



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2021 – 08:25 PM EST

PDB ID : 3G71
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.17.1

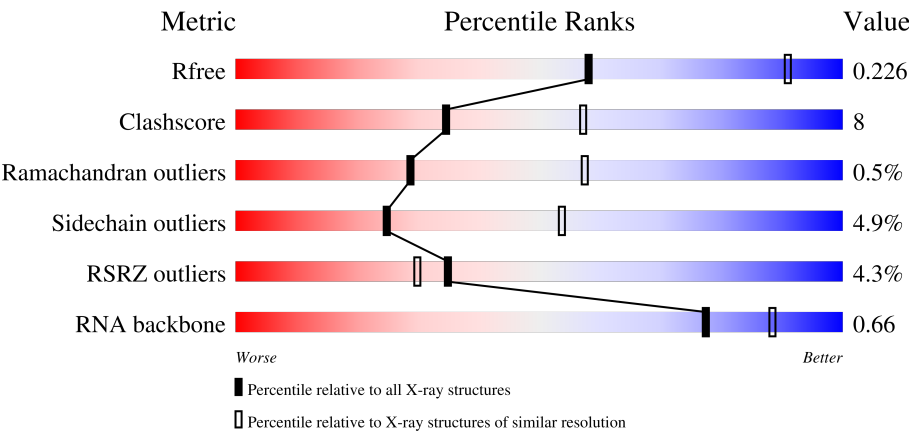
1 Overall quality at a glance i

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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

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	<div><div></div><div>54%34%5%6%</div></div>
2	A	237	<div><div>6%</div><div>84%14%</div></div>
3	B	337	<div><div></div><div>85%14%</div></div>
4	C	246	<div><div></div><div>84%13%</div></div>

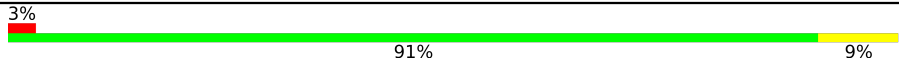

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	172	
7	F	119	
8	G	348	
9	H	177	
10	I	70	
11	J	142	
12	K	132	
13	L	165	
14	M	194	
15	N	186	
16	O	115	
17	P	143	
18	Q	95	
19	R	150	
20	S	81	
21	T	119	
22	U	53	
23	V	65	
24	W	154	
25	X	82	
26	Y	142	
27	Z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

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Mol	Chain	Length	Quality of chain
30	3	92	
31	9	122	

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
32	MG	0	8090	-	-	-	X
33	K	0	8401	-	-	-	X
34	NA	0	8524	-	-	-	X
34	NA	0	8527	-	-	-	X
34	NA	0	8542	-	-	-	X
34	NA	0	8549	-	-	-	X
34	NA	0	8554	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8560	-	-	-	X
34	NA	0	8566	-	-	-	X
34	NA	9	8572	-	-	-	X
34	NA	H	8518	-	-	-	X
36	SR	0	8913	-	-	-	X
36	SR	0	8982	-	-	-	X
36	SR	0	8996	-	-	-	X
36	SR	0	9006	-	-	-	X
36	SR	B	8987	-	-	-	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 (three-letter code: 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 (three-letter code: K) (formula: K).

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

- Molecule 34 is SODIUM ION (three-letter code: 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 (three-letter code: 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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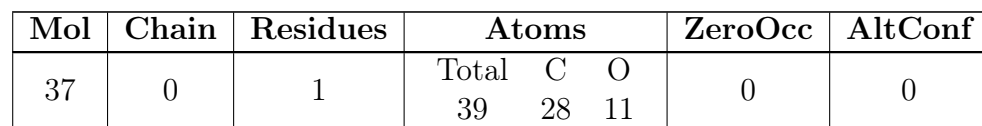
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: 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-{{(2E)-3,4-dimethylpent-2-enoyl}oxy}-3,11,12-trihydroxy-2,16-dioxo-13,20-epoxypicras-3-en-21-oate (three-letter code: 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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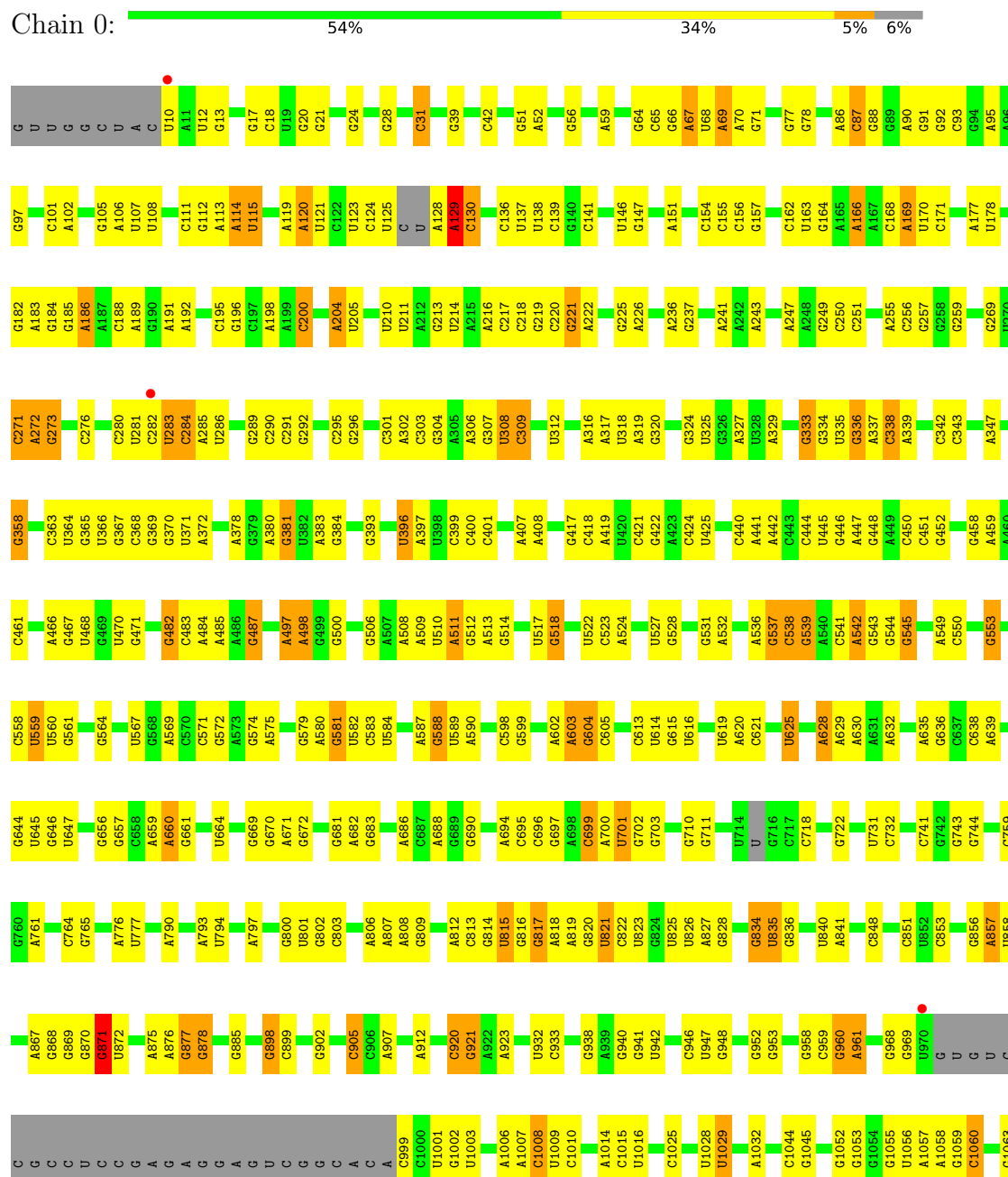
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	20	Total 20	O 20	0	0
39	Y	94	Total 94	O 94	0	0
39	Z	28	Total 28	O 28	0	0
39	1	52	Total 52	O 52	0	0
39	2	39	Total 39	O 39	0	0
39	3	66	Total 66	O 66	0	0
39	9	149	Total 149	O 149	0	0

