



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:38 AM UTC

PDB ID : 3G71 / pdb_00003g71
Title : Co-crystal structure of Bruceantin bound to the large ribosomal subunit
Authors : Gurel, G.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2009-02-09
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

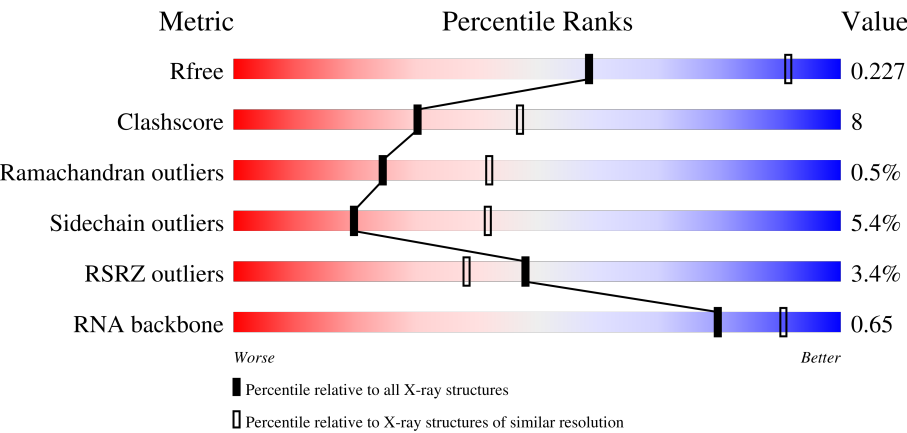
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

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

Mol	Chain	Length	Quality of chain
1	0	2923	54% 34% 5% 6%
2	A	237	3% 82% 16% .
3	B	337	% 80% 18% .
4	C	246	2% 80% 16% ..

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	172	
7	F	119	
8	G	348	
9	H	177	
10	I	70	
11	J	142	
12	K	132	
13	L	165	
14	M	194	
15	N	186	
16	O	115	
17	P	143	
18	Q	95	
19	R	150	
20	S	81	
21	T	119	
22	U	53	
23	V	65	
24	W	154	
25	X	82	
26	Y	142	
27	Z	73	
28	1	56	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	3% 88% 12%
31	9	122	2% 43% 42% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	8522	-	-	-	X
34	NA	0	8559	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 2 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 3 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 4 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 5 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 6 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	172	Total	C	N	O	S	0	0	0
			1358	840	224	290	4			

- Molecule 7 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 8 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 9 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 10 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	70	Total	C	N	O	S	0	0	0
			520	323	81	115	1			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	145	Total	C	N	O		0	0	0
			1118	670	222	226				

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	333	282	1			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O	0	0	0
			1137	683	229	225			

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	150	Total	C	N	O	S	0	0	0
			1150	713	209	224	4			

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	81	Total	C	N	O	S	0	0	0
			642	389	111	139	3			

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 22 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	53	Total	C	N	O	S	0	0	0
			411	244	75	87	5			

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S	0	0	0
			500	304	94	101	1			

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 25 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	X	82	Total	C	N	O	S	0	0	0
			655	402	129	123	1			

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Y	142	Total	C	N	O	0	0	0
			1131	686	228	217			

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			574	343	113	113	5			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	A	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	9	2	Total	Mg	0	0
			2	2		

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	C	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	J	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	K	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0

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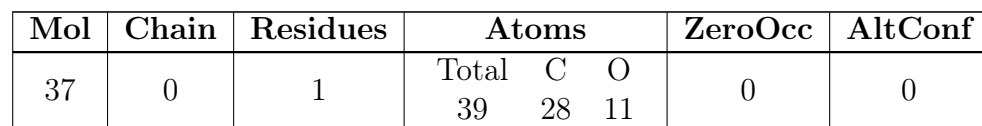
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	95	Total 95	Sr 95	0	0
36	A	2	Total 2	Sr 2	0	0
36	B	2	Total 2	Sr 2	0	0
36	F	1	Total 1	Sr 1	0	0
36	R	1	Total 1	Sr 1	0	0
36	S	1	Total 1	Sr 1	0	0
36	1	1	Total 1	Sr 1	0	0
36	3	2	Total 2	Sr 2	0	0
36	9	3	Total 3	Sr 3	0	0

- Molecule 37 is methyl (5beta,7alpha,9beta,10alpha,11alpha,12alpha,13beta,15alpha)-15-{[(2 E)-3,4-dimethylpent-2-enoyl]oxy}-3,11,12-trihydroxy-2,16-dioxo-13,20-epoxypicras-3-en-21-oate (CCD ID: WIN) (formula: C₂₈H₃₆O₁₁).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 38 | O | 1 | Total Cd
1 1 | 0 | 0 |
| 38 | U | 1 | Total Cd
1 1 | 0 | 0 |
| 38 | Z | 1 | Total Cd
1 1 | 0 | 0 |
| 38 | 1 | 1 | Total Cd
1 1 | 0 | 0 |
| 38 | 3 | 1 | Total Cd
1 1 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 39 | 0 | 5993 | Total O
5993 5993 | 0 | 0 |
| 39 | A | 107 | Total O
107 107 | 0 | 0 |
| 39 | B | 146 | Total O
146 146 | 0 | 0 |



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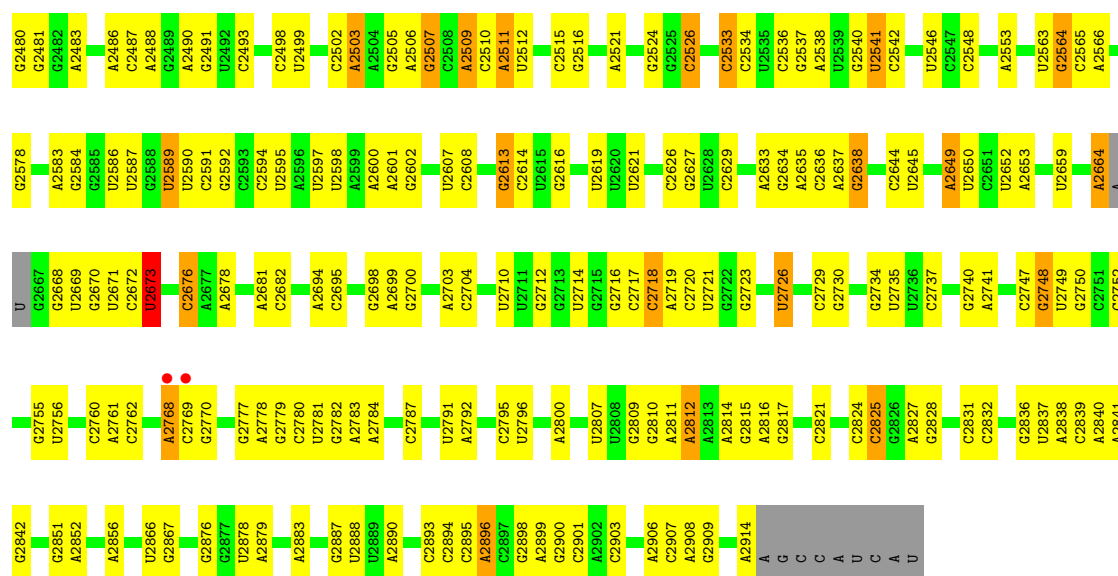
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	C	171	Total 171	O 171	0	0
39	D	45	Total 45	O 45	0	0
39	E	40	Total 40	O 40	0	0
39	F	25	Total 25	O 25	0	0
39	G	18	Total 18	O 18	0	0
39	H	62	Total 62	O 62	0	0
39	I	5	Total 5	O 5	0	0
39	J	52	Total 52	O 52	0	0
39	K	53	Total 53	O 53	0	0
39	L	79	Total 79	O 79	0	0
39	M	128	Total 128	O 128	0	0
39	N	62	Total 62	O 62	0	0
39	O	40	Total 40	O 40	0	0
39	P	65	Total 65	O 65	0	0
39	Q	43	Total 43	O 43	0	0
39	R	77	Total 77	O 77	0	0
39	S	28	Total 28	O 28	0	0
39	T	32	Total 32	O 32	0	0
39	U	27	Total 27	O 27	0	0
39	V	12	Total 12	O 12	0	0
39	W	65	Total 65	O 65	0	0

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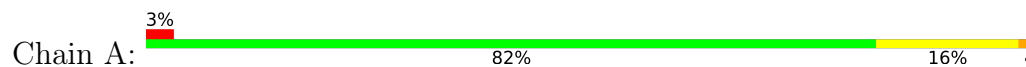
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	20	Total 20	O 20	0	0
39	Y	94	Total 94	O 94	0	0
39	Z	28	Total 28	O 28	0	0
39	1	52	Total 52	O 52	0	0
39	2	39	Total 39	O 39	0	0
39	3	66	Total 66	O 66	0	0
39	9	149	Total 149	O 149	0	0

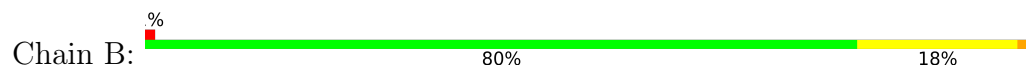
U2373	G2566	U2133	U2032	A1941	G1819	A1733	G1634	C1537	A1424	C1334	U1234	G1160	G1059
G2374	G2257	G2134	G2033	A1942	G1820	C1734	U1635	U1544	A1427	C1342	U1237	A1161	C1060
A2375	A2258	A2135	U2034	C1943	A1829	C1735	G1636	C1545	C1343	G1163	C1238	G1163	G1063
C2376	U2265	G2136	A2039	G1947	G1834	A1736	A1637	G1546	U1434	U1164	G1165	U1164	U1066
G2379	A2266	C	C2040	G1948	U1835	A1742	A1642	G1556	A1435	A1352	A1243	A1166	A1067
A2380	C2267	A	G2041	G1951	U1836	A1749	C1643	G1557	C1436	C1353	G1167	G1167	
C2381	C2268	U	U2042	U	U1838	G1752	G1644	C1558	C1439	A1357	U1244	U1169	G1071
A2382	C2269	C	G2045	A	A1839	G1759	U1645	U	U1440	C1360	U1245	U1170	A1072
G2385	G2270	C	G2046	A	A1840	G1760	U1652	U1561	A1442	U1361	A1246	G1171	G1074
U2387	C2271	C	C2047	C	G1844	A1755	A1653	C1562	A1443	U1362	U1249	G1172	G1075
C2388	U2272	C	G2050	A	A1845	G1756	U1654	C1566	G1444	G1363	C1250	A1173	G1076
U2389	C2281	A	A2054	U	U1846	A1759	G1655	G1567	G1445	G1364	C1251	G1174	G1077
C2392	U2282	C	G2057	G	G1848	G1761	A1657	U1568	U1446	C1365	G1175	A1177	A1078
A2401	A2291	C	U2064	C	G1849	C1762	A1658	U1569	U1447	C1366	C1257	C1176	A1081
A2402	A2300	U	G2070	C	G1855	C1763	A1664	G1570	G1453	G1370	U1258	U1180	
C2411	A2301	G	C2071	U1964	C1856	U1766	G1665	A1571	U1454	U1371	A1269	A1181	C1084
G2412	A2302	C	G2072	C1965	A1857	G1773	U1666	A1572	C1455	A1372	A1261	C1182	G1087
A2413	G2073	A	U1966	U1967	A1858	A1778	A1667	A1573	C1456		C1268	C1184	A1088
A2414	A2074	C	U1967	U1968	G1861	C1768	U1668	G1576	U1457	A1375	C1269	U1185	A1097
A2415	C2308	A	A1968	A1969	G1864	C1769	U1677	U1577	U1463	G1376	C1273	U1187	A1098
G2416	G2316	U	G2079	G1970	U1864	U1770	A1678	U1587	C1464	A1381	A1278	A1188	A1099
C2417	C2317	C	A2081	G1971	G1868	G1773	A1679	G1588	C1474	G1382	U1279	A1189	G1100
U2418	G2082	C	G2082	U1972	G1868	A1778	G1680	G1589	C1477	U1383	G1190	C1104	
G2419	A2083	C	A2083	A1973	G1873	A1779	A1682	G1593	U1478	C1384	G1289	A1192	C1105
G2420	U2320	C	C2087	G1974	G1877	U1783	A1683	C1594	A1482	G1385	A1290	A1193	A1106
G2421	A2321	C	C2088	A1978	G1877	U1784	A1684	C1595	C1483	G1386	A1291		
U2422	U2325	G	A2089	G1979	U1879	G1789	A1685	G1596	G1484	G1387	A1294	G1197	U1109
G2426	C2326	U	G2090	U1980	G1879	G1789	C1686	U1597	A1485	G1391	G1295	U1110	G1110
U2435	G2338	C	G2091	A1981	A1880	U1788	C1687	A1597		A1392	A1295	C1201	U1115
U2436	A	C	G2092	U1982	C1882	G1789	G1688	A1598	C1495	A1393	G1299	A1202	U1116
A2437	C	A	G2093	C1983	U1883	G1790		A1603	A1496	C1394	G1300	G1203	A1117
G2438	A2095	G	G2094	A1994	G1883	U1791		G1604	G1497	C1395		C1204	A1118
C2439	A2096	U	A2096	G1995	A1886	U1791		G1605	U1500	C1396	U1306	U1205	G1119
C2443	G2344	C	A2100	U1996	U1903	G1795	U1702	A1606		C1397	A1307	U1206	U1120
U2444	A2345	A	A2101	C2002	A1904	A1796		A1607	U1503	G1398	A1308	A1207	G1121
U2445	C2346	C	G2102	U2003	G1904	A1797	G1706	C1613	A1504	A1399	G1311	C1208	U1130
G2446	C2347	G	A2103	U2004	A1909	C1798	G1707	G1614	A1505	A1406	G1312	C1209	G1131
C2462	C2348	C	C2104	G2005	A1910	G1799		A1615	U1506	A1407	A1312	G1210	A1150
G2465	A2353	U	C2105	G2006	G1919	G1800		A1616	U1506	U1408	A1313	G1211	A1151
A2466	A2354	C	C2106	A2007	A1919	C1803	G1714	C1617	A1515	G1409	G1315	G1212	A1152
A2467	C2355	A	G2110	U2008	C1920	A1804	G1715	G1622	U1516	G1410	G1316	G1214	G1137
A2468	A2361	C	G2111	A2011	A1921	G1805	A1716	G1623	U1524	A1413	A1321	A1215	U1149
G2472	A2364	C	G2112	U2012	A1922	A1811	U1722	C1624	G1525	A1414	G1322	G1216	U1150
U2473	G2365	G	C2114	G2013	C1928	G1812	G1723	U1625	A1526	G1415	G1322	G1217	G1151
A2474	A2366	C	U2115	G2013	G1929	U1813	U1724	A1626	A1527	A1328	U1219	U1218	
C2475	C2367	C	U2116	U2016	G1937	G1814	C1725	G1627	U1528	G1329	U1220	U1219	A1154
C2476	A2368	C	G2121	U2017	U1938	A1815	G1725	A1631	A1529	A1330	A1330	G1155	
	A2252	U	C2122	U2022	U1939	U1816	G1730	A1632	G1536	C1420	C1331	C1229	G1158
	C2372	G			C1940	C1818	A1732	C1633		U1421	G1332	A1230	G1159



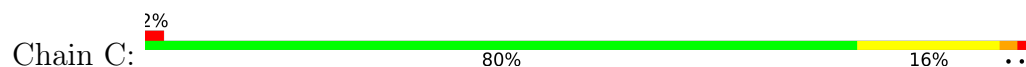
• Molecule 2: 50S ribosomal protein L2P

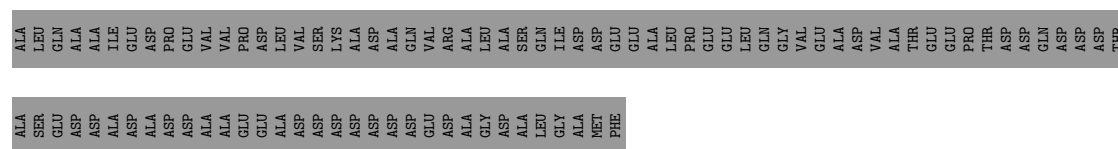


• Molecule 3: 50S ribosomal protein L3P

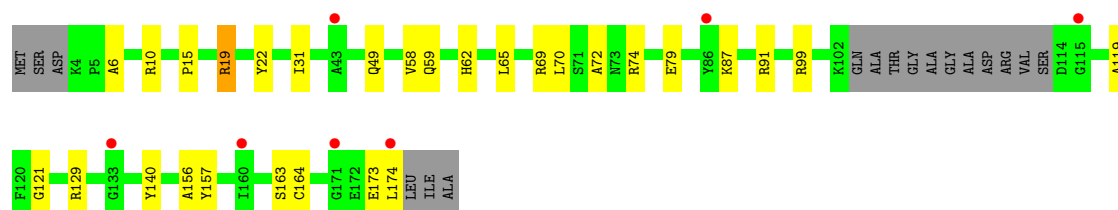


• Molecule 4: 50S ribosomal protein L4P

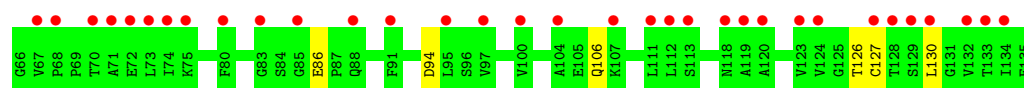




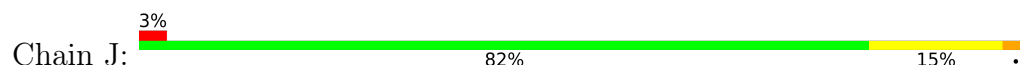
- Molecule 9: 50S ribosomal protein L10e



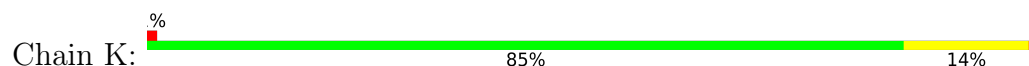
- Molecule 10: 50S ribosomal protein L11P



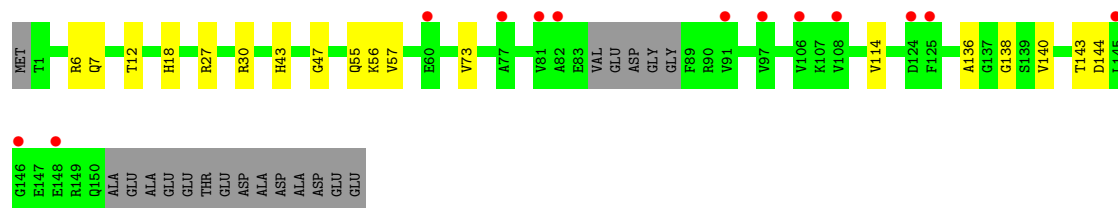
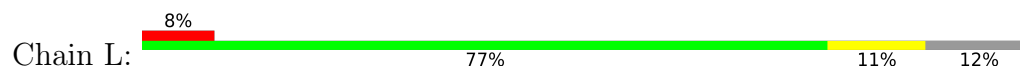
- Molecule 11: 50S ribosomal protein L13P



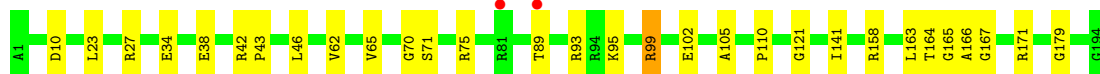
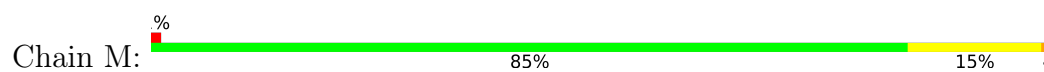
- Molecule 12: 50S ribosomal protein L14P



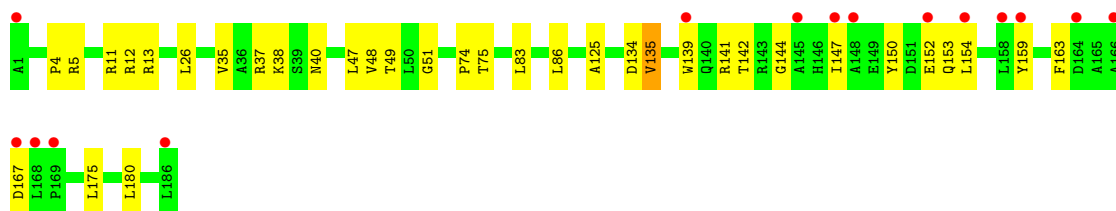
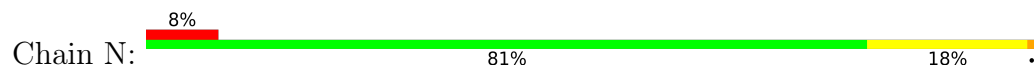
- Molecule 13: 50S ribosomal protein L15P



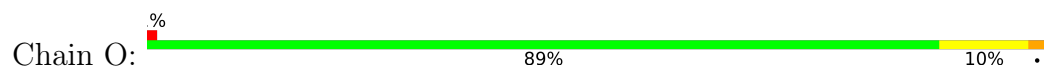
- Molecule 14: 50S ribosomal protein L15e



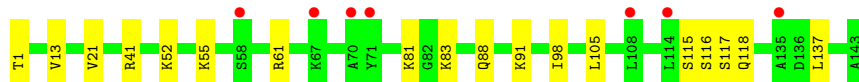
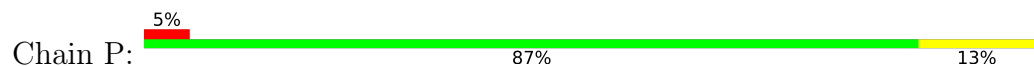
- Molecule 15: 50S ribosomal protein L18P



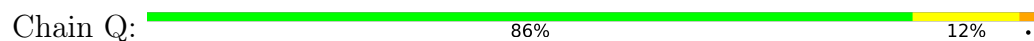
- Molecule 16: 50S ribosomal protein L18e



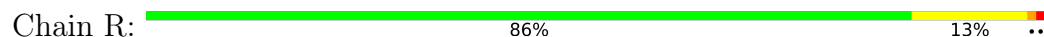
- Molecule 17: 50S ribosomal protein L19e



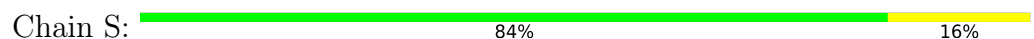
- Molecule 18: 50S ribosomal protein L21e



- Molecule 19: 50S ribosomal protein L22P

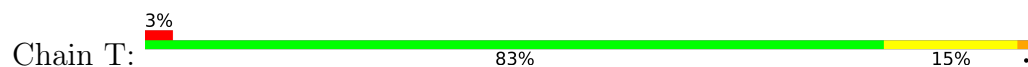


- Molecule 20: 50S ribosomal protein L23P

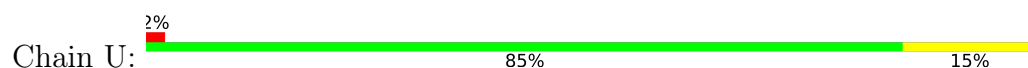




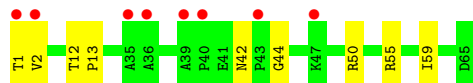
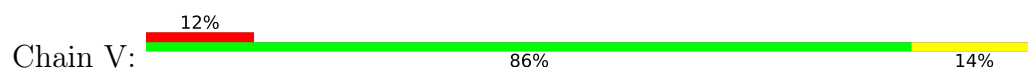
- Molecule 21: 50S ribosomal protein L24P



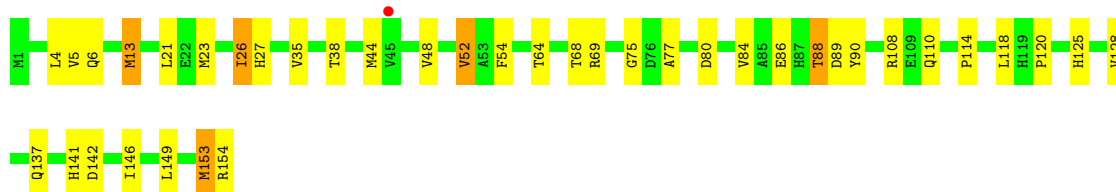
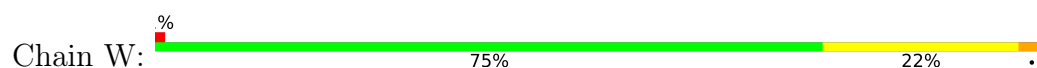
- Molecule 22: 50S ribosomal protein L24e



- Molecule 23: 50S ribosomal protein L29P



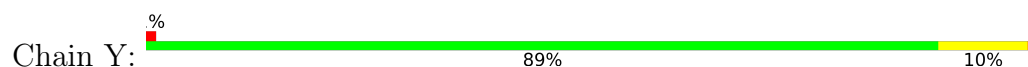
- Molecule 24: 50S ribosomal protein L30P



