
6	F	139	PRO
16	P	50	ALA
42	l	132	THR
3	C	271	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	220/221 (100%)	203 (92%)	17 (8%)	12	38
4	D	173/173 (100%)	156 (90%)	17 (10%)	7	31
5	E	168/168 (100%)	154 (92%)	14 (8%)	10	35
6	F	139/154 (90%)	100 (72%)	39 (28%)	0	3
7	G	123/153 (80%)	102 (83%)	21 (17%)	2	13
8	H	122/123 (99%)	109 (89%)	13 (11%)	6	28
9	I	100/100 (100%)	91 (91%)	9 (9%)	9	33
10	J	109/112 (97%)	99 (91%)	10 (9%)	8	33
11	K	108/114 (95%)	94 (87%)	14 (13%)	4	21
12	L	96/101 (95%)	96 (100%)	0	100	100
13	M	86/95 (90%)	74 (86%)	12 (14%)	3	19
14	N	93/100 (93%)	74 (80%)	19 (20%)	1	8
15	O	96/96 (100%)	91 (95%)	5 (5%)	21	48
16	P	84/86 (98%)	80 (95%)	4 (5%)	23	50
17	Q	89/94 (95%)	78 (88%)	11 (12%)	4	23
18	R	78/80 (98%)	67 (86%)	11 (14%)	3	19
19	S	81/88 (92%)	74 (91%)	7 (9%)	10	34
20	T	75/82 (92%)	65 (87%)	10 (13%)	4	21
21	U	60/64 (94%)	52 (87%)	8 (13%)	4	21
22	V	44/49 (90%)	38 (86%)	6 (14%)	3	20
23	W	58/60 (97%)	43 (74%)	15 (26%)	0	4
24	X	52/52 (100%)	47 (90%)	5 (10%)	8	32
25	Y	21/56 (38%)	17 (81%)	4 (19%)	1	9
26	Z	36/44 (82%)	36 (100%)	0	100	100
27	1	44/45 (98%)	34 (77%)	10 (23%)	1	6
28	2	39/39 (100%)	38 (97%)	1 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	3	55/55 (100%)	51 (93%)	4 (7%)	13	40
30	4	35/35 (100%)	31 (89%)	4 (11%)	5	26
32	b	194/201 (96%)	192 (99%)	2 (1%)	68	75
33	c	164/175 (94%)	163 (99%)	1 (1%)	78	79
34	d	174/175 (99%)	172 (99%)	2 (1%)	65	74
35	e	122/131 (93%)	117 (96%)	5 (4%)	27	53
36	f	83/86 (96%)	81 (98%)	2 (2%)	43	63
37	g	131/132 (99%)	122 (93%)	9 (7%)	14	41
38	h	112/113 (99%)	110 (98%)	2 (2%)	51	68
39	i	105/107 (98%)	102 (97%)	3 (3%)	37	60
40	j	87/91 (96%)	84 (97%)	3 (3%)	32	57
41	k	90/104 (86%)	88 (98%)	2 (2%)	45	65
42	l	117/130 (90%)	111 (95%)	6 (5%)	21	49
43	m	100/104 (96%)	98 (98%)	2 (2%)	48	66
44	n	52/53 (98%)	52 (100%)	0	100	100
45	o	79/81 (98%)	78 (99%)	1 (1%)	61	72
46	p	74/77 (96%)	72 (97%)	2 (3%)	39	61
47	q	75/82 (92%)	68 (91%)	7 (9%)	8	32
48	r	57/68 (84%)	55 (96%)	2 (4%)	32	57
49	s	71/91 (78%)	70 (99%)	1 (1%)	59	71
50	t	67/69 (97%)	67 (100%)	0	100	100
All	All	4438/4709 (94%)	4096 (92%)	342 (8%)	14	38

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	ILE
3	C	4	LYS
3	C	24	ILE
3	C	64	VAL
3	C	65	ILE
3	C	68	LYS
3	C	71	LYS
3	C	87	ARG
3	C	115	ILE

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Mol	Chain	Res	Type
3	C	116	VAL
3	C	123	ASP
3	C	125	LYS
3	C	144	ILE
3	C	243	ARG
3	C	245	SER
3	C	270	ILE
3	C	272	ARG
4	D	13	THR
4	D	18	GLU
4	D	21	GLU
4	D	22	LEU
4	D	27	VAL
4	D	54	GLU
4	D	100	GLU
4	D	106	SER
4	D	107	VAL
4	D	108	ASP
4	D	131	ILE
4	D	137	SER
4	D	158	SER
4	D	168	LYS
4	D	193	LYS
4	D	200	ASN
4	D	205	LYS
5	E	9	LEU
5	E	10	ASP
5	E	16	SER
5	E	17	ILE
5	E	46	GLN
5	E	74	ARG
5	E	84	ARG
5	E	117	LYS
5	E	130	ASN
5	E	137	LYS
5	E	140	LYS
5	E	143	LEU
5	E	161	VAL
5	E	176	THR
6	F	5	LYS
6	F	6	GLU
6	F	16	LEU

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Mol	Chain	Res	Type
6	F	17	MET
6	F	23	SER
6	F	24	SER
6	F	25	VAL
6	F	27	GLU
6	F	28	VAL
6	F	44	VAL
6	F	51	ASP
6	F	54	VAL
6	F	56	GLU
6	F	59	LEU
6	F	60	ILE
6	F	64	LYS
6	F	66	LEU
6	F	67	VAL
6	F	78	ARG
6	F	85	ILE
6	F	88	LYS
6	F	106	VAL
6	F	110	ARG
6	F	120	LYS
6	F	128	TYR
6	F	132	VAL
6	F	133	LYS
6	F	135	GLN
6	F	136	LEU
6	F	138	PHE
6	F	143	TYR
6	F	148	LYS
6	F	149	VAL
6	F	150	ARG
6	F	152	MET
6	F	154	ILE
6	F	156	ILE
6	F	168	GLU
6	F	170	LEU
7	G	25	THR
7	G	39	GLU
7	G	42	THR
7	G	49	THR
7	G	53	VAL
7	G	57	ASP

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Mol	Chain	Res	Type
7	G	58	SER
7	G	59	LYS
7	G	68	THR
7	G	79	VAL
7	G	81	GLN
7	G	84	VAL
7	G	98	MET
7	G	99	GLN
7	G	107	VAL
7	G	109	TYR
7	G	113	VAL
7	G	121	ILE
7	G	122	THR
7	G	124	SER
7	G	175	LYS
8	H	18	VAL
8	H	19	ILE
8	H	20	ASP
8	H	24	GLN
8	H	25	THR
8	H	36	ILE
8	H	58	ILE
8	H	63	ILE
8	H	86	LYS
8	H	125	VAL
8	H	139	GLU
8	H	140	ASN
8	H	143	LEU
9	I	14	SER
9	I	64	ARG
9	I	66	LYS
9	I	67	SER
9	I	69	VAL
9	I	94	ARG
9	I	98	ILE
9	I	102	VAL
9	I	122	LEU
10	J	91	VAL
10	J	92	THR
10	J	95	LEU
10	J	97	VAL
10	J	101	VAL

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Mol	Chain	Res	Type
10	J	102	VAL
10	J	103	LYS
10	J	104	ASN
10	J	106	LYS
10	J	131	SER
11	K	1	MET
11	K	2	LEU
11	K	3	LEU
11	K	7	VAL
11	K	18	THR
11	K	42	ILE
11	K	44	SER
11	K	45	ARG
11	K	47	ILE
11	K	54	MET
11	K	72	THR
11	K	102	ILE
11	K	103	LEU
11	K	130	LYS
13	M	6	ASP
13	M	9	LYS
13	M	11	ARG
13	M	13	LYS
13	M	33	VAL
13	M	45	ILE
13	M	58	SER
13	M	66	THR
13	M	74	THR
13	M	93	VAL
13	M	113	ARG
13	M	114	GLU
14	N	5	LYS
14	N	7	ILE
14	N	10	VAL
14	N	12	LYS
14	N	14	GLN
14	N	17	THR
14	N	27	THR
14	N	28	LEU
14	N	32	VAL
14	N	34	ILE
14	N	35	ILE

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Mol	Chain	Res	Type
14	N	41	ARG
14	N	57	VAL
14	N	63	VAL
14	N	65	LYS
14	N	78	LEU
14	N	82	LYS
14	N	85	LYS
14	N	87	GLU
15	O	8	THR
15	O	9	VAL
15	O	89	ASP
15	O	90	ILE
15	O	117	LEU
16	P	1	MET
16	P	47	LYS
16	P	53	VAL
16	P	83	LYS
17	Q	1	MET
17	Q	9	THR
17	Q	38	LEU
17	Q	43	SER
17	Q	51	LEU
17	Q	52	MET
17	Q	65	ASN
17	Q	67	ASP
17	Q	70	VAL
17	Q	81	THR
17	Q	111	LYS
18	R	13	THR
18	R	14	GLU
18	R	36	THR
18	R	63	LYS
18	R	65	MET
18	R	75	ARG
18	R	77	LYS
18	R	83	LYS
18	R	84	GLU
18	R	89	LEU
18	R	90	PHE
19	S	29	LYS
19	S	30	LYS
19	S	31	ASP

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Mol	Chain	Res	Type
19	S	34	VAL
19	S	35	VAL
19	S	38	VAL
19	S	77	GLU
20	T	7	ILE
20	T	8	ILE
20	T	9	ARG
20	T	21	LEU
20	T	22	ARG
20	T	23	LYS
20	T	24	SER
20	T	27	VAL
20	T	46	VAL
20	T	77	TYR
21	U	12	LYS
21	U	45	LEU
21	U	53	ILE
21	U	57	GLU
21	U	75	VAL
21	U	82	ARG
21	U	83	ASP
21	U	84	LYS
22	V	7	VAL
22	V	11	LYS
22	V	40	VAL
22	V	50	SER
22	V	52	ARG
22	V	58	LYS
23	W	10	THR
23	W	12	SER
23	W	15	GLU
23	W	16	GLU
23	W	17	GLN
23	W	19	LYS
23	W	22	LYS
23	W	29	ARG
23	W	30	PHE
23	W	34	THR
23	W	36	GLN
23	W	39	GLU
23	W	43	ILE
23	W	62	ILE

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Mol	Chain	Res	Type
23	W	65	SER
24	X	5	GLN
24	X	6	ILE
24	X	7	THR
24	X	10	ARG
24	X	18	THR
25	Y	3	GLN
25	Y	5	ILE
25	Y	8	GLU
25	Y	10	HIS
27	1	5	VAL
27	1	12	CYS
27	1	18	ILE
27	1	23	LYS
27	1	29	ARG
27	1	31	GLU
27	1	32	MET
27	1	40	ASN
27	1	41	LYS
27	1	48	THR
28	2	2	VAL
29	3	52	LYS
29	3	53	SER
29	3	56	LYS
29	3	62	LEU
30	4	3	VAL
30	4	8	LYS
30	4	12	GLU
30	4	15	LYS
32	b	6	MET
32	b	43	LEU
33	c	78	LYS
34	d	3	ARG
34	d	71	THR
35	e	10	GLU
35	e	12	GLU
35	e	70	ASP
35	e	152	ASP
35	e	164	LEU
36	f	17	ASP
36	f	81	LYS
37	g	9	LYS

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Mol	Chain	Res	Type
37	g	10	ARG
37	g	12	VAL
37	g	13	LEU
37	g	32	LEU
37	g	35	LYS
37	g	66	ILE
37	g	72	VAL
37	g	73	LEU
38	h	35	GLU
38	h	68	GLN
39	i	18	VAL
39	i	60	LYS
39	i	96	TYR
40	j	10	LEU
40	j	31	ARG
40	j	92	LEU
41	k	125	LYS
41	k	126	ARG
42	l	89	GLU
42	l	102	ASP
42	l	115	LEU
42	l	129	LEU
42	l	132	THR
42	l	133	LYS
43	m	27	THR
43	m	34	LEU
45	o	74	ASP
46	p	43	THR
46	p	81	MET
47	q	40	VAL
47	q	41	LYS
47	q	44	LYS
47	q	48	THR
47	q	63	ILE
47	q	69	LEU
47	q	84	SER
48	r	17	TYR
48	r	25	HIS
49	s	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	15	ASN
3	C	61	GLN
3	C	75	ASN
3	C	86	ASN
3	C	133	GLN
3	C	134	ASN
3	C	143	ASN
3	C	163	GLN
3	C	230	HIS
3	C	232	HIS
4	D	47	ASN
4	D	148	HIS
4	D	182	ASN
5	E	29	ASN
5	E	46	GLN
6	F	21	ASN
6	F	46	ASN
6	F	161	ASN
7	G	38	ASN
7	G	74	ASN
7	G	97	GLN
7	G	128	ASN
8	H	3	GLN
8	H	81	HIS
8	H	131	HIS
8	H	136	GLN
10	J	81	GLN
10	J	83	ASN
10	J	126	HIS
11	K	12	GLN
11	K	46	GLN
11	K	123	HIS
12	L	12	GLN
12	L	73	ASN
12	L	106	GLN
13	M	15	HIS
13	M	37	ASN
13	M	39	HIS
13	M	48	ASN
14	N	3	ASN
14	N	14	GLN
14	N	43	GLN
15	O	66	ASN