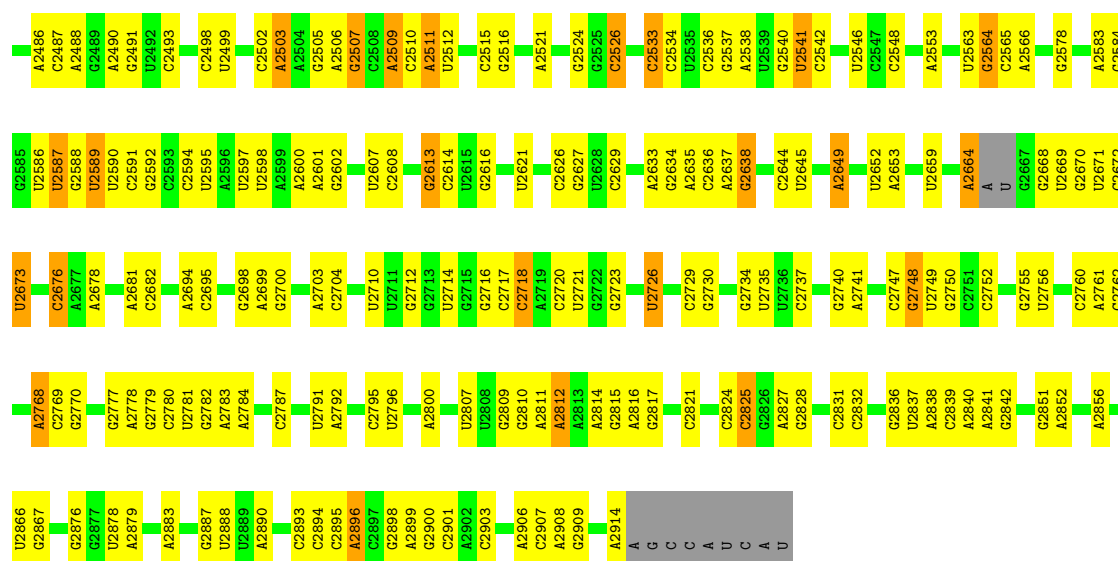
3 Residue-property plots

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

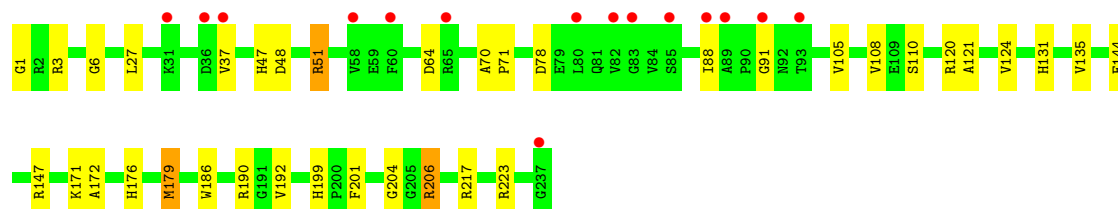
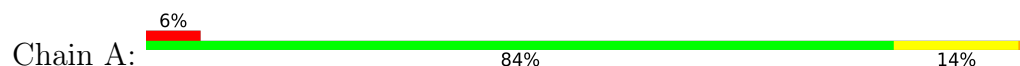
• Molecule 1: 23S ribosomal RNA



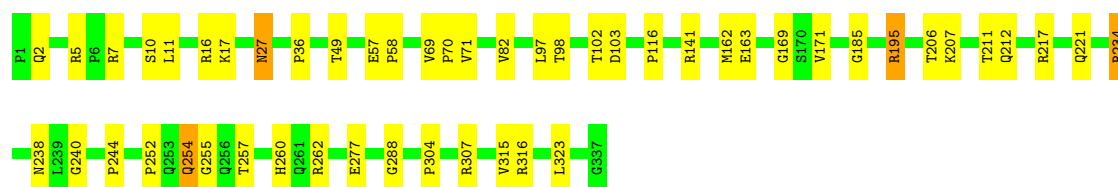
U2265	G2379	U2039	G1947	C1834	U1741	A1641	G1546	A1434	A1352	C1238	G1066
A2266	A2380	C2040	G1948	U1835	A1742	A1642	G1556	U1435	A1353	G1239	A1067
G2267	C2288	G2041	G1951	U1836	U1749	C1643	C1557	C1436	A1242	A1071	
C2268	C2269	C	U	U1838	G1752	U1644	C1558	C1439	C1357	G1072	
G2270	G2271	G2045	A	A1840	G1755	U1645	U	G1440	C1360	U1170	
G2271		G2046	A	A1841	A1756	C1652	U1561	G1441	C1361	A1073	
U2277		G2047	C	C1844	G1756	A1653	U1562	A1442	C1362	G1074	
U2386		G2050	U	A1845	G1759	G1654	C1566	G1443	U1249	G1075	
U2387		A	U	U1846	A1760	G1655	G1567	G1444	G1363	G1076	
C2388		A	G	G1847	U1761	A1656	G1568	G1445	G1364	G1077	
U2389		G2054	A	G1848	U1762	A1657	U1569	U1446	C1365	A1078	
U2392		U2064	C	G1849	C1763	A1658	U1570	U1447	C1366	A1177	
A2401		G2070	C	G1855	C1762	A1664	C1570	G1453	C1257	A1081	
A2402		C2071	C	C1856	C1763	A1665	A1572	U1454	G1258	C1084	
A2300		G2072	U1964	A1857	U1766	G1666	A1573	A1455	U1371		
A2301		G2073	C1965	A1858	A1767	A1667	A1573	C1456	G1259	G1087	
A2302		A2074	U1966	C1861	C1768	U1668	G1576	U1457	G1260	A1088	
U2308		C2079	U1967	C1862	C1769	U1677	U1577	U1463	C1268		
C2309		G2080	A1968	C1864	U1770	A1678	U1587	C1464	G1269	A1089	
G2316		A2081	G1970	C1864	G1773	C1679	U1588	U1464	C1273	G1099	
C2317		G2082	U1972	G1868	A1778	C1680	G1589	C1474	U1278	G1100	
U2320		A2083	A1973	G1873	A1779	G1681	G1592	C1477	U1279	C1104	
A2321		C2087	G1974	U1877	A1783	A1682	C1593	U1478	G1289	C1105	
U2325		G2088	A1978	G1878	U1784	G1683	C1594	A1482	A1291	A1106	
C2326		A2089	G1979	G1879	U1785	A1684	C1595	C1483	C1290		
G2326		G2090	U1980	U1879	C1787	C1686	U1596	G1484	G1291	G1118	
G2338		C2091	A1981	C1880	U1788	G1687	A1597	A1485	U1306	G1119	
A2344		G2092	U1982	A1881	U1789	C1688	A1598	C1486	A1307	U1120	
A2345		G2093	C1992	U1882	C1790	C1692	A1603	C1495	G1308	G1121	
C2346		G2094	A1994	U1883	U1791	C1692	G1604	G1496	G1311	U1130	
C2347		A2095	G1995	A1886	G1795	U1702	G1605	G1497	G1312	G1131	
C2348		U2096	U1996	U1903	A1796	G1706	A1607	U1500	G1313	A1132	
A2353		A2100	C2002	A1904	C1797	G1707	C1613	U1503	A1407	A1133	
A2354		A2101	U2003	A1909	G1798	G1707	G1614	A1504	U1408	G1137	
A2361		A2102	U2004	A1910	G1799	A1710	A1615	U1506	G1315		
A2362		C2104	G2005	A1910	G1800	A1714	A1616	A1515	G1316	U1149	
A2363		C2105	C2006	A1919	C1803	C1714	C1617	U1516	A1321	A1150	
A2364		C2106	A2007	C1920	A1804	C1715	G1622	U1524	G1322	G1151	
A2365		G2110	U2008	A1921	G1805	A1716	C1623	G1525	A1328		
A2366		G2111	A2011	A1922	C1811	C1716	A1624	A1526	G1329	A1154	
A2367		C2114	U2012	C1928	A1812	U1722	U1625	A1527	U1219	G1155	
A2368		U2115	G2013	G1929	U1813	U1723	A1626	G1528	C1421	G1158	
A2369		U2116	U2016	U1937	G1814	U1724	G1627	G1529	G1331	G1159	
A2372		G2121	U2017	G1938	C1816	C1725	G1631	G1535	C1332	G1160	
U2373		C2122	A2022	U1939	U1817	G1730	A1632	G1536	U1220	A1161	
U2374		U2133	U2032	C1940	C1818	A1732	C1633	G1537	C1333		
A2375		G2134	A1941	A1941	G1819	A1733	G1634	C1587	U1423		
A2376		A2135	U2034	C1943	G1820	C1735	U1635	U1644	A1424	U1234	
A2377		G2136	G2034	A1943	A1829	A1736	A1637	C1545	A1427	U1237	
A2378											
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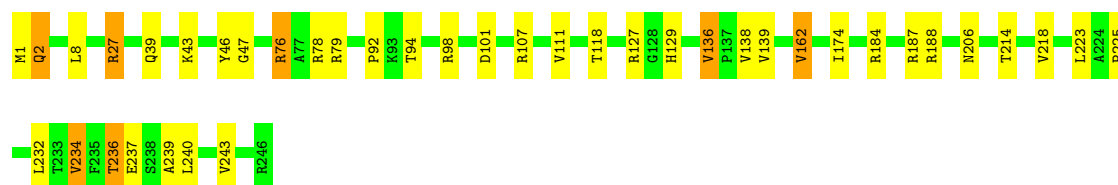
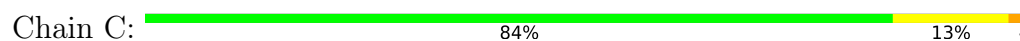
• Molecule 2: 50S ribosomal protein L2P