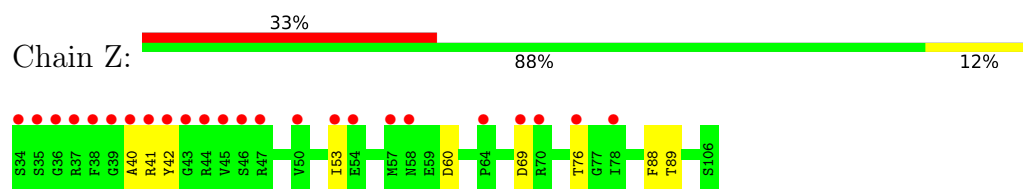
- Molecule 25: 50S ribosomal protein L31e



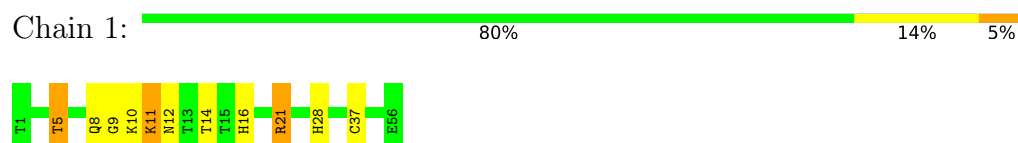
- Molecule 26: 50S ribosomal protein L32e



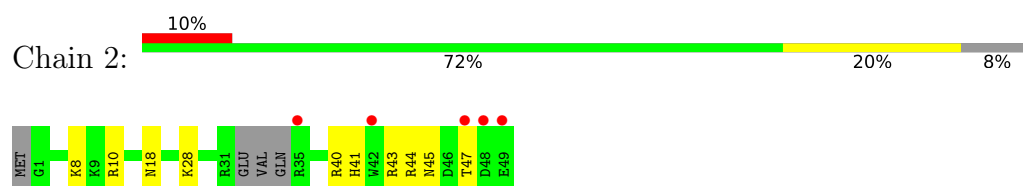
- Molecule 27: 50S ribosomal protein L37Ae



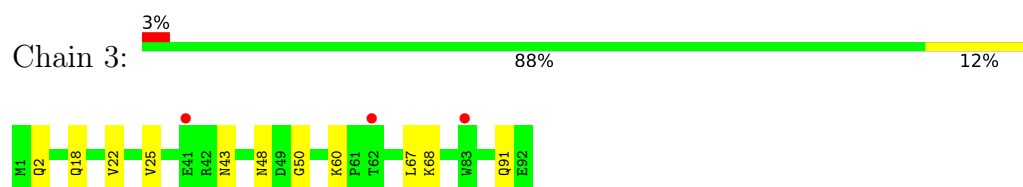
- Molecule 28: 50S ribosomal protein L37e



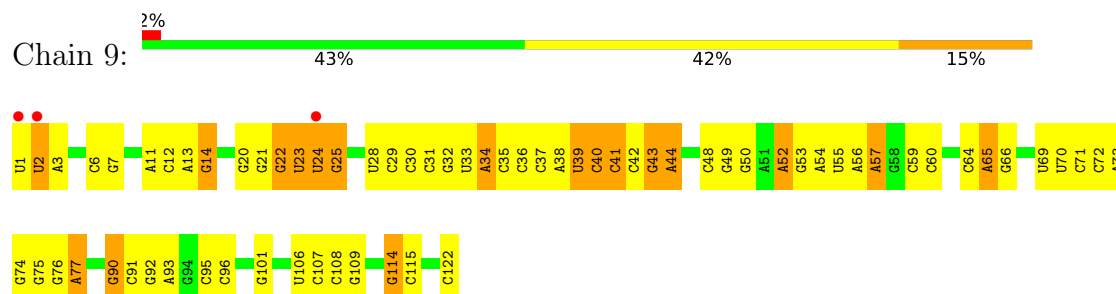
- Molecule 29: 50S ribosomal protein L39e



- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.21Å 299.54Å 574.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.85 49.76 – 2.85	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.76-2.85) 91.3 (49.76-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.186 , 0.233 0.183 , 0.227	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99174	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, OMU, 1MA, MG, PSU, WIN, UR3, K, OMG, NA, SR, CD

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	O	0.38	0/65958	0.60	17/102869 (0.0%)
2	A	0.65	0/1787	1.11	8/2408 (0.3%)
3	B	0.61	1/2690 (0.0%)	1.10	13/3652 (0.4%)
4	C	0.62	0/1885	1.14	11/2552 (0.4%)
5	D	0.70	0/1111	1.07	6/1498 (0.4%)
6	E	0.67	0/1383	1.01	4/1880 (0.2%)
7	F	0.69	1/901 (0.1%)	1.13	2/1224 (0.2%)
8	G	0.61	0/241	1.11	1/324 (0.3%)
9	H	0.65	0/1302	1.06	7/1743 (0.4%)
10	I	0.72	0/527	1.11	3/716 (0.4%)
11	J	0.62	1/1136 (0.1%)	1.11	2/1530 (0.1%)
12	K	0.59	0/1004	1.11	3/1351 (0.2%)
13	L	0.57	0/1130	1.07	6/1509 (0.4%)
14	M	0.56	0/1583	1.06	7/2116 (0.3%)
15	N	0.62	0/1474	1.18	10/1999 (0.5%)
16	O	0.59	0/874	1.06	3/1181 (0.3%)
17	P	0.54	0/1148	1.04	0/1528
18	Q	0.58	0/749	1.08	4/1005 (0.4%)
19	R	0.66	1/1173 (0.1%)	1.11	6/1578 (0.4%)
20	S	0.59	0/649	0.92	0/875
21	T	0.54	0/958	1.11	4/1289 (0.3%)
22	U	0.57	0/418	1.02	3/562 (0.5%)
23	V	0.59	0/503	1.15	2/675 (0.3%)
24	W	0.67	2/1219 (0.2%)	1.15	7/1655 (0.4%)
25	X	0.65	0/665	1.18	4/895 (0.4%)
26	Y	0.59	0/1147	1.06	2/1536 (0.1%)
27	Z	0.69	0/585	1.06	2/781 (0.3%)
28	1	0.54	0/438	1.06	4/578 (0.7%)
29	2	0.53	0/401	1.03	1/529 (0.2%)
30	3	0.56	0/771	0.92	3/1024 (0.3%)
31	9	0.37	0/2904	0.57	1/4526 (0.0%)
All	All	0.47	6/98714 (0.0%)	0.76	146/147588 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	31
24	W	0	1
31	9	0	1
All	All	0	33

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	109	MET	SD-CE	-9.34	1.56	1.79
7	F	63	ILE	CA-CB	8.59	1.58	1.54
3	B	162	MET	SD-CE	-6.69	1.62	1.79
24	W	13	MET	SD-CE	-6.38	1.63	1.79
11	J	19	MET	SD-CE	-5.66	1.65	1.79
24	W	153	MET	SD-CE	-5.30	1.66	1.79

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	170	TYR	N-CA-C	9.79	124.81	112.86
21	T	52	ARG	N-CA-C	9.77	125.75	113.43
15	N	163	PHE	N-CA-C	-9.42	99.50	112.12
24	W	75	GLY	N-CA-C	9.01	121.18	112.08
9	H	10	ARG	N-CA-C	8.04	120.04	111.28
8	G	27	ILE	N-CA-C	-7.94	105.47	111.90
3	B	222	LYS	N-CA-C	-7.82	99.25	110.59
4	C	205	ARG	N-CA-C	7.56	120.47	111.33
3	B	206	THR	N-CA-C	7.33	119.79	110.33
9	H	58	VAL	N-CA-C	7.25	117.67	108.82
14	M	121	GLY	N-CA-C	7.22	120.94	111.70
14	M	89	THR	N-CA-C	7.18	118.90	111.14
26	Y	143	TRP	N-CA-C	7.12	120.65	109.96
3	B	157	LYS	N-CA-C	-7.10	105.15	114.31
10	I	126	THR	N-CA-C	-7.05	106.58	114.62
3	B	175	LEU	N-CA-C	-7.00	103.73	111.36
27	Z	88	PHE	N-CA-C	6.80	118.84	109.18
13	L	73	VAL	N-CA-C	6.77	117.52	110.62
4	C	236	THR	N-CA-C	-6.74	99.32	110.17
9	H	119	ALA	N-CA-C	6.70	120.56	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	127	CYS	N-CA-C	6.62	118.29	111.14
18	Q	17	LYS	N-CA-C	-6.61	101.33	109.65
13	L	55	GLN	N-CA-C	6.51	120.09	111.75
15	N	48	VAL	N-CA-C	6.48	117.62	108.36
1	0	2726	U	N1-C1'-C2'	6.47	121.71	112.00
5	D	136	ARG	CA-C-N	6.27	127.68	119.84
5	D	136	ARG	C-N-CA	6.27	127.68	119.84
13	L	47	GLY	N-CA-C	6.25	118.47	111.85
31	9	39	U	N1-C1'-C2'	6.22	121.34	112.00
1	0	1504	A	N9-C1'-C2'	6.20	121.30	112.00
5	D	137	PRO	N-CA-C	6.20	125.23	112.47
19	R	13	THR	N-CA-C	6.11	118.47	109.24
1	0	834	G	C2'-C3'-O3'	-6.11	104.54	113.70
1	0	1942	A	C5'-C4'-C3'	6.08	125.13	116.00
1	0	871	G	C5'-C4'-O4'	-6.08	100.69	109.80
28	1	5	THR	CA-C-N	-6.08	113.42	119.56
28	1	5	THR	C-N-CA	-6.08	113.42	119.56
7	F	60	VAL	N-CA-CB	-6.04	105.57	112.21
21	T	3	GLN	CA-C-N	6.03	126.20	119.32
21	T	3	GLN	C-N-CA	6.03	126.20	119.32
29	2	44	ARG	N-CA-C	6.03	117.53	111.07
4	C	89	ALA	N-CA-C	6.02	118.36	111.02
13	L	12	THR	N-CA-C	6.02	120.46	113.18
27	Z	42	TYR	N-CA-C	6.00	123.57	110.80
14	M	110	PRO	N-CA-C	5.99	121.71	113.98
13	L	57	VAL	N-CA-C	-5.98	107.16	112.90
16	O	111	VAL	N-CA-C	5.98	116.73	108.12
2	A	135	VAL	N-CA-C	5.96	118.58	108.86
2	A	129	LEU	N-CA-C	5.94	120.05	111.02
12	K	122	GLY	N-CA-C	5.93	119.85	112.73
3	B	213	GLY	CA-C-N	5.91	125.78	119.28
3	B	213	GLY	C-N-CA	5.91	125.78	119.28
4	C	20	ASP	N-CA-C	5.90	119.30	111.75
4	C	134	ASP	N-CA-C	-5.89	105.10	112.93
25	X	79	GLU	N-CA-C	5.86	117.75	111.36
2	A	213	LYS	N-CA-C	5.86	118.61	111.82
6	E	13	ALA	N-CA-C	5.85	118.44	108.90
12	K	24	THR	N-CA-C	5.83	118.41	111.71
30	3	43	ASN	N-CA-C	5.83	120.12	113.19
10	I	106	GLN	N-CA-C	5.81	117.48	111.03
4	C	178	GLN	N-CA-C	5.81	120.10	113.19
19	R	106	GLY	N-CA-C	5.78	119.64	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	920	C	C2'-C3'-O3'	-5.77	105.04	113.70
16	O	25	VAL	CB-CA-C	-5.76	104.92	111.55
28	1	21	ARG	N-CA-C	5.75	118.41	111.40
15	N	135	VAL	N-CA-C	-5.75	107.17	113.43
15	N	150	TYR	N-CA-C	-5.74	106.41	113.41
3	B	113	LEU	N-CA-C	5.74	118.57	110.14
28	1	11	LYS	N-CA-C	5.73	118.49	108.52
13	L	7	GLN	N-CA-C	5.72	119.44	112.23
15	N	51	GLY	CA-C-N	5.72	125.58	119.28
15	N	51	GLY	C-N-CA	5.72	125.58	119.28
4	C	78	ARG	N-CA-C	5.71	116.91	108.86
1	0	1979	G	C4'-C3'-O3'	-5.68	104.48	113.00
24	W	77	ALA	N-CA-C	5.67	118.69	110.42
16	O	66	GLY	N-CA-C	5.66	126.60	113.18
11	J	45	VAL	N-CA-C	5.66	117.56	108.85
22	U	46	ALA	N-CA-C	5.65	118.98	111.75
25	X	60	ALA	N-CA-C	5.64	117.88	111.11
7	F	62	HIS	N-CA-C	5.63	119.32	112.23
19	R	82	GLU	N-CA-C	5.62	117.48	111.36
15	N	153	GLN	N-CA-C	-5.61	102.88	110.68
1	0	129	A	C2'-C3'-O3'	5.61	122.11	113.70
5	D	11	HIS	N-CA-C	5.60	118.32	111.82
3	B	323	LEU	N-CA-C	5.59	117.95	110.35
5	D	171	ASP	N-CA-C	5.59	116.45	108.74
15	N	13	ARG	N-CA-C	-5.59	106.59	113.41
24	W	26	ILE	CB-CA-C	5.58	118.07	111.32
1	0	1120	U	C5'-C4'-C3'	-5.54	107.68	116.00
2	A	25	ALA	N-CA-C	5.53	117.67	108.99
3	B	103	ASP	N-CA-C	-5.52	106.47	113.43
24	W	118	LEU	N-CA-C	5.51	117.99	110.55
9	H	164	CYS	N-CA-C	5.51	118.06	109.52
1	0	2291	A	N9-C1'-C2'	5.51	120.26	112.00
1	0	1592	G	N9-C1'-C2'	5.51	120.26	112.00
3	B	217	ARG	N-CA-C	5.49	117.35	111.36
25	X	77	PHE	N-CA-C	5.49	115.48	108.24
2	A	70	ALA	N-CA-C	5.48	117.53	109.42
3	B	230	GLN	N-CA-C	5.48	119.69	112.89
15	N	75	THR	N-CA-C	5.48	120.64	113.30
14	M	158	ARG	N-CA-C	5.44	118.72	111.75
9	H	121	GLY	N-CA-C	5.44	119.50	112.54
1	0	1979	G	N9-C1'-C2'	5.43	120.15	112.00
30	3	60	LYS	N-CA-C	-5.43	102.80	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	U	50	GLU	N-CA-C	5.43	118.11	111.82
1	0	2301	A	N9-C1'-C2'	5.42	120.13	112.00
4	C	177	GLY	N-CA-C	5.42	118.89	112.33
1	0	1819	G	C5'-C4'-C3'	5.41	124.12	116.00
4	C	19	PRO	N-CA-C	5.41	119.71	111.11
19	R	141	VAL	N-CA-C	5.38	116.34	108.53
18	Q	25	PRO	CA-C-N	5.38	124.90	119.19
18	Q	25	PRO	C-N-CA	5.38	124.90	119.19
22	U	18	GLY	N-CA-C	5.35	118.81	112.33
6	E	119	HIS	N-CA-C	5.33	117.40	108.23
18	Q	2	SER	N-CA-C	-5.29	107.20	113.97
24	W	69	ARG	N-CA-C	5.29	121.48	114.12
6	E	91	PHE	N-CA-C	5.28	116.58	109.24
4	C	162	VAL	N-CA-CB	-5.26	105.47	112.26
24	W	86	GLU	N-CA-C	5.26	119.42	112.89
25	X	25	ARG	N-CA-C	5.24	118.46	111.75
1	0	1261	A	N9-C1'-C2'	5.24	119.86	112.00
2	A	37	VAL	N-CA-C	5.24	120.24	109.34
26	Y	203	VAL	N-CA-C	5.24	116.03	108.48
19	R	76	ASP	N-CA-C	5.24	119.42	112.72
30	3	67	LEU	N-CA-C	5.21	118.09	109.85
2	A	166	ASP	N-CA-C	5.20	117.02	111.36
24	W	27	HIS	N-CA-C	5.20	119.89	113.50
3	B	114	ASP	N-CA-C	-5.18	98.86	108.24
2	A	198	ASP	N-CA-C	5.15	119.65	112.90
19	R	122	GLN	N-CA-C	-5.14	100.13	108.41
23	V	42	ASN	CA-C-N	5.14	124.93	119.28
23	V	42	ASN	C-N-CA	5.14	124.93	119.28
14	M	42	ARG	CA-C-N	5.13	125.05	119.76
14	M	42	ARG	C-N-CA	5.13	125.05	119.76
9	H	163	SER	N-CA-C	-5.13	102.89	110.48
15	N	152	GLU	N-CA-C	-5.10	105.81	112.23
6	E	11	VAL	N-CA-C	5.09	116.86	108.97
1	0	2316	G	C5'-C4'-C3'	-5.08	107.57	115.20
11	J	112	ASP	N-CA-C	-5.08	101.42	109.96
1	0	2673	U	N1-C1'-C2'	5.04	119.57	112.00
9	H	79	GLU	N-CA-C	5.04	118.59	112.23
21	T	92	ASP	N-CA-C	-5.03	101.11	109.46
12	K	5	GLY	N-CA-C	-5.03	106.84	115.08
4	C	215	ALA	N-CA-C	5.02	118.51	112.38
14	M	70	GLY	N-CA-C	5.00	118.92	111.76
3	B	23	THR	N-CA-C	-5.00	102.29	109.24

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1260	G	Sidechain
1	0	1635	U	Sidechain
1	0	1749	U	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1848	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1972	U	Sidechain
1	0	221	G	Sidechain
1	0	2308	U	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2607	U	Sidechain
1	0	2673	U	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	625	U	Sidechain
1	0	722	G	Sidechain
1	0	815	U	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
1	0	867	A	Sidechain
31	9	90	G	Sidechain
24	W	90	TYR	Sidechain

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	0	59021	0	29812	1013	0
2	A	1754	0	1766	26	0
3	B	2625	0	2533	34	0
4	C	1860	0	1813	23	0
5	D	1094	0	1085	14	0
6	E	1358	0	1266	10	0
7	F	890	0	843	2	0
8	G	240	0	231	1	0
9	H	1282	0	1292	14	0
10	I	520	0	500	2	0
11	J	1120	0	1098	18	0
12	K	994	0	1027	12	0
13	L	1118	0	1076	9	0
14	M	1559	0	1573	15	0
15	N	1445	0	1401	14	0
16	O	865	0	873	8	0
17	P	1137	0	1123	12	0
18	Q	735	0	729	7	0
19	R	1150	0	1122	11	0
20	S	642	0	605	7	0
21	T	950	0	924	9	0
22	U	411	0	364	3	0
23	V	500	0	511	6	0
24	W	1196	0	1137	22	0
25	X	655	0	653	8	0
26	Y	1131	0	1133	12	0
27	Z	574	0	534	6	0
28	1	431	0	426	10	0
29	2	396	0	413	8	0
30	3	755	0	729	5	0
31	9	2599	0	1325	77	0
32	0	85	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	9	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	K	1	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	95	0	0	0	0
36	1	1	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	2	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	39	0	36	13	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5993	0	0	125	0
39	1	52	0	0	0	0
39	2	39	0	0	0	0
39	3	66	0	0	0	0
39	9	149	0	0	7	0
39	A	107	0	0	3	0
39	B	146	0	0	1	0
39	C	171	0	0	5	0
39	D	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	E	40	0	0	0	0
39	F	25	0	0	0	0
39	G	18	0	0	0	0
39	H	62	0	0	2	0
39	I	5	0	0	1	0
39	J	52	0	0	1	0
39	K	53	0	0	0	0
39	L	79	0	0	3	0
39	M	128	0	0	0	0
39	N	62	0	0	0	0
39	O	40	0	0	2	0
39	P	65	0	0	0	0
39	Q	43	0	0	0	0
39	R	77	0	0	1	0
39	S	28	0	0	0	0
39	T	32	0	0	0	0
39	U	27	0	0	0	0
39	V	12	0	0	0	0
39	W	65	0	0	1	0
39	X	20	0	0	0	0
39	Y	94	0	0	3	0
39	Z	28	0	0	1	0
All	All	99174	0	59953	1250	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 8.