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Mol	Chain	Res	Type
15	O	72	HIS
16	P	18	GLN
17	Q	40	ASN
17	Q	57	ASN
18	R	37	GLN
18	R	54	ASN
19	S	44	HIS
20	T	20	GLN
20	T	38	ASN
20	T	88	HIS
27	1	4	ASN
27	1	16	ASN
27	1	22	ASN
27	1	25	ASN
27	1	26	ASN
27	1	40	ASN
27	1	45	HIS
28	2	7	GLN
28	2	17	HIS
29	3	7	HIS
29	3	35	ASN
29	3	43	GLN
32	b	15	HIS
32	b	75	GLN
32	b	77	GLN
33	c	88	ASN
33	c	185	HIS
34	d	85	ASN
34	d	146	GLN
37	g	28	ASN
37	g	122	ASN
37	g	130	ASN
37	g	148	ASN
38	h	68	GLN
39	i	77	GLN
41	k	119	ASN
42	l	39	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2921 (98%)	951 (33%)	78 (2%)
2	B	114/115 (99%)	46 (40%)	4 (3%)
31	a	1470/1548 (94%)	382 (25%)	0
All	All	4463/4584 (97%)	1379 (30%)	82 (1%)

All (1379) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	13	A
1	A	18	C
1	A	19	G
1	A	23	G
1	A	24	G
1	A	28	A
1	A	29	U
1	A	34	U
1	A	36	G
1	A	39	C
1	A	43	A
1	A	46	C
1	A	47	C
1	A	50	U
1	A	51	G
1	A	54	G
1	A	55	G
1	A	58	G
1	A	62	C
1	A	63	U
1	A	64	A
1	A	66	C
1	A	70	G
1	A	71	A
1	A	74	U
1	A	75	G
1	A	80	G
1	A	83	G
1	A	84	A
1	A	88	G
1	A	90	A
1	A	91	A

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Mol	Chain	Res	Type
1	A	92	G
1	A	93	U
1	A	94	A
1	A	96	G
1	A	100	U
1	A	101	G
1	A	102	A
1	A	103	U
1	A	104	C
1	A	105	C
1	A	106	A
1	A	117	A
1	A	118	A
1	A	119	U
1	A	122	G
1	A	124	A
1	A	125	A
1	A	135	G
1	A	140	A
1	A	153	G
1	A	158	G
1	A	162	A
1	A	163	U
1	A	164	A
1	A	165	C
1	A	166	A
1	A	167	U
1	A	169	G
1	A	170	C
1	A	171	A
1	A	173	A
1	A	176	A
1	A	177	G
1	A	179	A
1	A	180	G
1	A	183	A
1	A	184	C
1	A	185	A
1	A	199	A
1	A	200	A
1	A	202	A
1	A	203	U

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Mol	Chain	Res	Type
1	A	209	U
1	A	213	C
1	A	215	G
1	A	216	A
1	A	218	G
1	A	219	A
1	A	224	A
1	A	225	A
1	A	226	A
1	A	231	A
1	A	232	U
1	A	234	C
1	A	235	G
1	A	236	A
1	A	242	U
1	A	244	A
1	A	248	G
1	A	251	G
1	A	255	G
1	A	268	A
1	A	269	G
1	A	272	C
1	A	275	A
1	A	278	A
1	A	280	C
1	A	281	A
1	A	282	A
1	A	284	C
1	A	286	U
1	A	287	G
1	A	288	C
1	A	289	U
1	A	290	U
1	A	292	U
1	A	293	U
1	A	294	G
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	303	G
1	A	305	A

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Mol	Chain	Res	Type
1	A	309	U
1	A	310	C
1	A	311	U
1	A	312	A
1	A	318	A
1	A	321	U
1	A	324	A
1	A	326	A
1	A	327	G
1	A	328	G
1	A	329	A
1	A	333	C
1	A	335	U
1	A	336	U
1	A	353	A
1	A	354	A
1	A	360	A
1	A	372	A
1	A	388	A
1	A	390	A
1	A	392	U
1	A	393	G
1	A	397	U
1	A	399	U
1	A	401	U
1	A	403	U
1	A	404	U
1	A	405	G
1	A	406	A
1	A	411	A
1	A	417	A
1	A	432	G
1	A	434	G
1	A	440	C
1	A	447	A
1	A	448	A
1	A	449	U
1	A	451	U
1	A	452	G
1	A	459	C
1	A	460	C
1	A	461	A

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Mol	Chain	Res	Type
1	A	463	C
1	A	468	A
1	A	482	U
1	A	489	A
1	A	490	C
1	A	492	G
1	A	497	U
1	A	502	C
1	A	503	A
1	A	506	A
1	A	507	C
1	A	511	G
1	A	512	A
1	A	513	G
1	A	520	G
1	A	521	U
1	A	523	A
1	A	525	A
1	A	527	G
1	A	529	A
1	A	530	C
1	A	537	A
1	A	540	G
1	A	548	A
1	A	549	U
1	A	550	A
1	A	553	A
1	A	554	C
1	A	565	G
1	A	566	U
1	A	567	G
1	A	572	C
1	A	574	A
1	A	575	G
1	A	576	U
1	A	577	A
1	A	578	G
1	A	581	A
1	A	583	A
1	A	591	A
1	A	592	A
1	A	606	G

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Mol	Chain	Res	Type
1	A	608	C
1	A	616	G
1	A	617	A
1	A	618	A
1	A	619	U
1	A	621	A
1	A	623	C
1	A	629	A
1	A	630	G
1	A	644	C
1	A	645	A
1	A	646	A
1	A	647	G
1	A	659	A
1	A	661	U
1	A	666	A
1	A	672	A
1	A	673	G
1	A	676	A
1	A	679	G
1	A	682	A
1	A	690	U
1	A	691	A
1	A	696	G
1	A	698	U
1	A	699	U
1	A	700	A
1	A	715	A
1	A	716	C
1	A	720	A
1	A	722	A
1	A	731	U
1	A	746	G
1	A	749	G
1	A	775	A
1	A	792	5MU
1	A	797	A
1	A	802	G
1	A	805	G
1	A	809	A
1	A	810	A
1	A	815	G

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Mol	Chain	Res	Type
1	A	816	G
1	A	820	G
1	A	821	C
1	A	822	G
1	A	827	A
1	A	828	A
1	A	829	U
1	A	830	U
1	A	834	A
1	A	835	U
1	A	837	G
1	A	838	A
1	A	850	G
1	A	856	U
1	A	857	C
1	A	868	A
1	A	872	U
1	A	873	U
1	A	890	G
1	A	891	A
1	A	899	U
1	A	904	G
1	A	911	A
1	A	917	U
1	A	922	G
1	A	925	G
1	A	926	G
1	A	927	G
1	A	928	C
1	A	938	G
1	A	939	U
1	A	940	U
1	A	942	C
1	A	943	C
1	A	944	G
1	A	945	A
1	A	951	G
1	A	952	A
1	A	955	A
1	A	957	C
1	A	960	C
1	A	964	U

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Mol	Chain	Res	Type
1	A	965	G
1	A	970	U
1	A	971	U
1	A	973	A
1	A	975	U
1	A	977	A
1	A	985	A
1	A	989	A
1	A	990	G
1	A	992	A
1	A	993	C
1	A	1003	A
1	A	1005	G
1	A	1012	G
1	A	1017	A
1	A	1018	A
1	A	1019	A
1	A	1024	A
1	A	1027	A
1	A	1028	G
1	A	1029	C
1	A	1033	G
1	A	1034	A
1	A	1035	C
1	A	1037	A
1	A	1040	A
1	A	1043	U
1	A	1046	G
1	A	1047	G
1	A	1056	U
1	A	1057	A
1	A	1061	G
1	A	1063	U
1	A	1064	A
1	A	1066	G
1	A	1070	A
1	A	1071	A
1	A	1077	U
1	A	1083	G
1	A	1086	G
1	A	1089	C
1	A	1090	A

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Mol	Chain	Res	Type
1	A	1091	G
1	A	1092	A
1	A	1093	C
1	A	1094	A
1	A	1095	A
1	A	1096	C
1	A	1097	U
1	A	1098	A
1	A	1100	G
1	A	1101	A
1	A	1105	U
1	A	1106	G
1	A	1109	U
1	A	1111	A
1	A	1113	A
1	A	1114	A
1	A	1115	G
1	A	1116	C
1	A	1117	A
1	A	1118	G
1	A	1119	C
1	A	1120	C
1	A	1125	U
1	A	1126	U
1	A	1127	U
1	A	1130	A
1	A	1131	G
1	A	1132	A
1	A	1133	G
1	A	1135	G
1	A	1138	U
1	A	1143	G
1	A	1145	U
1	A	1147	A
1	A	1148	C
1	A	1149	U
1	A	1151	G
1	A	1153	C
1	A	1154	G
1	A	1155	A
1	A	1156	G
1	A	1157	U

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Mol	Chain	Res	Type
1	A	1159	A
1	A	1160	C
1	A	1163	U
1	A	1166	G
1	A	1174	U
1	A	1175	G
1	A	1176	U
1	A	1177	A
1	A	1179	C
1	A	1180	G
1	A	1183	G
1	A	1185	U
1	A	1186	A
1	A	1192	A
1	A	1200	A
1	A	1201	G
1	A	1208	A
1	A	1215	U
1	A	1217	U
1	A	1220	A
1	A	1225	G
1	A	1234	G
1	A	1245	G
1	A	1258	A
1	A	1265	G
1	A	1273	G
1	A	1274	G
1	A	1275	A
1	A	1276	G
1	A	1284	A
1	A	1286	G
1	A	1287	U
1	A	1290	G
1	A	1291	A
1	A	1294	G
1	A	1304	G
1	A	1309	G
1	A	1310	A
1	A	1312	A
1	A	1337	A
1	A	1338	U
1	A	1339	U

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Mol	Chain	Res	Type
1	A	1340	G
1	A	1341	A
1	A	1342	C
1	A	1344	A
1	A	1348	U
1	A	1349	U
1	A	1357	G
1	A	1358	A
1	A	1360	G
1	A	1361	G
1	A	1362	C
1	A	1366	U
1	A	1370	C
1	A	1378	U
1	A	1384	G
1	A	1387	C
1	A	1396	A
1	A	1397	G
1	A	1402	A
1	A	1405	G
1	A	1415	A
1	A	1416	U
1	A	1421	A
1	A	1422	A
1	A	1432	A
1	A	1433	U
1	A	1434	U
1	A	1440	A
1	A	1443	A
1	A	1450	A
1	A	1451	U
1	A	1454	U
1	A	1455	U
1	A	1457	U
1	A	1458	A
1	A	1459	A
1	A	1460	U
1	A	1462	G
1	A	1463	A
1	A	1464	U
1	A	1465	G
1	A	1471	A

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Mol	Chain	Res	Type
1	A	1472	C
1	A	1476	G
1	A	1477	U
1	A	1478	A
1	A	1479	G
1	A	1481	A
1	A	1482	U
1	A	1484	G
1	A	1487	G
1	A	1488	A
1	A	1489	A
1	A	1490	G
1	A	1493	U
1	A	1494	G
1	A	1497	A
1	A	1498	U
1	A	1499	U
1	A	1500	G
1	A	1504	U
1	A	1505	G
1	A	1506	C
1	A	1507	A
1	A	1508	C
1	A	1509	G
1	A	1511	C
1	A	1512	U
1	A	1513	A
1	A	1517	A
1	A	1522	G
1	A	1523	G
1	A	1524	C
1	A	1525	U
1	A	1526	G
1	A	1528	G
1	A	1532	U
1	A	1538	A
1	A	1539	A
1	A	1540	U
1	A	1542	C
1	A	1550	G
1	A	1551	U
1	A	1552	U

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Mol	Chain	Res	Type
1	A	1553	A
1	A	1554	A
1	A	1555	G
1	A	1556	G
1	A	1557	C
1	A	1558	U
1	A	1560	A
1	A	1562	C
1	A	1568	U
1	A	1569	G
1	A	1571	G
1	A	1575	A
1	A	1576	A
1	A	1577	G
1	A	1578	A
1	A	1579	C
1	A	1580	A
1	A	1581	U
1	A	1582	U
1	A	1583	G
1	A	1584	U
1	A	1585	G
1	A	1586	U
1	A	1587	C
1	A	1588	U
1	A	1589	U
1	A	1590	C
1	A	1591	G
1	A	1592	A
1	A	1593	G
1	A	1594	U
1	A	1596	G
1	A	1598	U
1	A	1599	G
1	A	1602	U
1	A	1605	A
1	A	1606	C
1	A	1613	G
1	A	1616	A
1	A	1623	U
1	A	1624	C
1	A	1625	U

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Mol	Chain	Res	Type
1	A	1627	G
1	A	1628	A
1	A	1629	U
1	A	1630	A
1	A	1631	G
1	A	1632	A
1	A	1633	A
1	A	1634	A
1	A	1635	A
1	A	1636	U
1	A	1637	A
1	A	1639	G
1	A	1641	G
1	A	1651	C
1	A	1652	A
1	A	1653	A
1	A	1654	A
1	A	1656	C
1	A	1657	G
1	A	1658	A
1	A	1660	A
1	A	1661	C
1	A	1662	A
1	A	1666	A
1	A	1678	A
1	A	1679	A
1	A	1687	G
1	A	1690	A
1	A	1691	G
1	A	1692	C
1	A	1707	U
1	A	1717	G
1	A	1718	G
1	A	1719	C
1	A	1737	U
1	A	1740	G
1	A	1757	U
1	A	1758	A
1	A	1759	G
1	A	1760	G
1	A	1761	G
1	A	1762	U