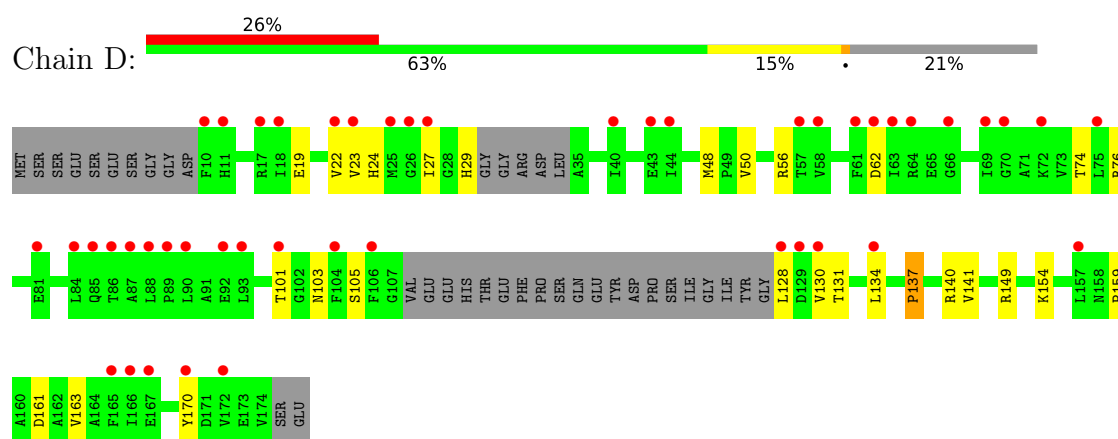
• Molecule 3: 50S ribosomal protein L3P



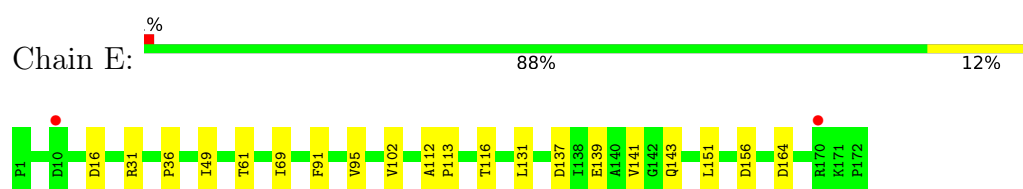
• Molecule 4: 50S ribosomal protein L4P



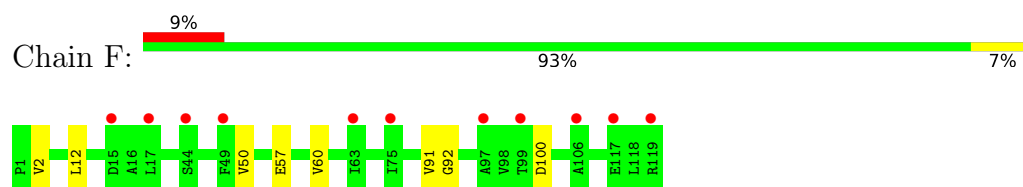
• Molecule 5: 50S ribosomal protein L5P



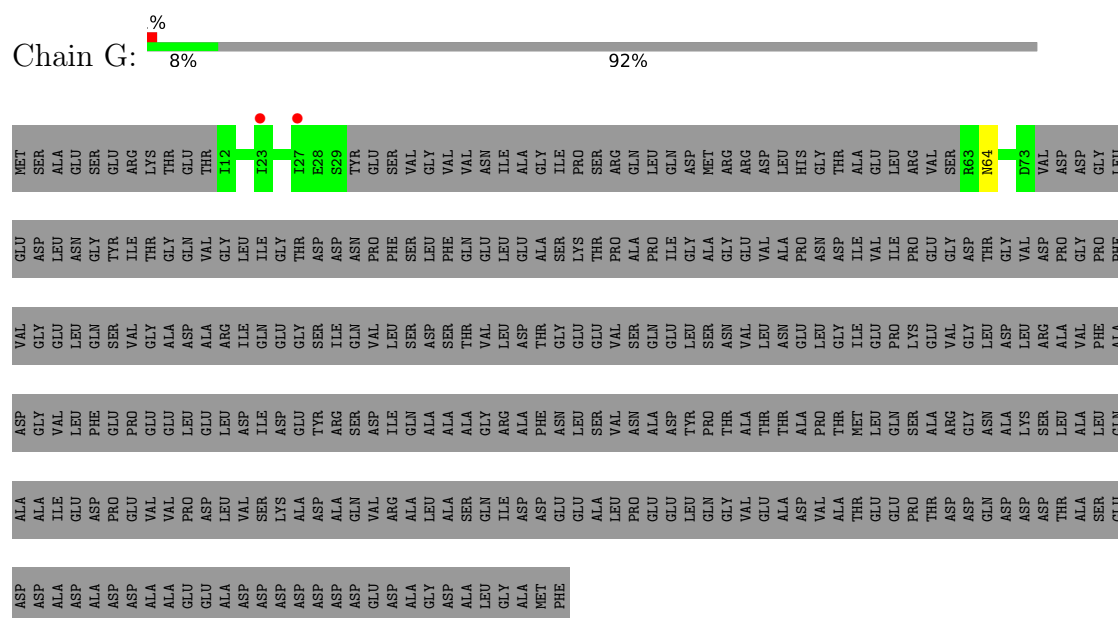
- Molecule 6: 50S ribosomal protein L6P



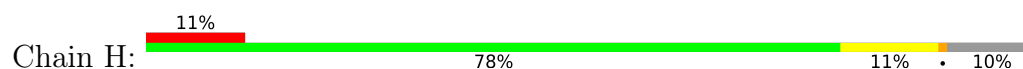
- Molecule 7: 50S ribosomal protein L7Ae

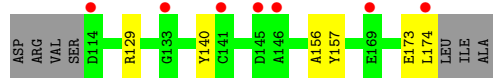


- Molecule 8: 50S ribosomal protein L10E

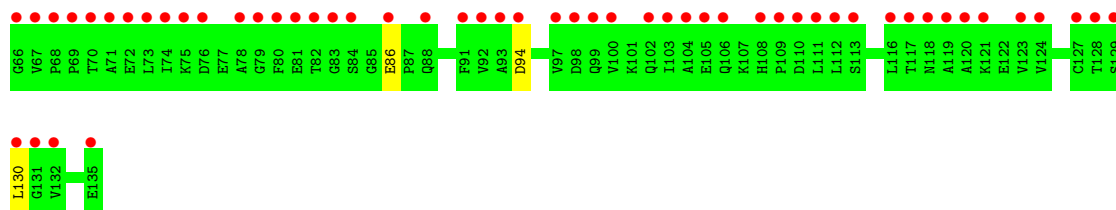
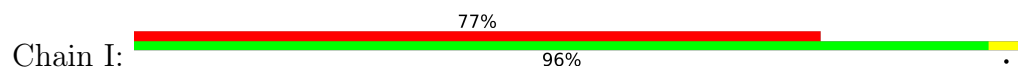


- Molecule 9: 50S ribosomal protein L10e

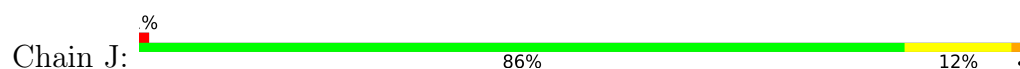




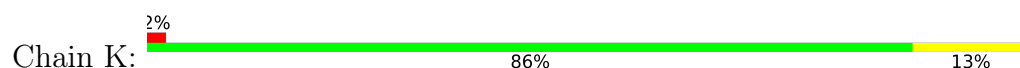
• Molecule 10: 50S ribosomal protein L11P



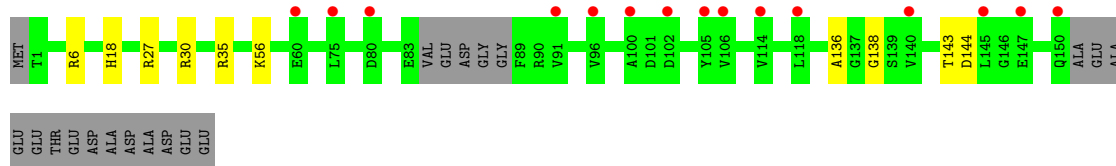
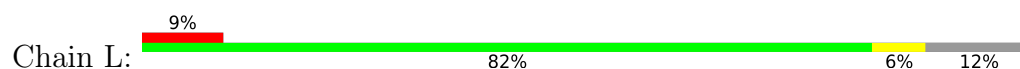
• Molecule 11: 50S ribosomal protein L13P



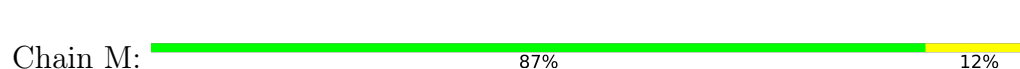
• Molecule 12: 50S ribosomal protein L14P



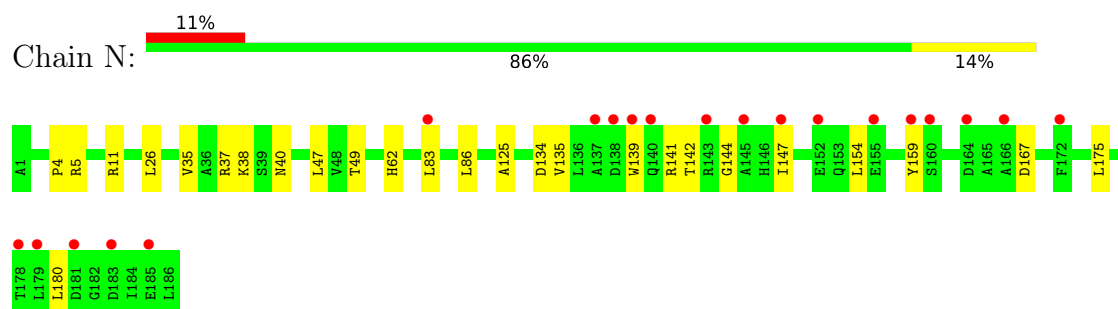
• Molecule 13: 50S ribosomal protein L15P



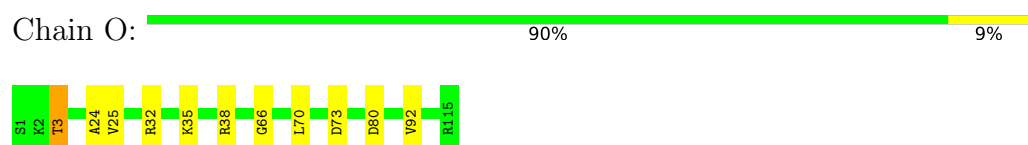
• Molecule 14: 50S ribosomal protein L15e