All (1250) 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)
1:0:871:G:H5'	1:0:871:G:H8	1.10	1.15
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12
1:0:871:G:H5'	1:0:871:G:C8	1.88	1.08
31:9:76:G:H3'	31:9:77:A:H5''	1.36	1.05
31:9:56:A:H2'	31:9:57:A:H5''	1.37	1.04
1:0:156:C:H5''	14:M:171:ARG:HD3	1.43	0.99
1:0:1701:A:H4'	1:0:1702:U:H5''	1.49	0.94
1:0:656:G:H5'	16:O:3:THR:HG22	1.48	0.94
1:0:542:A:H5'	1:0:542:A:H8	1.33	0.93
1:0:1242:A:H5'	11:J:82:THR:HG23	1.47	0.93
1:0:545:G:H5'	1:0:545:G:H8	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2540:G:H4'	37:0:9101:WIN:H1O	1.50	0.91
1:0:870:G:H2'	1:0:871:G:H5''	1.53	0.91
1:0:2717:C:C2'	1:0:2718:C:H5''	2.02	0.90
1:0:1666:C:C2'	1:0:1667:A:H5''	2.02	0.90
15:N:37:ARG:NH1	31:9:6:C:H5''	1.87	0.90
1:0:2506:A:HO2'	1:0:2507:G:H8	0.94	0.89
1:0:381:G:H5''	39:0:2945:HOH:O	1.74	0.86
12:K:10:GLN:H	12:K:10:GLN:HE21	1.18	0.86
1:0:1603:A:H5'	1:0:1605:G:O4'	1.74	0.86
17:P:115:SER:H	17:P:118:GLN:HE21	1.22	0.86
1:0:1474:C:H5'	1:0:1474:C:H6	1.40	0.85
24:W:5:VAL:HG11	24:W:153:MET:HE1	1.56	0.85
1:0:2586:U:H3	1:0:2592:G:H22	1.22	0.85
1:0:1119:G:H2'	11:J:52:GLN:NE2	1.92	0.85
1:0:1160:G:C5'	1:0:1161:A:H5'	2.06	0.84
1:0:2812:A:H2	1:0:2814:A:H62	1.26	0.84
1:0:1160:G:H5'	1:0:1161:A:C5'	2.06	0.84
1:0:1372:A:H3'	39:0:6923:HOH:O	1.76	0.84
1:0:2717:C:H2'	1:0:2718:C:H5''	1.57	0.84
1:0:541:C:H2'	1:0:542:A:H5''	1.59	0.83
1:0:877:G:H5'	1:0:878:G:OP1	1.79	0.83
1:0:1205:U:H2'	1:0:1206:U:H5''	1.59	0.82
1:0:1593:C:H5'	17:P:116:SER:O	1.79	0.82
1:0:823:U:H3'	39:0:3123:HOH:O	1.78	0.82
1:0:2487:C:C2	37:0:9101:WIN:H1F	2.15	0.82
1:0:1666:C:H2'	1:0:1667:A:H5''	1.61	0.82
31:9:29:C:H2'	31:9:30:C:H5'	1.62	0.81
1:0:657:G:OP1	4:C:27:ARG:NH2	2.14	0.81
1:0:506:G:H22	1:0:509:A:C5'	1.94	0.81
31:9:56:A:C2'	31:9:57:A:H5''	2.11	0.81
1:0:506:G:H22	1:0:509:A:H5''	1.46	0.79
1:0:1118:A:H3'	1:0:1118:A:H8	1.47	0.79
1:0:500:G:H21	19:R:98:ASN:HD21	1.26	0.79
1:0:541:C:C2'	1:0:542:A:H5''	2.13	0.78
1:0:1205:U:H2'	1:0:1206:U:C5'	2.12	0.78
1:0:1835:U:H5	1:0:1840:A:N7	1.81	0.78
1:0:1118:A:H62	1:0:1244:U:H3	1.29	0.78
1:0:1118:A:H3'	1:0:1118:A:C8	2.19	0.77
1:0:2637:A:H5'	39:0:3948:HOH:O	1.84	0.77
1:0:157:G:H4'	14:M:95:LYS:HE2	1.66	0.77
1:0:1666:C:O2'	1:0:1667:A:H5''	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H8	1:0:871:G:C5'	1.96	0.77
1:0:1300:G:H1'	39:0:3448:HOH:O	1.83	0.77
1:0:2756:U:H3	1:0:2896:A:H2	1.33	0.76
1:0:1474:C:H5'	1:0:1474:C:C6	2.20	0.76
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.49	0.76
1:0:2533:C:H6	1:0:2533:C:H5'	1.50	0.76
1:0:870:G:C2'	1:0:871:G:H5''	2.16	0.75
1:0:1116:U:HO2'	1:0:1118:A:H2	1.31	0.75
31:9:24:U:H3'	31:9:25:G:H5'	1.67	0.75
1:0:545:G:H5'	1:0:545:G:C8	2.17	0.75
1:0:681:G:N3	1:0:681:G:H5'	2.01	0.75
1:0:2506:A:O2'	1:0:2507:G:H8	1.70	0.75
1:0:1667:A:H5'	1:0:1667:A:H8	1.52	0.75
1:0:1701:A:H5'	39:0:5659:HOH:O	1.86	0.74
1:0:1116:U:H3	1:0:1246:A:H62	1.31	0.74
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.70	0.74
31:9:73:A:H61	31:9:108:C:H42	1.33	0.74
31:9:92:G:H2'	31:9:93:A:C8	2.22	0.73
21:T:24:ARG:HH21	21:T:39:ASN:HD22	1.35	0.73
1:0:1666:C:H2'	1:0:1667:A:C5'	2.18	0.73
1:0:2005:G:OP2	1:0:2005:G:H3'	1.89	0.73
1:0:1206:U:H6	1:0:1206:U:H5'	1.54	0.73
1:0:2420:G:O2'	1:0:2421:G:H5'	1.89	0.73
1:0:281:U:H2'	1:0:282:C:O4'	1.89	0.72
1:0:2717:C:O2'	1:0:2718:C:H5''	1.89	0.72
1:0:182:G:H5'	39:0:4102:HOH:O	1.90	0.72
1:0:559:U:H6	1:0:559:U:H5'	1.55	0.71
1:0:2291:A:C8	1:0:2309:C:H5'	2.25	0.71
1:0:2578:G:H5'	1:0:2578:G:H8	1.55	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.73	0.71
31:9:14:G:H5'	31:9:14:G:H8	1.56	0.70
1:0:12:U:H2'	1:0:13:G:H5'	1.74	0.70
1:0:1116:U:O2'	1:0:1118:A:H2	1.74	0.69
1:0:541:C:H2'	1:0:542:A:C5'	2.22	0.69
1:0:1278:A:H4'	1:0:1279:U:C4	2.28	0.69
1:0:1701:A:H4'	1:0:1702:U:C5'	2.21	0.69
1:0:2635:A:O2'	1:0:2636:C:H5'	1.93	0.69
1:0:450:C:OP1	4:C:184:ARG:NH2	2.24	0.69
1:0:542:A:H5'	1:0:542:A:C8	2.22	0.69
1:0:853:C:H3'	39:0:3276:HOH:O	1.91	0.69
1:0:93:C:H5''	23:V:1:THR:HB	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1834:C:H2'	1:0:1840:A:N6	2.07	0.68
1:0:603:A:H5''	1:0:604:G:OP1	1.93	0.68
1:0:2769:C:C2'	1:0:2770:G:H5'	2.24	0.68
1:0:2502:C:H2'	1:0:2503:A:H5'	1.76	0.68
1:0:2768:A:H2'	1:0:2769:C:O4'	1.93	0.67
1:0:1189:A:H1'	1:0:1209:C:O4'	1.94	0.67
1:0:2716:G:H5''	3:B:206:THR:HG21	1.74	0.67
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.58	0.67
1:0:1632:A:H2'	1:0:1633:C:H5'	1.76	0.67
3:B:238:ASN:HD22	3:B:240:GLY:H	1.43	0.67
1:0:2502:C:C2'	1:0:2503:A:H5'	2.25	0.67
24:W:149:LEU:HG	24:W:153:MET:HE2	1.77	0.67
3:B:221:GLN:HE22	12:K:42:ASN:HD22	1.41	0.67
1:0:1119:G:N2	1:0:1246:A:C2	2.60	0.67
1:0:20:G:H21	19:R:117:HIS:HD2	1.41	0.66
1:0:1625:U:H4'	39:0:3427:HOH:O	1.94	0.66
1:0:1189:A:H1'	1:0:1209:C:C1'	2.24	0.66
1:0:188:C:H5''	14:M:163:LEU:HD21	1.77	0.66
1:0:1377:C:H6	1:0:1377:C:H5'	1.61	0.66
1:0:2908:A:H2'	1:0:2909:G:O4'	1.96	0.66
39:0:4058:HOH:O	35:K:8812:CL:CL	2.50	0.65
1:0:2443:C:H1'	13:L:56:LYS:HE3	1.76	0.65
1:0:2468:A:H61	30:3:48:ASN:HD21	1.44	0.65
1:0:2320:U:H4'	1:0:2321:A:O4'	1.97	0.65
15:N:141:ARG:HH21	31:9:48:C:H4'	1.59	0.65
1:0:671:A:O2'	1:0:672:G:H2'	1.97	0.65
1:0:2710:U:H1'	39:0:7520:HOH:O	1.96	0.65
1:0:1973:A:H2'	1:0:1974:G:O4'	1.96	0.65
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.79	0.65
31:9:49:G:O2'	31:9:50:G:H5'	1.97	0.65
1:0:308:U:H5'	1:0:309:C:OP1	1.96	0.65
1:0:821:U:H2'	1:0:822:C:H6	1.61	0.65
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.45	0.64
31:9:39:U:H1'	31:9:44:A:H61	1.61	0.64
1:0:136:C:H2'	1:0:137:U:O4'	1.97	0.64
1:0:871:G:C8	1:0:871:G:C5'	2.74	0.64
1:0:1181:A:H2'	1:0:1182:C:H5'	1.78	0.64
1:0:1184:C:H1'	39:0:7308:HOH:O	1.98	0.64
31:9:75:G:H1	31:9:106:U:H3	1.45	0.64
1:0:1947:G:H2'	1:0:1948:G:H8	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:3:A:N6	31:9:22:G:H1'	2.13	0.64
1:0:1183:C:N4	1:0:1184:C:H41	1.94	0.64
1:0:2787:C:H5	39:0:3383:HOH:O	1.81	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.97	0.64
30:3:2:GLN:HE21	30:3:91:GLN:HE21	1.45	0.63
1:0:371:U:H2'	1:0:372:A:H8	1.63	0.63
1:0:1641:A:H2'	1:0:1642:A:H5'	1.80	0.63
1:0:2491:G:H1'	39:0:6473:HOH:O	1.97	0.63
1:0:1166:A:H1'	1:0:1192:A:C2	2.33	0.63
1:0:1165:G:H4'	1:0:1174:A:O2'	1.99	0.63
31:9:7:G:H5'	39:9:5071:HOH:O	1.98	0.63
1:0:2896:A:H5''	39:0:5399:HOH:O	1.99	0.62
14:M:164:THR:HG22	14:M:166:ALA:H	1.63	0.62
1:0:2533:C:H5'	1:0:2533:C:C6	2.33	0.62
39:0:4183:HOH:O	12:K:39:GLY:HA2	1.99	0.62
1:0:482:G:H4'	1:0:508:A:N1	2.15	0.62
1:0:272:A:H5'	1:0:273:G:OP2	1.99	0.62
1:0:2419:U:H5''	1:0:2420:G:H5'	1.81	0.62
1:0:1835:U:C5	1:0:1840:A:N7	2.67	0.62
1:0:1886:A:H4'	39:Z:395:HOH:O	1.99	0.62
1:0:1762:C:H2'	1:0:1763:C:H6	1.64	0.62
1:0:2486:A:H3'	39:0:3735:HOH:O	1.99	0.62
1:0:2748:G:H2'	39:0:7410:HOH:O	2.00	0.62
15:N:141:ARG:NH2	31:9:48:C:H4'	2.15	0.62
31:9:1:U:H4'	31:9:3:A:OP1	1.99	0.61
1:0:1800:G:H1'	17:P:88:GLN:NE2	2.15	0.61
1:0:1819:G:H5'	39:0:3491:HOH:O	1.99	0.61
1:0:285:A:H2'	1:0:286:U:O4'	2.00	0.61
1:0:2401:A:H2'	1:0:2402:A:C8	2.35	0.61
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.81	0.61
1:0:440:C:H2'	1:0:441:A:C8	2.36	0.61
1:0:56:G:H5''	23:V:50:ARG:NH1	2.15	0.61
1:0:1741:U:H5'	1:0:1742:A:OP1	2.00	0.61
16:O:32:ARG:HE	16:O:35:LYS:HD2	1.66	0.61
1:0:282:C:H1'	1:0:368:C:N4	2.15	0.61
1:0:820:G:H3'	39:0:6936:HOH:O	2.01	0.61
31:9:76:G:H3'	31:9:77:A:C5'	2.22	0.61
1:0:553:G:P	26:Y:204:ARG:HH22	2.24	0.60
1:0:656:G:H1'	39:C:7042:HOH:O	2.00	0.60
1:0:1201:C:H5''	39:0:5584:HOH:O	1.99	0.60
1:0:1528:A:H2'	1:0:1529:G:O4'	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.83	0.60
1:0:1015:C:H2'	1:0:1016:U:H6	1.66	0.60
1:0:1097:A:H5''	24:W:125:HIS:NE2	2.16	0.60
1:0:558:C:C2'	1:0:559:U:H5''	2.32	0.60
1:0:1187:U:O2'	1:0:1189:A:H2	1.83	0.60
1:0:1213:C:O2'	1:0:1214:G:H5'	2.02	0.60
1:0:2054:A:N3	19:R:128:ARG:NH2	2.49	0.60
1:0:1189:A:H3'	39:0:7609:HOH:O	2.02	0.60
1:0:1209:C:H2'	1:0:1210:G:H8	1.65	0.60
1:0:2472:C:O2'	1:0:2634:G:H4'	2.01	0.60
31:9:12:C:H5'	31:9:70:U:O4'	2.00	0.60
1:0:814:G:H4'	39:0:7240:HOH:O	2.01	0.60
31:9:24:U:H3'	31:9:25:G:C5'	2.31	0.60
15:N:11:ARG:HD3	31:9:114:G:O6	2.02	0.59
1:0:2426:G:H1'	39:0:5391:HOH:O	2.01	0.59
1:0:1166:A:H61	1:0:1180:U:H3	1.50	0.59
1:0:1972:U:H2'	1:0:1973:A:H5'	1.85	0.59
1:0:2563:U:H2'	1:0:2565:C:O5'	2.02	0.59
1:0:282:C:O2'	1:0:283:U:H5'	2.02	0.59
1:0:338:C:H4'	4:C:174:ILE:CD1	2.32	0.59
1:0:399:C:H5'	14:M:179:GLY:O	2.03	0.59
1:0:1120:U:C6	1:0:1120:U:H5''	2.38	0.59
4:C:127:ARG:NH2	4:C:225:PRO:HG2	2.18	0.59
7:F:91:VAL:HG12	7:F:92:GLY:H	1.68	0.59
1:0:2712:G:H5'	39:0:4183:HOH:O	2.02	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.03	0.59
1:0:2616:G:H1'	39:0:8327:HOH:O	2.03	0.58
1:0:2781:U:H1'	6:E:139:GLU:OE2	2.03	0.58
31:9:13:A:O2'	31:9:14:G:H5''	2.02	0.58
1:0:56:G:H5''	23:V:50:ARG:HH12	1.67	0.58
1:0:1446:U:H2'	20:S:55:GLN:NE2	2.17	0.58
1:0:2252:A:C5	1:0:2253:G:H1'	2.38	0.58
31:9:39:U:H3'	31:9:40:C:H5''	1.85	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.03	0.58
1:0:1189:A:H1'	1:0:1209:C:H1'	1.84	0.58
1:0:1328:A:OP1	26:Y:169:ARG:HD2	2.03	0.58
1:0:1363:G:P	4:C:76:ARG:HH22	2.26	0.58
1:0:2241:C:H2'	1:0:2242:U:C6	2.38	0.58
1:0:2270:G:H4'	2:A:223:ARG:NH1	2.18	0.58
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.83	0.58
1:0:821:U:H2'	1:0:822:C:C6	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:902:G:N7	13:L:18:HIS:HD2	2.02	0.58
1:0:67:A:H5''	1:0:69:A:C8	2.39	0.58
1:0:960:G:H4'	39:0:7253:HOH:O	2.04	0.58
1:0:1165:G:H1'	1:0:1174:A:H1'	1.85	0.58
1:0:1441:G:O2'	1:0:1442:A:H5'	2.04	0.58
1:0:1790:C:H2'	1:0:1791:U:H6	1.68	0.58
1:0:1679:C:H5'	39:0:4173:HOH:O	2.04	0.58
1:0:2524:G:H21	1:0:2526:C:N4	2.02	0.58
1:0:2783:A:H3'	39:0:4201:HOH:O	2.03	0.58
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.21	0.58
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.84	0.58
1:0:952:G:N3	1:0:2302:A:H2'	2.19	0.57
1:0:1973:A:H5'	1:0:1973:A:H8	1.68	0.57
1:0:2894:C:O2'	1:0:2895:C:H5'	2.04	0.57
3:B:36:PRO:HG3	3:B:169:GLY:H	1.68	0.57
22:U:39:ASN:ND2	22:U:44:ARG:HH11	2.02	0.57
1:0:1118:A:C8	1:0:1118:A:C3'	2.83	0.57
1:0:1733:A:H4'	3:B:212:GLN:HA	1.85	0.57
1:0:2670:G:O2'	1:0:2671:U:H5'	2.03	0.57
1:0:407:A:H5'	39:0:5296:HOH:O	2.04	0.57
1:0:1419:U:H2'	1:0:1685:A:C2	2.39	0.57
1:0:2769:C:H2'	1:0:2770:G:O4'	2.04	0.57
1:0:2769:C:H2'	1:0:2770:G:H5'	1.85	0.57
1:0:1441:G:H1'	39:0:7717:HOH:O	2.03	0.57
1:0:2769:C:O2'	1:0:2770:G:H5'	2.04	0.57
5:D:154:LYS:H	5:D:154:LYS:HD2	1.69	0.57
31:9:14:G:H5'	31:9:14:G:C8	2.38	0.57
11:J:19:MET:HE3	11:J:132:LEU:HD11	1.86	0.57
1:0:1994:A:P	12:K:66:ARG:HH22	2.28	0.57
5:D:140:ARG:HB3	31:9:29:C:H5''	1.86	0.57
1:0:1015:C:H2'	1:0:1016:U:C6	2.40	0.57
1:0:1838:U:O2'	1:0:2644:C:H5'	2.05	0.57
1:0:2780:C:H1'	6:E:143:GLN:HE21	1.69	0.57
31:9:55:U:H4'	31:9:56:A:C8	2.39	0.57
1:0:1166:A:P	1:0:1174:A:H4'	2.44	0.57
1:0:1819:G:H2'	1:0:1820:G:H4'	1.86	0.57
1:0:68:U:O2'	1:0:69:A:H5''	2.05	0.57
1:0:2365:G:H4'	18:Q:45:PRO:O	2.05	0.57
1:0:1008:C:H5''	9:H:19:ARG:HH12	1.68	0.57
1:0:1667:A:H5'	1:0:1667:A:C8	2.37	0.57
1:0:2781:U:O2'	1:0:2782:G:H5'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2900:G:H2'	1:0:2901:C:O4'	2.05	0.56
1:0:625:U:H3'	39:0:7631:HOH:O	2.04	0.56
1:0:969:G:H1	1:0:999:C:H42	1.53	0.56
1:0:1132:A:N6	1:0:1229:C:H2'	2.20	0.56
17:P:115:SER:H	17:P:118:GLN:NE2	1.99	0.56
1:0:2534:C:H1'	39:0:8179:HOH:O	2.04	0.56
1:0:65:C:O2'	1:0:66:G:H5'	2.04	0.56
1:0:119:A:H2'	1:0:120:A:H5''	1.86	0.56
1:0:794:U:H3	1:0:819:A:H61	1.54	0.56
1:0:95:A:H5''	1:0:97:G:O4'	2.05	0.56
1:0:560:U:H2'	1:0:561:G:H8	1.69	0.56
31:9:38:A:H2'	31:9:39:U:C6	2.41	0.56
1:0:69:A:H5'	1:0:69:A:H8	1.69	0.56
1:0:797:A:N6	1:0:816:G:H1'	2.20	0.56
1:0:2755:G:H1'	39:0:3447:HOH:O	2.06	0.56
25:X:61:ARG:HH12	25:X:67:PRO:HD3	1.70	0.56
1:0:1279:U:H2'	1:0:1279:U:O2	2.05	0.56
1:0:2032:U:H5'	39:0:3222:HOH:O	2.04	0.56
1:0:2760:C:H5''	39:0:4329:HOH:O	2.06	0.56
5:D:103:ASN:HD22	5:D:134:LEU:H	1.54	0.56
1:0:1634:G:H3'	39:0:8650:HOH:O	2.06	0.56
1:0:2756:U:N3	1:0:2896:A:H2	2.02	0.56
15:N:144:GLY:O	15:N:147:ILE:HG22	2.05	0.56
1:0:162:C:H2'	1:0:163:U:H5'	1.88	0.55
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.55
1:0:731:U:H2'	1:0:732:C:C6	2.41	0.55
1:0:1845:A:OP2	2:A:190:ARG:NH1	2.39	0.55
1:0:196:G:H2'	39:0:6170:HOH:O	2.05	0.55
1:0:613:C:H2'	1:0:614:U:H6	1.71	0.55
1:0:1205:U:C2'	1:0:1206:U:H5''	2.34	0.55
1:0:1330:A:H5''	39:Y:7277:HOH:O	2.06	0.55
4:C:139:VAL:HG13	39:C:6251:HOH:O	2.06	0.55
1:0:2597:U:H1'	39:0:4058:HOH:O	2.05	0.55
1:0:2769:C:H2'	1:0:2770:G:C5'	2.36	0.55
1:0:1422:U:H2'	1:0:1423:C:C6	2.41	0.55
1:0:1497:G:H4'	1:0:1627:G:O2'	2.07	0.55
1:0:1654:U:H2'	2:A:47:HIS:HD2	1.71	0.55
31:9:29:C:C2'	31:9:30:C:H5'	2.33	0.55
31:9:55:U:H4'	31:9:56:A:H8	1.71	0.55
1:0:317:A:OP1	21:T:52:ARG:O	2.24	0.55
1:0:776:A:OP1	28:1:28:HIS:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1701:A:H5''	1:0:1702:U:H3'	1.88	0.55
5:D:76:ARG:NH2	31:9:44:A:H1'	2.21	0.55
31:9:95:C:O2'	31:9:96:C:H5'	2.06	0.55
1:0:31:C:H2'	39:0:7619:HOH:O	2.05	0.55
1:0:306:A:P	21:T:38:ARG:HH21	2.30	0.55
1:0:371:U:H2'	1:0:372:A:C8	2.42	0.55
1:0:468:U:H3'	39:0:7448:HOH:O	2.05	0.55
1:0:559:U:H5'	1:0:559:U:C6	2.40	0.55
1:0:1182:C:H1'	1:0:1192:A:H8	1.71	0.55
9:H:72:ALA:HB2	9:H:156:ALA:HB2	1.87	0.55
1:0:1364:G:H1'	39:0:3619:HOH:O	2.06	0.55
1:0:2509:A:H2'	1:0:2510:C:O4'	2.07	0.55
1:0:2613:G:O2'	1:0:2614:C:H5'	2.07	0.55
4:C:162:VAL:HG22	4:C:232:LEU:HD21	1.89	0.55
9:H:59:GLN:HE21	9:H:129:ARG:HE	1.55	0.55
11:J:19:MET:HE1	11:J:78:ILE:HG22	1.88	0.55
1:0:588:G:O6	24:W:154:ARG:NH1	2.40	0.55
1:0:1118:A:H8	1:0:1119:G:H5''	1.71	0.55
1:0:1173:A:H4'	1:0:1174:A:C8	2.41	0.55
1:0:1632:A:C2'	1:0:1633:C:H5'	2.37	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.22	0.55
1:0:2050:G:H5''	19:R:80:TYR:O	2.06	0.55
1:0:1527:A:H1'	1:0:1528:A:C8	2.42	0.54
1:0:1741:U:O2'	1:0:2723:G:H4'	2.07	0.54
1:0:1979:G:H2'	39:0:3969:HOH:O	2.07	0.54
1:0:2064:U:H5'	1:0:2652:U:H4'	1.89	0.54
11:J:41:ALA:HB3	39:J:5907:HOH:O	2.06	0.54
16:O:38:ARG:NH1	39:O:7674:HOH:O	2.40	0.54
1:0:69:A:C8	1:0:69:A:H5'	2.43	0.54
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.39	0.54
2:A:48:ASP:HB3	39:A:5706:HOH:O	2.07	0.54
1:0:121:U:OP2	29:2:10:ARG:NH2	2.38	0.54
1:0:841:A:H5''	39:0:6534:HOH:O	2.07	0.54
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.89	0.54
1:0:128:A:O2'	1:0:129:A:H5'	2.07	0.54
1:0:1191:A:H2	1:0:1206:U:H3	1.56	0.54
1:0:1790:C:H2'	1:0:1791:U:C6	2.42	0.54
1:0:1855:G:H4'	1:0:1856:C:O5'	2.07	0.54
1:0:836:G:H5''	39:0:3971:HOH:O	2.07	0.54
1:0:1053:G:OP1	9:H:15:PRO:HG3	2.08	0.54
1:0:1787:C:H4'	1:0:2883:A:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2435:U:H1'	39:0:4462:HOH:O	2.07	0.54
1:0:2524:G:H21	1:0:2526:C:H41	1.56	0.54
1:0:2672:C:H1'	39:0:6210:HOH:O	2.07	0.54
31:9:92:G:H2'	31:9:93:A:H8	1.70	0.54
1:0:1762:C:H2'	1:0:1763:C:C6	2.43	0.54
1:0:10:U:O4	1:0:532:A:OP2	2.25	0.54
1:0:90:A:H2'	1:0:91:G:O4'	2.08	0.54
1:0:1594:C:O2'	1:0:1607:A:H4'	2.08	0.54
1:0:2414:A:H2'	1:0:2415:A:C8	2.42	0.54
1:0:2505:G:O2'	1:0:2506:A:H5'	2.08	0.54
1:0:2779:G:H21	6:E:143:GLN:NE2	2.06	0.54
1:0:2878:U:H2'	1:0:2879:A:O4'	2.08	0.54
1:0:506:G:H22	1:0:509:A:H5'	1.69	0.53
1:0:1921:A:O2'	1:0:1922:A:H5'	2.07	0.53
37:0:9101:WIN:H1FB	37:0:9101:WIN:H1OA	1.89	0.53
29:2:41:HIS:H	29:2:45:ASN:HD22	1.56	0.53
1:0:694:A:H2'	1:0:695:C:H5'	1.90	0.53
1:0:1206:U:H2'	1:0:1207:A:O4'	2.08	0.53
1:0:1972:U:H2'	1:0:1973:A:C5'	2.39	0.53
1:0:2700:G:H3'	39:0:8266:HOH:O	2.08	0.53
2:A:121:ALA:O	2:A:124:VAL:HG22	2.08	0.53
6:E:95:VAL:HG11	6:E:131:LEU:HD11	1.90	0.53
1:0:445:U:H2'	1:0:446:G:H8	1.72	0.53
1:0:1119:G:H8	11:J:52:GLN:HE22	1.55	0.53
1:0:2487:C:C6	37:0:9101:WIN:O1K	2.61	0.53
20:S:33:SER:O	20:S:37:VAL:HG23	2.07	0.53
31:9:64:C:H2'	31:9:65:A:H5'	1.91	0.53
1:0:87:C:H2'	29:2:28:LYS:O	2.08	0.53
1:0:558:C:H2'	1:0:559:U:C5'	2.38	0.53
1:0:1119:G:H22	1:0:1246:A:H2	1.51	0.53
1:0:1477:C:H5'	1:0:1868:G:C5'	2.38	0.53
5:D:103:ASN:ND2	5:D:134:LEU:H	2.07	0.53
31:9:23:U:O2'	31:9:24:U:H4'	2.09	0.53
1:0:316:A:N3	1:0:336:G:O2'	2.38	0.53
1:0:2445:U:H2'	1:0:2446:G:C8	2.43	0.53
2:A:179:MET:HG2	2:A:186:TRP:HB2	1.91	0.53
1:0:1947:G:H2'	1:0:1948:G:C8	2.43	0.53
1:0:2111:G:H1'	39:0:3082:HOH:O	2.07	0.53
1:0:2344:G:N3	1:0:2344:G:H2'	2.23	0.53
1:0:447:A:O2'	1:0:448:G:H5'	2.09	0.53
1:0:635:A:H2'	1:0:636:G:H5''	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:848:C:H5'	39:0:7034:HOH:O	2.09	0.53
1:0:1299:G:O6	13:L:6:ARG:HD3	2.08	0.53
1:0:1878:G:O2'	1:0:1879:U:OP2	2.27	0.53
31:9:2:U:OP2	31:9:3:A:H5'	2.08	0.53
1:0:947:U:O2'	1:0:948:G:H5'	2.09	0.53
1:0:2795:C:O2'	1:0:2796:U:H5'	2.09	0.53
31:9:71:C:H2'	31:9:72:C:H6	1.74	0.53
1:0:407:A:H2'	1:0:408:A:C8	2.44	0.53
1:0:195:C:H2'	1:0:196:G:H5'	1.90	0.52
1:0:450:C:H4'	4:C:46:TYR:CE1	2.43	0.52
1:0:1803:C:H2'	1:0:1804:A:C8	2.44	0.52
13:L:136:ALA:HB3	39:L:6166:HOH:O	2.07	0.52
1:0:1181:A:C2'	1:0:1182:C:H5'	2.39	0.52
1:0:1375:A:C2'	1:0:1376:G:H5'	2.39	0.52
1:0:1603:A:H5''	1:0:1605:G:H5'	1.91	0.52
1:0:2364:A:H5''	18:Q:15:LYS:HD3	1.91	0.52
1:0:2387:U:H2'	1:0:2388:C:C6	2.44	0.52
6:E:137:ASP:O	6:E:141:VAL:HG23	2.10	0.52
1:0:1180:U:H4'	10:I:86:GLU:HG2	1.91	0.52
1:0:1268:C:H2'	1:0:1269:G:H8	1.74	0.52
1:0:2103:A:H2'	1:0:2104:C:H5'	1.90	0.52
39:0:6217:HOH:O	21:T:38:ARG:NH1	2.42	0.52
1:0:790:A:H1'	1:0:1710:A:H2'	1.91	0.52
1:0:1427:A:H61	1:0:1440:U:H1'	1.73	0.52
1:0:2039:A:OP2	3:B:234:ARG:NH2	2.43	0.52
1:0:247:A:H2'	39:0:8680:HOH:O	2.09	0.52
1:0:1333:U:H2'	1:0:1334:C:C6	2.44	0.52
31:9:34:A:H2'	31:9:35:C:O4'	2.10	0.52
1:0:10:U:O4	1:0:531:G:H2'	2.10	0.52
1:0:522:U:O2'	1:0:1366:C:H5'	2.09	0.52
1:0:944:G:H21	24:W:44:MET:HE2	1.75	0.52
37:0:9101:WIN:H1A	37:0:9101:WIN:H1BA	1.92	0.52
11:J:127:ILE:HG22	35:J:8801:CL:CL	2.46	0.52
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.91	0.52
3:B:217:ARG:HG3	3:B:257:THR:HG22	1.92	0.52
28:1:8:GLN:HE22	28:1:11:LYS:NZ	2.08	0.52
1:0:303:C:H2'	1:0:304:G:O4'	2.10	0.52
1:0:1596:U:H2'	1:0:1598:A:OP2	2.10	0.52
1:0:2542:C:H1'	39:0:6378:HOH:O	2.08	0.52
1:0:821:U:H3'	39:0:8455:HOH:O	2.10	0.52
1:0:1060:C:H6	1:0:1060:C:H5'	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1167:G:H2'	1:0:1168:C:C6	2.45	0.52
1:0:2248:C:H3'	39:0:4476:HOH:O	2.10	0.52
1:0:2256:G:O2'	1:0:2257:G:H5'	2.10	0.52
1:0:2717:C:H2'	1:0:2718:C:C5'	2.34	0.52
1:0:249:G:O2'	1:0:250:C:H5'	2.10	0.52
3:B:221:GLN:HE22	12:K:42:ASN:ND2	2.08	0.52
30:3:2:GLN:HE21	30:3:91:GLN:NE2	2.07	0.52
1:0:564:G:H1'	39:0:5694:HOH:O	2.10	0.51
1:0:1928:C:H2'	1:0:1929:G:O4'	2.10	0.51
1:0:2584:G:H4'	39:0:6824:HOH:O	2.09	0.51
5:D:141:VAL:HG21	31:9:57:A:H8	1.75	0.51
1:0:1175:G:H1'	1:0:1193:A:H2'	1.92	0.51
1:0:1940:C:H4'	39:0:7130:HOH:O	2.10	0.51
4:C:118:THR:O	4:C:136:VAL:HG13	2.09	0.51
13:L:143:THR:HG22	13:L:144:ASP:H	1.75	0.51
1:0:497:A:H2'	1:0:498:A:C5'	2.40	0.51
1:0:1313:A:H5'	26:Y:208:LYS:O	2.10	0.51
1:0:1444:G:H5''	20:S:11:THR:HG22	1.92	0.51
1:0:105:G:O2'	1:0:106:A:H5'	2.11	0.51
1:0:154:C:H2'	1:0:155:C:H6	1.76	0.51
1:0:905:C:H3'	39:0:4139:HOH:O	2.10	0.51
1:0:1181:A:N1	1:0:1192:A:O2'	2.42	0.51
1:0:1205:U:H2'	1:0:1206:U:H5'	1.91	0.51
1:0:2271:G:H2'	1:0:2271:G:N3	2.24	0.51
1:0:2271:G:H5'	39:A:3548:HOH:O	2.09	0.51
1:0:1029:U:O2'	1:0:1273:C:OP1	2.26	0.51
1:0:1183:C:H41	1:0:1192:A:P	2.34	0.51
1:0:200:C:H2'	39:0:8130:HOH:O	2.11	0.51
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.93	0.51
1:0:2597:U:H2'	1:0:2598:U:H5'	1.91	0.51
1:0:1165:G:H4'	1:0:1174:A:HO2'	1.73	0.51
1:0:1299:G:N7	13:L:6:ARG:NH1	2.59	0.51
1:0:1856:C:H5'	1:0:1858:A:O4'	2.11	0.51
1:0:2088:C:H1'	1:0:2841:A:N1	2.26	0.51
1:0:958:G:H2'	1:0:959:C:C6	2.45	0.51
1:0:1566:C:H2'	1:0:1567:G:C8	2.46	0.51
1:0:2353:A:H4'	1:0:2354:A:O5'	2.10	0.51
14:M:99:ARG:HD2	14:M:167:GLY:HA2	1.93	0.51
27:Z:60:ASP:HB3	27:Z:69:ASP:HB3	1.93	0.51
1:0:1391:G:H2'	1:0:1392:A:H5'	1.93	0.51
1:0:1634:G:H2'	1:0:1635:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2510:C:H42	1:0:2564:G:H22	1.58	0.51
24:W:64:THR:O	24:W:68:THR:HG22	2.11	0.51
1:0:364:U:H2'	1:0:365:G:O4'	2.11	0.51
1:0:527:U:H2'	1:0:528:G:C8	2.46	0.51
1:0:1234:U:N3	3:B:244:PRO:HB3	2.25	0.50
1:0:1636:G:O2'	1:0:1637:A:H5'	2.10	0.50
1:0:1603:A:C5'	1:0:1605:G:H5'	2.41	0.50
1:0:1755:A:H2'	1:0:1756:G:O4'	2.11	0.50
31:9:90:G:H3'	39:9:2357:HOH:O	2.10	0.50
1:0:1130:U:H4'	39:0:5437:HOH:O	2.11	0.50
2:A:199:HIS:HD2	2:A:201:PHE:H	1.59	0.50
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.93	0.50
1:0:1118:A:C8	1:0:1119:G:H5''	2.45	0.50
1:0:1525:G:H5'	1:0:1526:A:OP2	2.11	0.50
1:0:1864:C:C5	14:M:75:ARG:NH1	2.79	0.50
1:0:2002:C:H2'	1:0:2003:U:H5'	1.94	0.50
7:F:2:VAL:HG22	7:F:57:GLU:OE1	2.11	0.50
25:X:30:MET:HE1	25:X:58:ALA:HB3	1.92	0.50
1:0:10:U:H3'	1:0:10:U:H6	1.76	0.50
1:0:280:C:H2'	1:0:281:U:O4'	2.11	0.50
1:0:1980:U:O2	1:0:2008:U:H4'	2.10	0.50
1:0:324:G:O2'	1:0:325:U:H5'	2.12	0.50
1:0:899:C:H5'	39:0:7471:HOH:O	2.11	0.50
1:0:1189:A:O2'	1:0:1208:C:H2'	2.12	0.50
1:0:1413:A:H2'	1:0:1414:A:O4'	2.12	0.50
1:0:338:C:H4'	4:C:174:ILE:HD11	1.94	0.50
1:0:441:A:O5'	1:0:441:A:H8	1.95	0.50
1:0:485:A:N3	1:0:487:G:H5''	2.27	0.50
1:0:656:G:H5'	16:O:3:THR:CG2	2.33	0.50
1:0:1406:A:H4'	1:0:1407:A:H5''	1.92	0.50
1:0:1566:C:H2'	1:0:1567:G:H8	1.76	0.50
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.47	0.50
1:0:2467:A:O2'	1:0:2468:A:H2'	2.11	0.50
1:0:380:A:H2'	39:0:6974:HOH:O	2.11	0.50
1:0:1066:U:H2'	1:0:1067:A:C8	2.47	0.50
1:0:1116:U:O2'	1:0:1118:A:C2	2.50	0.50
1:0:2659:U:H5''	39:0:8896:HOH:O	2.11	0.50
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.50
1:0:2135:A:O2'	1:0:2136:G:H5'	2.12	0.50
1:0:2511:A:H2'	1:0:2512:U:O4'	2.12	0.50
1:0:2898:G:H4'	3:B:288:GLY:HA2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:536:A:H3'	39:0:3958:HOH:O	2.11	0.49
1:0:969:G:H1	1:0:999:C:N4	2.10	0.49
1:0:1864:C:H5	14:M:75:ARG:NH1	2.10	0.49
1:0:1878:G:H1'	39:0:5431:HOH:O	2.12	0.49
1:0:2703:A:H2'	1:0:2704:C:H6	1.77	0.49
1:0:21:G:H4'	19:R:2:ILE:HG22	1.93	0.49
1:0:170:U:H2'	1:0:171:C:H5'	1.94	0.49
1:0:319:A:H4'	1:0:338:C:C5	2.47	0.49
1:0:711:G:H1'	39:0:6793:HOH:O	2.11	0.49
1:0:920:C:H4'	1:0:921:G:C2	2.47	0.49
1:0:1589:G:H22	1:0:1605:G:H1'	1.77	0.49
1:0:1644:C:H2'	1:0:1645:U:H6	1.77	0.49
1:0:2345:A:H3'	1:0:2346:C:C6	2.47	0.49
1:0:2415:A:H2'	1:0:2416:G:H5'	1.93	0.49
1:0:459:A:H4'	39:0:4687:HOH:O	2.12	0.49
1:0:857:A:H4'	2:A:176:HIS:CD2	2.46	0.49
1:0:941:G:C5	1:0:942:U:C4	3.00	0.49
1:0:1307:A:H2'	1:0:1308:A:C8	2.47	0.49
1:0:2521:A:OP2	9:H:6:ALA:HB3	2.11	0.49
13:L:138:GLY:HA3	39:L:4360:HOH:O	2.11	0.49
31:9:114:G:H2'	31:9:115:C:C6	2.48	0.49
1:0:451:C:O2'	1:0:452:G:H5'	2.12	0.49
1:0:500:G:H21	19:R:98:ASN:ND2	2.05	0.49
1:0:797:A:H61	1:0:816:G:H1'	1.77	0.49
1:0:2720:C:O2	12:K:87:ARG:NH2	2.45	0.49
1:0:2103:A:N6	37:0:9101:WIN:O1G	2.41	0.49
1:0:2538:A:H1'	37:0:9101:WIN:O1M	2.12	0.49
1:0:2578:G:H5'	1:0:2578:G:C8	2.43	0.49
1:0:2781:U:C2'	1:0:2782:G:H5'	2.42	0.49
1:0:660:A:H4'	1:0:661:G:O5'	2.13	0.49
1:0:932:U:H2'	1:0:933:C:C6	2.48	0.49
1:0:1115:U:O2'	1:0:1116:U:H5'	2.11	0.49
1:0:1172:G:H5''	39:0:7015:HOH:O	2.12	0.49
1:0:2807:U:P	3:B:27:ASN:HD21	2.34	0.49
1:0:1181:A:H2'	1:0:1182:C:C5'	2.42	0.49
1:0:1398:G:O2'	1:0:1399:A:H5'	2.13	0.49
1:0:2072:G:H3'	1:0:2073:G:C5'	2.43	0.49
14:M:23:LEU:HD13	14:M:27:ARG:HH21	1.78	0.49
31:9:64:C:C2'	31:9:65:A:H5'	2.43	0.49
1:0:281:U:O2'	1:0:282:C:H5'	2.13	0.49
1:0:941:G:O2'	1:0:942:U:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1244:U:OP1	11:J:18:ILE:HD13	2.13	0.49
1:0:1453:G:H2'	1:0:1454:U:O4'	2.13	0.49
1:0:2325:U:O2'	1:0:2411:C:H1'	2.13	0.49
1:0:2498:C:O2'	1:0:2499:U:H5'	2.12	0.49
1:0:2821:C:H4'	3:B:116:PRO:HG3	1.95	0.49
1:0:28:G:H1'	39:0:3446:HOH:O	2.13	0.49
1:0:2032:U:H2'	1:0:2033:G:C5'	2.43	0.49
1:0:2510:C:H5'	1:0:2511:A:OP2	2.13	0.49
1:0:2524:G:N2	1:0:2526:C:H41	2.11	0.49
1:0:2729:C:O2'	1:0:2730:G:H5'	2.12	0.49
31:9:73:A:H61	31:9:108:C:N4	2.06	0.49
1:0:250:C:O2'	1:0:251:C:H5'	2.13	0.49
1:0:669:G:O2'	1:0:670:G:H5'	2.12	0.49
1:0:946:C:H2'	1:0:947:U:C6	2.47	0.49
1:0:1423:C:O2'	1:0:1424:A:H5'	2.13	0.49
1:0:1589:G:N2	1:0:1605:G:H1'	2.27	0.49
4:C:127:ARG:HD3	4:C:129:HIS:HE1	1.77	0.49
1:0:12:U:C2'	1:0:13:G:H5'	2.42	0.48
1:0:589:U:H2'	1:0:590:A:H8	1.78	0.48
1:0:1333:U:H2'	1:0:1334:C:H6	1.78	0.48
1:0:1603:A:H5'	1:0:1605:G:C4'	2.43	0.48
1:0:1735:C:OP2	3:B:234:ARG:HG3	2.13	0.48
1:0:2887:G:H2'	1:0:2888:U:C6	2.47	0.48
8:G:64:ASN:N	8:G:64:ASN:HD22	2.10	0.48
1:0:1980:U:O2'	1:0:1981:A:H5'	2.13	0.48
39:0:7291:HOH:O	3:B:211:THR:HG21	2.12	0.48
1:0:64:G:H2'	1:0:65:C:O4'	2.13	0.48
1:0:130:C:H2'	39:0:7324:HOH:O	2.13	0.48
1:0:271:C:H41	1:0:378:A:H2	1.61	0.48
1:0:1495:C:H1'	1:0:1573:A:H1'	1.94	0.48
1:0:2269:C:H2'	1:0:2270:G:H5'	1.95	0.48
1:0:2375:A:H2'	1:0:2376:C:C6	2.47	0.48
14:M:102:GLU:OE1	14:M:164:THR:HG21	2.13	0.48
15:N:40:ASN:ND2	31:9:28:U:H5''	2.28	0.48
1:0:583:C:H2'	1:0:584:U:H6	1.78	0.48
1:0:1120:U:H5'	1:0:1121:G:OP2	2.12	0.48
31:9:73:A:N6	31:9:108:C:H42	2.06	0.48
31:9:107:C:H5	39:9:3167:HOH:O	1.96	0.48
1:0:1058:A:H2'	1:0:1060:C:H5''	1.95	0.48
1:0:1797:A:H4'	1:0:1798:C:C5	2.49	0.48
37:0:9101:WIN:H1FA	37:0:9101:WIN:O1L	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:108:ARG:HH21	24:W:114:PRO:HG2	1.79	0.48
31:9:107:C:O2'	31:9:108:C:H5'	2.14	0.48
1:0:24:G:N2	1:0:518:G:H1'	2.29	0.48
1:0:120:A:N3	1:0:120:A:H2'	2.28	0.48
1:0:137:U:H2'	1:0:139:C:C5	2.49	0.48
1:0:210:U:H2'	1:0:211:U:C6	2.48	0.48
1:0:659:A:H5''	39:0:6799:HOH:O	2.13	0.48
1:0:1250:C:O2'	1:0:1251:C:H5'	2.13	0.48
1:0:2563:U:O2'	1:0:2564:G:H3'	2.13	0.48
1:0:2768:A:O2'	1:0:2769:C:H5'	2.12	0.48
14:M:34:GLU:HB3	14:M:38:GLU:HG3	1.95	0.48
1:0:816:G:H5'	1:0:1598:A:H4'	1.95	0.48
1:0:961:A:H4'	39:0:6342:HOH:O	2.13	0.48
1:0:1714:C:O2'	1:0:1715:C:H5'	2.13	0.48
1:0:2893:C:O2'	1:0:2894:C:H5'	2.13	0.48
19:R:40:ALA:O	19:R:44:VAL:HG23	2.14	0.48
1:0:107:U:H2'	1:0:108:U:H5'	1.96	0.48
1:0:368:C:H2'	1:0:369:G:H5'	1.96	0.48
1:0:1104:C:H4'	11:J:88:PRO:HD3	1.96	0.48
1:0:1183:C:H42	1:0:1184:C:H41	1.62	0.48
1:0:1209:C:H2'	1:0:1210:G:C8	2.49	0.48
1:0:1268:C:H2'	1:0:1269:G:C8	2.48	0.48
1:0:2072:G:C6	1:0:2533:C:H1'	2.49	0.48
1:0:2269:C:C2'	1:0:2270:G:H5'	2.44	0.48
1:0:2507:G:H2'	1:0:2510:C:H42	1.78	0.48
1:0:2717:C:OP1	3:B:207:LYS:HG3	2.13	0.48
1:0:2839:C:H2'	1:0:2840:A:H5''	1.94	0.48
1:0:292:G:H2'	1:0:358:G:N2	2.28	0.48
1:0:301:C:H2'	1:0:302:A:H8	1.79	0.48
1:0:877:G:C5'	1:0:878:G:OP1	2.58	0.48
1:0:1603:A:H5''	1:0:1604:G:H3'	1.95	0.48
1:0:2379:G:H5'	1:0:2381:C:O4'	2.14	0.48
1:0:2540:G:H4'	37:0:9101:WIN:C1O	2.35	0.48
1:0:2718:C:H5'	1:0:2718:C:H6	1.79	0.48
3:B:212:GLN:HB2	3:B:257:THR:HG21	1.96	0.48
5:D:159:PRO:O	5:D:163:VAL:HG23	2.14	0.48
1:0:214:U:H5'	39:0:5454:HOH:O	2.14	0.48
1:0:710:G:H1'	39:O:1484:HOH:O	2.14	0.48
1:0:812:A:H2'	1:0:813:C:C6	2.48	0.48
1:0:1641:A:C2'	1:0:1642:A:H5'	2.44	0.48
1:0:2073:G:H5''	39:0:8581:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2270:G:H4'	2:A:223:ARG:HH12	1.79	0.48
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.14	0.47
1:0:1289:C:O2'	1:0:1290:G:H5'	2.14	0.47
1:0:1845:A:P	2:A:190:ARG:HH11	2.37	0.47
1:0:123:U:H2'	1:0:124:C:C6	2.49	0.47
1:0:1185:U:H2'	1:0:1186:C:C6	2.49	0.47
1:0:2487:C:O2	37:0:9101:WIN:H1F	2.13	0.47
1:0:226:A:H1'	1:0:393:G:C5	2.49	0.47
1:0:1477:C:O2'	1:0:1478:U:H5'	2.14	0.47
1:0:1559:A:H4'	39:0:5067:HOH:O	2.14	0.47
1:0:1568:G:O2'	1:0:1569:U:H5'	2.14	0.47
1:0:1903:U:O2'	1:0:1904:A:N7	2.46	0.47
1:0:2090:G:H2'	1:0:2091:G:C8	2.49	0.47
14:M:43:PRO:HG3	14:M:62:VAL:HG21	1.96	0.47