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Mol	Chain	Res	Type
1	A	1763	U
1	A	1764	A
1	A	1766	C
1	A	1769	C
1	A	1770	C
1	A	1771	A
1	A	1790	G
1	A	1791	G
1	A	1796	A
1	A	1797	G
1	A	1800	A
1	A	1803	G
1	A	1805	U
1	A	1806	U
1	A	1808	U
1	A	1809	C
1	A	1811	A
1	A	1813	A
1	A	1827	C
1	A	1828	U
1	A	1829	A
1	A	1835	U
1	A	1843	U
1	A	1844	G
1	A	1856	A
1	A	1870	C
1	A	1871	U
1	A	1874	A
1	A	1876	G
1	A	1883	A
1	A	1886	A
1	A	1893	A
1	A	1894	G
1	A	1897	U
1	A	1898	C
1	A	1899	U
1	A	1903	A
1	A	1904	A
1	A	1905	G
1	A	1908	A
1	A	1909	C
1	A	1912	A

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Mol	Chain	Res	Type
1	A	1919	C
1	A	1923	A
1	A	1933	G
1	A	1934	G
1	A	1938	U
1	A	1939	A
1	A	1945	A
1	A	1946	A
1	A	1948	G
1	A	1950	U
1	A	1951	C
1	A	1954	A
1	A	1956	G
1	A	1957	G
1	A	1958	U
1	A	1964	A
1	A	1965	A
1	A	1966	5MU
1	A	1967	U
1	A	1982	U
1	A	1992	C
1	A	1994	C
1	A	1996	A
1	A	1997	A
1	A	1998	A
1	A	1999	G
1	A	2003	U
1	A	2008	A
1	A	2009	U
1	A	2018	U
1	A	2019	G
1	A	2020	U
1	A	2023	C
1	A	2024	A
1	A	2029	G
1	A	2048	G
1	A	2050	A
1	A	2057	A
1	A	2058	A
1	A	2059	G
1	A	2060	A
1	A	2061	U

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Mol	Chain	Res	Type
1	A	2062	G
1	A	2070	C
1	A	2075	G
1	A	2076	A
1	A	2078	A
1	A	2082	C
1	A	2083	G
1	A	2087	A
1	A	2088	G
1	A	2089	A
1	A	2090	C
1	A	2095	U
1	A	2096	G
1	A	2107	G
1	A	2109	A
1	A	2114	G
1	A	2117	A
1	A	2119	U
1	A	2120	G
1	A	2127	G
1	A	2128	G
1	A	2129	C
1	A	2130	A
1	A	2132	A
1	A	2133	G
1	A	2134	C
1	A	2135	U
1	A	2136	U
1	A	2137	G
1	A	2138	U
1	A	2139	A
1	A	2140	C
1	A	2143	G
1	A	2144	A
1	A	2145	U
1	A	2146	A
1	A	2147	G
1	A	2148	G
1	A	2149	U
1	A	2153	A
1	A	2155	C
1	A	2156	C

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Mol	Chain	Res	Type
1	A	2158	U
1	A	2159	U
1	A	2161	A
1	A	2163	A
1	A	2164	C
1	A	2169	G
1	A	2170	C
1	A	2172	C
1	A	2173	U
1	A	2175	G
1	A	2177	U
1	A	2185	A
1	A	2186	G
1	A	2188	C
1	A	2190	C
1	A	2193	G
1	A	2194	U
1	A	2195	G
1	A	2196	G
1	A	2198	A
1	A	2200	A
1	A	2204	C
1	A	2205	C
1	A	2206	C
1	A	2208	A
1	A	2209	G
1	A	2210	C
1	A	2211	U
1	A	2212	G
1	A	2214	G
1	A	2215	U
1	A	2217	G
1	A	2221	U
1	A	2224	U
1	A	2225	A
1	A	2226	A
1	A	2230	G
1	A	2231	C
1	A	2232	A
1	A	2235	A
1	A	2238	U
1	A	2239	A

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Mol	Chain	Res	Type
1	A	2240	U
1	A	2241	C
1	A	2245	G
1	A	2252	A
1	A	2265	G
1	A	2266	G
1	A	2287	C
1	A	2296	A
1	A	2306	G
1	A	2310	C
1	A	2311	U
1	A	2312	C
1	A	2313	A
1	A	2314	A
1	A	2315	A
1	A	2326	G
1	A	2328	A
1	A	2329	U
1	A	2330	G
1	A	2331	G
1	A	2332	U
1	A	2333	U
1	A	2334	G
1	A	2335	G
1	A	2336	A
1	A	2337	A
1	A	2338	A
1	A	2339	U
1	A	2342	U
1	A	2345	A
1	A	2346	U
1	A	2347	A
1	A	2348	G
1	A	2349	A
1	A	2350	G
1	A	2352	G
1	A	2353	U
1	A	2354	A
1	A	2358	G
1	A	2360	A
1	A	2362	A
1	A	2364	G

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Mol	Chain	Res	Type
1	A	2370	U
1	A	2371	U
1	A	2372	G
1	A	2374	C
1	A	2377	C
1	A	2388	A
1	A	2396	A
1	A	2397	G
1	A	2398	G
1	A	2399	G
1	A	2404	A
1	A	2408	C
1	A	2410	G
1	A	2411	A
1	A	2412	C
1	A	2416	G
1	A	2417	U
1	A	2418	G
1	A	2430	C
1	A	2433	C
1	A	2434	A
1	A	2437	G
1	A	2441	G
1	A	2450	U
1	A	2451	C
1	A	2452	A
1	A	2453	A
1	A	2455	G
1	A	2456	G
1	A	2457	A
1	A	2461	A
1	A	2463	G
1	A	2468	C
1	A	2474	G
1	A	2475	A
1	A	2493	C
1	A	2497	G
1	A	2505	A
1	A	2506	U
1	A	2508	G
1	A	2521	G
1	A	2525	C

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Mol	Chain	Res	Type
1	A	2528	C
1	A	2529	G
1	A	2530	2MA
1	A	2531	U
1	A	2532	G
1	A	2533	U
1	A	2534	C
1	A	2543	G
1	A	2545	A
1	A	2547	C
1	A	2552	G
1	A	2554	C
1	A	2556	G
1	A	2558	A
1	A	2559	G
1	A	2562	G
1	A	2568	A
1	A	2569	A
1	A	2570	G
1	A	2574	U
1	A	2579	U
1	A	2580	G
1	A	2589	U
1	A	2592	A
1	A	2593	A
1	A	2594	G
1	A	2599	A
1	A	2600	C
1	A	2601	G
1	A	2605	G
1	A	2609	G
1	A	2612	U
1	A	2613	C
1	A	2626	G
1	A	2629	A
1	A	2636	U
1	A	2640	U
1	A	2642	U
1	A	2648	G
1	A	2649	U
1	A	2650	G
1	A	2656	A

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Mol	Chain	Res	Type
1	A	2661	A
1	A	2668	A
1	A	2672	G
1	A	2673	C
1	A	2681	A
1	A	2682	G
1	A	2683	U
1	A	2684	A
1	A	2685	C
1	A	2687	A
1	A	2692	A
1	A	2693	C
1	A	2694	C
1	A	2695	G
1	A	2696	G
1	A	2700	G
1	A	2709	U
1	A	2712	G
1	A	2716	U
1	A	2728	U
1	A	2729	G
1	A	2733	A
1	A	2741	G
1	A	2745	G
1	A	2753	U
1	A	2755	U
1	A	2756	G
1	A	2760	A
1	A	2761	C
1	A	2769	G
1	A	2771	G
1	A	2776	A
1	A	2777	A
1	A	2781	U
1	A	2782	C
1	A	2783	U
1	A	2784	A
1	A	2787	C
1	A	2788	A
1	A	2792	A
1	A	2794	C
1	A	2803	A

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Mol	Chain	Res	Type
1	A	2804	G
1	A	2805	A
1	A	2806	U
1	A	2807	G
1	A	2817	A
1	A	2818	A
1	A	2819	C
1	A	2820	U
1	A	2821	U
1	A	2824	G
1	A	2826	U
1	A	2827	A
1	A	2828	U
1	A	2829	A
1	A	2830	A
1	A	2832	A
1	A	2838	C
1	A	2840	A
1	A	2844	U
1	A	2846	A
1	A	2851	G
1	A	2853	U
1	A	2855	A
1	A	2887	G
1	A	2888	A
1	A	2892	G
1	A	2899	A
1	A	2900	C
1	A	2904	U
1	A	2905	C
1	A	2906	G
1	A	2913	G
1	A	2914	A
1	A	2916	U
1	A	2919	A
1	A	2920	U
2	B	3	U
2	B	6	U
2	B	10	U
2	B	14	G
2	B	16	A
2	B	17	A

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Mol	Chain	Res	Type
2	B	22	G
2	B	23	U
2	B	24	C
2	B	25	A
2	B	26	C
2	B	27	A
2	B	30	U
2	B	31	G
2	B	33	U
2	B	36	C
2	B	37	A
2	B	39	G
2	B	40	C
2	B	41	C
2	B	42	G
2	B	43	A
2	B	45	C
2	B	49	G
2	B	50	A
2	B	51	A
2	B	52	G
2	B	53	U
2	B	54	U
2	B	55	A
2	B	56	A
2	B	58	C
2	B	62	U
2	B	63	U
2	B	64	A
2	B	65	G
2	B	87	C
2	B	88	G
2	B	101	A
2	B	102	G
2	B	105	C
2	B	106	G
2	B	107	U
2	B	111	C
2	B	113	G
2	B	115	C
31	a	8	G
31	a	10	G

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Mol	Chain	Res	Type
31	a	31	U
31	a	32	G
31	a	33	A
31	a	40	G
31	a	43	G
31	a	45	G
31	a	48	C
31	a	49	C
31	a	52	A
31	a	62	G
31	a	65	G
31	a	67	G
31	a	69	G
31	a	71	A
31	a	72	C
31	a	76	C
31	a	94	G
31	a	95	A
31	a	98	U
31	a	99	U
31	a	100	A
31	a	118	A
31	a	119	A
31	a	120	C
31	a	129	A
31	a	130	A
31	a	136	C
31	a	142	G
31	a	151	A
31	a	157	G
31	a	158	G
31	a	159	G
31	a	163	C
31	a	167	A
31	a	168	G
31	a	171	A
31	a	173	U
31	a	174	A
31	a	184	A
31	a	185	U
31	a	188	U
31	a	189	G

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Mol	Chain	Res	Type
31	a	194	G
31	a	197	U
31	a	200	U
31	a	201	U
31	a	203	A
31	a	204	A
31	a	209	G
31	a	211	A
31	a	215	C
31	a	217	G
31	a	226	U
31	a	227	C
31	a	230	U
31	a	233	U
31	a	234	A
31	a	239	G
31	a	248	U
31	a	251	A
31	a	255	G
31	a	256	C
31	a	259	G
31	a	268	G
31	a	269	U
31	a	274	G
31	a	275	C
31	a	278	A
31	a	279	C
31	a	297	G
31	a	301	A
31	a	327	G
31	a	329	A
31	a	336	C
31	a	337	A
31	a	338	C
31	a	352	A
31	a	355	G
31	a	359	G
31	a	360	C
31	a	362	G
31	a	363	C
31	a	375	U
31	a	380	C

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Mol	Chain	Res	Type
31	a	390	A
31	a	396	G
31	a	401	A
31	a	405	A
31	a	406	C
31	a	412	G
31	a	414	G
31	a	415	A
31	a	421	G
31	a	422	A
31	a	423	A
31	a	424	G
31	a	427	C
31	a	429	U
31	a	430	C
31	a	431	G
31	a	437	U
31	a	440	A
31	a	442	C
31	a	443	U
31	a	447	U
31	a	452	A
31	a	456	A
31	a	459	A
31	a	460	A
31	a	461	C
31	a	466	G
31	a	468	G
31	a	473	U
31	a	484	A
31	a	485	U
31	a	486	C
31	a	487	U
31	a	488	U
31	a	489	G
31	a	492	G
31	a	499	A
31	a	501	U
31	a	503	A
31	a	504	G
31	a	508	G
31	a	514	G

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Mol	Chain	Res	Type
31	a	517	A
31	a	519	C
31	a	526	C
31	a	529	G
31	a	532	G
31	a	535	G
31	a	538	G
31	a	539	U
31	a	540	A
31	a	541	A
31	a	542	U
31	a	543	A
31	a	544	C
31	a	548	G
31	a	553	C
31	a	555	A
31	a	567	A
31	a	572	U
31	a	578	G
31	a	580	A
31	a	581	A
31	a	584	C
31	a	585	G
31	a	587	G
31	a	590	U
31	a	591	A
31	a	596	G
31	a	604	A
31	a	612	G
31	a	634	U
31	a	640	G
31	a	641	U
31	a	642	C
31	a	649	A
31	a	650	A
31	a	660	U
31	a	661	U
31	a	664	G
31	a	673	A
31	a	691	G
31	a	694	U
31	a	701	G