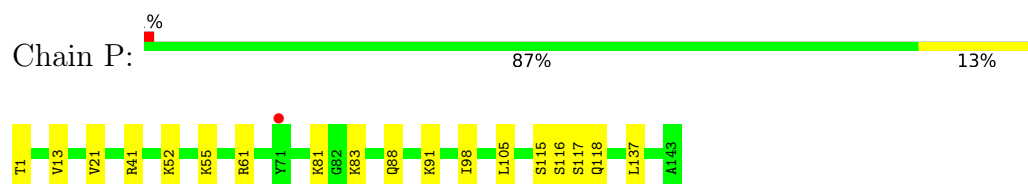
- Molecule 15: 50S ribosomal protein L18P



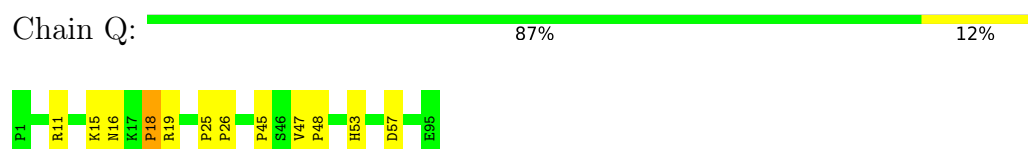
- Molecule 16: 50S ribosomal protein L18e



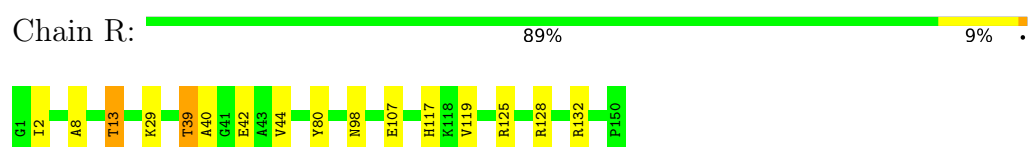
- Molecule 17: 50S ribosomal protein L19e



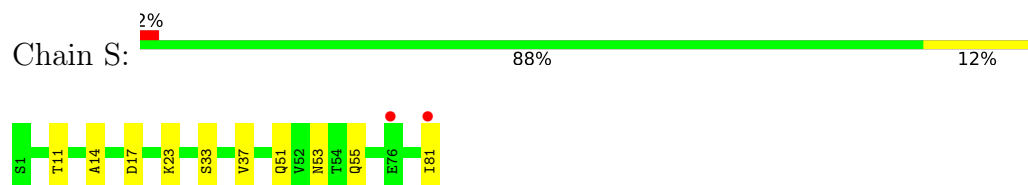
- Molecule 18: 50S ribosomal protein L21e



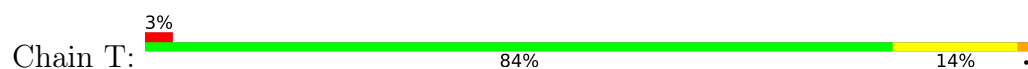
- Molecule 19: 50S ribosomal protein L22P

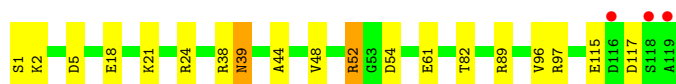


- Molecule 20: 50S ribosomal protein L23P



- Molecule 21: 50S ribosomal protein L24P

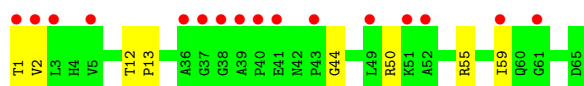
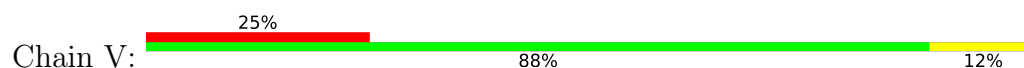




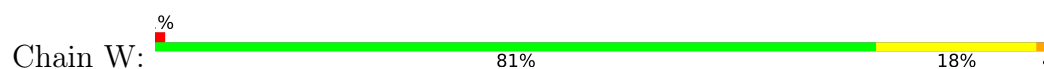
- Molecule 22: 50S ribosomal protein L24e



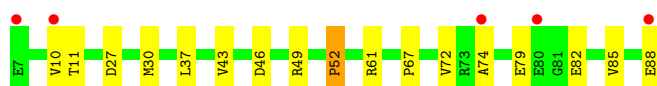
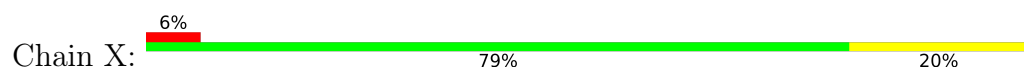
- Molecule 23: 50S ribosomal protein L29P



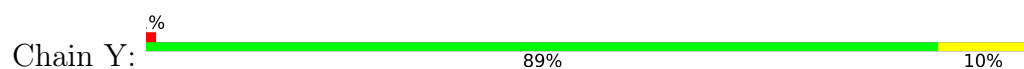
- Molecule 24: 50S ribosomal protein L30P



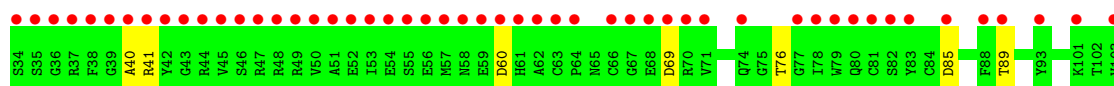
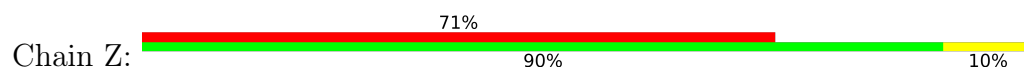
- Molecule 25: 50S ribosomal protein L31e




- Molecule 26: 50S ribosomal protein L32e

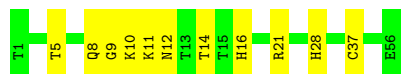


- Molecule 27: 50S ribosomal protein L37Ae




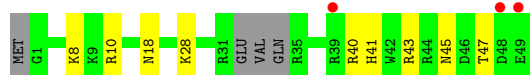
- Molecule 28: 50S ribosomal protein L37e

Chain 1:  80% 20%




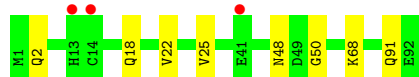
- Molecule 29: 50S ribosomal protein L39e

Chain 2:  6% 74% 18% 8%



- Molecule 30: 50S ribosomal protein L44E

Chain 3:  3% 91% 9%



- Molecule 31: 5S ribosomal RNA

Chain 9:  2% 43% 42% 15%



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 85.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.76-2.85) 91.0 (85.61-2.40)	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 0.181 , 0.226	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 , 80.7	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: OMG, OMU, PSU, CD, WIN, SR, 1MA, NA, CL, MG, K, UR3

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	0	0.39	0/65958	0.68	10/102869 (0.0%)
2	A	0.51	1/1787 (0.1%)	0.76	0/2408
3	B	0.53	0/2690	0.77	0/3652
4	C	0.56	0/1885	0.79	0/2552
5	D	0.63	0/1111	0.71	2/1498 (0.1%)
6	E	0.60	0/1383	0.68	0/1880
7	F	0.54	0/901	0.70	0/1224
8	G	0.50	0/241	0.66	0/324
9	H	0.61	0/1302	0.76	0/1743
10	I	0.58	0/527	0.63	0/716
11	J	0.62	0/1136	0.73	0/1530
12	K	0.49	0/1004	0.80	0/1351
13	L	0.52	0/1130	0.74	0/1509
14	M	0.51	0/1583	0.74	0/2116
15	N	0.55	0/1474	0.75	0/1999
16	O	0.50	0/874	0.72	1/1181 (0.1%)
17	P	0.53	0/1148	0.66	0/1528
18	Q	0.51	0/749	0.75	0/1005
19	R	0.57	0/1173	0.76	0/1578
20	S	0.54	0/649	0.65	0/875
21	T	0.47	0/958	0.76	1/1289 (0.1%)
22	U	0.58	0/418	0.68	0/562
23	V	0.43	0/503	0.68	0/675
24	W	0.52	0/1219	0.77	1/1655 (0.1%)
25	X	0.52	0/665	0.75	0/895
26	Y	0.51	0/1147	0.72	0/1536
27	Z	0.68	0/585	0.71	0/781
28	1	0.55	0/438	0.73	0/578
29	2	0.45	0/401	0.70	0/529
30	3	0.56	0/771	0.67	0/1024
31	9	0.33	0/2904	0.69	1/4526 (0.0%)
All	All	0.44	1/98714 (0.0%)	0.70	16/147588 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	192	VAL	CB-CG1	-5.05	1.42	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.01	100.69	109.10
1	0	2726	U	N1-C1'-C2'	5.93	121.71	114.00
1	0	1942	A	C5'-C4'-C3'	5.70	125.13	116.00
1	0	1504	A	C1'-O4'-C4'	-5.67	105.36	109.90
31	9	39	U	N1-C1'-C2'	5.64	121.34	114.00
1	0	1504	A	N9-C1'-C2'	5.62	121.30	114.00
21	T	52	ARG	N-CA-C	5.46	125.75	111.00
16	O	66	GLY	N-CA-C	5.40	126.60	113.10
1	0	2316	G	C5'-C4'-C3'	-5.27	107.57	116.00
1	0	129	A	C2'-C3'-O3'	5.25	122.11	113.70
1	0	1165	G	C5'-C4'-O4'	5.24	115.39	109.10
1	0	1120	U	C5'-C4'-C3'	-5.20	107.68	116.00
5	D	170	TYR	N-CA-C	5.11	124.81	111.00
24	W	4	LEU	CA-CB-CG	5.10	127.04	115.30
1	0	1819	G	C5'-C4'-C3'	5.07	124.12	116.00
5	D	137	PRO	N-CA-C	5.05	125.23	112.10