19:R:39:THR:HG23	19:R:107:GLU:O	2.14	0.47
31:9:42:C:H5'	31:9:43:G:OP2	2.14	0.47
1:0:189:A:OP1	14:M:171:ARG:NH2	2.46	0.47
1:0:816:G:C6	1:0:817:G:N1	2.82	0.47
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.47
1:0:1014:A:H2'	1:0:1015:C:H5'	1.94	0.47
1:0:1370:G:H5''	39:R:4608:HOH:O	2.14	0.47
1:0:1419:U:H5'	1:0:1420:C:OP2	2.15	0.47
1:0:1484:G:H3'	39:0:7776:HOH:O	2.15	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.96	0.47
1:0:1815:A:H2'	1:0:1816:C:O4'	2.14	0.47
1:0:2100:A:H5'	39:C:7192:HOH:O	2.14	0.47
12:K:32:ILE:HD11	12:K:56:SER:HB3	1.96	0.47
26:Y:177:LYS:HD3	26:Y:181:GLY:O	2.15	0.47
1:0:960:G:H3'	1:0:960:G:N3	2.28	0.47
1:0:1028:U:H1'	39:0:8330:HOH:O	2.14	0.47
1:0:1071:G:H4'	26:Y:154:ARG:NH2	2.30	0.47
1:0:1415:G:H5'	28:1:12:ASN:O	2.14	0.47
1:0:1861:C:H4'	2:A:6:GLY:O	2.15	0.47
1:0:2437:A:H2'	1:0:2438:G:C8	2.50	0.47
11:J:107:ASN:HD22	11:J:109:TYR:H	1.61	0.47
23:V:55:ARG:O	23:V:59:ILE:HG12	2.15	0.47
1:0:571:C:H6	1:0:571:C:O5'	1.96	0.47
1:0:2134:G:N2	1:0:2242:U:C2	2.82	0.47
1:0:2598:U:O2	1:0:2600:A:H8	1.98	0.47
1:0:307:G:H3'	39:0:6217:HOH:O	2.14	0.47
1:0:396:U:H1'	39:0:7529:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:960:G:N3	1:0:960:G:C2'	2.77	0.47
1:0:1056:U:H2'	1:0:1057:A:O4'	2.14	0.47
1:0:2372:A:H2'	1:0:2373:U:C6	2.50	0.47
1:0:2389:U:H4'	18:Q:53:HIS:CD2	2.48	0.47
1:0:2509:A:OP2	1:0:2510:C:H5	1.98	0.47
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.97	0.47
1:0:366:U:H2'	1:0:367:G:O4'	2.14	0.47
1:0:1120:U:H5''	1:0:1120:U:H6	1.78	0.47
1:0:1496:A:H5'	1:0:1572:A:H1'	1.96	0.47
1:0:2338:G:H1'	5:D:105:SER:OG	2.15	0.47
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.48	0.47
1:0:421:C:H2'	1:0:422:G:H8	1.80	0.47
1:0:470:U:O2'	28:1:16:HIS:HD2	1.98	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
1:0:1666:C:C2'	1:0:1667:A:C5'	2.80	0.47
1:0:1342:C:C2'	1:0:1343:C:H5'	2.45	0.47
1:0:1409:G:C2	1:0:1410:G:C8	3.03	0.47
1:0:2281:C:C2'	1:0:2282:U:H5'	2.44	0.47
39:0:5919:HOH:O	6:E:31:ARG:NH1	2.43	0.47
1:0:396:U:O2'	1:0:418:C:H4'	2.14	0.46
1:0:506:G:N2	1:0:509:A:H5''	2.24	0.46
1:0:690:G:H4'	1:0:741:C:O2	2.15	0.46
1:0:821:U:H4'	27:Z:41:ARG:HH12	1.80	0.46
1:0:1130:U:H5'	39:0:7596:HOH:O	2.14	0.46
1:0:2005:G:O2'	1:0:2008:U:OP2	2.33	0.46
1:0:2241:C:O2'	1:0:2242:U:H5'	2.16	0.46
1:0:2445:U:H2'	1:0:2446:G:H8	1.78	0.46
1:0:558:C:H2'	1:0:559:U:H5''	1.96	0.46
1:0:946:C:H2'	1:0:947:U:H6	1.81	0.46
1:0:1427:A:H61	1:0:1440:U:C1'	2.28	0.46
1:0:1735:C:O2'	1:0:1736:A:H5'	2.15	0.46
1:0:2541:U:H4'	39:0:4427:HOH:O	2.15	0.46
1:0:2598:U:O2	1:0:2600:A:C8	2.69	0.46
6:E:116:THR:HG22	6:E:151:LEU:HD22	1.96	0.46
31:9:20:G:O2'	31:9:21:G:H5'	2.15	0.46
31:9:39:U:H3	31:9:42:C:H5''	1.81	0.46
1:0:213:G:N2	1:0:225:G:H2'	2.31	0.46
1:0:1363:G:OP1	4:C:76:ARG:NH2	2.48	0.46
1:0:1942:A:O2'	1:0:1943:C:H5'	2.15	0.46
1:0:2382:A:H5'	39:0:3538:HOH:O	2.14	0.46
1:0:1052:G:N3	1:0:1052:G:H2'	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1773:G:C8	27:Z:40:ALA:HA	2.50	0.46
1:0:2668:G:H2'	1:0:2669:U:C6	2.50	0.46
1:0:1201:C:H2'	1:0:1202:A:H5'	1.97	0.46
1:0:1545:C:H2'	1:0:1546:G:O4'	2.16	0.46
1:0:2326:C:H4'	1:0:2412:G:H4'	1.98	0.46
1:0:2348:C:H5'	5:D:22:VAL:HG11	1.97	0.46
1:0:2594:C:O2'	1:0:2595:U:H5'	2.15	0.46
1:0:2866:U:H4'	1:0:2867:G:H5'	1.96	0.46
1:0:146:U:O2'	1:0:147:G:H5'	2.16	0.46
1:0:164:G:H3'	39:0:8328:HOH:O	2.16	0.46
1:0:216:A:O2'	1:0:217:C:H5'	2.15	0.46
1:0:256:C:H2'	1:0:257:G:O4'	2.16	0.46
1:0:512:G:O3'	1:0:513:A:H8	1.99	0.46
1:0:700:A:H5''	1:0:701:U:H5'	1.97	0.46
1:0:1025:C:H5'	24:W:23:MET:O	2.15	0.46
1:0:1063:G:H5''	39:0:6221:HOH:O	2.16	0.46
1:0:1158:G:O2'	1:0:1159:G:H5'	2.16	0.46
1:0:1422:U:H2'	1:0:1423:C:H6	1.78	0.46
1:0:2100:A:C2	37:0:9101:WIN:H1DB	2.51	0.46
1:0:2392:C:H4'	39:0:9136:HOH:O	2.15	0.46
1:0:255:A:H2'	1:0:256:C:C6	2.49	0.46
1:0:517:U:H2'	1:0:518:G:H5'	1.97	0.46
1:0:1384:C:H5'	25:X:30:MET:HG2	1.96	0.46
1:0:2629:C:H41	2:A:206:ARG:HH21	1.64	0.46
1:0:2638:G:H5'	39:0:3790:HOH:O	2.15	0.46
1:0:2851:G:C2'	1:0:2852:A:H5'	2.45	0.46
4:C:1:MET:HG2	4:C:2:GLN:H	1.81	0.46
9:H:49:GLN:HE21	9:H:140:TYR:HE2	1.63	0.46
15:N:159:TYR:HE1	31:9:50:G:H5''	1.80	0.46
24:W:4:LEU:HD22	24:W:52:VAL:HG21	1.97	0.46
1:0:236:A:H8	1:0:236:A:OP1	1.99	0.46
1:0:682:A:H2'	1:0:683:G:O4'	2.15	0.46
1:0:1919:A:H4'	39:0:3679:HOH:O	2.16	0.46
1:0:2548:C:H5'	3:B:252:PRO:HD2	1.98	0.46
1:0:2896:A:H2'	1:0:2896:A:N3	2.31	0.46
1:0:2899:A:O2'	1:0:2900:G:H5'	2.16	0.46
3:B:17:LYS:O	3:B:260:HIS:HD2	1.99	0.46
1:0:183:A:O2'	1:0:184:G:H5'	2.16	0.46
1:0:602:A:O2'	1:0:605:C:H4'	2.15	0.46
1:0:800:G:H2'	1:0:801:U:C6	2.50	0.46
1:0:1667:A:H2'	1:0:1668:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:199:HIS:CD2	2:A:201:PHE:H	2.33	0.46
20:S:11:THR:H	20:S:14:ALA:HB3	1.79	0.46
31:9:29:C:H2'	31:9:30:C:C5'	2.40	0.46
1:0:101:C:H2'	1:0:102:A:C8	2.51	0.46
1:0:523:C:H2'	1:0:524:A:C8	2.51	0.46
1:0:1716:A:H4'	17:P:55:LYS:HD3	1.97	0.46
1:0:1769:C:O2'	1:0:1770:U:H5'	2.15	0.46
1:0:168:C:H6	1:0:168:C:O5'	1.98	0.45
1:0:466:A:H2'	1:0:467:G:O4'	2.16	0.45
1:0:960:G:N3	1:0:960:G:H2'	2.31	0.45
1:0:1314:U:H5''	1:0:1316:G:O4'	2.16	0.45
1:0:1731:C:H1'	39:0:5883:HOH:O	2.16	0.45
1:0:1834:C:H2'	1:0:1840:A:H62	1.80	0.45
17:P:105:LEU:HD21	17:P:137:LEU:HD11	1.98	0.45
31:9:108:C:O2'	31:9:109:G:H5'	2.17	0.45
1:0:364:U:H2'	1:0:365:G:C8	2.51	0.45
1:0:702:G:O2'	1:0:703:G:H5'	2.17	0.45
1:0:1160:G:H5'	1:0:1161:A:C4'	2.46	0.45
1:0:1204:C:H2'	1:0:1205:U:O4'	2.16	0.45
1:0:1562:C:H2'	1:0:1562:C:O2	2.16	0.45
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.45
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.45
4:C:47:GLY:HA2	4:C:92:PRO:HB2	1.97	0.45
1:0:204:A:H2'	1:0:205:U:H5'	1.98	0.45
1:0:834:G:H4'	1:0:835:U:OP2	2.15	0.45
1:0:1007:A:H2'	9:H:22:TYR:CZ	2.52	0.45
1:0:1500:U:P	17:P:41:ARG:HH22	2.39	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.16	0.45
1:0:2348:C:H1'	5:D:131:THR:HG21	1.96	0.45
31:9:31:C:H2'	31:9:32:G:O4'	2.17	0.45
1:0:820:G:C5	2:A:171:LYS:HB2	2.51	0.45
1:0:1362:U:H5'	39:0:7682:HOH:O	2.16	0.45
1:0:1593:C:OP1	17:P:117:SER:HB3	2.16	0.45
1:0:2256:G:C2'	1:0:2257:G:H5'	2.47	0.45
25:X:61:ARG:NH1	25:X:67:PRO:HD3	2.31	0.45
1:0:397:A:O2'	1:0:417:G:N3	2.46	0.45
1:0:657:G:P	4:C:27:ARG:HH22	2.40	0.45
1:0:1131:G:C6	1:0:1230:A:C4	3.04	0.45
1:0:2269:C:H2'	1:0:2270:G:C5'	2.46	0.45
1:0:2694:A:H4'	6:E:91:PHE:CE1	2.51	0.45
12:K:74:VAL:HG12	12:K:75:ARG:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:51:G:O2'	1:0:52:A:H5'	2.17	0.45
1:0:1220:U:H4'	9:H:174:LEU:HD21	1.98	0.45
1:0:1375:A:H2'	1:0:1376:G:H5'	1.99	0.45
1:0:1687:C:O2	28:1:9:GLY:HA2	2.17	0.45
1:0:1706:G:C6	1:0:1707:G:C6	3.05	0.45
1:0:2740:G:H2'	1:0:2741:A:O4'	2.16	0.45
3:B:238:ASN:HD22	3:B:240:GLY:N	2.12	0.45
3:B:315:VAL:HG23	3:B:316:ARG:HG2	1.99	0.45
13:L:30:ARG:NH1	39:L:165:HOH:O	2.48	0.45
1:0:59:A:H5'	39:0:2959:HOH:O	2.16	0.45
1:0:569:A:H5''	1:0:587:A:N1	2.32	0.45
26:Y:144:ARG:NH1	39:Y:4909:HOH:O	2.49	0.45
1:0:221:G:H2'	1:0:222:A:C8	2.51	0.45
1:0:243:A:H61	1:0:269:G:C1'	2.30	0.45
1:0:527:U:H2'	1:0:528:G:H8	1.81	0.45
1:0:558:C:H2'	1:0:559:U:H5'	1.99	0.45
1:0:1202:A:H2'	1:0:1203:G:H5'	1.98	0.45
24:W:6:GLN:HB2	24:W:26:ILE:HD11	1.99	0.45
1:0:334:G:H2'	1:0:335:U:O4'	2.16	0.45
1:0:363:C:O2'	1:0:364:U:H5'	2.17	0.45
1:0:1616:A:H5''	1:0:1617:C:OP1	2.17	0.45
4:C:188:ARG:HD3	39:C:2507:HOH:O	2.15	0.45
31:9:22:G:H5'	31:9:23:U:OP1	2.17	0.45
1:0:664:U:O4	1:0:681:G:H5''	2.16	0.45
1:0:820:G:OP1	27:Z:41:ARG:NH2	2.50	0.45
1:0:1149:U:H5''	1:0:1151:G:O4'	2.17	0.45
1:0:1375:A:O2'	1:0:1376:G:H5'	2.17	0.45
1:0:1439:C:H5''	29:2:41:HIS:HE1	1.82	0.45
1:0:1849:G:H1'	1:0:2011:A:N1	2.32	0.45
1:0:1937:U:O2'	1:0:1938:G:H5'	2.17	0.45
1:0:2083:A:N6	11:J:90:LYS:HE3	2.32	0.45
31:9:36:C:C5	31:9:37:C:C5	3.05	0.45
1:0:193:A:N1	1:0:413:G:O2'	2.47	0.44
1:0:424:C:H2'	1:0:425:U:C6	2.51	0.44
1:0:558:C:C2'	1:0:559:U:C5'	2.95	0.44
1:0:646:G:H2'	1:0:647:U:C6	2.51	0.44
1:0:1783:A:O2'	1:0:1784:U:H5'	2.17	0.44
1:0:2291:A:N9	1:0:2309:C:H5'	2.32	0.44
20:S:51:GLN:HE21	20:S:53:ASN:HD21	1.64	0.44
1:0:319:A:H4'	1:0:338:C:C4	2.52	0.44
1:0:538:C:OP2	26:Y:134:HIS:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:629:A:H2'	1:0:630:A:O4'	2.17	0.44
1:0:711:G:C2	1:0:718:C:C2	3.06	0.44
1:0:807:A:O2'	1:0:808:A:H5'	2.18	0.44
1:0:1249:U:H2'	1:0:1250:C:C6	2.52	0.44
1:0:1398:G:H2'	1:0:1399:A:C8	2.52	0.44
1:0:1447:U:H3'	1:0:1506:U:O2	2.16	0.44
1:0:1506:U:H6	1:0:1506:U:H5'	1.82	0.44
1:0:2121:G:O2'	1:0:2122:C:H5'	2.16	0.44
1:0:2241:C:H2'	1:0:2242:U:H6	1.79	0.44
5:D:141:VAL:HG21	31:9:57:A:C8	2.52	0.44
15:N:37:ARG:NH1	31:9:6:C:OP1	2.45	0.44
1:0:383:A:H2'	1:0:384:G:O4'	2.18	0.44
1:0:483:C:C4	1:0:484:A:C6	3.06	0.44
1:0:583:C:H2'	1:0:584:U:C6	2.53	0.44
1:0:793:A:H5''	17:P:83:LYS:HG2	1.99	0.44
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.44
1:0:1098:A:H2'	1:0:1099:G:O4'	2.17	0.44
1:0:1768:C:H2'	1:0:1769:C:O4'	2.18	0.44
1:0:2004:U:H4'	39:0:4302:HOH:O	2.18	0.44
1:0:2510:C:H42	1:0:2564:G:N2	2.16	0.44
1:0:2678:A:H4'	39:0:6889:HOH:O	2.18	0.44
19:R:39:THR:HG22	19:R:42:GLU:H	1.83	0.44
1:0:645:U:O2	1:0:761:A:H2	2.01	0.44
1:0:802:G:O2'	1:0:803:C:H5'	2.17	0.44
1:0:1626:A:H2'	1:0:1627:G:C5'	2.48	0.44
1:0:1634:G:H2'	1:0:1635:U:H6	1.82	0.44
1:0:2256:G:H2'	1:0:2257:G:C5'	2.48	0.44
1:0:2831:C:C2'	1:0:2832:C:H5'	2.48	0.44
5:D:22:VAL:HG22	5:D:74:THR:HG22	2.00	0.44
24:W:80:ASP:O	24:W:84:VAL:HG23	2.18	0.44
31:9:3:A:OP2	31:9:25:G:N2	2.51	0.44
1:0:177:A:H2'	1:0:178:U:O4'	2.17	0.44
1:0:1445:G:N2	1:0:1678:A:H1'	2.33	0.44
1:0:1622:G:H2'	1:0:1623:C:H5'	1.98	0.44
1:0:2105:C:H2'	1:0:2106:C:C6	2.52	0.44
3:B:254:GLN:HG2	3:B:255:GLY:N	2.32	0.44
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.99	0.44
31:9:52:A:H2'	31:9:53:G:O4'	2.18	0.44
1:0:628:1MA:H4'	39:0:7268:HOH:O	2.18	0.44
1:0:815:U:O2'	1:0:1598:A:H4'	2.17	0.44
1:0:1197:G:H1'	1:0:1203:G:N2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1535:G:H2'	1:0:1536:C:C6	2.53	0.44
1:0:2838:A:OP1	3:B:307:ARG:NH2	2.50	0.44
23:V:1:THR:HG23	23:V:2:VAL:HG23	2.00	0.44
24:W:48:VAL:HG12	24:W:52:VAL:HB	1.98	0.44
31:9:2:U:OP2	31:9:2:U:H4'	2.18	0.44
1:0:517:U:C2'	1:0:518:G:H5'	2.47	0.44
1:0:920:C:H5''	1:0:921:G:O5'	2.18	0.44
1:0:1311:G:C2	1:0:1312:G:C8	3.06	0.44
1:0:1439:C:O5'	1:0:1439:C:H6	2.00	0.44
1:0:1664:A:H8	1:0:1664:A:OP1	2.01	0.44
1:0:1994:A:OP1	12:K:66:ARG:NH2	2.51	0.44
13:L:27:ARG:HH21	13:L:30:ARG:HG2	1.82	0.44
1:0:271:C:H4'	1:0:272:A:OP1	2.17	0.44
1:0:333:G:O2'	1:0:334:G:H5'	2.18	0.44
1:0:1330:A:C5'	39:Y:7277:HOH:O	2.65	0.44
1:0:1515:A:H2'	1:0:1516:U:C6	2.53	0.44
1:0:1666:C:H2'	1:0:1667:A:H5'	1.97	0.44
1:0:2041:G:O2'	1:0:2042:U:H5'	2.17	0.44
1:0:2094:G:O6	1:0:2649:A:H2	2.00	0.44
1:0:2626:C:H2'	1:0:2627:G:C8	2.53	0.44
1:0:2824:C:H5''	1:0:2825:C:H5'	1.99	0.44
2:A:51:ARG:NH1	2:A:120:ARG:O	2.51	0.44
2:A:70:ALA:HB1	27:Z:89:THR:HG21	2.00	0.44
31:9:59:C:H2'	31:9:60:C:C6	2.52	0.44
1:0:39:G:N2	1:0:444:C:C2	2.86	0.44
1:0:445:U:H2'	1:0:446:G:C8	2.52	0.44
1:0:1088:A:C6	1:0:1291:A:H1'	2.53	0.44
1:0:1170:U:H2'	1:0:1172:G:OP2	2.18	0.44
1:0:1587:U:H2'	1:0:1588:G:O4'	2.17	0.44
1:0:1844:C:H6	1:0:1844:C:O5'	2.01	0.44
1:0:2281:C:H2'	1:0:2282:U:H5'	2.00	0.44
1:0:2809:G:H2'	1:0:2810:G:O4'	2.18	0.44
39:0:2979:HOH:O	28:1:10:LYS:HG3	2.18	0.44
1:0:638:C:H2'	1:0:639:A:C8	2.53	0.43
1:0:764:C:H2'	1:0:765:G:O4'	2.18	0.43
1:0:851:C:O2	1:0:2022:A:H2	2.01	0.43
1:0:1592:G:O2'	1:0:1593:C:O5'	2.36	0.43
1:0:2502:C:H2'	1:0:2503:A:C5'	2.47	0.43
1:0:2634:G:OP2	2:A:204:GLY:N	2.48	0.43
1:0:2856:A:H4'	25:X:11:THR:HB	1.99	0.43
1:0:169:A:H5''	39:0:5578:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:241:A:C2	1:0:378:A:H4'	2.53	0.43
1:0:635:A:H2	39:0:3734:HOH:O	2.00	0.43
1:0:1119:G:H8	11:J:52:GLN:NE2	2.16	0.43
1:0:1321:A:H2'	1:0:1322:G:C8	2.53	0.43
1:0:1361:C:H2'	1:0:1362:U:C6	2.53	0.43
1:0:1544:U:H2'	1:0:1545:C:C6	2.54	0.43
3:B:141:ARG:HD2	3:B:163:GLU:OE2	2.18	0.43
24:W:125:HIS:HE1	39:W:3071:HOH:O	2.01	0.43
1:0:101:C:H2'	1:0:102:A:H8	1.84	0.43
1:0:329:A:OP2	4:C:206:ASN:HB2	2.17	0.43
1:0:1003:U:H4'	9:H:91:ARG:O	2.18	0.43
1:0:1654:U:H2'	2:A:47:HIS:CD2	2.51	0.43
1:0:1759:A:N3	1:0:1818:C:H2'	2.33	0.43
1:0:2831:C:H2'	1:0:2832:C:H5'	2.00	0.43
1:0:111:C:O2'	1:0:112:G:H5'	2.18	0.43
1:0:694:A:C2'	1:0:695:C:H5'	2.48	0.43
1:0:1406:A:H4'	1:0:1407:A:C5'	2.48	0.43
1:0:1595:G:O2'	1:0:1596:U:H5'	2.19	0.43
1:0:2438:G:H2'	1:0:2439:C:O4'	2.18	0.43
1:0:2649:A:H5'	1:0:2649:A:H8	1.83	0.43
6:E:112:ALA:HA	6:E:113:PRO:HD3	1.90	0.43
15:N:83:LEU:HD13	15:N:175:LEU:HD23	2.00	0.43
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.57	0.43
1:0:106:A:H2'	1:0:107:U:O4'	2.19	0.43
1:0:289:G:O2'	1:0:290:C:H5'	2.19	0.43
1:0:419:A:H1'	1:0:1921:A:C2	2.53	0.43
1:0:1734:C:OP1	3:B:234:ARG:HD3	2.19	0.43
1:0:1881:A:OP1	2:A:199:HIS:HE1	2.02	0.43
1:0:1883:U:H5'	1:0:2012:U:OP2	2.19	0.43
1:0:2698:G:H2'	1:0:2699:A:C8	2.54	0.43
1:0:2783:A:H2'	1:0:2784:A:C8	2.53	0.43
1:0:92:G:H4'	23:V:44:GLY:HA3	1.99	0.43
1:0:271:C:C2	1:0:273:G:O4'	2.72	0.43
1:0:312:U:C2	1:0:320:G:N2	2.87	0.43
1:0:820:G:H5'	1:0:821:U:H5'	1.99	0.43
1:0:1427:A:N6	1:0:1440:U:H1'	2.33	0.43
1:0:1504:A:H4'	1:0:1506:U:C5	2.53	0.43
1:0:1626:A:H2'	1:0:1627:G:H5'	2.00	0.43
1:0:2488:A:H1'	39:0:3241:HOH:O	2.19	0.43
1:0:2633:A:H5'	39:0:5222:HOH:O	2.18	0.43
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:74:ALA:HB2	25:X:85:VAL:HG13	2.01	0.43
31:9:49:G:H5''	39:9:4707:HOH:O	2.19	0.43
1:0:111:C:H2'	1:0:112:G:O4'	2.18	0.43
1:0:1211:G:H2'	1:0:1212:C:C6	2.53	0.43
1:0:1439:C:H5''	29:2:41:HIS:CE1	2.52	0.43
1:0:1622:G:C2'	1:0:1623:C:H5'	2.48	0.43
1:0:2114:C:OP1	2:A:1:GLY:HA2	2.19	0.43
1:0:2507:G:H2'	1:0:2510:C:N4	2.33	0.43
1:0:2591:C:H2'	1:0:2592:G:O4'	2.19	0.43
31:9:3:A:H2	31:9:21:G:N3	2.17	0.43
1:0:42:C:H1'	39:0:3438:HOH:O	2.18	0.43
1:0:138:U:OP2	1:0:139:C:H5	2.01	0.43
1:0:447:A:P	21:T:1:SER:HB2	2.59	0.43
1:0:1184:C:O2'	1:0:1185:U:OP2	2.30	0.43
1:0:1294:A:H2'	1:0:1295:G:O4'	2.18	0.43
1:0:1571:G:H1'	1:0:1627:G:N2	2.34	0.43
1:0:1846:U:O2'	2:A:172:ALA:HB2	2.17	0.43
1:0:2073:G:OP2	1:0:2490:A:H5'	2.19	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
1:0:2716:G:H5'	3:B:262:ARG:HG3	2.00	0.43
15:N:4:PRO:HG3	31:9:69:U:OP1	2.19	0.43
1:0:571:C:H2'	1:0:572:G:O4'	2.18	0.43
1:0:661:G:C5	1:0:686:A:C2	3.07	0.43
1:0:1001:U:O2'	1:0:1002:G:H5'	2.19	0.43
1:0:1200:A:H3'	39:0:4912:HOH:O	2.18	0.43
1:0:1202:A:C2'	1:0:1203:G:H5'	2.49	0.43
1:0:2837:U:H2'	39:0:6433:HOH:O	2.17	0.43
1:0:836:G:H1'	39:0:7509:HOH:O	2.18	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.18	0.43
1:0:1592:G:H2'	1:0:1593:C:C6	2.54	0.43
1:0:2070:G:H2'	1:0:2072:G:OP1	2.18	0.43
1:0:2266:A:H2'	1:0:2267:G:C8	2.54	0.43
1:0:2781:U:H2'	1:0:2782:G:C5'	2.48	0.43
1:0:255:A:H2'	1:0:256:C:H6	1.84	0.42
1:0:369:G:H2'	1:0:370:G:H8	1.84	0.42
1:0:696:C:H2'	1:0:697:G:O4'	2.19	0.42
1:0:699:C:C2	1:0:743:G:N2	2.87	0.42
1:0:1845:A:O2'	1:0:1846:U:H5'	2.19	0.42
1:0:1966:U:H2'	1:0:1967:U:C6	2.54	0.42
1:0:2438:G:H5'	39:0:5494:HOH:O	2.18	0.42
1:0:2566:A:H2	1:0:2695:C:O2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:42:GLU:O	11:J:131:THR:HG23	2.19	0.42
1:0:538:C:H5''	1:0:539:G:C8	2.53	0.42
1:0:912:A:C4	1:0:1294:A:C2	3.07	0.42
1:0:1119:G:N2	1:0:1246:A:N1	2.67	0.42
1:0:1205:U:C2'	1:0:1206:U:C5'	2.89	0.42
1:0:1245:C:H6	1:0:1245:C:O5'	2.02	0.42
1:0:1381:A:N3	1:0:1382:G:H1'	2.34	0.42
1:0:1386:G:O2'	1:0:1387:G:H5'	2.19	0.42
1:0:1421:C:O2'	1:0:1422:U:H5'	2.19	0.42
1:0:1434:A:H2'	1:0:1436:C:C5	2.54	0.42
1:0:1562:C:N4	39:0:5067:HOH:O	2.52	0.42
1:0:1613:C:H2'	1:0:1614:G:O4'	2.18	0.42
1:0:1795:G:H2'	1:0:1796:A:O4'	2.19	0.42
1:0:1803:C:H2'	1:0:1804:A:H8	1.83	0.42
1:0:2045:G:H2'	1:0:2046:G:O4'	2.19	0.42
1:0:2102:G:C2	1:0:2104:C:C4	3.08	0.42
1:0:2816:A:H5''	1:0:2817:G:H5'	2.01	0.42
31:9:1:U:O2'	31:9:3:A:H5''	2.19	0.42
1:0:615:G:H2'	1:0:616:U:C6	2.54	0.42
1:0:1407:A:O2'	1:0:1408:U:H3'	2.19	0.42
31:9:91:C:H2'	31:9:92:G:O4'	2.19	0.42
1:0:276:C:H6	1:0:276:C:O5'	2.03	0.42
1:0:1010:C:OP1	15:N:5:ARG:NH1	2.53	0.42
1:0:1130:U:H2'	1:0:1131:G:O4'	2.18	0.42
1:0:1393:A:H2'	1:0:1394:C:C6	2.54	0.42
1:0:1968:A:H2'	1:0:1969:A:C8	2.55	0.42
1:0:2079:G:H2'	1:0:2080:G:O4'	2.19	0.42
1:0:2239:C:H2'	1:0:2240:U:C6	2.54	0.42
1:0:2252:A:H2'	1:0:2253:G:O4'	2.19	0.42
1:0:2487:C:H2'	1:0:2488:A:O4'	2.18	0.42
1:0:2546:U:H4'	39:B:3923:HOH:O	2.20	0.42
4:C:218:VAL:HG12	39:C:5065:HOH:O	2.19	0.42
18:Q:19:ARG:HH21	31:9:11:A:P	2.42	0.42
28:1:8:GLN:HE22	28:1:11:LYS:HZ1	1.67	0.42
1:0:295:C:H2'	1:0:296:G:O4'	2.20	0.42
1:0:308:U:C4	1:0:342:C:H1'	2.54	0.42
1:0:524:A:H5''	19:R:29:LYS:HD3	2.00	0.42
1:0:1396:C:H1'	17:P:1:THR:O	2.19	0.42
1:0:1761:U:H5'	17:P:81:LYS:O	2.20	0.42
1:0:1992:U:H2'	1:0:1994:A:OP2	2.19	0.42
1:0:2039:A:H4'	1:0:2760:C:O2'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2345:A:H3'	1:0:2346:C:H6	1.83	0.42
16:O:32:ARG:HH21	16:O:35:LYS:NZ	2.17	0.42
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	2.00	0.42
1:0:272:A:H3'	39:O:7395:HOH:O	2.19	0.42
1:0:470:U:O2'	28:1:16:HIS:CD2	2.72	0.42
1:0:542:A:H2'	1:0:543:G:O4'	2.19	0.42
1:0:567:U:H6	1:0:567:U:O5'	2.02	0.42
1:0:670:G:H2'	1:0:671:A:C8	2.54	0.42
1:0:699:C:C2	1:0:744:G:C2	3.07	0.42
1:0:812:A:H2'	1:0:813:C:O4'	2.19	0.42
1:0:876:A:N3	1:0:876:A:H2'	2.34	0.42
1:0:2589:U:H2'	1:0:2590:U:C6	2.54	0.42
1:0:2777:G:O2'	1:0:2778:A:H5'	2.20	0.42
14:M:164:THR:HG22	14:M:165:GLY:N	2.34	0.42
30:3:48:ASN:ND2	30:3:50:GLY:H	2.17	0.42
1:0:342:C:H2'	1:0:343:C:H6	1.84	0.42
1:0:574:G:O2'	1:0:575:A:H5'	2.20	0.42
1:0:958:G:H2'	1:0:959:C:H6	1.84	0.42
1:0:1055:G:OP2	9:H:99:ARG:NH1	2.53	0.42
1:0:1211:G:H2'	1:0:1212:C:H6	1.83	0.42
1:0:1218:U:H2'	1:0:1219:U:C6	2.54	0.42
1:0:1463:U:H2'	1:0:1464:C:C6	2.55	0.42
1:0:1788:U:C2	1:0:1805:G:N2	2.88	0.42
1:0:2649:A:H5'	1:0:2649:A:C8	2.55	0.42
9:H:69:ARG:HD3	39:H:6314:HOH:O	2.20	0.42
15:N:35:VAL:HG11	31:9:6:C:H4'	2.01	0.42
21:T:18:GLU:O	21:T:21:LYS:HG2	2.20	0.42
1:0:113:A:H2'	1:0:115:U:O4	2.20	0.42
1:0:204:A:C2'	1:0:205:U:H5'	2.49	0.42
1:0:447:A:OP1	21:T:2:LYS:HG2	2.20	0.42
1:0:825:U:H5''	1:0:826:U:OP1	2.19	0.42
1:0:1576:G:H2'	1:0:1577:U:C6	2.55	0.42
2:A:70:ALA:HA	2:A:71:PRO:HD3	1.88	0.42
11:J:80:LYS:HE3	11:J:101:VAL:O	2.20	0.42
1:0:210:U:H2'	1:0:211:U:H6	1.84	0.42
1:0:482:G:O4'	1:0:511:A:C2	2.72	0.42
1:0:907:A:H4'	1:0:1328:A:C2	2.55	0.42
1:0:1074:G:H4'	1:0:1260:G:C6	2.54	0.42
1:0:1099:G:H2'	1:0:1100:G:O4'	2.20	0.42
1:0:1154:A:H2'	1:0:1155:G:C8	2.55	0.42
1:0:1202:A:H2'	1:0:1203:G:C5'	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1819:G:H2'	1:0:1820:G:C5'	2.50	0.42
1:0:2419:U:H5''	1:0:2420:G:C5'	2.50	0.42
2:A:71:PRO:HG2	2:A:91:GLY:HA2	2.02	0.42
1:0:138:U:OP1	1:0:259:G:H5'	2.20	0.42
1:0:812:A:H1'	39:0:8714:HOH:O	2.19	0.42
1:0:1556:G:O2'	1:0:1557:G:H5'	2.19	0.42
1:0:1682:A:H5''	39:0:4695:HOH:O	2.20	0.42
1:0:1706:G:C5	1:0:1707:G:C6	3.08	0.42
1:0:1789:G:H2'	1:0:1790:C:O5'	2.20	0.42
1:0:1873:G:H3'	39:0:4169:HOH:O	2.19	0.42
1:0:1878:G:O2'	1:0:1879:U:P	2.78	0.42
1:0:2416:G:H2'	1:0:2417:C:C6	2.55	0.42
1:0:17:G:H2'	1:0:18:C:C6	2.56	0.41
1:0:185:G:H4'	1:0:186:A:H4'	2.02	0.41
1:0:218:C:C5	1:0:220:C:C4	3.07	0.41
1:0:581:G:O2'	1:0:582:U:H5'	2.20	0.41
1:0:1942:A:H4'	39:A:241:HOH:O	2.19	0.41
1:0:2039:A:H2'	1:0:2040:C:C6	2.54	0.41
16:O:73:ASP:HA	16:O:92:VAL:O	2.20	0.41
31:9:56:A:C3'	31:9:57:A:H5''	2.50	0.41
1:0:1819:G:H2'	1:0:1820:G:C4'	2.50	0.41
1:0:1855:G:H8	2:A:144:GLU:OE2	2.04	0.41
1:0:2533:C:H6	1:0:2533:C:C5'	2.27	0.41
1:0:2564:G:OP2	1:0:2565:C:H5''	2.20	0.41
1:0:2583:A:H5'	39:0:6007:HOH:O	2.21	0.41
9:H:59:GLN:NE2	9:H:129:ARG:HE	2.15	0.41
1:0:107:U:C2'	1:0:108:U:H5'	2.51	0.41
1:0:283:U:H5	1:0:284:C:C4	2.37	0.41
1:0:1098:A:OP1	24:W:128:VAL:HG22	2.20	0.41
1:0:1166:A:OP1	1:0:1174:A:H4'	2.19	0.41
1:0:1268:C:O2'	1:0:1269:G:H5'	2.20	0.41
1:0:1909:A:H2'	1:0:1910:A:C8	2.56	0.41
1:0:2540:G:O2'	37:0:9101:WIN:H2G	2.20	0.41
4:C:107:ARG:O	4:C:111:VAL:HG23	2.20	0.41
9:H:31:ILE:HG23	39:H:6314:HOH:O	2.19	0.41
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.87	0.41
1:0:168:C:H5'	1:0:2277:U:OP1	2.21	0.41
1:0:710:G:OP1	16:O:24:ALA:HB3	2.21	0.41
1:0:1014:A:H5''	31:9:101:G:O2'	2.20	0.41
1:0:1741:U:C4	1:0:2033:G:C8	3.08	0.41
1:0:1766:U:O2	1:0:1778:A:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2016:U:H2'	1:0:2017:U:O4'	2.20	0.41
1:0:2251:G:H2'	1:0:2252:A:C8	2.54	0.41
1:0:2354:A:C2	1:0:2367:A:C8	3.09	0.41
16:O:70:LEU:O	16:O:92:VAL:HG21	2.21	0.41
22:U:14:GLU:O	22:U:17:THR:HB	2.20	0.41
31:9:39:U:H3'	31:9:40:C:C5'	2.49	0.41
1:0:317:A:H4'	39:0:8457:HOH:O	2.19	0.41
1:0:1706:G:C6	1:0:1707:G:N1	2.88	0.41
1:0:2087:C:O2'	1:0:2088:C:H5'	2.20	0.41
1:0:2103:A:H2'	1:0:2104:C:C5'	2.51	0.41
1:0:2473:U:O3'	1:0:2474:A:H3'	2.20	0.41
1:0:2538:A:O2'	37:0:9101:WIN:H1AB	2.21	0.41
1:0:2714:U:H4'	3:B:10:SER:HB2	2.02	0.41
1:0:2815:G:N7	11:J:80:LYS:NZ	2.69	0.41
4:C:39:GLN:O	4:C:43:LYS:HD3	2.20	0.41
4:C:138:VAL:O	4:C:234:VAL:HA	2.21	0.41
12:K:130:MET:SD	22:U:25:ASP:O	2.78	0.41
1:0:125:U:H2'	39:0:8451:HOH:O	2.21	0.41
1:0:1684:A:O2'	1:0:1685:A:H5''	2.20	0.41
1:0:2092:G:H2'	1:0:2613:G:OP1	2.21	0.41
1:0:2265:U:H2'	1:0:2266:A:C8	2.55	0.41
1:0:2906:A:H5'	1:0:2907:C:O4'	2.20	0.41
18:Q:25:PRO:HB2	39:9:4350:HOH:O	2.19	0.41
20:S:57:THR:C	20:S:59:ASP:H	2.28	0.41
24:W:48:VAL:HG12	24:W:48:VAL:O	2.20	0.41
24:W:137:GLN:NE2	24:W:141:HIS:HE1	2.14	0.41
31:9:28:U:H2'	31:9:29:C:C6	2.55	0.41
1:0:318:U:H5'	1:0:339:A:N3	2.36	0.41
1:0:579:G:H2'	1:0:580:A:C8	2.56	0.41
1:0:1306:U:H5''	4:C:184:ARG:HD2	2.03	0.41
1:0:1456:C:H2'	1:0:1457:U:C6	2.55	0.41
1:0:1688:G:O2'	28:1:5:THR:HG23	2.20	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.21	0.41
1:0:2664:A:H8	1:0:2664:A:OP1	2.03	0.41
1:0:2734:G:O2'	1:0:2735:U:H5'	2.21	0.41
3:B:41:PHE:CD1	3:B:79:MET:HE2	2.56	0.41
3:B:304:PRO:HD2	3:B:307:ARG:NE	2.36	0.41
4:C:236:THR:HG22	4:C:239:ALA:H	1.86	0.41
9:H:70:LEU:O	9:H:74:ARG:HB2	2.20	0.41
1:0:185:G:H4'	1:0:186:A:OP1	2.21	0.41
1:0:400:C:O2'	1:0:401:C:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:549:A:O2'	1:0:550:C:H5'	2.21	0.41
1:0:559:U:H2'	1:0:560:U:O4'	2.20	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.21	0.41
1:0:1076:G:C2	1:0:1084:C:C2	3.09	0.41
1:0:1290:G:H3'	39:0:4115:HOH:O	2.20	0.41
1:0:1624:A:H5'	1:0:1626:A:O4'	2.21	0.41
1:0:1736:A:H1'	39:0:7468:HOH:O	2.20	0.41
1:0:1973:A:H5'	1:0:1973:A:C8	2.53	0.41
1:0:2326:C:H4'	1:0:2412:G:C4'	2.51	0.41
14:M:65:VAL:HG21	14:M:105:ALA:HB2	2.03	0.41
1:0:10:U:H3'	1:0:10:U:C6	2.56	0.41
1:0:282:C:H1'	1:0:368:C:H41	1.83	0.41
1:0:291:C:H2'	1:0:292:G:O4'	2.21	0.41
1:0:318:U:H5'	1:0:339:A:C4	2.56	0.41
1:0:327:A:H4'	1:0:329:A:C8	2.56	0.41
1:0:1165:G:O3'	1:0:1174:A:H4'	2.20	0.41
1:0:1167:G:H4'	10:I:130:LEU:HD21	2.03	0.41
1:0:1185:U:H5'	39:0:7308:HOH:O	2.21	0.41
1:0:1383:U:H5'	25:X:27:ASP:OD1	2.21	0.41
1:0:1631:A:H2'	1:0:1632:A:C8	2.56	0.41
1:0:1762:C:O2'	1:0:1763:C:H5'	2.20	0.41
1:0:2089:A:O2'	1:0:2090:G:H5'	2.21	0.41
1:0:2812:A:C2	1:0:2814:A:N6	2.75	0.41
3:B:102:THR:HB	3:B:103:ASP:H	1.71	0.41
5:D:23:VAL:HG12	5:D:130:VAL:HG22	2.02	0.41
31:9:35:C:H5''	39:9:4078:HOH:O	2.20	0.41
1:0:1652:C:H4'	27:Z:76:THR:HG21	2.03	0.41
1:0:1811:A:C2	1:0:2752:C:H1'	2.56	0.41
1:0:2047:C:H5'	39:0:6092:HOH:O	2.21	0.41
1:0:2074:A:H1'	39:0:6299:HOH:O	2.21	0.41
1:0:2385:G:H2'	1:0:2386:U:C6	2.56	0.41
1:0:2481:G:H5''	39:0:3267:HOH:O	2.20	0.41
1:0:2908:A:O5'	1:0:2908:A:H8	2.04	0.41
3:B:10:SER:O	3:B:16:ARG:NH1	2.53	0.41
3:B:69:VAL:HA	3:B:70:PRO:HD3	1.92	0.41
24:W:88:THR:HG22	24:W:89:ASP:H	1.86	0.41
1:0:856:G:H2'	39:0:4459:HOH:O	2.22	0.40
1:0:1159:G:H21	1:0:1189:A:H8	1.69	0.40
1:0:1778:A:H2'	1:0:1779:A:H5'	2.03	0.40
1:0:2121:G:H1'	39:0:3302:HOH:O	2.20	0.40
1:0:2548:C:OP2	3:B:5:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2672:C:H2'	1:0:2673:U:H6	1.85	0.40
3:B:195:ARG:HG2	3:B:323:LEU:HD22	2.02	0.40
1:0:283:U:H5	1:0:284:C:N3	2.18	0.40
1:0:304:G:H1'	1:0:347:A:N6	2.36	0.40
1:0:327:A:H4'	1:0:329:A:N7	2.37	0.40
1:0:383:A:H4'	39:0:4330:HOH:O	2.21	0.40
1:0:1072:G:OP2	26:Y:154:ARG:NH2	2.55	0.40
1:0:1342:C:O2'	1:0:1343:C:H5'	2.21	0.40
1:0:1972:U:C2'	1:0:1973:A:C5'	3.00	0.40
1:0:2002:C:C2'	1:0:2003:U:H5'	2.51	0.40
1:0:2114:C:O2'	1:0:2115:U:H5'	2.21	0.40
2:A:135:VAL:HG11	2:A:147:ARG:NH2	2.36	0.40
18:Q:47:VAL:HA	18:Q:48:PRO:HD3	1.94	0.40
26:Y:134:HIS:CD2	26:Y:134:HIS:H	2.39	0.40
31:9:54:A:O2'	31:9:55:U:H5'	2.21	0.40
31:9:73:A:H2'	31:9:74:G:O4'	2.20	0.40
1:0:10:U:C4	1:0:532:A:C8	3.10	0.40
1:0:1183:C:H5	1:0:1192:A:OP1	2.03	0.40
1:0:1804:A:H2'	1:0:1805:G:C8	2.56	0.40
3:B:57:GLU:HA	3:B:58:PRO:HD2	1.98	0.40
15:N:86:LEU:HD12	15:N:125:ALA:HB2	2.03	0.40
1:0:137:U:OP1	1:0:259:G:O2'	2.40	0.40
1:0:282:C:O2'	1:0:283:U:C5'	2.70	0.40
1:0:308:U:H5'	21:T:97:ARG:NH2	2.36	0.40
1:0:537:G:O4'	1:0:538:C:C5	2.75	0.40
1:0:598:C:H2'	1:0:599:G:H8	1.86	0.40
1:0:1008:C:O2'	1:0:1009:U:H5'	2.21	0.40
1:0:1016:U:H1'	39:0:8342:HOH:O	2.20	0.40
1:0:1132:A:H2'	1:0:1133:A:C8	2.57	0.40
1:0:1361:C:H2'	1:0:1362:U:H6	1.86	0.40
1:0:1788:U:O2'	1:0:1789:G:H5'	2.22	0.40
1:0:1812:G:H4'	1:0:1814:G:O4'	2.22	0.40
6:E:49:ILE:HD11	6:E:69:ILE:HD12	2.02	0.40
1:0:77:G:C2'	1:0:78:G:H5'	2.51	0.40
1:0:113:A:OP2	1:0:114:A:H2'	2.21	0.40
1:0:316:A:H5'	21:T:54:ASP:OD2	2.22	0.40
1:0:827:A:H2'	1:0:828:G:O4'	2.22	0.40
1:0:1167:G:H1'	39:I:6825:HOH:O	2.21	0.40
1:0:1175:G:H1'	1:0:1193:A:C2'	2.51	0.40
1:0:1211:G:O2'	1:0:1212:C:H5'	2.22	0.40
1:0:1257:C:O2'	1:0:1258:G:H5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1331:G:OP2	26:Y:142:SER:OG	2.33	0.40
1:0:1537:C:H1'	39:0:6076:HOH:O	2.22	0.40
1:0:1594:C:O2'	1:0:1595:G:H5'	2.22	0.40
1:0:1657:A:H2'	1:0:1658:A:C8	2.56	0.40
1:0:2245:C:O5'	1:0:2245:C:H6	2.04	0.40
1:0:2401:A:H2'	1:0:2402:A:H8	1.82	0.40
1:0:2629:C:N4	2:A:206:ARG:HH21	2.18	0.40
5:D:48:MET:HB3	31:9:41:C:H4'	2.04	0.40
31:9:33:U:H2'	39:9:3797:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	235/237 (99%)	218 (93%)	14 (6%)	3 (1%)	9	21
3	B	335/337 (99%)	307 (92%)	26 (8%)	2 (1%)	21	38
4	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	16	31
5	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	5	12
6	E	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
7	F	117/119 (98%)	109 (93%)	7 (6%)	1 (1%)	14	28
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	150 (96%)	5 (3%)	1 (1%)	21	38
10	I	68/70 (97%)	58 (85%)	10 (15%)	0	100	100
11	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
12	K	130/132 (98%)	125 (96%)	4 (3%)	1 (1%)	16	31
13	L	141/165 (86%)	127 (90%)	14 (10%)	0	100	100
14	M	192/194 (99%)	187 (97%)	4 (2%)	1 (0%)	24	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	N	184/186 (99%)	173 (94%)	8 (4%)	3 (2%)	7	17
16	O	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
17	P	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
18	Q	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	11	24
19	R	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
20	S	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
21	T	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	14	28
22	U	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
23	V	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
24	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
25	X	80/82 (98%)	77 (96%)	2 (2%)	1 (1%)	9	21
26	Y	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
27	Z	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
28	1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4172 (89%)	3503 (94%)	182 (5%)	20 (0%)	24	42