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Mol	Chain	Res	Type
31	a	703	A
31	a	708	G
31	a	726	A
31	a	730	G
31	a	732	G
31	a	741	G
31	a	757	A
31	a	763	G
31	a	785	A
31	a	788	A
31	a	789	A
31	a	790	A
31	a	793	G
31	a	794	G
31	a	796	U
31	a	801	U
31	a	802	A
31	a	803	C
31	a	817	G
31	a	820	G
31	a	823	A
31	a	825	C
31	a	826	G
31	a	827	A
31	a	829	G
31	a	836	A
31	a	864	G
31	a	868	C
31	a	869	A
31	a	879	U
31	a	880	U
31	a	881	A
31	a	894	G
31	a	911	G
31	a	923	A
31	a	934	G
31	a	935	G
31	a	936	G
31	a	937	G
31	a	940	C
31	a	942	G
31	a	943	C

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Mol	Chain	Res	Type
31	a	948	G
31	a	949	C
31	a	953	G
31	a	969	U
31	a	970	U
31	a	973	A
31	a	978	A
31	a	980	G
31	a	983	A
31	a	984	A
31	a	986	A
31	a	987	A
31	a	991	U
31	a	993	C
31	a	998	U
31	a	1000	U
31	a	1001	U
31	a	1002	G
31	a	1005	A
31	a	1007	C
31	a	1008	C
31	a	1029	A
31	a	1055	A
31	a	1060	U
31	a	1064	G
31	a	1067	U
31	a	1075	G
31	a	1076	U
31	a	1092	G
31	a	1097	U
31	a	1105	G
31	a	1110	G
31	a	1112	A
31	a	1113	A
31	a	1119	G
31	a	1120	C
31	a	1122	A
31	a	1124	C
31	a	1128	A
31	a	1132	U
31	a	1135	G
31	a	1137	U

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Mol	Chain	Res	Type
31	a	1139	C
31	a	1140	C
31	a	1141	A
31	a	1143	C
31	a	1144	A
31	a	1152	G
31	a	1155	C
31	a	1156	A
31	a	1167	A
31	a	1168	C
31	a	1169	U
31	a	1172	C
31	a	1174	G
31	a	1175	U
31	a	1177	A
31	a	1178	C
31	a	1179	A
31	a	1182	C
31	a	1187	G
31	a	1189	A
31	a	1194	G
31	a	1203	G
31	a	1205	C
31	a	1206	A
31	a	1207	A
31	a	1218	C
31	a	1222	U
31	a	1223	A
31	a	1225	G
31	a	1235	A
31	a	1236	C
31	a	1237	A
31	a	1239	A
31	a	1246	A
31	a	1248	A
31	a	1250	U
31	a	1254	C
31	a	1255	A
31	a	1256	A
31	a	1264	G
31	a	1266	C
31	a	1268	G

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Mol	Chain	Res	Type
31	a	1269	C
31	a	1270	G
31	a	1271	A
31	a	1278	G
31	a	1279	A
31	a	1280	G
31	a	1283	C
31	a	1289	A
31	a	1290	A
31	a	1292	C
31	a	1296	U
31	a	1297	A
31	a	1298	A
31	a	1303	G
31	a	1307	U
31	a	1308	C
31	a	1310	G
31	a	1312	U
31	a	1313	C
31	a	1315	G
31	a	1326	G
31	a	1329	A
31	a	1330	C
31	a	1331	U
31	a	1332	C
31	a	1333	G
31	a	1334	A
31	a	1335	C
31	a	1338	C
31	a	1341	G
31	a	1346	U
31	a	1347	G
31	a	1356	A
31	a	1357	G
31	a	1358	U
31	a	1363	G
31	a	1374	U
31	a	1380	G
31	a	1384	A
31	a	1385	A
31	a	1387	A
31	a	1388	C

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Mol	Chain	Res	Type
31	a	1389	G
31	a	1390	U
31	a	1391	U
31	a	1393	C
31	a	1397	G
31	a	1401	U
31	a	1404	A
31	a	1407	C
31	a	1408	A
31	a	1409	C
31	a	1410	C
31	a	1415	G
31	a	1420	A
31	a	1429	G
31	a	1445	G
31	a	1451	G
31	a	1452	G
31	a	1456	A
31	a	1457	A
31	a	1460	U
31	a	1474	C
31	a	1475	G
31	a	1476	U
31	a	1490	A
31	a	1498	G
31	a	1500	G
31	a	1504	A
31	a	1505	G
31	a	1508	G
31	a	1510	A
31	a	1514	A
31	a	1515	G
31	a	1517	U
31	a	1518	A
31	a	1528	G
31	a	1529	A
31	a	1530	A
31	a	1532	G
31	a	1540	G
31	a	1541	G
31	a	1547	C
31	a	1548	U

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Mol	Chain	Res	Type
31	a	1549	C
31	a	1550	C

All (82) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	63	U
1	A	82	G
1	A	90	A
1	A	98	U
1	A	104	C
1	A	199	A
1	A	202	A
1	A	291	G
1	A	299	U
1	A	327	G
1	A	328	G
1	A	337	A
1	A	373	A
1	A	403	U
1	A	502	C
1	A	513	G
1	A	520	G
1	A	548	A
1	A	576	U
1	A	577	A
1	A	614	U
1	A	672	A
1	A	690	U
1	A	715	A
1	A	809	A
1	A	890	G
1	A	910	C
1	A	1017	A
1	A	1028	G
1	A	1077	U
1	A	1096	C
1	A	1097	U
1	A	1130	A
1	A	1153	C
1	A	1312	A
1	A	1357	G

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Mol	Chain	Res	Type
1	A	1361	G
1	A	1433	U
1	A	1434	U
1	A	1455	U
1	A	1458	A
1	A	1525	U
1	A	1552	U
1	A	1554	A
1	A	1555	G
1	A	1577	G
1	A	1581	U
1	A	1591	G
1	A	1593	G
1	A	1605	A
1	A	1628	A
1	A	1629	U
1	A	1634	A
1	A	1652	A
1	A	1757	U
1	A	1760	G
1	A	1789	A
1	A	1826	G
1	A	2089	A
1	A	2094	G
1	A	2137	G
1	A	2224	U
1	A	2225	A
1	A	2238	U
1	A	2329	U
1	A	2347	A
1	A	2353	U
1	A	2409	G
1	A	2457	A
1	A	2495	A
1	A	2505	A
1	A	2533	U
1	A	2599	A
1	A	2628	C
1	A	2672	G
1	A	2829	A
1	A	2887	G
1	A	2912	A

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Mol	Chain	Res	Type
2	B	22	G
2	B	37	A
2	B	50	A
2	B	105	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MG	A	2472	1	23,26,27	1.37	3 (13%)	33,38,41	2.75	12 (36%)
1	2MA	A	2530	1,52	22,25,26	1.47	5 (22%)	32,37,40	2.45	9 (28%)
1	5MU	A	792	1	19,22,23	1.47	5 (26%)	27,32,35	2.28	8 (29%)
1	OMG	A	2278	1	23,26,27	1.28	4 (17%)	32,38,41	2.07	7 (21%)
1	5MU	A	1966	1	19,22,23	1.66	5 (26%)	27,32,35	2.35	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	2472	1	-	0/9/27/28	0/3/3/3
1	2MA	A	2530	1,52	-	0/7/25/26	0/3/3/3
1	5MU	A	792	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2278	1	-	1/9/27/28	0/3/3/3
1	5MU	A	1966	1	-	0/7/25/26	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2530	2MA	C5-C4	4.00	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2472	2MG	C6-N1	-3.40	1.32	1.38
1	A	792	5MU	C4-N3	-3.25	1.32	1.38
1	A	1966	5MU	C4-N3	-3.20	1.32	1.38
1	A	1966	5MU	C6-C5	3.14	1.39	1.34
1	A	1966	5MU	C2-N3	-3.08	1.32	1.38
1	A	2278	OMG	C6-N1	-3.04	1.33	1.38
1	A	2472	2MG	C5-N7	-2.85	1.33	1.39
1	A	2530	2MA	C5-N7	-2.79	1.34	1.39
1	A	792	5MU	C2-N3	-2.73	1.33	1.38
1	A	2472	2MG	C4-N9	-2.70	1.31	1.38
1	A	792	5MU	C6-N1	-2.68	1.33	1.38
1	A	2278	OMG	C5-C4	2.59	1.45	1.38
1	A	1966	5MU	C2-N1	2.54	1.42	1.38
1	A	2278	OMG	C5-N7	-2.47	1.34	1.39
1	A	2530	2MA	C5-C6	2.40	1.47	1.41
1	A	1966	5MU	C4-C5	2.29	1.48	1.44
1	A	792	5MU	C2-N1	2.16	1.41	1.38
1	A	792	5MU	C6-C5	2.15	1.38	1.34
1	A	2530	2MA	C4-N9	-2.15	1.33	1.37
1	A	2278	OMG	C4-N9	-2.11	1.32	1.38
1	A	2530	2MA	C8-N9	-2.02	1.34	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2472	2MG	C2-N3-C4	8.90	123.13	112.00
1	A	2530	2MA	C5-C4-N3	-8.26	118.48	127.18
1	A	2472	2MG	N1-C2-N2	7.09	123.80	116.56
1	A	2530	2MA	N3-C4-N9	6.93	135.78	126.99
1	A	2278	OMG	C5-C4-N3	-6.16	118.58	128.39
1	A	1966	5MU	N3-C2-N1	6.02	122.73	114.89
1	A	2472	2MG	C5-C4-N3	-5.60	119.48	128.39
1	A	792	5MU	N3-C2-N1	5.41	121.93	114.89
1	A	1966	5MU	C5-C4-N3	5.31	119.94	115.32
1	A	2278	OMG	C2-N3-C4	5.30	121.42	112.30
1	A	1966	5MU	C4-N3-C2	-5.12	120.62	127.34
1	A	792	5MU	C4-N3-C2	-5.00	120.79	127.34
1	A	2278	OMG	N9-C4-N3	4.50	134.96	125.95
1	A	2472	2MG	C6-C5-N7	4.29	138.10	130.29
1	A	792	5MU	O4-C4-C5	-4.01	120.33	124.92
1	A	792	5MU	C5-C4-N3	3.90	118.72	115.32
1	A	2472	2MG	N9-C4-N3	3.53	133.01	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	792	5MU	C5-C6-N1	-3.37	119.65	123.31
1	A	2278	OMG	C6-C5-N7	3.36	136.41	130.29
1	A	1966	5MU	O4-C4-C5	-3.31	121.13	124.92
1	A	1966	5MU	O2-C2-N3	-3.28	115.45	121.49
1	A	2530	2MA	C4-C5-N7	-3.19	106.94	110.58
1	A	2530	2MA	N6-C6-N1	3.16	121.29	117.03
1	A	2472	2MG	N2-C2-N3	-3.13	116.53	120.51
1	A	2530	2MA	C4-N9-C8	3.11	109.00	105.74
1	A	792	5MU	C3'-C2'-C1'	2.99	107.13	101.46
1	A	1966	5MU	O4'-C1'-N1	2.89	114.90	108.36
1	A	2472	2MG	C4-C5-N7	-2.78	106.27	110.67
1	A	2530	2MA	C2-N1-C6	2.71	122.27	118.10
1	A	2530	2MA	C5-N7-C8	2.62	107.56	103.45
1	A	1966	5MU	C6-N1-C2	-2.60	118.72	121.30
1	A	792	5MU	C1'-N1-C2	2.59	122.25	117.59
1	A	792	5MU	O2-C2-N3	-2.51	116.87	121.49
1	A	2278	OMG	O6-C6-C5	-2.49	119.97	126.53
1	A	1966	5MU	C5-C6-N1	-2.47	120.63	123.31
1	A	2472	2MG	N1-C2-N3	-2.39	119.66	123.68
1	A	2278	OMG	C4-C5-N7	-2.33	106.98	110.67
1	A	2278	OMG	C5-C6-N1	2.26	119.00	113.25
1	A	2530	2MA	N9-C8-N7	-2.24	110.75	113.94
1	A	2472	2MG	C5-C6-N1	2.22	118.90	113.25
1	A	2472	2MG	C6-C5-C4	-2.13	115.62	118.83
1	A	2472	2MG	O6-C6-C5	-2.11	120.95	126.53
1	A	2530	2MA	C6-C5-N7	2.11	136.15	132.09
1	A	2472	2MG	C8-N7-C5	2.03	107.87	104.26

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2278	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	A1D6G	A	3000	52	72,73,73	2.43	25 (34%)	97,107,107	1.84	30 (30%)