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

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Mol	Chain	Res	Type	Group
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	1012	0
2	A	1754	0	1766	26	0
3	B	2625	0	2533	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	16	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	6	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	20	0
25	X	655	0	653	7	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
34	H	1	0	0	0	0
34	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
39	E	40	0	0	0	0
39	F	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1243	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 (1243) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1205: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
1:0:1183: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
1:0:1299: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
1:0:1029:U:O2'	1:0:1273:C:OP1	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:657: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:424: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:282:C:HO2'	1:0:368:C:N4	2.15	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
28:1:8:GLN:HE22	28:1:11:LYS:HZ2	1.65	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:166:A:O2'	1:0:898:G:O6	2.36	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
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
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'	39:0:7395: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1181:A:N1	1:0:1192:A:O2'	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:940:G:O2'	1:0:1032:A:N1	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
24:W:5:VAL:HG11	24:W:153:MET:CE	2.52	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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	235/237 (99%)	218 (93%)	14 (6%)	3 (1%)	12	33
3	B	335/337 (99%)	307 (92%)	26 (8%)	2 (1%)	25	53
4	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	19	46
5	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	6	21
6	E	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
7	F	117/119 (98%)	109 (93%)	7 (6%)	1 (1%)	17	43
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	150 (96%)	5 (3%)	1 (1%)	25	53
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%)	19	46
13	L	141/165 (86%)	127 (90%)	14 (10%)	0	100	100
14	M	192/194 (99%)	187 (97%)	4 (2%)	1 (0%)	29	57
15	N	184/186 (99%)	173 (94%)	8 (4%)	3 (2%)	9	28
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%)	14	38
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%)	17	43
22	U	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
23	V	63/65 (97%)	61 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
25	X	80/82 (98%)	77 (96%)	2 (2%)	1 (1%)	12	33
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%)	29	57

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
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%)	168 (94%)	11 (6%)	18	43
3	B	282/282 (100%)	268 (95%)	14 (5%)	24	53
4	C	193/193 (100%)	176 (91%)	17 (9%)	10	26
5	D	117/148 (79%)	108 (92%)	9 (8%)	13	32
6	E	152/152 (100%)	146 (96%)	6 (4%)	32	63
7	F	93/93 (100%)	90 (97%)	3 (3%)	39	69
8	G	27/282 (10%)	27 (100%)	0	100	100
9	H	134/145 (92%)	128 (96%)	6 (4%)	27	57
10	I	58/58 (100%)	57 (98%)	1 (2%)	60	83
11	J	118/118 (100%)	110 (93%)	8 (7%)	16	38
12	K	106/106 (100%)	100 (94%)	6 (6%)	20	47
13	L	113/127 (89%)	112 (99%)	1 (1%)	78	92
14	M	158/158 (100%)	152 (96%)	6 (4%)	33	64
15	N	149/149 (100%)	140 (94%)	9 (6%)	19	45
16	O	93/93 (100%)	90 (97%)	3 (3%)	39	69
17	P	113/113 (100%)	108 (96%)	5 (4%)	28	58
18	Q	79/79 (100%)	75 (95%)	4 (5%)	24	52
19	R	117/117 (100%)	112 (96%)	5 (4%)	29	59
20	S	71/71 (100%)	70 (99%)	1 (1%)	67	86
21	T	105/105 (100%)	96 (91%)	9 (9%)	10	27
22	U	44/44 (100%)	44 (100%)	0	100	100
23	V	51/51 (100%)	49 (96%)	2 (4%)	32	63
24	W	130/130 (100%)	123 (95%)	7 (5%)	22	49
25	X	66/66 (100%)	57 (86%)	9 (14%)	3	9
26	Y	120/120 (100%)	116 (97%)	4 (3%)	38	68
27	Z	60/60 (100%)	59 (98%)	1 (2%)	60	83
28	1	46/46 (100%)	45 (98%)	1 (2%)	52	79
29	2	42/46 (91%)	41 (98%)	1 (2%)	49	77
30	3	79/79 (100%)	77 (98%)	2 (2%)	47	76
All	All	3095/3410 (91%)	2944 (95%)	151 (5%)	25	54

All (151) 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	78	ASP
2	A	105	VAL
2	A	108	VAL
2	A	110	SER
2	A	131	HIS
2	A	179	MET
2	A	206	ARG
2	A	217	ARG
3	B	7	ARG
3	B	11	LEU
3	B	27	ASN
3	B	49	THR
3	B	71	VAL
3	B	82	VAL
3	B	97	LEU
3	B	98	THR
3	B	162	MET
3	B	171	VAL
3	B	195	ARG
3	B	234	ARG
3	B	254	GLN
3	B	277	GLU
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	101	ASP
4	C	136	VAL
4	C	162	VAL
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

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Mol	Chain	Res	Type
5	D	19	GLU
5	D	24	HIS
5	D	29	HIS
5	D	50	VAL
5	D	62	ASP
5	D	101	THR
5	D	128	LEU
5	D	149	ARG
5	D	161	ASP
6	E	16	ASP
6	E	36	PRO
6	E	61	THR
6	E	102	VAL
6	E	156	ASP
6	E	164	ASP
7	F	12	LEU
7	F	50	VAL
7	F	60	VAL
9	H	62	HIS
9	H	65	LEU
9	H	87	LYS
9	H	91	ARG
9	H	157	TYR
9	H	173	GLU
10	I	94	ASP
11	J	39	VAL
11	J	45	VAL
11	J	52	GLN
11	J	79	PHE
11	J	107	ASN
11	J	120	SER
11	J	130	VAL
11	J	131	THR
12	K	10	GLN
12	K	19	THR
12	K	49	LEU
12	K	98	VAL
12	K	107	THR
12	K	119	GLN
13	L	35	ARG
14	M	10	ASP
14	M	46	LEU

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Mol	Chain	Res	Type
14	M	68	ARG
14	M	93	ARG
14	M	99	ARG
14	M	116	ASN
15	N	26	LEU
15	N	38	LYS
15	N	47	LEU
15	N	49	THR
15	N	62	HIS
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	80	ASP
17	P	13	VAL
17	P	21	VAL
17	P	52	LYS
17	P	91	LYS
17	P	98	ILE
18	Q	11	ARG
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	125	ARG
19	R	132	ARG
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	115	GLU
21	T	117	ASP
23	V	12	THR
23	V	13	PRO

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Mol	Chain	Res	Type
24	W	35	VAL
24	W	38	THR
24	W	52	VAL
24	W	120	PRO
24	W	125	HIS
24	W	142	ASP
24	W	146	ILE
25	X	10	VAL
25	X	43	VAL
25	X	46	ASP
25	X	49	ARG
25	X	52	PRO
25	X	72	VAL
25	X	79	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	85	ASP
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 (66) 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	145	HIS
3	B	238	ASN
3	B	260	HIS
3	B	320	GLN
3	B	332	ASN
4	C	2	GLN
4	C	67	GLN
4	C	73	GLN
4	C	129	HIS

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Mol	Chain	Res	Type
5	D	103	ASN
6	E	143	GLN
8	G	64	ASN
9	H	49	GLN
9	H	59	GLN
10	I	102	GLN
11	J	52	GLN
11	J	107	ASN
12	K	10	GLN
12	K	42	ASN
13	L	18	HIS
13	L	41	HIS
14	M	24	GLN
14	M	58	GLN
14	M	137	ASN
14	M	170	ASN
15	N	40	ASN
15	N	107	ASN
17	P	50	GLN
17	P	66	GLN
17	P	88	GLN
17	P	89	ASN
17	P	118	GLN
18	Q	40	HIS
19	R	94	ASN
19	R	98	ASN
19	R	117	HIS
19	R	123	GLN
20	S	51	GLN
20	S	55	GLN
21	T	39	ASN
22	U	39	ASN
22	U	48	ASN
23	V	60	GLN
24	W	110	GLN
24	W	119	HIS
24	W	125	HIS
24	W	141	HIS
25	X	23	HIS
26	Y	119	GLN
26	Y	129	ASN
26	Y	134	HIS

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Mol	Chain	Res	Type
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	41	HIS
29	2	45	ASN
30	3	2	GLN
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%)	238 (8%)	26 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	27 (0%)

All (255) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	0	2608	C
1	0	2613	G
1	0	2638	G
1	0	2645	U
1	0	2649	A
1	0	2664	A
1	0	2676	C
1	0	2681	A
1	0	2682	C
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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	1MA	0	628	34,1	15,25,26	0.82	0	15,37,40	1.42	1 (6%)
1	UR3	0	2619	1	14,22,23	0.77	0	15,32,35	0.58	0
1	PSU	0	2621	1	17,21,22	1.68	3 (17%)	20,30,33	5.49	5 (25%)
1	OMU	0	2587	34,1	14,22,23	1.03	1 (7%)	14,31,34	1.14	1 (7%)
1	OMG	0	2588	1	18,26,27	1.05	2 (11%)	20,38,41	2.60	5 (25%)