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	37	VAL
5	D	137	PRO
15	N	154	LEU
15	N	139	TRP
3	B	2	GLN
5	D	56	ARG
12	K	127	ALA
15	N	167	ASP
2	A	27	LEU
3	B	185	GLY
4	C	8	LEU
7	F	100	ASP
14	M	71	SER
9	H	19	ARG
21	T	44	ALA

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Mol	Chain	Res	Type
4	C	79	ARG
5	D	27	ILE
18	Q	18	PRO
2	A	88	ILE
25	X	52	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	179/179 (100%)	167 (93%)	12 (7%)	15	31
3	B	282/282 (100%)	261 (93%)	21 (7%)	13	26
4	C	193/193 (100%)	176 (91%)	17 (9%)	9	20
5	D	117/148 (79%)	103 (88%)	14 (12%)	5	9
6	E	152/152 (100%)	145 (95%)	7 (5%)	24	48
7	F	93/93 (100%)	88 (95%)	5 (5%)	20	42
8	G	27/282 (10%)	27 (100%)	0	100	100
9	H	134/145 (92%)	129 (96%)	5 (4%)	30	55
10	I	58/58 (100%)	57 (98%)	1 (2%)	53	75
11	J	118/118 (100%)	110 (93%)	8 (7%)	14	30
12	K	106/106 (100%)	101 (95%)	5 (5%)	23	47
13	L	113/127 (89%)	110 (97%)	3 (3%)	39	63
14	M	158/158 (100%)	153 (97%)	5 (3%)	34	59
15	N	149/149 (100%)	139 (93%)	10 (7%)	15	31
16	O	93/93 (100%)	89 (96%)	4 (4%)	26	50
17	P	113/113 (100%)	108 (96%)	5 (4%)	25	49
18	Q	79/79 (100%)	76 (96%)	3 (4%)	29	54
19	R	117/117 (100%)	113 (97%)	4 (3%)	32	58
20	S	71/71 (100%)	69 (97%)	2 (3%)	38	62
21	T	105/105 (100%)	97 (92%)	8 (8%)	12	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	44/44 (100%)	44 (100%)	0	100	100
23	V	51/51 (100%)	49 (96%)	2 (4%)	28	54
24	W	130/130 (100%)	122 (94%)	8 (6%)	16	34
25	X	66/66 (100%)	56 (85%)	10 (15%)	3	5
26	Y	120/120 (100%)	116 (97%)	4 (3%)	33	58
27	Z	60/60 (100%)	59 (98%)	1 (2%)	53	75
28	1	46/46 (100%)	45 (98%)	1 (2%)	45	69
29	2	42/46 (91%)	41 (98%)	1 (2%)	43	67
30	3	79/79 (100%)	77 (98%)	2 (2%)	42	66
All	All	3095/3410 (91%)	2927 (95%)	168 (5%)	20	42