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
51	A1D6G	A	3000	52	-	11/82/113/113	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	3000	A1D6G	C65-N64	8.81	1.45	1.33
51	A	3000	A1D6G	C11-N13	7.40	1.49	1.34
51	A	3000	A1D6G	O67-C65	4.89	1.43	1.36
51	A	3000	A1D6G	O10-C11	4.81	1.43	1.35
51	A	3000	A1D6G	C22-C21	4.62	1.55	1.44
51	A	3000	A1D6G	O67-C68	-4.40	1.41	1.47
51	A	3000	A1D6G	O04-C03	-4.32	1.39	1.46
51	A	3000	A1D6G	C19-C20	3.81	1.56	1.47
51	A	3000	A1D6G	C25-C26	-3.80	1.40	1.48
51	A	3000	A1D6G	O04-C05	3.55	1.42	1.34
51	A	3000	A1D6G	C35-N33	-3.16	1.33	1.39
51	A	3000	A1D6G	C50-C46	-3.13	1.47	1.53
51	A	3000	A1D6G	C28-C29	3.13	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	3000	A1D6G	O42-C41	3.03	1.49	1.41
51	A	3000	A1D6G	C32-N33	-3.02	1.32	1.35
51	A	3000	A1D6G	C63-N64	-2.95	1.40	1.45
51	A	3000	A1D6G	C25-C35	-2.74	1.36	1.41
51	A	3000	A1D6G	O10-C09	-2.49	1.41	1.44
51	A	3000	A1D6G	O54-C52	-2.38	1.39	1.44
51	A	3000	A1D6G	C45-C46	-2.31	1.48	1.53
51	A	3000	A1D6G	O27-C26	-2.28	1.18	1.23
51	A	3000	A1D6G	O60-C59	-2.20	1.18	1.21
51	A	3000	A1D6G	C28-C26	-2.11	1.39	1.44
51	A	3000	A1D6G	O42-C43	2.09	1.48	1.44
51	A	3000	A1D6G	C56-C52	2.06	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	A	3000	A1D6G	C63-N64-C65	-4.34	106.72	112.39
51	A	3000	A1D6G	O10-C11-N13	4.31	118.03	111.01
51	A	3000	A1D6G	O42-C43-C45	4.30	115.49	109.34
51	A	3000	A1D6G	C52-C39-C37	-4.09	107.29	113.54
51	A	3000	A1D6G	C02-C03-C68	-3.97	109.76	115.23
51	A	3000	A1D6G	C44-C43-C45	-3.90	107.37	113.27
51	A	3000	A1D6G	C41-O42-C43	3.78	118.74	112.91
51	A	3000	A1D6G	O04-C05-C07	3.30	118.59	111.53
51	A	3000	A1D6G	C35-N33-C32	3.14	123.12	120.03
51	A	3000	A1D6G	O66-C65-N64	-3.07	125.56	129.19
51	A	3000	A1D6G	O30-C29-C28	3.07	122.87	115.69
51	A	3000	A1D6G	O67-C68-C69	3.03	112.15	106.80
51	A	3000	A1D6G	O67-C65-O66	3.00	125.54	121.64
51	A	3000	A1D6G	C03-O04-C05	-2.97	113.01	118.20
51	A	3000	A1D6G	O10-C11-O12	-2.85	120.36	124.55
51	A	3000	A1D6G	C28-C32-N33	-2.61	119.61	123.31
51	A	3000	A1D6G	C14-N13-C11	-2.61	117.55	121.98
51	A	3000	A1D6G	C38-C37-C09	-2.59	106.84	111.40
51	A	3000	A1D6G	C56-C52-C39	-2.36	107.34	110.18
51	A	3000	A1D6G	C45-C46-N47	-2.31	109.09	115.59
51	A	3000	A1D6G	C53-C52-C39	2.25	113.09	109.79
51	A	3000	A1D6G	O12-C11-N13	-2.21	121.60	124.93
51	A	3000	A1D6G	O30-C29-O31	-2.16	118.76	123.90
51	A	3000	A1D6G	C69-C68-C03	-2.15	108.54	112.36
51	A	3000	A1D6G	C57-C59-C61	2.13	122.72	119.13
51	A	3000	A1D6G	O42-C41-C50	2.11	114.70	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	A	3000	A1D6G	O31-C29-C28	-2.08	118.37	122.67
51	A	3000	A1D6G	C56-C57-C59	-2.04	109.89	113.32
51	A	3000	A1D6G	O40-C39-C52	2.04	111.18	106.44
51	A	3000	A1D6G	C15-C14-N13	-2.03	106.50	112.20

There are no chirality outliers.

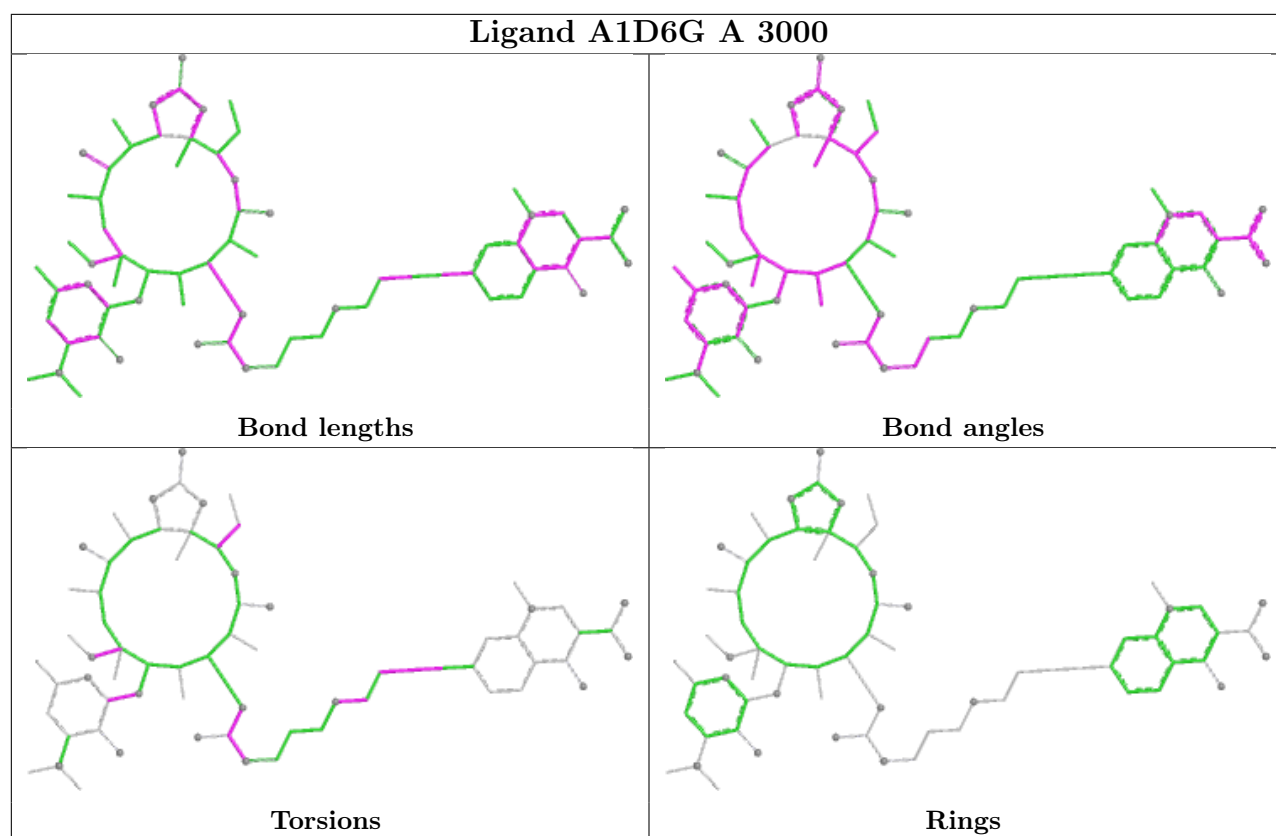
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	A	3000	A1D6G	O10-C11-N13-C14
51	A	3000	A1D6G	O12-C11-N13-C14
51	A	3000	A1D6G	C18-C19-C20-C21
51	A	3000	A1D6G	C19-C20-C21-C22
51	A	3000	A1D6G	N13-C11-O10-C09
51	A	3000	A1D6G	O42-C41-O40-C39
51	A	3000	A1D6G	C01-C02-C03-O04
51	A	3000	A1D6G	O12-C11-O10-C09
51	A	3000	A1D6G	C19-C18-O17-C16
51	A	3000	A1D6G	C50-C41-O40-C39
51	A	3000	A1D6G	C56-C52-O54-C55

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

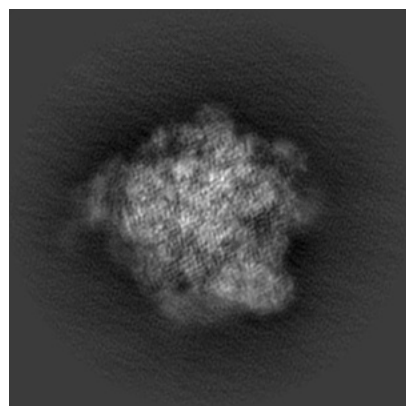
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38876. These allow visual inspection of the internal detail of the map and identification of artifacts.

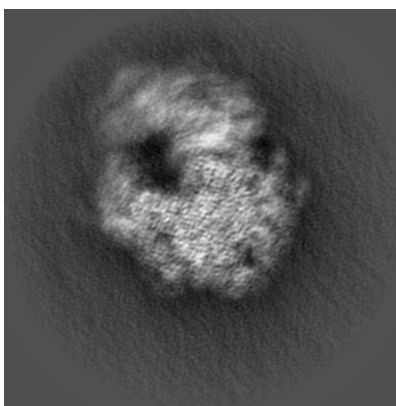
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

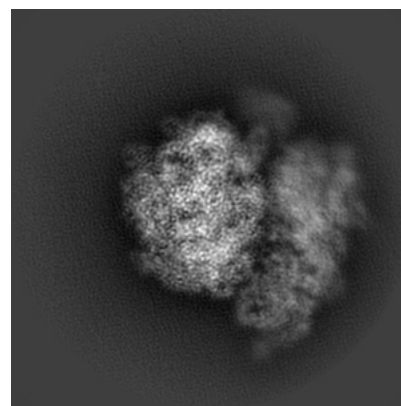
6.1.1 Primary map



X

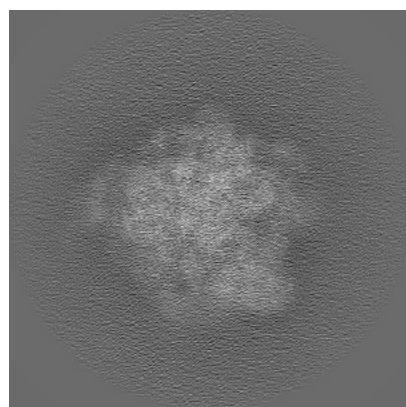


Y

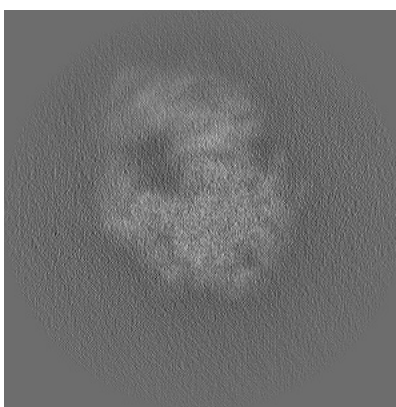


Z

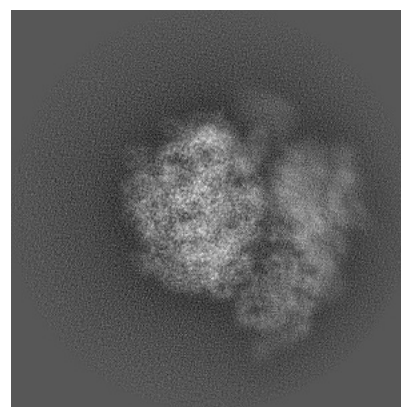
6.1.2 Raw map



X



Y

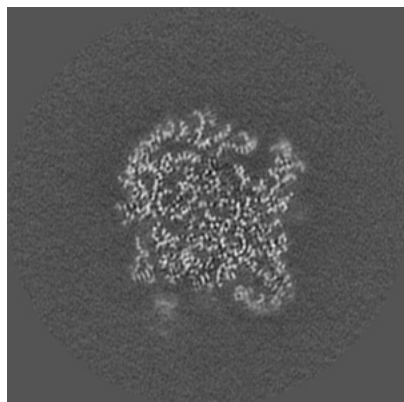


Z

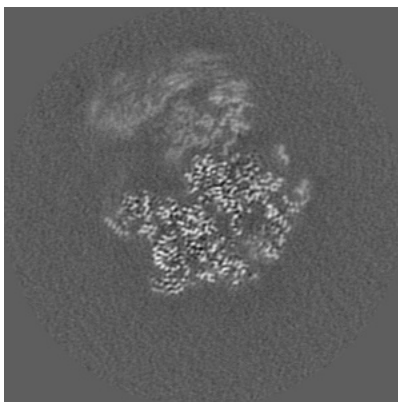
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