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	1MA	0	628	34,1	-	0/3/25/26	0/3/3/3
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMU	0	2587	34,1	-	0/7/27/28	0/2/2/2
1	OMG	0	2588	1	-	1/5/27/28	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.25	1.47	1.52
1	0	2588	OMG	C6-N1	3.40	1.39	1.33
1	0	2621	PSU	C4-N3	2.72	1.37	1.33
1	0	2621	PSU	C2-N1	2.65	1.43	1.38
1	0	2587	OMU	C4-N3	2.48	1.37	1.33
1	0	2588	OMG	C8-N7	-2.13	1.30	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.57	114.46	128.43
1	0	2621	PSU	C4-N3-C2	14.34	127.25	115.14
1	0	2588	OMG	C5-C6-N1	-8.61	111.66	123.43
1	0	2621	PSU	C5-C4-N3	-8.03	115.01	125.36
1	0	2588	OMG	C6-N1-C2	5.81	125.17	115.93
1	0	628	1MA	C2-N3-C4	-4.68	110.73	116.58
1	0	2587	OMU	C5-C4-N3	-3.87	114.79	123.31
1	0	2588	OMG	C2-N3-C4	-3.01	111.92	115.36
1	0	2621	PSU	C6-N1-C2	2.67	119.76	115.36
1	0	2588	OMG	N3-C2-N1	-2.48	123.91	127.22
1	0	2588	OMG	C6-C5-C4	-2.22	118.68	120.80
1	0	2621	PSU	C5-C1'-C2'	-2.01	111.74	115.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	628	1MA	1	0
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	-	41,43,43	1.87	9 (21%)	50,71,71	3.82	29 (58%)

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	-	-	6/20/110/110	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	C2M-C2G	5.40	1.61	1.53
37	0	9101	WIN	C1N-C1V	5.32	1.41	1.33
37	0	9101	WIN	C2B-C1X	-4.08	1.40	1.46
37	0	9101	WIN	C1C-C1Y	3.64	1.56	1.50
37	0	9101	WIN	C1N-C1W	-2.95	1.39	1.46
37	0	9101	WIN	O1U-C1Z	2.41	1.38	1.34
37	0	9101	WIN	O1U-C2G	2.33	1.49	1.46
37	0	9101	WIN	C2H-C1Y	2.14	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	WIN	C1B-C1V	2.14	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	9.27	125.14	111.41
37	0	9101	WIN	C2F-O1T-C1W	-9.15	104.94	116.94
37	0	9101	WIN	C1O-C2M-C2G	6.67	123.74	112.79
37	0	9101	WIN	O1J-C2A-C2L	-6.55	111.90	123.67
37	0	9101	WIN	O1U-C1Z-O1I	6.15	127.45	118.47
37	0	9101	WIN	C1P-C2I-C2H	6.14	114.32	107.80
37	0	9101	WIN	C2I-C2H-C1Y	5.85	120.23	112.18
37	0	9101	WIN	C1P-C1X-C2B	5.83	126.51	117.06
37	0	9101	WIN	C1V-C1N-C1W	5.82	142.36	126.75
37	0	9101	WIN	C1C-C1Y-C2H	5.75	130.28	116.23
37	0	9101	WIN	C1O-C2M-C2K	-5.08	92.00	100.97
37	0	9101	WIN	O1U-C1Z-C2F	-5.02	106.04	117.93
37	0	9101	WIN	O1H-C1X-C1P	-4.94	111.59	120.44
37	0	9101	WIN	O1U-C2G-C1Q	-4.90	96.58	104.84
37	0	9101	WIN	O1T-C1W-O1G	-4.80	115.53	123.35
37	0	9101	WIN	C1Q-C2G-C2M	3.90	121.06	113.78
37	0	9101	WIN	C1A-O1R-C2A	3.52	121.87	115.94
37	0	9101	WIN	C2H-C1Q-C2G	-3.26	102.67	111.37
37	0	9101	WIN	C2M-C2J-C2D	3.22	116.06	109.96
37	0	9101	WIN	O1L-C2D-C2J	-3.17	101.83	111.92
37	0	9101	WIN	O1T-C2F-C2K	-2.93	102.92	109.79
37	0	9101	WIN	C1F-C2I-C2J	-2.91	106.07	113.09
37	0	9101	WIN	C1F-C2I-C2H	2.90	114.87	109.88
37	0	9101	WIN	C2I-C2J-C2D	2.49	120.98	115.07
37	0	9101	WIN	O1K-C2B-C1X	2.34	120.02	115.66
37	0	9101	WIN	O1S-C1O-C2M	-2.27	103.02	105.67
37	0	9101	WIN	O1T-C1W-C1N	2.08	116.16	111.27
37	0	9101	WIN	O1I-C1Z-C2F	-2.07	118.54	122.22
37	0	9101	WIN	C1D-C2C-C1V	-2.05	107.96	111.89

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	0	9101	WIN	C1B-C1V-C2C-C1E
37	0	9101	WIN	O1J-C2A-C2L-O1S
37	0	9101	WIN	O1R-C2A-C2L-O1S

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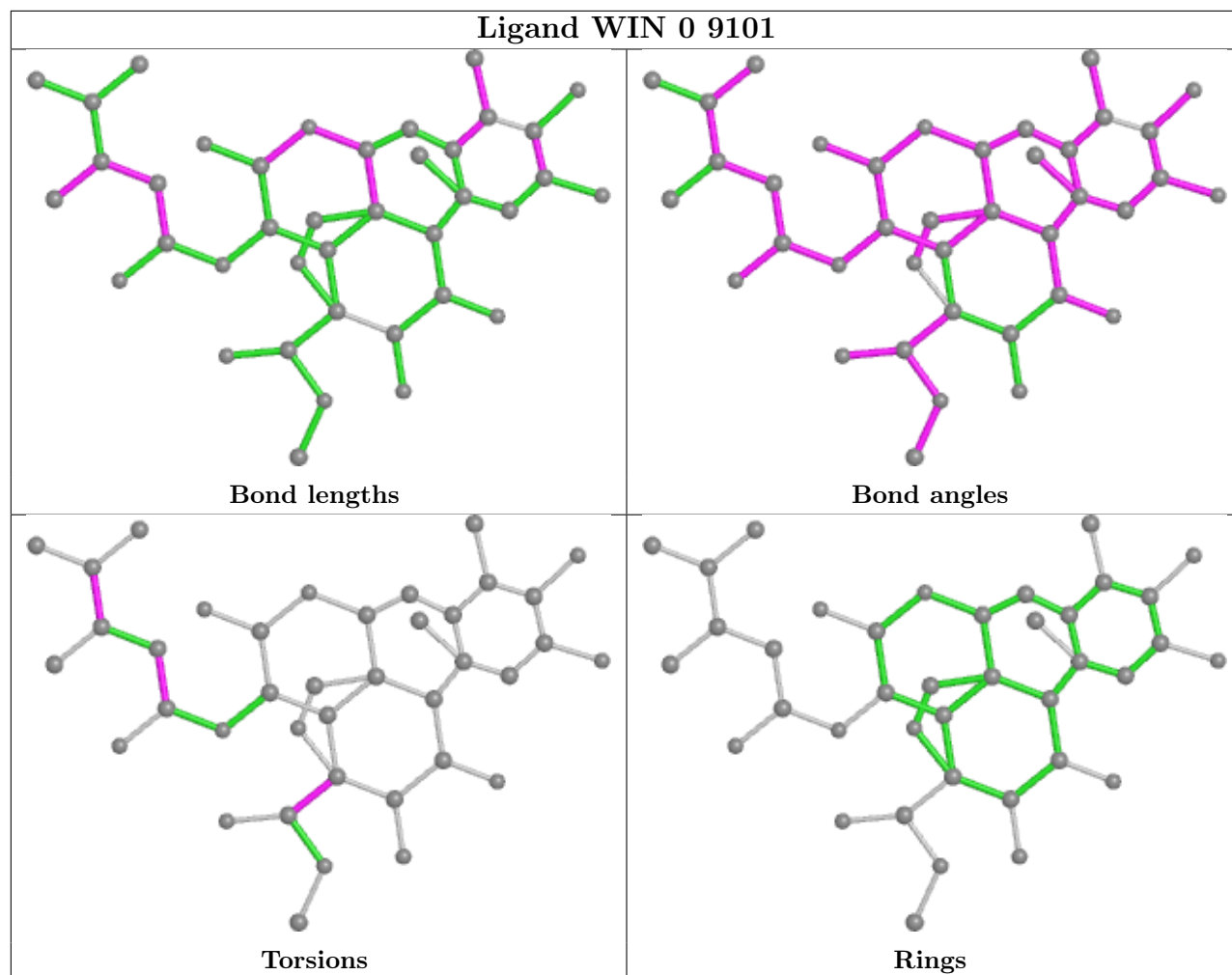
Mol	Chain	Res	Type	Atoms
37	0	9101	WIN	C1V-C1N-C1W-O1T
37	0	9101	WIN	O1R-C2A-C2L-C2K
37	0	9101	WIN	C1V-C1N-C1W-O1G