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	ARG
2	A	51	ARG
2	A	64	ASP
2	A	94	LEU
2	A	105	VAL
2	A	108	VAL
2	A	110	SER
2	A	131	HIS
2	A	175	LYS
2	A	179	MET
2	A	200	PRO
2	A	217	ARG
3	B	7	ARG
3	B	11	LEU
3	B	27	ASN
3	B	49	THR
3	B	53	LEU
3	B	71	VAL
3	B	82	VAL
3	B	84	LEU
3	B	97	LEU
3	B	98	THR
3	B	151	VAL
3	B	162	MET
3	B	171	VAL

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Mol	Chain	Res	Type
3	B	195	ARG
3	B	234	ARG
3	B	251	VAL
3	B	254	GLN
3	B	267	LYS
3	B	277	GLU
3	B	280	VAL
3	B	301	VAL
4	C	2	GLN
4	C	27	ARG
4	C	76	ARG
4	C	78	ARG
4	C	94	THR
4	C	98	ARG
4	C	136	VAL
4	C	162	VAL
4	C	171	GLU
4	C	187	ARG
4	C	214	THR
4	C	223	LEU
4	C	234	VAL
4	C	236	THR
4	C	237	GLU
4	C	240	LEU
4	C	243	VAL
5	D	19	GLU
5	D	23	VAL
5	D	24	HIS
5	D	29	HIS
5	D	50	VAL
5	D	58	VAL
5	D	62	ASP
5	D	69	ILE
5	D	73	VAL
5	D	101	THR
5	D	128	LEU
5	D	137	PRO
5	D	149	ARG
5	D	161	ASP
6	E	16	ASP
6	E	36	PRO
6	E	61	THR

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Mol	Chain	Res	Type
6	E	86	VAL
6	E	102	VAL
6	E	133	VAL
6	E	156	ASP
7	F	12	LEU
7	F	46	GLU
7	F	50	VAL
7	F	60	VAL
7	F	91	VAL
9	H	62	HIS
9	H	65	LEU
9	H	87	LYS
9	H	157	TYR
9	H	173	GLU
10	I	94	ASP
11	J	35	THR
11	J	39	VAL
11	J	45	VAL
11	J	46	ILE
11	J	120	SER
11	J	127	ILE
11	J	130	VAL
11	J	131	THR
12	K	10	GLN
12	K	19	THR
12	K	98	VAL
12	K	107	THR
12	K	119	GLN
13	L	43	HIS
13	L	114	VAL
13	L	140	VAL
14	M	10	ASP
14	M	46	LEU
14	M	93	ARG
14	M	99	ARG
14	M	141	ILE
15	N	12	ARG
15	N	26	LEU
15	N	38	LYS
15	N	47	LEU
15	N	49	THR
15	N	74	PRO

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Mol	Chain	Res	Type
15	N	134	ASP
15	N	135	VAL
15	N	142	THR
15	N	180	LEU
16	O	3	THR
16	O	25	VAL
16	O	69	VAL
16	O	80	ASP
17	P	13	VAL
17	P	21	VAL
17	P	52	LYS
17	P	91	LYS
17	P	98	ILE
18	Q	16	ASN
18	Q	18	PRO
18	Q	57	ASP
19	R	13	THR
19	R	39	THR
19	R	119	VAL
19	R	143	VAL
20	S	10	VAL
20	S	81	ILE
21	T	5	ASP
21	T	39	ASN
21	T	48	VAL
21	T	61	GLU
21	T	82	THR
21	T	89	ARG
21	T	96	VAL
21	T	117	ASP
23	V	12	THR
23	V	13	PRO
24	W	13	MET
24	W	35	VAL
24	W	38	THR
24	W	52	VAL
24	W	88	THR
24	W	120	PRO
24	W	142	ASP
24	W	146	ILE
25	X	10	VAL
25	X	43	VAL

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Mol	Chain	Res	Type
25	X	46	ASP
25	X	49	ARG
25	X	52	PRO
25	X	72	VAL
25	X	79	GLU
25	X	80	GLU
25	X	82	GLU
25	X	88	GLU
26	Y	154	ARG
26	Y	174	VAL
26	Y	189	ASN
26	Y	203	VAL
27	Z	53	ILE
28	1	14	THR
29	2	18	ASN
30	3	18	GLN
30	3	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	47	HIS
2	A	176	HIS
2	A	199	HIS
3	B	27	ASN
3	B	55	ASN
3	B	177	HIS
3	B	221	GLN
3	B	238	ASN
3	B	243	ASN
3	B	260	HIS
3	B	320	GLN
3	B	332	ASN
4	C	2	GLN
4	C	39	GLN
4	C	67	GLN
4	C	73	GLN
4	C	129	HIS
4	C	163	HIS
5	D	47	GLN
5	D	103	ASN
6	E	55	ASN