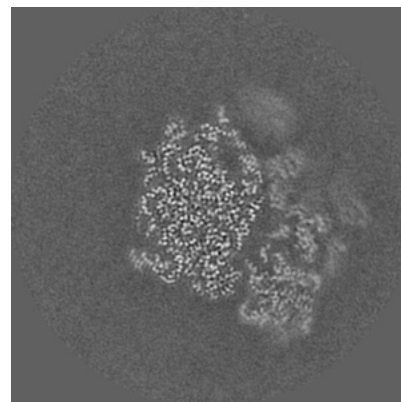
6.2.1 Primary map



X Index: 240

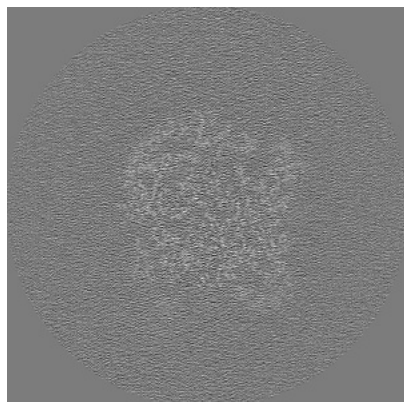


Y Index: 240

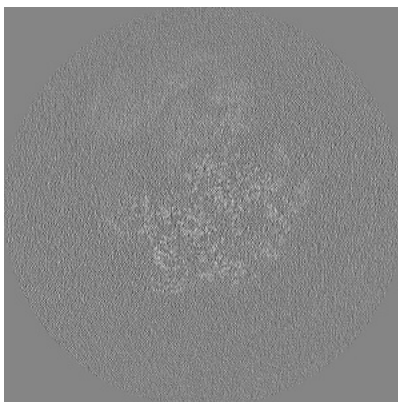


Z Index: 240

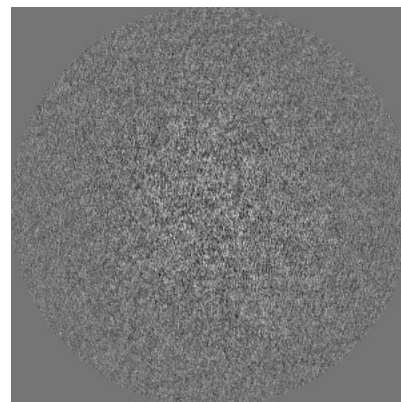
6.2.2 Raw map



X Index: 240



Y Index: 240

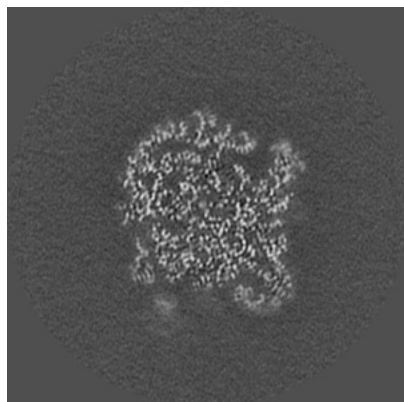


Z Index: 240

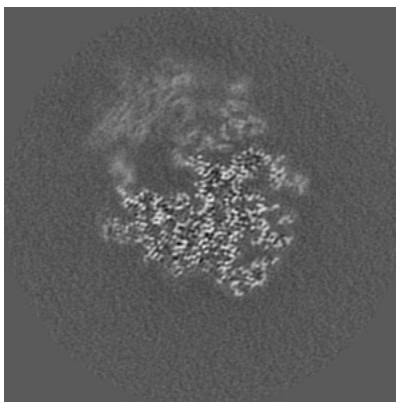
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

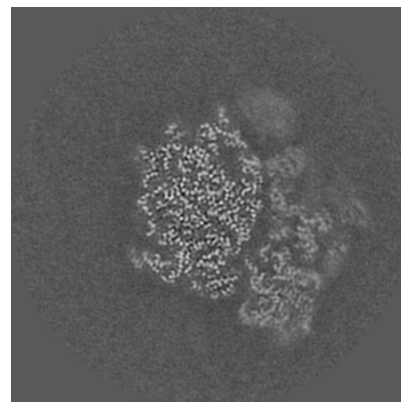
6.3.1 Primary map



X Index: 239

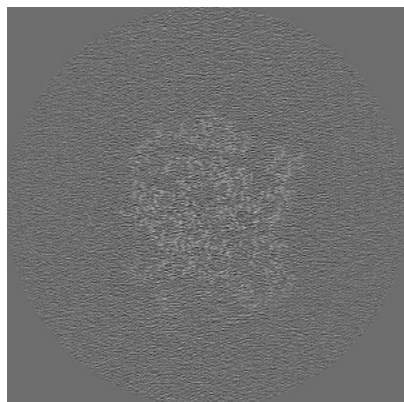


Y Index: 256

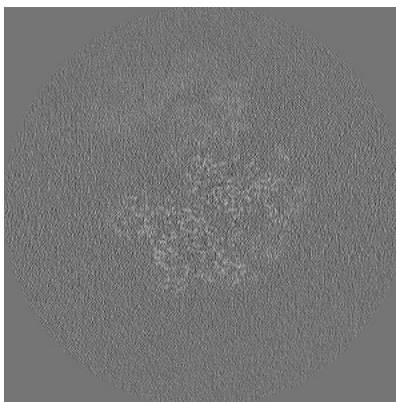


Z Index: 242

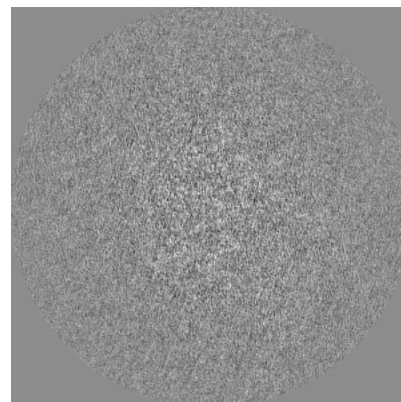
6.3.2 Raw map



X Index: 233



Y Index: 241

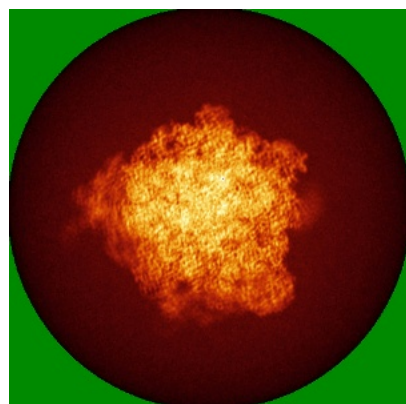


Z Index: 245

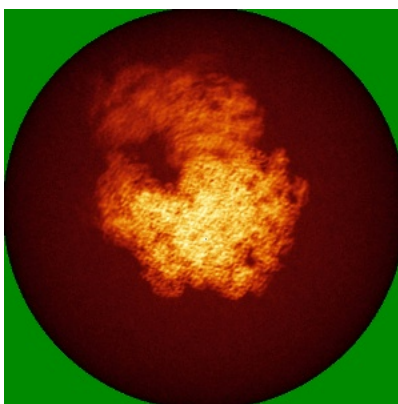
The images above show the largest variance slices of the map in three orthogonal directions.

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

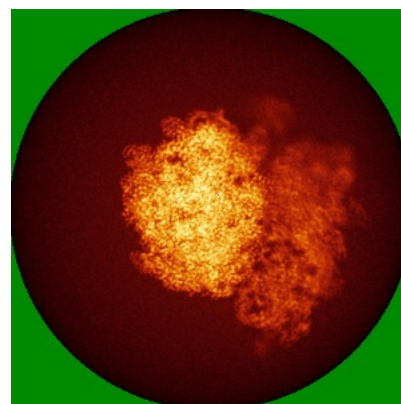
6.4.1 Primary map



X

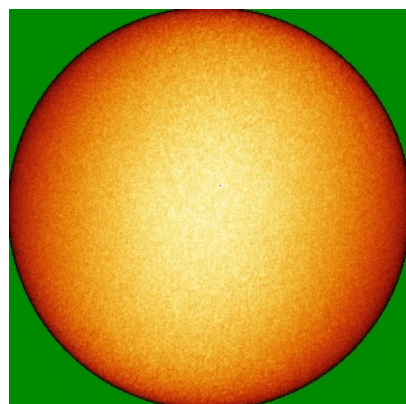


Y

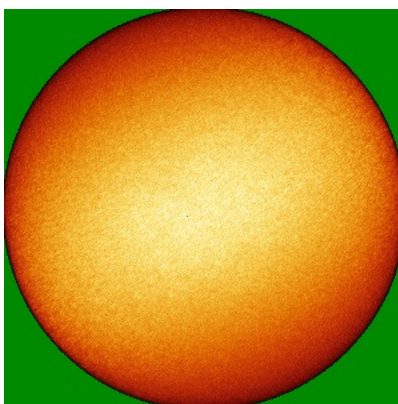


Z

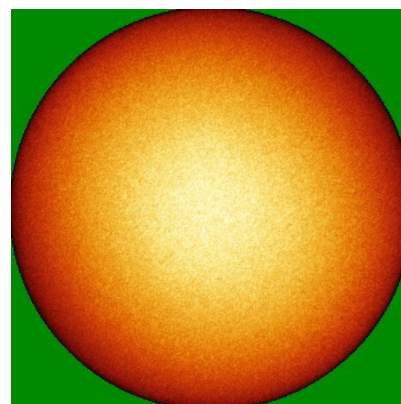
6.4.2 Raw map



X



Y

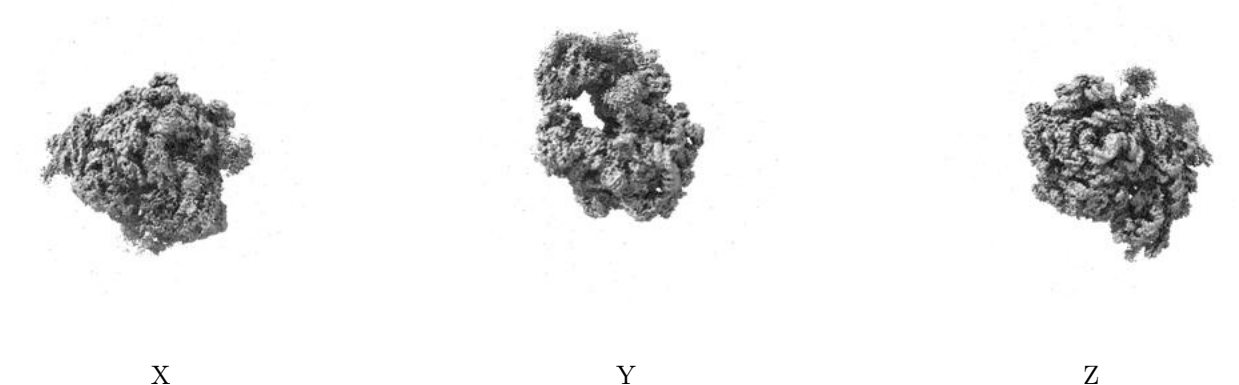


Z

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

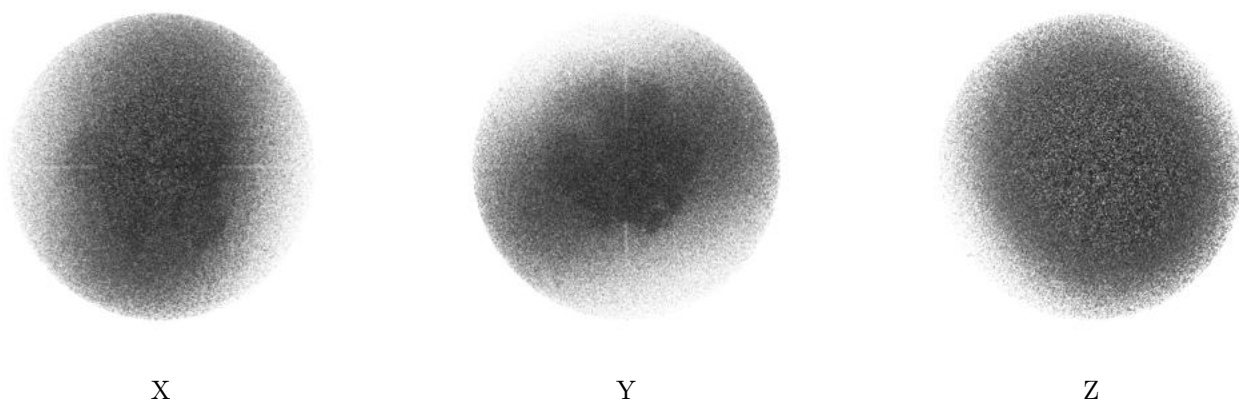
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

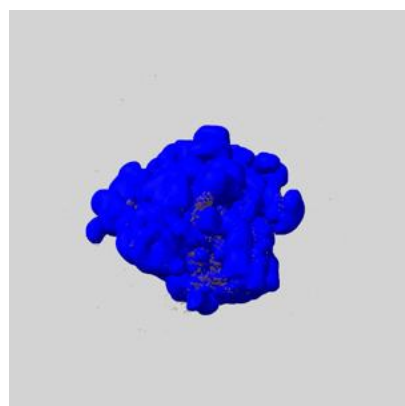
6.6 Mask visualisation [i](#)

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

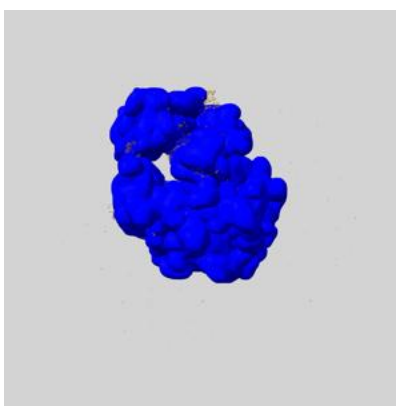
A mask typically either:

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

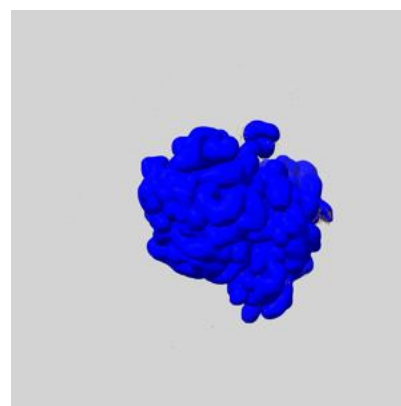
6.6.1 emd_38876_msk_1.map [i](#)