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%)	-0.68	10 (0%)	92	92	24, 56, 105, 182	0
2	A	237/237 (100%)	0.07	15 (6%)	20	15	35, 71, 114, 133	0
3	B	337/337 (100%)	-0.43	0	100	100	34, 65, 95, 108	0
4	C	246/246 (100%)	-0.42	0	100	100	31, 56, 80, 91	0
5	D	140/177 (79%)	1.44	46 (32%)	0	0	80, 120, 142, 152	0
6	E	172/172 (100%)	-0.15	2 (1%)	79	78	55, 81, 105, 112	0
7	F	119/119 (100%)	0.64	11 (9%)	9	6	64, 90, 122, 137	0
8	G	29/348 (8%)	0.83	2 (6%)	16	12	89, 109, 116, 119	0
9	H	160/177 (90%)	0.64	20 (12%)	3	2	57, 84, 120, 128	0
10	I	70/70 (100%)	3.82	54 (77%)	0	0	142, 164, 183, 184	0
11	J	142/142 (100%)	-0.43	1 (0%)	87	87	47, 60, 82, 104	0
12	K	132/132 (100%)	-0.42	2 (1%)	73	72	44, 61, 86, 90	0
13	L	145/165 (87%)	0.43	15 (10%)	6	4	35, 87, 131, 142	0
14	M	194/194 (100%)	-0.43	0	100	100	38, 55, 75, 82	0
15	N	186/186 (100%)	0.38	20 (10%)	5	4	55, 83, 139, 146	0
16	O	115/115 (100%)	-0.41	0	100	100	43, 66, 84, 88	0
17	P	143/143 (100%)	-0.26	1 (0%)	87	87	50, 70, 86, 94	0
18	Q	95/95 (100%)	-0.50	0	100	100	49, 60, 76, 89	0
19	R	150/150 (100%)	-0.57	0	100	100	38, 56, 78, 84	0
20	S	81/81 (100%)	0.01	2 (2%)	57	54	56, 76, 100, 108	0
21	T	119/119 (100%)	-0.06	3 (2%)	57	54	48, 71, 100, 127	0
22	U	53/53 (100%)	-0.28	0	100	100	56, 72, 95, 102	0
23	V	65/65 (100%)	1.51	16 (24%)	0	0	66, 94, 137, 144	0
24	W	154/154 (100%)	-0.45	1 (0%)	89	89	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%)	-0.08	5 (6%) 21 17	55, 71, 97, 111	0
26	Y	142/142 (100%)	-0.58	1 (0%) 87 87	31, 53, 80, 102	0
27	Z	73/73 (100%)	4.55	52 (71%) 0 0	99, 132, 149, 150	0
28	1	56/56 (100%)	-0.48	0 100 100	33, 41, 52, 62	0
29	2	46/50 (92%)	0.04	3 (6%) 18 14	48, 79, 112, 122	0
30	3	92/92 (100%)	0.28	3 (3%) 46 41	58, 85, 99, 109	0
31	9	122/122 (100%)	-0.82	2 (1%) 72 70	46, 78, 108, 156	0
All	All	6646/7217 (92%)	-0.24	287 (4%) 35 30	24, 64, 122, 184	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	46	SER	18.3
27	Z	58	ASN	18.3
27	Z	35	SER	17.0
27	Z	50	VAL	14.0
23	V	1	THR	13.9
10	I	74	ILE	13.8
27	Z	43	GLY	11.0
23	V	39	ALA	10.6
27	Z	55	SER	10.3
27	Z	53	ILE	9.9
27	Z	47	ARG	9.9
10	I	128	THR	9.7
27	Z	45	VAL	9.5
27	Z	42	TYR	9.1
5	D	63	ILE	8.7
27	Z	44	ARG	8.6
27	Z	69	ASP	8.4
27	Z	59	GLU	7.9
10	I	70	THR	7.8
23	V	40	PRO	7.6
27	Z	38	PHE	7.5
27	Z	49	ARG	7.5
10	I	72	GLU	7.1
10	I	104	ALA	6.9
27	Z	34	SER	6.9
10	I	71	ALA	6.7
15	N	166	ALA	6.7
10	I	83	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
27	Z	48	ARG	6.6
27	Z	54	GLU	6.5
10	I	97	VAL	6.5
27	Z	57	MET	6.2
10	I	102	GLN	6.1
10	I	66	GLY	5.9
10	I	132	VAL	5.9
27	Z	51	ALA	5.8
5	D	88	LEU	5.7
10	I	106	GLN	5.6
10	I	93	ALA	5.5
10	I	91	PHE	5.5
10	I	100	VAL	5.5
27	Z	68	GLU	5.4
23	V	43	PRO	5.3
2	A	85	SER	5.3
7	F	106	ALA	5.2
5	D	69	ILE	5.2
2	A	37	VAL	5.1
10	I	111	LEU	5.1
10	I	108	HIS	5.1
27	Z	82	SER	5.1
10	I	79	GLY	5.1
10	I	99	GLN	5.1
10	I	105	GLU	5.1
5	D	57	THR	5.0
5	D	90	LEU	5.0
10	I	73	LEU	4.8
31	9	1	U	4.7
5	D	27	ILE	4.7
20	S	81	ILE	4.6
27	Z	81	CYS	4.6
5	D	172	VAL	4.6
5	D	89	PRO	4.6
10	I	112	LEU	4.6
27	Z	62	ALA	4.6
5	D	87	ALA	4.5
5	D	10	PHE	4.5
5	D	18	ILE	4.5
27	Z	40	ALA	4.5
10	I	80	PHE	4.4
9	H	141	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
10	I	127	CYS	4.3
21	T	119	ALA	4.3
27	Z	52	GLU	4.3
27	Z	37	ARG	4.3
5	D	25	MET	4.3
5	D	44	ILE	4.3
27	Z	56	GLU	4.2
27	Z	36	GLY	4.2
13	L	60	GLU	4.2
27	Z	78	ILE	4.2
10	I	92	VAL	4.2
5	D	26	GLY	4.2
27	Z	70	ARG	4.2
23	V	38	GLY	4.2
10	I	116	LEU	4.1
13	L	80	ASP	4.0
10	I	113	SER	4.0
27	Z	39	GLY	4.0
10	I	110	ASP	4.0
27	Z	60	ASP	4.0
10	I	88	GLN	4.0
27	Z	83	TYR	4.0
27	Z	77	GLY	4.0
15	N	145	ALA	3.9
5	D	85	GLN	3.9
10	I	130	LEU	3.9
7	F	49	PHE	3.9
2	A	237	GLY	3.9
10	I	69	PRO	3.9
5	D	40	ILE	3.8
5	D	61	PHE	3.8
13	L	106	VAL	3.7
10	I	94	ASP	3.7
10	I	98	ASP	3.7
10	I	75	LYS	3.7
10	I	78	ALA	3.7
27	Z	63	CYS	3.7
27	Z	67	GLY	3.7
2	A	80	LEU	3.6
5	D	130	VAL	3.6
5	D	134	LEU	3.6
10	I	117	THR	3.6