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Mol	Chain	Res	Type
6	E	96	ASN
6	E	106	ASN
6	E	119	HIS
6	E	143	GLN
6	E	155	ASN
7	F	55	GLN
8	G	64	ASN
9	H	40	GLN
9	H	49	GLN
9	H	59	GLN
9	H	75	HIS
10	I	102	GLN
11	J	25	GLN
11	J	52	GLN
11	J	107	ASN
11	J	126	ASN
12	K	10	GLN
12	K	67	GLN
12	K	119	GLN
13	L	18	HIS
13	L	41	HIS
14	M	24	GLN
14	M	26	GLN
14	M	58	GLN
14	M	129	HIS
14	M	170	ASN
15	N	21	HIS
15	N	40	ASN
15	N	107	ASN
15	N	140	GLN
17	P	66	GLN
17	P	73	HIS
17	P	88	GLN
17	P	89	ASN
17	P	118	GLN
18	Q	16	ASN
18	Q	40	HIS
19	R	22	GLN
19	R	94	ASN
19	R	98	ASN
19	R	102	GLN
19	R	117	HIS

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Mol	Chain	Res	Type
20	S	7	HIS
20	S	9	HIS
20	S	21	GLN
20	S	53	ASN
20	S	55	GLN
21	T	39	ASN
22	U	39	ASN
22	U	48	ASN
23	V	60	GLN
24	W	14	HIS
24	W	110	GLN
24	W	141	HIS
25	X	23	HIS
26	Y	98	GLN
26	Y	119	GLN
26	Y	129	ASN
26	Y	134	HIS
26	Y	149	GLN
26	Y	189	ASN
28	1	8	GLN
28	1	16	HIS
28	1	28	HIS
29	2	16	ASN
29	2	18	ASN
29	2	36	ASN
29	2	37	HIS
29	2	41	HIS
29	2	45	ASN
30	3	2	GLN
30	3	18	GLN
30	3	20	HIS
30	3	30	GLN
30	3	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	241 (8%)	26 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	258 (9%)	27 (0%)

All (258) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	198	A
1	0	200	C
1	0	204	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A

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Mol	Chain	Res	Type
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	938	G
1	0	953	G
1	0	960	G
1	0	961	A

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Mol	Chain	Res	Type
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1106	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1151	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1205	U
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	G
1	0	1342	C
1	0	1353	C
1	0	1357	A
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C

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Mol	Chain	Res	Type
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1535	G
1	0	1592	G
1	0	1617	C
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1965	C
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U

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Mol	Chain	Res	Type
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2133	U
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2291	A
1	0	2317	C
1	0	2320	U
1	0	2321	A
1	0	2345	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G

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Mol	Chain	Res	Type
1	0	2608	C
1	0	2613	G
1	0	2638	G
1	0	2645	U
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2676	C
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2836	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	34	A
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A

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Mol	Chain	Res	Type
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1165	G
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1474	C
1	0	1667	A
1	0	1684	A
1	0	1979	G
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
31	9	65	A

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	OMU	0	2587	34,1	19,22,23	0.34	0	25,31,34	0.36	0
1	PSU	0	2621	1	18,21,22	1.59	2 (11%)	21,30,33	1.41	3 (14%)
1	OMG	0	2588	1	23,26,27	0.28	0	32,38,41	0.43	0
1	1MA	0	628	34,1	21,25,26	0.74	1 (4%)	30,37,40	0.84	2 (6%)
1	UR3	0	2619	1	19,22,23	0.50	0	26,32,35	0.68	1 (3%)

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	OMU	0	2587	34,1	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	1/9/27/28	0/3/3/3
1	1MA	0	628	34,1	-	2/7/25/26	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.19	1.43	1.36
1	0	2621	PSU	C6-C5	2.96	1.38	1.35
1	0	628	1MA	C6-N6	2.55	1.34	1.28

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.46	120.51	118.17
1	0	2621	PSU	C6-N1-C2	-3.16	119.76	122.69
1	0	2621	PSU	O2-C2-N1	3.00	125.87	122.79
1	0	628	1MA	N1-C2-N3	2.84	129.37	126.00
1	0	2619	UR3	C4-N3-C2	2.68	126.74	124.58
1	0	628	1MA	CM1-N1-C6	2.09	123.39	120.15

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4
1	0	2588	OMG	C3'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	628	1MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 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
37	WIN	0	9101	-	40,43,43	1.93	9 (22%)	51,71,71	3.63	29 (56%)

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
37	WIN	0	9101	-	-	9/20/110/110	0/6/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	WIN	C1N-C1V	5.72	1.41	1.33
37	0	9101	WIN	C2M-C2G	5.40	1.61	1.53
37	0	9101	WIN	C2B-C1X	-4.24	1.40	1.46
37	0	9101	WIN	C1C-C1Y	3.69	1.56	1.50
37	0	9101	WIN	C1N-C1W	-2.98	1.39	1.46
37	0	9101	WIN	O1U-C1Z	2.46	1.38	1.34
37	0	9101	WIN	O1U-C2G	2.38	1.49	1.46
37	0	9101	WIN	C2H-C1Y	2.24	1.56	1.52
37	0	9101	WIN	C1B-C1V	2.17	1.54	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	WIN	O1R-C2A-C2L	9.00	125.14	111.46
37	0	9101	WIN	O1J-C2A-C2L	-6.63	111.90	123.67
37	0	9101	WIN	C1O-C2M-C2G	6.43	123.74	112.86
37	0	9101	WIN	C1P-C1X-C2B	6.30	126.51	117.19
37	0	9101	WIN	O1U-C1Z-O1I	6.17	127.45	118.52
37	0	9101	WIN	C1V-C1N-C1W	6.17	142.36	126.67
37	0	9101	WIN	C2I-C2H-C1Y	5.92	120.23	112.19
37	0	9101	WIN	C1C-C1Y-C2H	5.66	130.28	116.10
37	0	9101	WIN	C1P-C2I-C2H	5.62	114.32	107.64
37	0	9101	WIN	O1U-C1Z-C2F	-5.51	106.04	118.04
37	0	9101	WIN	O1U-C2G-C1Q	-4.97	96.58	104.80
37	0	9101	WIN	O1T-C1W-O1G	-4.88	115.53	123.34
37	0	9101	WIN	O1H-C1X-C1P	-4.84	111.59	120.41
37	0	9101	WIN	C1O-C2M-C2K	-4.79	92.00	100.89
37	0	9101	WIN	O1T-C2F-C1Z	-4.30	99.88	108.00
37	0	9101	WIN	C1Q-C2G-C2M	3.92	121.06	113.76
37	0	9101	WIN	C1A-O1R-C2A	3.63	121.87	115.91
37	0	9101	WIN	O1T-C2F-C2K	-3.44	102.92	110.59
37	0	9101	WIN	O1L-C2D-C2J	-3.37	101.83	111.94
37	0	9101	WIN	C2H-C1Q-C2G	-3.30	102.67	111.35
37	0	9101	WIN	C2M-C2J-C2D	3.24	116.06	109.87
37	0	9101	WIN	C1F-C2I-C2H	2.97	114.87	109.89
37	0	9101	WIN	C1F-C2I-C2J	-2.88	106.07	113.19
37	0	9101	WIN	C2I-C2J-C2D	2.57	120.98	115.04
37	0	9101	WIN	O1K-C2B-C1X	2.40	120.02	115.74
37	0	9101	WIN	O1S-C1O-C2M	-2.24	103.02	105.72
37	0	9101	WIN	C1D-C2C-C1V	-2.20	107.96	111.63
37	0	9101	WIN	O1T-C1W-C1N	2.14	116.16	111.20
37	0	9101	WIN	O1I-C1Z-C2F	-2.13	118.54	122.29

There are no chirality outliers.

All (9) torsion outliers are listed below:

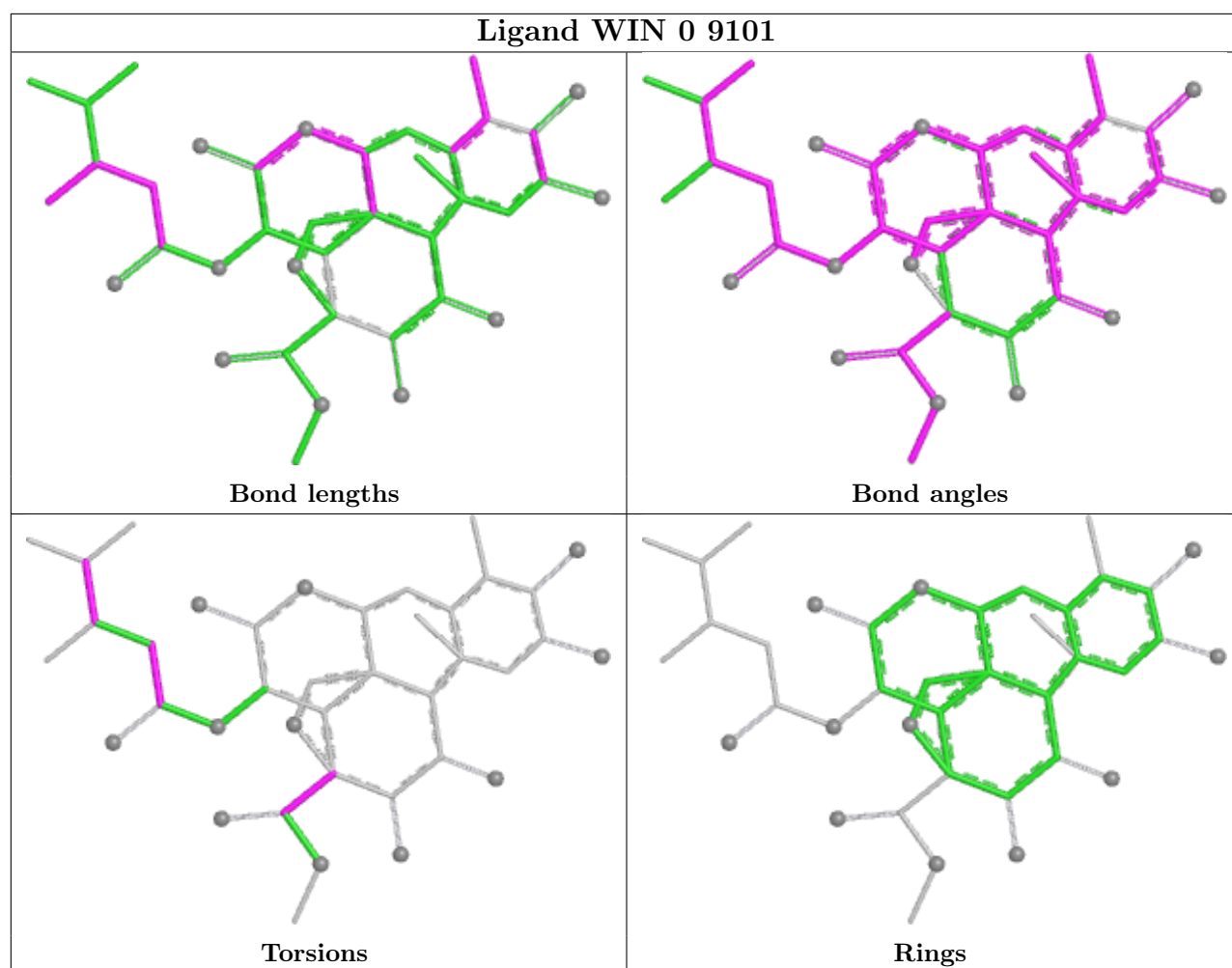
Mol	Chain	Res	Type	Atoms
37	0	9101	WIN	C1N-C1V-C2C-C1D
37	0	9101	WIN	C1N-C1V-C2C-C1E
37	0	9101	WIN	C1B-C1V-C2C-C1D
37	0	9101	WIN	O1J-C2A-C2L-O1S
37	0	9101	WIN	O1R-C2A-C2L-O1S
37	0	9101	WIN	C1V-C1N-C1W-O1T
37	0	9101	WIN	O1R-C2A-C2L-C2K
37	0	9101	WIN	C1V-C1N-C1W-O1G
37	0	9101	WIN	C1B-C1V-C2C-C1E

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	9101	WIN	13	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2923 (94%)	-0.51	14 (0%) 87 85	24, 56, 105, 182	0
2	A	237/237 (100%)	0.35	8 (3%) 48 38	35, 71, 114, 133	0
3	B	337/337 (100%)	0.22	3 (0%) 81 76	34, 65, 95, 108	0
4	C	246/246 (100%)	0.17	5 (2%) 65 57	31, 56, 80, 91	0
5	D	140/177 (79%)	1.45	36 (25%) 1 1	80, 120, 142, 152	0
6	E	172/172 (100%)	0.51	7 (4%) 41 32	55, 81, 105, 112	0
7	F	119/119 (100%)	0.74	8 (6%) 24 17	64, 90, 122, 137	0
8	G	29/348 (8%)	0.99	7 (24%) 2 1	89, 109, 116, 119	0
9	H	160/177 (90%)	0.49	7 (4%) 39 30	57, 84, 120, 128	0
10	I	70/70 (100%)	2.22	33 (47%) 0 0	142, 164, 183, 184	0
11	J	142/142 (100%)	0.17	4 (2%) 55 46	47, 60, 82, 104	0
12	K	132/132 (100%)	0.12	1 (0%) 82 78	44, 61, 86, 90	0
13	L	145/165 (87%)	0.69	13 (8%) 15 12	35, 87, 131, 142	0
14	M	194/194 (100%)	0.14	2 (1%) 79 74	38, 55, 75, 82	0
15	N	186/186 (100%)	0.72	15 (8%) 18 13	55, 83, 139, 146	0
16	O	115/115 (100%)	0.40	1 (0%) 81 76	43, 66, 84, 88	0
17	P	143/143 (100%)	0.52	7 (4%) 35 27	50, 70, 86, 94	0
18	Q	95/95 (100%)	0.09	0 100 100	49, 60, 76, 89	0
19	R	150/150 (100%)	-0.12	0 100 100	38, 56, 78, 84	0
20	S	81/81 (100%)	0.25	0 100 100	56, 76, 100, 108	0
21	T	119/119 (100%)	0.39	4 (3%) 48 38	48, 71, 100, 127	0
22	U	53/53 (100%)	0.30	1 (1%) 66 59	56, 72, 95, 102	0
23	V	65/65 (100%)	0.96	8 (12%) 8 6	66, 94, 137, 144	0
24	W	154/154 (100%)	0.15	1 (0%) 85 82	44, 60, 79, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/82 (100%)	0.46	6 (7%) 21 15	55, 71, 97, 111	0
26	Y	142/142 (100%)	-0.06	2 (1%) 73 67	31, 53, 80, 102	0
27	Z	73/73 (100%)	1.95	24 (32%) 1 1	99, 132, 149, 150	0
28	1	56/56 (100%)	-0.39	0 100 100	33, 41, 52, 62	0
29	2	46/50 (92%)	0.66	5 (10%) 10 8	48, 79, 112, 122	0
30	3	92/92 (100%)	0.47	3 (3%) 49 40	58, 85, 99, 109	0
31	9	122/122 (100%)	-0.17	3 (2%) 58 49	46, 78, 108, 156	0
All	All	6646/7217 (92%)	0.03	228 (3%) 48 38	24, 64, 122, 184	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	11.0
27	Z	46	SER	8.1
10	I	128	THR	7.5
27	Z	36	GLY	6.4
10	I	71	ALA	6.0
27	Z	42	TYR	5.7
27	Z	35	SER	5.3
27	Z	45	VAL	5.3
10	I	74	ILE	5.0
10	I	112	LEU	5.0
10	I	127	CYS	4.9
10	I	120	ALA	4.8
27	Z	43	GLY	4.7
27	Z	58	ASN	4.7
27	Z	50	VAL	4.7
27	Z	39	GLY	4.6
5	D	107	GLY	4.5
10	I	70	THR	4.5
23	V	2	VAL	4.3
15	N	168	LEU	4.3
31	9	1	U	4.3
5	D	69	ILE	4.3
27	Z	40	ALA	4.3
10	I	113	SER	4.2
5	D	55	LYS	4.0
5	D	10	PHE	3.9
5	D	26	GLY	3.9
5	D	90	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
10	I	130	LEU	3.8
6	E	154	ILE	3.8
15	N	166	ALA	3.8
2	A	32	VAL	3.7
21	T	119	ALA	3.7
27	Z	38	PHE	3.7
23	V	39	ALA	3.7
5	D	18	ILE	3.6
10	I	95	LEU	3.6
15	N	154	LEU	3.6
10	I	72	GLU	3.5
1	O	10	U	3.5
23	V	40	PRO	3.5
27	Z	37	ARG	3.5
14	M	89	THR	3.5
5	D	35	ALA	3.5
5	D	174	VAL	3.4
27	Z	34	SER	3.4
15	N	159	TYR	3.4
5	D	63	ILE	3.4
8	G	12	ILE	3.4
29	2	49	GLU	3.4
10	I	132	VAL	3.4
5	D	44	ILE	3.4
27	Z	53	ILE	3.4
13	L	146	GLY	3.3
5	D	172	VAL	3.3
10	I	124	VAL	3.3
7	F	101	ALA	3.3
10	I	104	ALA	3.3
13	L	82	ALA	3.3
9	H	174	LEU	3.3
10	I	85	GLY	3.3
21	T	40	VAL	3.3
25	X	85	VAL	3.3
5	D	40	ILE	3.2
5	D	70	GLY	3.2
23	V	43	PRO	3.2
5	D	134	LEU	3.1
5	D	171	ASP	3.1
27	Z	41	ARG	3.0
1	O	1161	A	3.0

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Mol	Chain	Res	Type	RSRZ
5	D	37	ALA	3.0
25	X	83	ALA	3.0
31	9	24	U	3.0
2	A	82	VAL	3.0
27	Z	47	ARG	2.9
29	2	48	ASP	2.9
10	I	100	VAL	2.9
5	D	104	PHE	2.9
1	0	138	U	2.9
9	H	171	GLY	2.9
27	Z	54	GLU	2.9
15	N	145	ALA	2.9
13	L	60	GLU	2.8
13	L	148	GLU	2.8
30	3	41	GLU	2.8
5	D	135	VAL	2.8
17	P	135	ALA	2.8
6	E	100	ASP	2.8
2	A	85	SER	2.8
15	N	158	LEU	2.8
5	D	130	VAL	2.8
25	X	87	ALA	2.8
10	I	91	PHE	2.8
11	J	70	PHE	2.8
31	9	2	U	2.8
10	I	129	SER	2.8
10	I	107	LYS	2.8
7	F	102	GLY	2.8
5	D	89	PRO	2.8
10	I	123	VAL	2.8
1	0	1171	A	2.7
7	F	17	LEU	2.7
2	A	211	LYS	2.7
6	E	45	ASP	2.7
5	D	53	LYS	2.7
27	Z	57	MET	2.7
10	I	111	LEU	2.7
15	N	169	PRO	2.7
15	N	167	ASP	2.7
10	I	88	GLN	2.7
10	I	134	ILE	2.6
2	A	37	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
17	P	58	SER	2.6
13	L	91	VAL	2.6
13	L	108	VAL	2.6
2	A	88	ILE	2.6
15	N	147	ILE	2.6
8	G	63	ARG	2.6
27	Z	78	ILE	2.6
15	N	1	ALA	2.6
23	V	35	ALA	2.6
16	O	47	ARG	2.6
5	D	58	VAL	2.6
13	L	125	PHE	2.6
6	E	10	ASP	2.6
27	Z	70	ARG	2.5
29	2	42	TRP	2.5
7	F	47	LEU	2.5
1	0	1160	G	2.5
27	Z	64	PRO	2.5
30	3	83	TRP	2.5
7	F	75	ILE	2.5
7	F	111	ILE	2.5
10	I	119	ALA	2.5
29	2	35	ARG	2.5
7	F	15	ASP	2.5
5	D	57	THR	2.5
23	V	36	ALA	2.5
1	0	1184	C	2.5
10	I	68	PRO	2.4
9	H	133	GLY	2.4
10	I	67	VAL	2.4
5	D	25	MET	2.4
10	I	73	LEU	2.4
8	G	23	ILE	2.4
13	L	124	ASP	2.4
21	T	114	SER	2.4
27	Z	44	ARG	2.4
10	I	133	THR	2.4
5	D	166	ILE	2.4
10	I	75	LYS	2.4
9	H	115	GLY	2.4
2	A	36	ASP	2.4
7	F	106	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
11	J	92	GLN	2.3
2	A	68	ILE	2.3
5	D	62	ASP	2.3
5	D	75	LEU	2.3
5	D	128	LEU	2.3
9	H	160	ILE	2.3
4	C	101	ASP	2.3
5	D	88	LEU	2.3
22	U	51	TRP	2.3
3	B	1	PRO	2.3
10	I	83	GLY	2.3
10	I	97	VAL	2.2
1	0	1162	G	2.2
21	T	25	ALA	2.2
1	0	735	C	2.2
25	X	65	ASN	2.2
15	N	164	ASP	2.2
27	Z	69	ASP	2.2
4	C	61	PHE	2.2
23	V	47	LYS	2.2
13	L	77	ALA	2.2
10	I	118	ASN	2.2
1	0	1186	C	2.2
13	L	145	LEU	2.2
15	N	186	LEU	2.2
6	E	81	GLU	2.2
17	P	70	ALA	2.2
5	D	27	ILE	2.1
4	C	16	VAL	2.1
13	L	97	VAL	2.1
8	G	73	ASP	2.1
3	B	208	GLY	2.1
5	D	86	THR	2.1
11	J	79	PHE	2.1
1	0	1279	U	2.1
11	J	144	THR	2.1
17	P	114	LEU	2.1
9	H	43	ALA	2.1
15	N	148	ALA	2.1
17	P	71	TYR	2.1
4	C	245	GLU	2.1
6	E	134	SER	2.1