X



Y

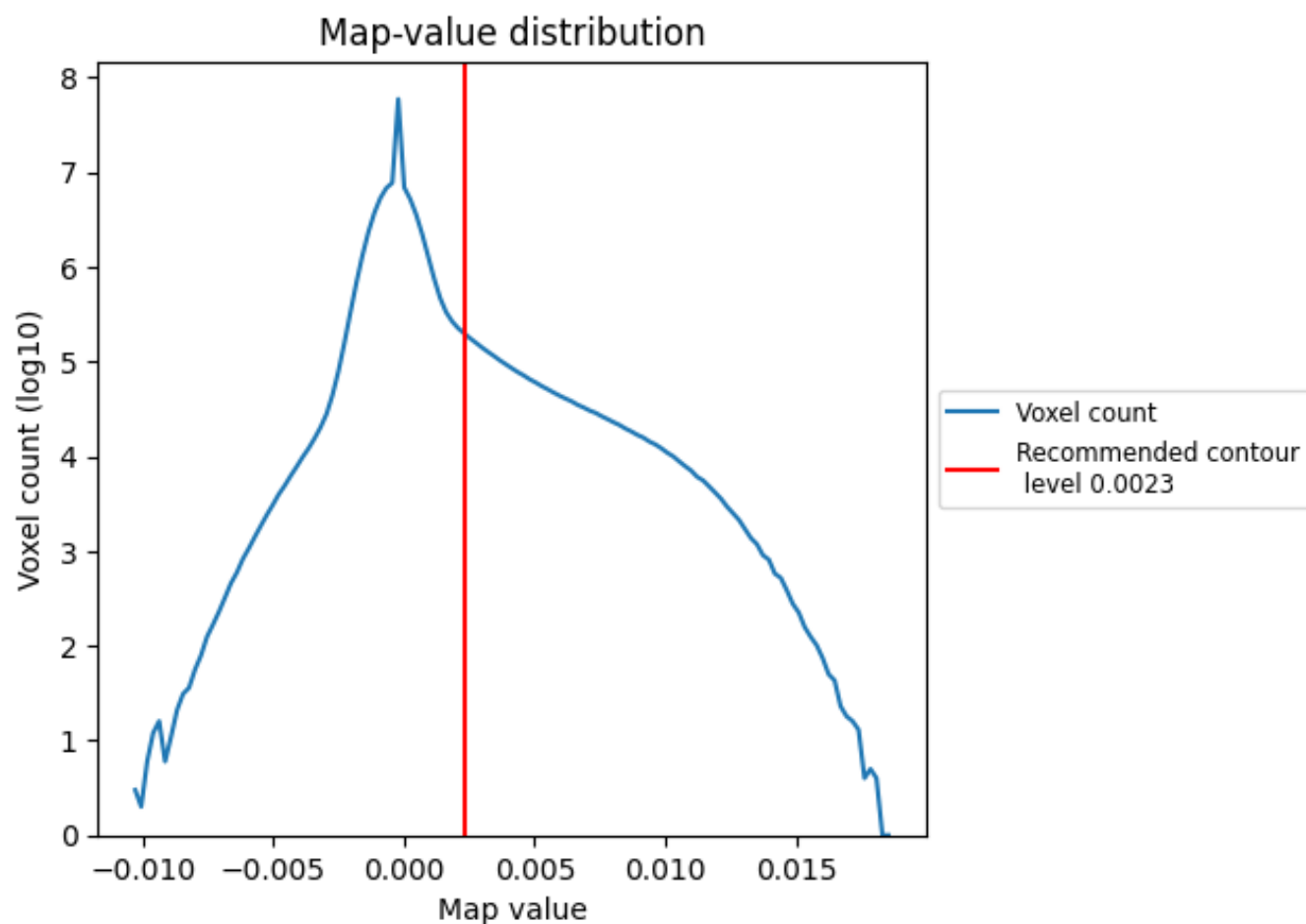


Z

7 Map analysis [i](#)

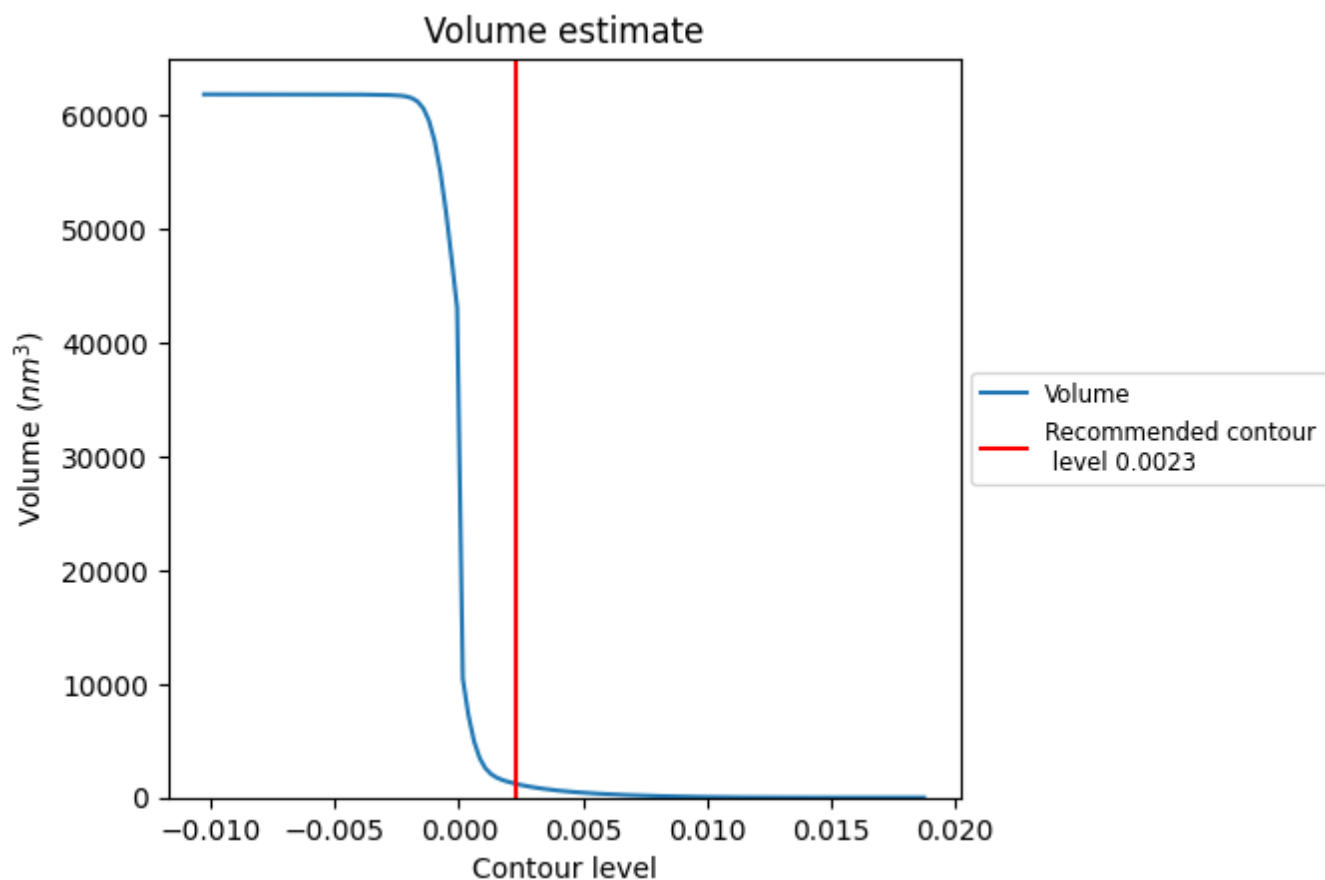
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

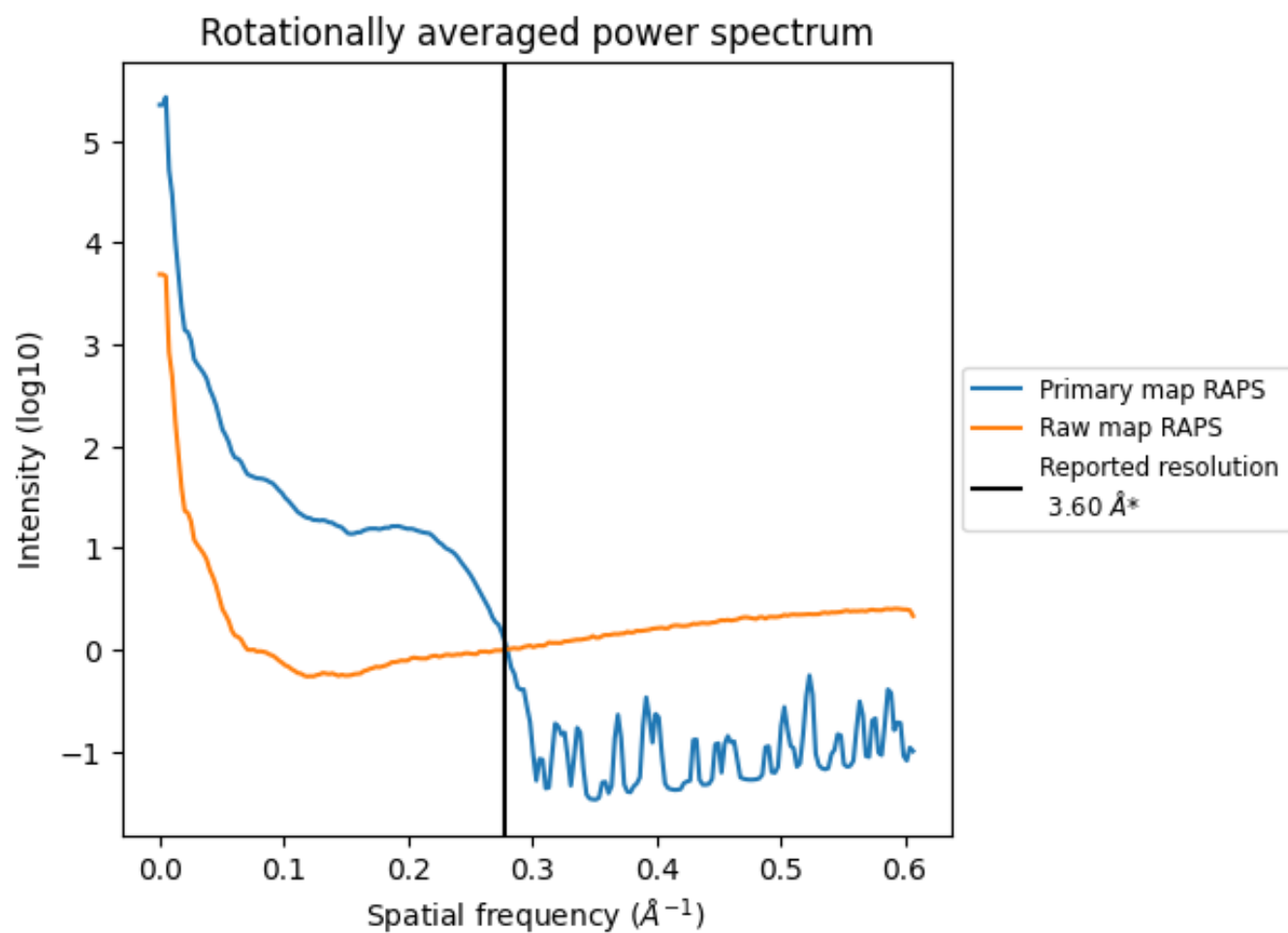
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1208 nm³; this corresponds to an approximate mass of 1091 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

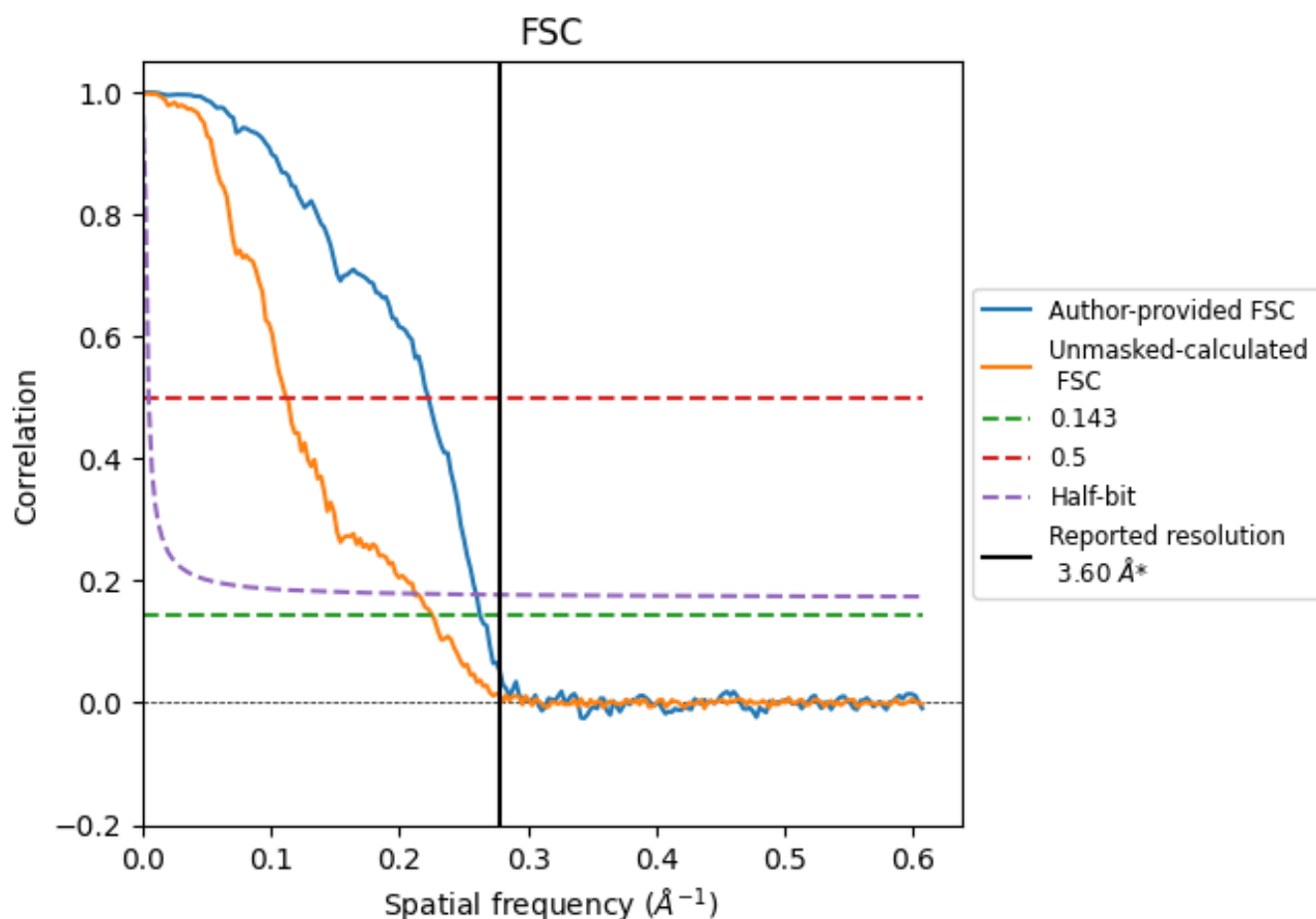


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

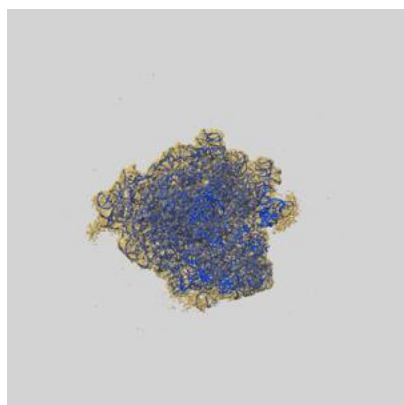
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.80	4.49	3.85
Unmasked-calculated*	4.43	8.90	4.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.43 differs from the reported value 3.6 by more than 10 %

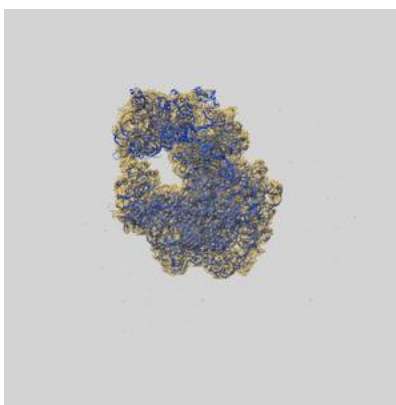
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38876 and PDB model 8Y39. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

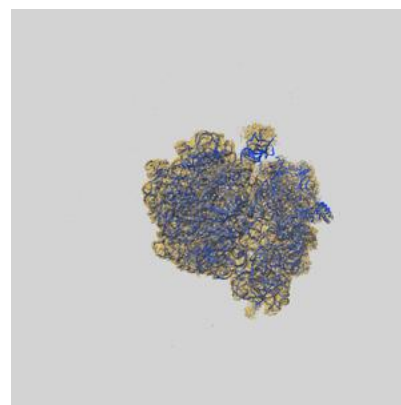
9.1 Map-model overlay [i](#)



X



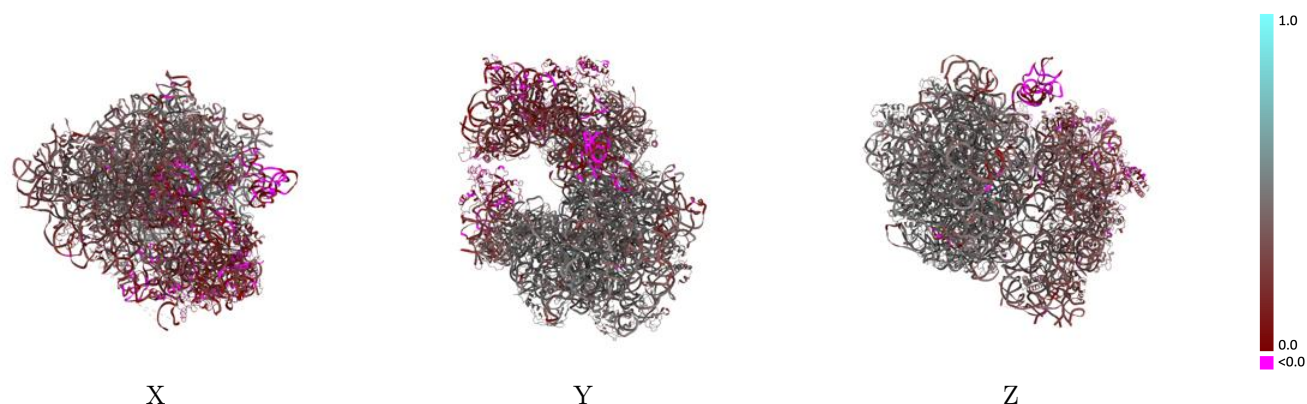
Y



Z

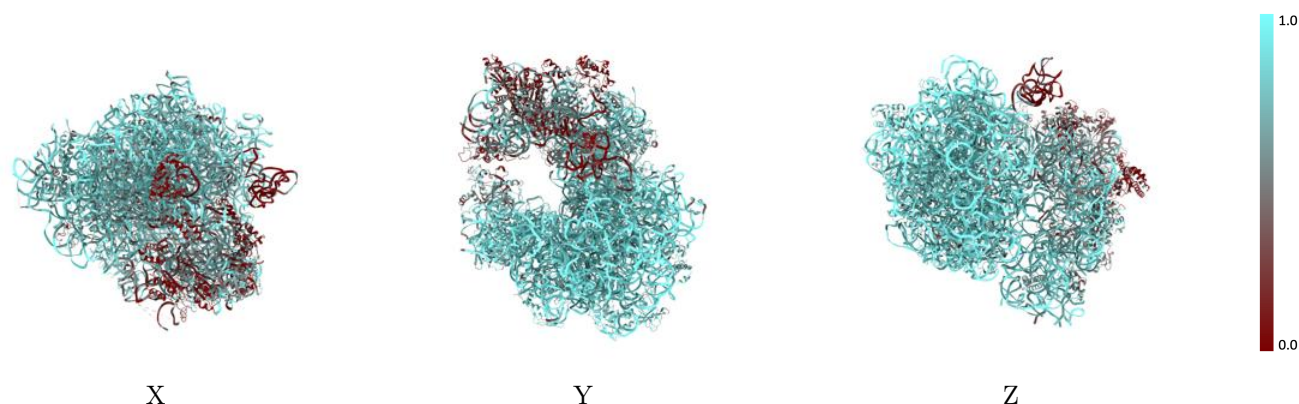
The images above show the 3D surface view of the map at the recommended contour level 0.0023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



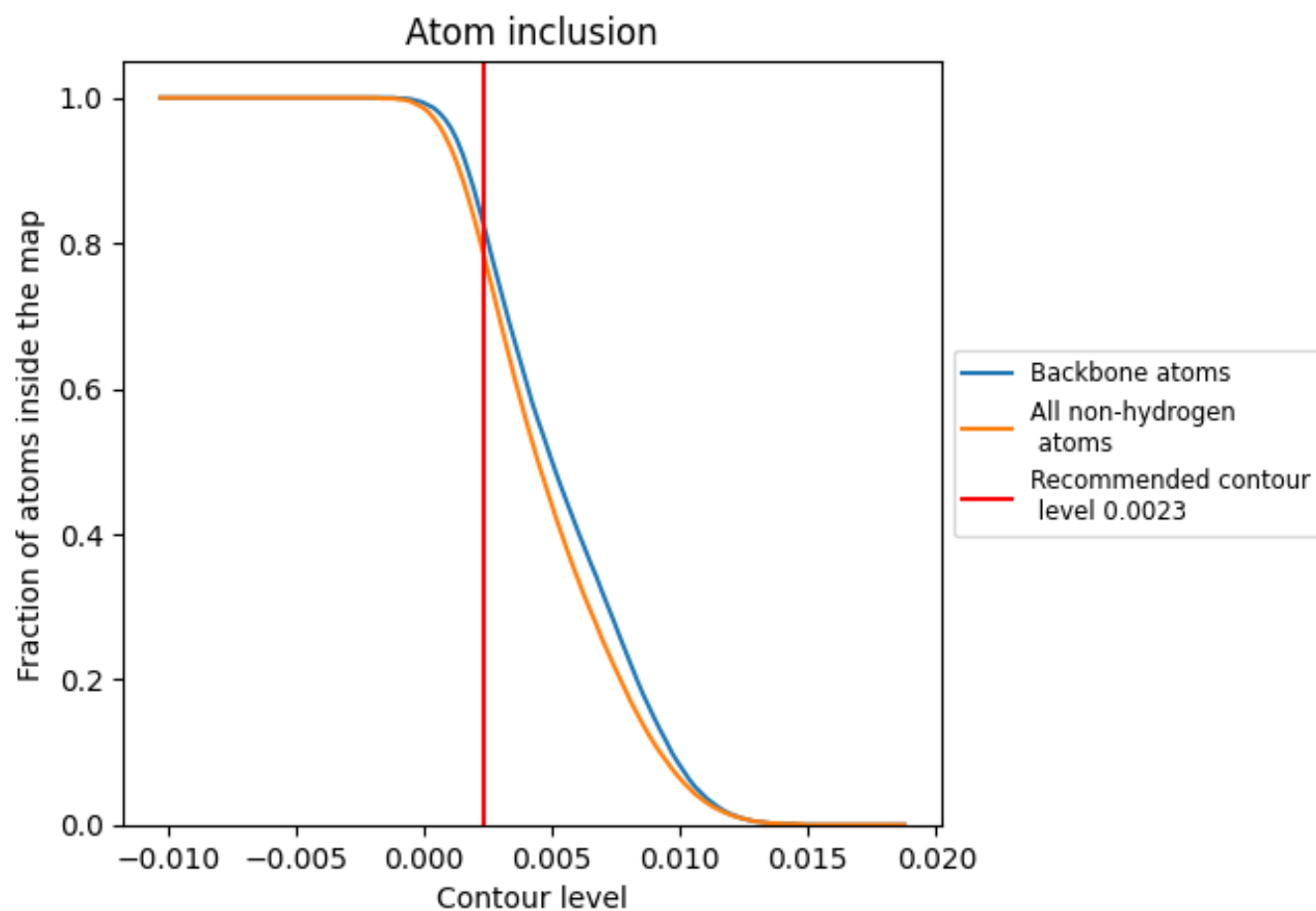
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7890	 0.3530
1	 0.8800	 0.4430
2	 0.8320	 0.4650
3	 0.8630	 0.4810
4	 0.8410	 0.4670
A	 0.8940	 0.3980
B	 0.8810	 0.3200
C	 0.8170	 0.4580
D	 0.8650	 0.4710
E	 0.8380	 0.4500
F	 0.5710	 0.1650
G	 0.8380	 0.3990
H	 0.8600	 0.4600
I	 0.8040	 0.4570
J	 0.8710	 0.4650
K	 0.8670	 0.4650
L	 0.8410	 0.4630
M	 0.7790	 0.3250
N	 0.8170	 0.4400
O	 0.8910	 0.4530
P	 0.8550	 0.4650
Q	 0.8350	 0.4530
R	 0.7940	 0.4240
S	 0.7880	 0.4100
T	 0.7760	 0.3820
U	 0.8370	 0.4330
V	 0.8370	 0.4500
W	 0.7730	 0.3910
X	 0.8440	 0.4680
Y	 0.5380	 0.0990
Z	 0.8850	 0.4820
a	 0.7660	 0.2860
b	 0.1700	 0.1330
c	 0.1650	 0.2070
d	 0.5540	 0.2560



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Chain	Atom inclusion	Q-score
e	 0.5530	 0.2670
f	 0.6340	 0.3250
g	 0.1960	 0.1510
h	 0.6320	 0.3110
i	 0.2380	 0.0840
j	 0.1470	 0.1500
k	 0.5070	 0.2320
l	 0.5110	 0.3050
m	 0.2340	 0.1690
n	 0.3020	 0.1990
o	 0.6880	 0.3160
p	 0.6290	 0.3350
q	 0.6230	 0.3290
r	 0.6590	 0.2740
s	 0.3360	 0.1510
t	 0.6480	 0.3450