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Mol	Chain	Res	Type	RSRZ
8	G	27	ILE	2.1
1	0	2769	C	2.1
5	D	72	LYS	2.1
13	L	106	VAL	2.1
24	W	45	VAL	2.1
3	B	305	ASP	2.1
10	I	80	PHE	2.1
14	M	81	ARG	2.1
26	Y	216	ARG	2.1
26	Y	235	GLU	2.1
1	0	2768	A	2.1
1	0	1176	C	2.1
4	C	139	VAL	2.1
12	K	110	LYS	2.1
17	P	67	LYS	2.1
5	D	68	PRO	2.1
8	G	13	PRO	2.1
8	G	71	LEU	2.1
17	P	108	LEU	2.1
5	D	17	ARG	2.1
29	2	47	THR	2.1
25	X	84	ILE	2.1
1	0	1175	G	2.0
30	3	62	THR	2.0
6	E	53	GLU	2.0
15	N	139	TRP	2.0
15	N	152	GLU	2.0
5	D	59	GLY	2.0
25	X	66	THR	2.0
27	Z	76	THR	2.0
9	H	86	TYR	2.0
13	L	81	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMG	0	2588	24/25	0.97	0.06	42,44,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	UR3	0	2619	21/22	0.97	0.07	45,48,51,54	0
1	1MA	0	628	23/24	0.98	0.06	34,36,38,39	0
1	OMU	0	2587	21/22	0.98	0.06	43,44,46,48	0
1	PSU	0	2621	20/21	0.98	0.06	30,35,50,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8525	1/1	0.22	0.39	93,93,93,93	0
34	NA	0	8573	1/1	0.58	0.23	87,87,87,87	0
34	NA	9	8572	1/1	0.59	0.26	117,117,117,117	0
36	SR	0	8983	1/1	0.59	0.23	199,199,199,199	0
32	MG	0	8090	1/1	0.62	0.31	121,121,121,121	0
34	NA	0	8557	1/1	0.63	0.36	74,74,74,74	0
34	NA	0	8559	1/1	0.64	0.53	95,95,95,95	0
34	NA	0	8571	1/1	0.66	0.32	98,98,98,98	0
34	NA	0	8556	1/1	0.66	0.39	68,68,68,68	0
36	SR	0	8996	1/1	0.66	0.23	200,200,200,200	0
36	SR	0	8991	1/1	0.69	0.21	195,195,195,195	0
32	MG	0	8063	1/1	0.70	0.29	80,80,80,80	0
32	MG	0	8049	1/1	0.71	0.30	116,116,116,116	0
34	NA	0	8511	1/1	0.72	0.17	67,67,67,67	0
36	SR	0	8977	1/1	0.74	0.08	197,197,197,197	0
34	NA	0	8548	1/1	0.74	0.34	67,67,67,67	0
34	NA	J	8538	1/1	0.75	0.20	67,67,67,67	0
34	NA	0	8522	1/1	0.75	0.84	108,108,108,108	0
34	NA	0	8509	1/1	0.77	0.35	77,77,77,77	0
34	NA	H	8518	1/1	0.77	0.27	95,95,95,95	0
36	SR	0	9006	1/1	0.77	0.35	200,200,200,200	0
36	SR	0	8959	1/1	0.78	0.09	181,181,181,181	0
34	NA	0	8554	1/1	0.78	0.16	70,70,70,70	0
36	SR	0	9000	1/1	0.78	0.22	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8920	1/1	0.78	0.24	185,185,185,185	0
36	SR	0	8933	1/1	0.79	0.18	143,143,143,143	0
36	SR	0	8997	1/1	0.79	0.28	200,200,200,200	0
36	SR	9	9003	1/1	0.79	0.14	187,187,187,187	0
36	SR	0	8917	1/1	0.80	0.20	151,151,151,151	0
36	SR	0	8944	1/1	0.80	0.19	178,178,178,178	0
36	SR	0	8947	1/1	0.80	0.24	200,200,200,200	0
36	SR	9	8978	1/1	0.80	0.15	169,169,169,169	0
36	SR	0	8927	1/1	0.80	0.16	167,167,167,167	0
36	SR	0	8993	1/1	0.81	0.14	178,178,178,178	0
34	NA	0	8533	1/1	0.81	0.31	72,72,72,72	0
32	MG	0	8072	1/1	0.81	0.18	82,82,82,82	0
32	MG	0	8091	1/1	0.81	0.12	89,89,89,89	0
36	SR	0	8982	1/1	0.81	0.31	200,200,200,200	0
36	SR	0	8934	1/1	0.81	0.24	166,166,166,166	0
36	SR	0	8919	1/1	0.81	0.16	179,179,179,179	0
34	NA	0	8501	1/1	0.82	0.14	54,54,54,54	0
32	MG	0	8080	1/1	0.82	0.08	87,87,87,87	0
36	SR	0	8956	1/1	0.82	0.11	187,187,187,187	0
36	SR	0	8989	1/1	0.82	0.23	185,185,185,185	0
34	NA	0	8524	1/1	0.82	0.22	73,73,73,73	0
36	SR	0	8971	1/1	0.82	0.15	185,185,185,185	0
34	NA	0	8506	1/1	0.83	0.12	76,76,76,76	0
34	NA	0	8535	1/1	0.83	0.23	63,63,63,63	0
36	SR	0	8941	1/1	0.83	0.17	131,131,131,131	0
32	MG	0	8092	1/1	0.83	0.12	80,80,80,80	0
32	MG	0	8031	1/1	0.83	0.13	73,73,73,73	0
34	NA	0	8561	1/1	0.84	0.53	90,90,90,90	0
36	SR	0	8942	1/1	0.84	0.17	144,144,144,144	0
36	SR	0	8922	1/1	0.84	0.18	156,156,156,156	0
34	NA	0	8536	1/1	0.84	0.12	65,65,65,65	0
36	SR	0	8984	1/1	0.84	0.13	143,143,143,143	0
32	MG	9	8074	1/1	0.84	0.25	101,101,101,101	0
36	SR	9	8980	1/1	0.84	0.09	175,175,175,175	0
32	MG	0	8071	1/1	0.84	0.31	71,71,71,71	0
36	SR	A	8930	1/1	0.85	0.21	169,169,169,169	0
36	SR	B	8987	1/1	0.85	0.41	200,200,200,200	0
36	SR	0	8976	1/1	0.85	0.17	200,200,200,200	0
36	SR	0	9002	1/1	0.85	0.16	183,183,183,183	0
34	NA	0	8562	1/1	0.85	0.51	82,82,82,82	0
36	SR	0	9001	1/1	0.86	0.11	184,184,184,184	0
36	SR	0	8986	1/1	0.86	0.27	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	9004	1/1	0.86	0.22	200,200,200,200	0
34	NA	0	8564	1/1	0.86	0.23	95,95,95,95	0
36	SR	0	8951	1/1	0.86	0.07	149,149,149,149	0
36	SR	B	8950	1/1	0.86	0.16	119,119,119,119	0
36	SR	0	8955	1/1	0.86	0.23	198,198,198,198	0
34	NA	0	8574	1/1	0.86	0.38	69,69,69,69	0
33	K	0	8401	1/1	0.86	0.39	123,123,123,123	0
36	SR	0	8965	1/1	0.86	0.14	151,151,151,151	0
34	NA	0	8558	1/1	0.87	0.14	63,63,63,63	0
36	SR	0	8979	1/1	0.87	0.11	195,195,195,195	0
36	SR	0	8995	1/1	0.87	0.16	142,142,142,142	0
36	SR	0	8908	1/1	0.87	0.32	175,175,175,175	0
36	SR	0	8949	1/1	0.87	0.16	146,146,146,146	0
36	SR	0	8913	1/1	0.87	0.31	200,200,200,200	0
36	SR	0	8975	1/1	0.87	0.12	154,154,154,154	0
34	NA	0	8575	1/1	0.87	0.35	87,87,87,87	0
37	WIN	0	9101	39/39	0.87	0.27	125,127,128,129	0
34	NA	0	8560	1/1	0.88	0.23	97,97,97,97	0
36	SR	0	8957	1/1	0.88	0.20	200,200,200,200	0
34	NA	0	8507	1/1	0.88	0.14	46,46,46,46	0
36	SR	0	8964	1/1	0.88	0.10	139,139,139,139	0
34	NA	M	8539	1/1	0.88	0.20	53,53,53,53	0
36	SR	0	8967	1/1	0.88	0.12	147,147,147,147	0
34	NA	Q	8540	1/1	0.88	0.12	58,58,58,58	0
34	NA	R	8532	1/1	0.88	0.32	59,59,59,59	0
34	NA	0	8514	1/1	0.88	0.28	54,54,54,54	0
36	SR	0	8928	1/1	0.88	0.14	151,151,151,151	0
34	NA	0	8520	1/1	0.88	0.21	55,55,55,55	0
36	SR	0	8931	1/1	0.89	0.12	136,136,136,136	0
34	NA	0	8541	1/1	0.89	0.20	70,70,70,70	0
32	MG	0	8039	1/1	0.89	0.14	63,63,63,63	0
36	SR	0	8969	1/1	0.89	0.31	173,173,173,173	0
35	CL	A	8809	1/1	0.89	0.36	96,96,96,96	0
36	SR	0	8973	1/1	0.89	0.11	141,141,141,141	0
32	MG	0	8033	1/1	0.89	0.14	63,63,63,63	0
34	NA	0	8555	1/1	0.89	0.23	53,53,53,53	0
36	SR	0	8916	1/1	0.89	0.15	129,129,129,129	0
32	MG	0	8037	1/1	0.89	0.30	80,80,80,80	0
34	NA	0	8527	1/1	0.89	0.27	86,86,86,86	0
34	NA	0	8529	1/1	0.89	0.19	50,50,50,50	0
34	NA	0	8502	1/1	0.89	0.31	66,66,66,66	0
36	SR	F	9005	1/1	0.89	0.10	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	3	8999	1/1	0.89	0.12	140,140,140,140	0
36	SR	0	8985	1/1	0.89	0.17	148,148,148,148	0
34	NA	0	8516	1/1	0.89	0.08	37,37,37,37	0
36	SR	0	8988	1/1	0.89	0.08	158,158,158,158	0
32	MG	A	8051	1/1	0.89	0.09	98,98,98,98	0
34	NA	0	8569	1/1	0.90	0.14	61,61,61,61	0
34	NA	0	8526	1/1	0.90	0.07	45,45,45,45	0
34	NA	0	8515	1/1	0.90	0.07	50,50,50,50	0
32	MG	0	8066	1/1	0.90	0.33	88,88,88,88	0
36	SR	0	8958	1/1	0.90	0.11	121,121,121,121	0
34	NA	0	8519	1/1	0.90	0.12	50,50,50,50	0
32	MG	0	8089	1/1	0.90	0.08	64,64,64,64	0
36	SR	0	8924	1/1	0.90	0.17	149,149,149,149	0
32	MG	0	8056	1/1	0.90	0.17	62,62,62,62	0
34	NA	0	8537	1/1	0.90	0.09	50,50,50,50	0
32	MG	0	8035	1/1	0.90	0.22	70,70,70,70	0
34	NA	0	8547	1/1	0.90	0.24	71,71,71,71	0
36	SR	0	9007	1/1	0.90	0.43	199,199,199,199	0
36	SR	A	8929	1/1	0.90	0.20	142,142,142,142	0
34	NA	S	8510	1/1	0.90	0.10	50,50,50,50	0
36	SR	0	8937	1/1	0.90	0.12	125,125,125,125	0
36	SR	0	8938	1/1	0.90	0.11	191,191,191,191	0
36	SR	0	8939	1/1	0.90	0.11	145,145,145,145	0
34	NA	0	8563	1/1	0.90	0.27	82,82,82,82	0
35	CL	0	8815	1/1	0.90	0.14	83,83,83,83	0
32	MG	0	8073	1/1	0.90	0.30	80,80,80,80	0
35	CL	J	8802	1/1	0.90	0.11	79,79,79,79	0
34	NA	0	8566	1/1	0.90	0.14	59,59,59,59	0
34	NA	0	8570	1/1	0.91	0.20	59,59,59,59	0
34	NA	0	8531	1/1	0.91	0.23	50,50,50,50	0
34	NA	0	8551	1/1	0.91	0.18	60,60,60,60	0
33	K	0	8402	1/1	0.91	0.17	90,90,90,90	0
36	SR	0	8945	1/1	0.91	0.14	131,131,131,131	0
36	SR	0	8998	1/1	0.91	0.18	175,175,175,175	0
36	SR	S	8961	1/1	0.91	0.11	145,145,145,145	0
34	NA	9	8543	1/1	0.91	0.26	57,57,57,57	0
34	NA	0	8534	1/1	0.91	0.16	47,47,47,47	0
36	SR	0	8936	1/1	0.91	0.11	108,108,108,108	0
34	NA	0	8568	1/1	0.91	0.17	57,57,57,57	0
32	MG	9	8040	1/1	0.91	0.15	97,97,97,97	0
36	SR	0	8901	1/1	0.92	0.09	96,96,96,96	0
32	MG	Y	8086	1/1	0.92	0.06	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8521	1/1	0.92	0.07	71,71,71,71	0
36	SR	0	8943	1/1	0.92	0.11	95,95,95,95	0
36	SR	0	8914	1/1	0.92	0.19	127,127,127,127	0
32	MG	0	8082	1/1	0.92	0.14	81,81,81,81	0
36	SR	0	9008	1/1	0.92	0.11	111,111,111,111	0
32	MG	T	8057	1/1	0.92	0.17	72,72,72,72	0
36	SR	0	8968	1/1	0.92	0.12	165,165,165,165	0
36	SR	0	8948	1/1	0.92	0.12	122,122,122,122	0
36	SR	0	8970	1/1	0.92	0.11	135,135,135,135	0
36	SR	0	8992	1/1	0.92	0.21	137,137,137,137	0
34	NA	0	8550	1/1	0.92	0.24	59,59,59,59	0
36	SR	0	8994	1/1	0.92	0.31	199,199,199,199	0
35	CL	J	8801	1/1	0.92	0.11	82,82,82,82	0
36	SR	0	8974	1/1	0.92	0.21	179,179,179,179	0
36	SR	0	8954	1/1	0.92	0.08	109,109,109,109	0
34	NA	0	8530	1/1	0.92	0.17	60,60,60,60	0
34	NA	0	8528	1/1	0.93	0.09	60,60,60,60	0
36	SR	0	8915	1/1	0.93	0.11	136,136,136,136	0
34	NA	0	8567	1/1	0.93	0.32	87,87,87,87	0
36	SR	0	8960	1/1	0.93	0.08	151,151,151,151	0
36	SR	0	8946	1/1	0.93	0.10	129,129,129,129	0
36	SR	0	8981	1/1	0.93	0.19	158,158,158,158	0
32	MG	2	8060	1/1	0.93	0.14	65,65,65,65	0
34	NA	0	8552	1/1	0.93	0.15	80,80,80,80	0
32	MG	0	8038	1/1	0.93	0.07	70,70,70,70	0
32	MG	0	8064	1/1	0.93	0.09	51,51,51,51	0
34	NA	0	8512	1/1	0.93	0.23	48,48,48,48	0
36	SR	0	8926	1/1	0.93	0.12	142,142,142,142	0
32	MG	0	8017	1/1	0.93	0.07	34,34,34,34	0
32	MG	0	8078	1/1	0.94	0.11	54,54,54,54	0
35	CL	3	8804	1/1	0.94	0.08	76,76,76,76	0
32	MG	0	8044	1/1	0.94	0.04	55,55,55,55	0
34	NA	0	8549	1/1	0.94	0.34	60,60,60,60	0
36	SR	0	8910	1/1	0.94	0.13	106,106,106,106	0
32	MG	0	8001	1/1	0.94	0.05	26,26,26,26	0
32	MG	0	8069	1/1	0.94	0.08	49,49,49,49	0
36	SR	0	8972	1/1	0.94	0.18	164,164,164,164	0
32	MG	B	8042	1/1	0.94	0.19	62,62,62,62	0
34	NA	0	8542	1/1	0.94	0.33	62,62,62,62	0
35	CL	0	8805	1/1	0.94	0.09	76,76,76,76	0
36	SR	1	8952	1/1	0.94	0.08	93,93,93,93	0
34	NA	0	8544	1/1	0.94	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	C	8503	1/1	0.94	0.10	46,46,46,46	0
34	NA	0	8545	1/1	0.94	0.14	48,48,48,48	0
36	SR	0	8923	1/1	0.94	0.09	112,112,112,112	0
36	SR	0	8963	1/1	0.94	0.05	133,133,133,133	0
36	SR	0	8909	1/1	0.95	0.09	99,99,99,99	0
36	SR	0	8966	1/1	0.95	0.08	120,120,120,120	0
32	MG	0	8068	1/1	0.95	0.11	67,67,67,67	0
34	NA	0	8517	1/1	0.95	0.06	36,36,36,36	0
32	MG	0	8083	1/1	0.95	0.10	74,74,74,74	0
32	MG	0	8085	1/1	0.95	0.19	69,69,69,69	0
32	MG	0	8036	1/1	0.95	0.12	60,60,60,60	0
32	MG	0	8070	1/1	0.95	0.15	64,64,64,64	0
32	MG	0	8053	1/1	0.95	0.12	69,69,69,69	0
34	NA	0	8546	1/1	0.95	0.13	85,85,85,85	0
36	SR	0	8921	1/1	0.95	0.07	99,99,99,99	0
34	NA	0	8505	1/1	0.95	0.37	44,44,44,44	0
32	MG	0	8029	1/1	0.95	0.21	69,69,69,69	0
36	SR	0	8953	1/1	0.95	0.10	164,164,164,164	0
35	CL	0	8814	1/1	0.95	0.11	66,66,66,66	0
32	MG	0	8093	1/1	0.95	0.05	45,45,45,45	0
35	CL	0	8816	1/1	0.95	0.14	75,75,75,75	0
32	MG	0	8008	1/1	0.95	0.10	32,32,32,32	0
32	MG	0	8075	1/1	0.95	0.09	58,58,58,58	0
32	MG	0	8002	1/1	0.95	0.06	26,26,26,26	0
34	NA	0	8513	1/1	0.95	0.21	56,56,56,56	0
36	SR	0	8962	1/1	0.95	0.15	180,180,180,180	0
36	SR	0	8990	1/1	0.95	0.10	116,116,116,116	0
32	MG	0	8024	1/1	0.95	0.07	54,54,54,54	0
32	MG	0	8081	1/1	0.95	0.21	81,81,81,81	0
38	CD	Z	8703	1/1	0.95	0.10	172,172,172,172	0
36	SR	0	8918	1/1	0.96	0.09	94,94,94,94	0
32	MG	0	8061	1/1	0.96	0.09	36,36,36,36	0
32	MG	0	8062	1/1	0.96	0.12	61,61,61,61	0
32	MG	0	8032	1/1	0.96	0.05	42,42,42,42	0
35	CL	0	8813	1/1	0.96	0.06	54,54,54,54	0
34	NA	0	8523	1/1	0.96	0.12	65,65,65,65	0
32	MG	0	8011	1/1	0.96	0.10	30,30,30,30	0
32	MG	0	8084	1/1	0.96	0.09	36,36,36,36	0
35	CL	0	8822	1/1	0.96	0.25	86,86,86,86	0
32	MG	0	8065	1/1	0.96	0.07	41,41,41,41	0
35	CL	B	8819	1/1	0.96	0.09	57,57,57,57	0
32	MG	0	8034	1/1	0.96	0.05	47,47,47,47	0

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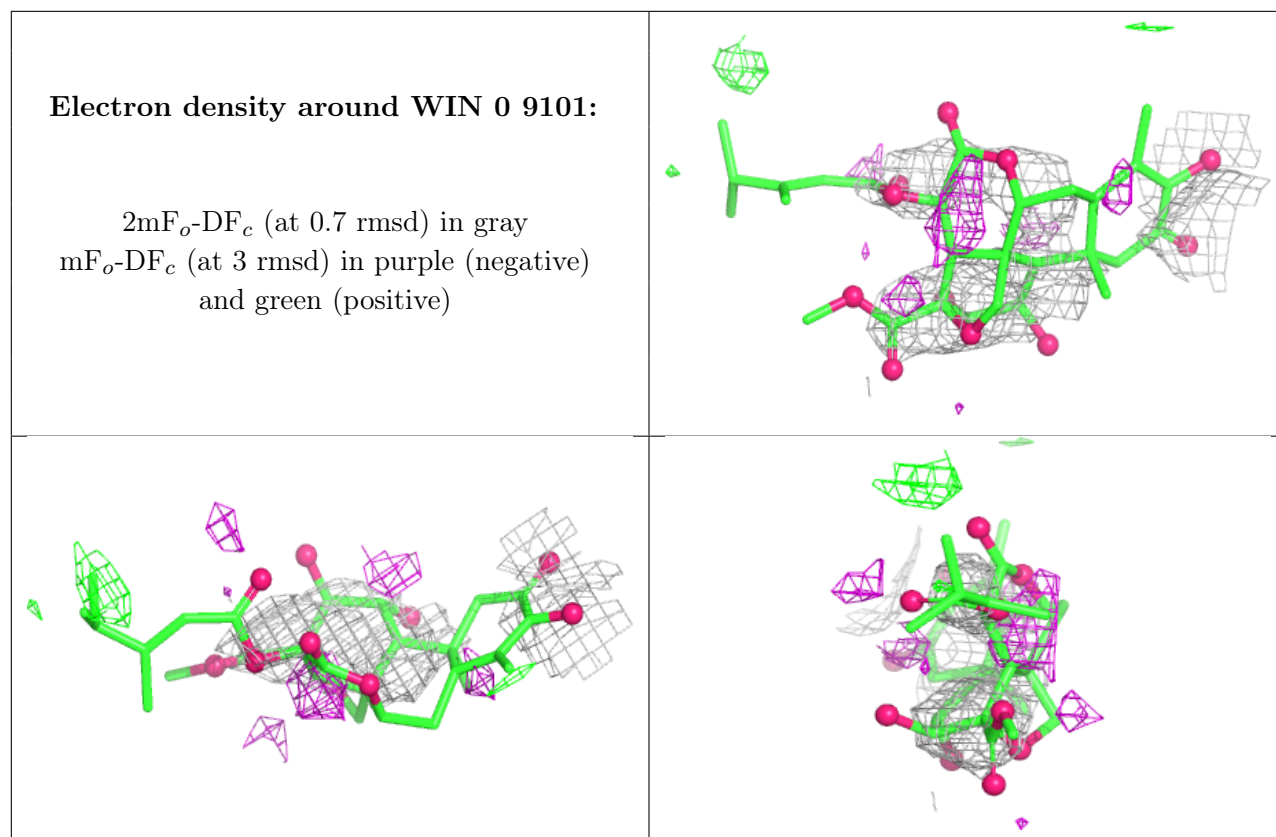
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8045	1/1	0.96	0.06	30,30,30,30	0
35	CL	J	8821	1/1	0.96	0.08	78,78,78,78	0
35	CL	K	8812	1/1	0.96	0.13	57,57,57,57	0
35	CL	L	8810	1/1	0.96	0.14	69,69,69,69	0
35	CL	O	8808	1/1	0.96	0.13	79,79,79,79	0
36	SR	0	8940	1/1	0.96	0.06	94,94,94,94	0
35	CL	Y	8820	1/1	0.96	0.07	46,46,46,46	0
32	MG	0	8009	1/1	0.96	0.23	42,42,42,42	0
34	NA	0	8553	1/1	0.96	0.12	69,69,69,69	0
32	MG	0	8050	1/1	0.96	0.15	74,74,74,74	0
32	MG	0	8052	1/1	0.96	0.07	58,58,58,58	0
32	MG	0	8030	1/1	0.96	0.19	79,79,79,79	0
36	SR	3	8932	1/1	0.96	0.05	94,94,94,94	0
36	SR	0	8911	1/1	0.96	0.05	95,95,95,95	0
32	MG	0	8055	1/1	0.96	0.10	49,49,49,49	0
32	MG	0	8018	1/1	0.96	0.15	54,54,54,54	0
32	MG	0	8076	1/1	0.96	0.04	38,38,38,38	0
32	MG	0	8059	1/1	0.96	0.10	52,52,52,52	0
32	MG	0	8079	1/1	0.96	0.17	67,67,67,67	0
32	MG	0	8067	1/1	0.97	0.09	34,34,34,34	0
35	CL	N	8807	1/1	0.97	0.07	72,72,72,72	0
34	NA	0	8508	1/1	0.97	0.12	63,63,63,63	0
35	CL	0	8817	1/1	0.97	0.05	68,68,68,68	0
34	NA	0	8565	1/1	0.97	0.16	100,100,100,100	0
36	SR	0	8935	1/1	0.97	0.06	93,93,93,93	0
32	MG	0	8020	1/1	0.97	0.20	57,57,57,57	0
36	SR	0	8902	1/1	0.97	0.07	70,70,70,70	0
32	MG	0	8046	1/1	0.97	0.14	53,53,53,53	0
34	NA	0	8504	1/1	0.97	0.19	46,46,46,46	0
35	CL	0	8811	1/1	0.97	0.10	72,72,72,72	0
32	MG	0	8047	1/1	0.97	0.16	71,71,71,71	0
36	SR	0	8925	1/1	0.97	0.06	95,95,95,95	0
38	CD	O	8705	1/1	0.97	0.06	105,105,105,105	0
32	MG	0	8010	1/1	0.97	0.05	34,34,34,34	0
32	MG	0	8087	1/1	0.98	0.04	36,36,36,36	0
32	MG	0	8088	1/1	0.98	0.12	46,46,46,46	0
35	CL	M	8818	1/1	0.98	0.06	49,49,49,49	0
35	CL	0	8803	1/1	0.98	0.05	62,62,62,62	0
32	MG	0	8023	1/1	0.98	0.11	30,30,30,30	0
35	CL	R	8806	1/1	0.98	0.05	55,55,55,55	0
32	MG	0	8013	1/1	0.98	0.05	30,30,30,30	0
32	MG	0	8048	1/1	0.98	0.11	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8077	1/1	0.98	0.03	43,43,43,43	0
36	SR	R	8912	1/1	0.98	0.07	93,93,93,93	0
32	MG	0	8026	1/1	0.98	0.12	55,55,55,55	0
36	SR	0	8904	1/1	0.98	0.09	64,64,64,64	0
32	MG	0	8014	1/1	0.98	0.13	33,33,33,33	0
32	MG	0	8015	1/1	0.98	0.07	33,33,33,33	0
32	MG	K	8054	1/1	0.98	0.14	47,47,47,47	0
32	MG	0	8006	1/1	0.98	0.06	33,33,33,33	0
32	MG	0	8041	1/1	0.98	0.08	32,32,32,32	0
32	MG	0	8043	1/1	0.98	0.12	58,58,58,58	0
32	MG	0	8007	1/1	0.98	0.07	40,40,40,40	0
32	MG	0	8003	1/1	0.98	0.06	35,35,35,35	0
32	MG	0	8028	1/1	0.99	0.09	30,30,30,30	0
32	MG	0	8058	1/1	0.99	0.04	23,23,23,23	0
32	MG	0	8016	1/1	0.99	0.04	30,30,30,30	0
32	MG	0	8021	1/1	0.99	0.09	43,43,43,43	0
32	MG	0	8022	1/1	0.99	0.10	37,37,37,37	0
32	MG	0	8012	1/1	0.99	0.06	26,26,26,26	0
32	MG	0	8005	1/1	0.99	0.07	35,35,35,35	0
32	MG	0	8019	1/1	0.99	0.12	30,30,30,30	0
36	SR	0	8903	1/1	0.99	0.13	66,66,66,66	0
32	MG	0	8027	1/1	0.99	0.07	47,47,47,47	0
36	SR	0	8905	1/1	0.99	0.15	73,73,73,73	0
36	SR	0	8906	1/1	0.99	0.08	67,67,67,67	0
36	SR	0	8907	1/1	0.99	0.05	62,62,62,62	0
38	CD	3	8704	1/1	0.99	0.03	94,94,94,94	0
38	CD	U	8701	1/1	1.00	0.03	71,71,71,71	0
32	MG	0	8025	1/1	1.00	0.04	37,37,37,37	0
38	CD	1	8702	1/1	1.00	0.02	72,72,72,72	0
32	MG	0	8004	1/1	1.00	0.05	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.