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Mol	Chain	Res	Type	RSRZ
10	I	109	PRO	3.6
10	I	103	ILE	3.6
7	F	99	THR	3.5
9	H	40	GLN	3.5
27	Z	64	PRO	3.5
15	N	185	GLU	3.5
8	G	23	ILE	3.5
10	I	124	VAL	3.5
10	I	81	GLU	3.5
10	I	84	SER	3.5
9	H	77	ILE	3.5
15	N	178	THR	3.5
15	N	179	LEU	3.5
2	A	82	VAL	3.5
27	Z	41	ARG	3.4
5	D	128	LEU	3.4
7	F	75	ILE	3.4
2	A	31	LYS	3.4
9	H	133	GLY	3.4
15	N	147	ILE	3.4
27	Z	79	TRP	3.4
9	H	146	ALA	3.4
5	D	64	ARG	3.4
13	L	91	VAL	3.3
10	I	121	LYS	3.3
9	H	90	LEU	3.3
31	9	24	U	3.3
9	H	86	TYR	3.3
7	F	119	ARG	3.2
29	2	49	GLU	3.2
10	I	76	ASP	3.2
5	D	92	GLU	3.2
27	Z	80	GLN	3.2
27	Z	61	HIS	3.1
27	Z	66	CYS	3.1
27	Z	93	TYR	3.1
5	D	104	PHE	3.1
29	2	39	ARG	3.1
1	0	1198	U	3.1
5	D	58	VAL	3.1
1	0	1172	G	3.1
2	A	83	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
26	Y	235	GLU	3.1
7	F	15	ASP	3.0
5	D	170	TYR	3.0
10	I	120	ALA	3.0
5	D	106	PHE	3.0
2	A	65	ARG	3.0
10	I	86	GLU	3.0
5	D	84	LEU	3.0
27	Z	89	THR	3.0
23	V	2	VAL	3.0
5	D	22	VAL	2.9
5	D	86	THR	2.9
29	2	48	ASP	2.9
2	A	88	ILE	2.9
2	A	60	PHE	2.9
13	L	96	VAL	2.9
15	N	155	GLU	2.9
7	F	44	SER	2.9
13	L	147	GLU	2.8
15	N	160	SER	2.8
5	D	166	ILE	2.8
9	H	76	LEU	2.8
25	X	88	GLU	2.8
8	G	27	ILE	2.8
23	V	52	ALA	2.8
25	X	80	GLU	2.8
5	D	62	ASP	2.8
9	H	35	LYS	2.7
23	V	51	LYS	2.7
23	V	59	ILE	2.7
9	H	48	VAL	2.7
9	H	114	ASP	2.7
10	I	67	VAL	2.7
13	L	102	ASP	2.7
15	N	138	ASP	2.7
23	V	41	GLU	2.7
5	D	75	LEU	2.7
9	H	174	LEU	2.7
13	L	75	LEU	2.7
23	V	37	GLY	2.7
5	D	81	GLU	2.7
10	I	135	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
21	T	116	ASP	2.7
1	0	282	C	2.7
27	Z	104	ARG	2.7
13	L	114	VAL	2.6
9	H	37	GLY	2.6
15	N	172	PHE	2.6
7	F	17	LEU	2.6
24	W	96	LEU	2.6
13	L	100	ALA	2.6
21	T	118	SER	2.6
2	A	58	VAL	2.6
11	J	70	PHE	2.6
5	D	23	VAL	2.6
25	X	10	VAL	2.6
5	D	66	GLY	2.5
12	K	132	VAL	2.5
2	A	91	GLY	2.5
9	H	145	ASP	2.5
10	I	82	THR	2.5
13	L	118	LEU	2.5
30	3	14	CYS	2.5
10	I	131	GLY	2.4
5	D	43	GLU	2.4
27	Z	85	ASP	2.4
1	0	1169	U	2.4
1	0	1199	A	2.4
10	I	68	PRO	2.4
5	D	70	GLY	2.4
6	E	10	ASP	2.4
10	I	118	ASN	2.4
15	N	137	ALA	2.4
13	L	140	VAL	2.4
27	Z	71	VAL	2.4
15	N	140	GLN	2.3
7	F	97	ALA	2.3
15	N	83	LEU	2.3
27	Z	88	PHE	2.3
10	I	123	VAL	2.3
1	0	1171	A	2.3
9	H	89	THR	2.3
1	0	970	U	2.3
12	K	110	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
23	V	3	LEU	2.3
7	F	117	GLU	2.3
27	Z	101	LYS	2.2
25	X	7	GLU	2.2
15	N	181	ASP	2.2
13	L	150	GLN	2.2
5	D	157	LEU	2.2
5	D	11	HIS	2.2
23	V	36	ALA	2.2
9	H	87	LYS	2.2
5	D	93	LEU	2.1
15	N	183	ASP	2.1
9	H	169	GLU	2.1
2	A	36	ASP	2.1
15	N	164	ASP	2.1
5	D	17	ARG	2.1
15	N	139	TRP	2.1
1	0	1948	G	2.1
15	N	152	GLU	2.1
1	0	10	U	2.1
15	N	143	ARG	2.1
13	L	105	TYR	2.1
27	Z	74	GLN	2.1
5	D	72	LYS	2.1
23	V	5	VAL	2.1
9	H	66	GLU	2.1
2	A	89	ALA	2.1
10	I	119	ALA	2.1
23	V	61	GLY	2.1
6	E	170	ARG	2.1
30	3	41	GLU	2.1
7	F	63	ILE	2.0
9	H	50	ILE	2.0
9	H	85	ASP	2.0
15	N	159	TYR	2.0
17	P	71	TYR	2.0
25	X	74	ALA	2.0
27	Z	103	VAL	2.0
10	I	129	SER	2.0
1	0	1177	A	2.0
5	D	165	PHE	2.0
30	3	13	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
5	D	167	GLU	2.0
2	A	93	THR	2.0
5	D	101	THR	2.0
13	L	145	LEU	2.0
5	D	129	ASP	2.0
20	S	76	GLU	2.0
23	V	49	LEU	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(Å ²)	Q<0.9
1	1MA	0	628	23/24	0.98	0.15	34,36,38,39	0
1	UR3	0	2619	21/22	0.98	0.13	45,48,51,54	0
1	PSU	0	2621	20/21	0.98	0.12	30,35,50,51	0
1	OMU	0	2587	21/22	0.99	0.10	43,44,46,48	0
1	OMG	0	2588	24/25	0.99	0.12	42,44,46,48	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
32	MG	0	8090	1/1	-0.02	0.56	121,121,121,121	0
36	SR	0	8977	1/1	0.10	0.06	197,197,197,197	0
36	SR	0	8944	1/1	0.34	0.16	178,178,178,178	0
34	NA	0	8525	1/1	0.36	0.27	93,93,93,93	0
34	NA	0	8554	1/1	0.43	0.42	70,70,70,70	0
36	SR	9	9003	1/1	0.45	0.06	187,187,187,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	0	8966	1/1	0.49	0.14	120,120,120,120	0
34	NA	9	8572	1/1	0.49	0.49	117,117,117,117	0
34	NA	0	8556	1/1	0.49	1.51	68,68,68,68	0
34	NA	0	8506	1/1	0.52	0.21	76,76,76,76	0
36	SR	0	8998	1/1	0.54	0.25	175,175,175,175	0
36	SR	0	8913	1/1	0.55	0.82	200,200,200,200	0
34	NA	C	8503	1/1	0.55	0.25	46,46,46,46	0
34	NA	0	8524	1/1	0.55	0.61	73,73,73,73	0
36	SR	0	9006	1/1	0.56	0.58	200,200,200,200	0
36	SR	0	8917	1/1	0.56	0.22	151,151,151,151	0
34	NA	0	8522	1/1	0.57	0.14	108,108,108,108	0
32	MG	0	8091	1/1	0.59	0.13	89,89,89,89	0
36	SR	0	8941	1/1	0.59	0.23	131,131,131,131	0
36	SR	0	8982	1/1	0.62	0.95	200,200,200,200	0
36	SR	0	8938	1/1	0.62	0.06	191,191,191,191	0
36	SR	0	8933	1/1	0.63	0.09	143,143,143,143	0
36	SR	0	8996	1/1	0.64	0.44	200,200,200,200	0
36	SR	0	8983	1/1	0.64	0.12	199,199,199,199	0
32	MG	0	8089	1/1	0.65	0.16	64,64,64,64	0
36	SR	0	8959	1/1	0.65	0.26	181,181,181,181	0
36	SR	0	8949	1/1	0.66	0.20	146,146,146,146	0
36	SR	0	8915	1/1	0.66	0.10	136,136,136,136	0
34	NA	0	8560	1/1	0.67	0.53	97,97,97,97	0
36	SR	0	8972	1/1	0.68	0.14	164,164,164,164	0
36	SR	0	8976	1/1	0.68	0.22	200,200,200,200	0
34	NA	0	8504	1/1	0.68	0.34	46,46,46,46	0
34	NA	0	8502	1/1	0.69	0.20	66,66,66,66	0
32	MG	0	8072	1/1	0.69	0.31	82,82,82,82	0
32	MG	9	8040	1/1	0.69	0.36	97,97,97,97	0
34	NA	0	8527	1/1	0.69	0.56	86,86,86,86	0
36	SR	0	8928	1/1	0.70	0.08	151,151,151,151	0
36	SR	0	8910	1/1	0.71	0.11	106,106,106,106	0
36	SR	0	9001	1/1	0.71	0.16	184,184,184,184	0
36	SR	0	8991	1/1	0.71	0.25	195,195,195,195	0
32	MG	0	8050	1/1	0.71	0.19	74,74,74,74	0
32	MG	0	8075	1/1	0.72	0.11	58,58,58,58	0
34	NA	0	8563	1/1	0.72	0.24	82,82,82,82	0
34	NA	0	8559	1/1	0.72	0.24	95,95,95,95	0
36	SR	0	8955	1/1	0.73	0.10	198,198,198,198	0
36	SR	0	8965	1/1	0.73	0.11	151,151,151,151	0
35	CL	3	8804	1/1	0.74	0.07	76,76,76,76	0
34	NA	0	8531	1/1	0.75	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	0	8984	1/1	0.75	0.07	143,143,143,143	0
36	SR	0	8942	1/1	0.75	0.18	144,144,144,144	0
36	SR	B	8950	1/1	0.75	0.12	119,119,119,119	0
34	NA	0	8566	1/1	0.75	0.59	59,59,59,59	0
36	SR	0	9000	1/1	0.76	0.21	200,200,200,200	0
34	NA	0	8548	1/1	0.76	0.28	67,67,67,67	0
36	SR	0	8951	1/1	0.76	0.05	149,149,149,149	0
36	SR	0	9008	1/1	0.76	0.24	111,111,111,111	0
34	NA	H	8518	1/1	0.76	0.50	95,95,95,95	0
36	SR	0	8958	1/1	0.76	0.12	121,121,121,121	0
34	NA	0	8549	1/1	0.77	0.91	60,60,60,60	0
32	MG	0	8038	1/1	0.77	0.09	70,70,70,70	0
34	NA	0	8529	1/1	0.77	0.06	50,50,50,50	0
36	SR	B	8987	1/1	0.77	0.53	200,200,200,200	0
36	SR	0	8924	1/1	0.77	0.21	149,149,149,149	0
36	SR	0	8995	1/1	0.78	0.14	142,142,142,142	0
36	SR	0	8956	1/1	0.78	0.10	187,187,187,187	0
33	K	0	8401	1/1	0.78	0.88	123,123,123,123	0
34	NA	0	8523	1/1	0.78	0.16	65,65,65,65	0
36	SR	9	8978	1/1	0.78	0.12	169,169,169,169	0
36	SR	9	8980	1/1	0.78	0.05	175,175,175,175	0
32	MG	0	8030	1/1	0.78	0.33	79,79,79,79	0
36	SR	0	8994	1/1	0.80	0.40	199,199,199,199	0
36	SR	0	8964	1/1	0.80	0.10	139,139,139,139	0
34	NA	0	8555	1/1	0.80	0.58	53,53,53,53	0
36	SR	0	8997	1/1	0.80	1.19	200,200,200,200	0
34	NA	0	8542	1/1	0.80	0.70	62,62,62,62	0
34	NA	0	8557	1/1	0.80	0.04	74,74,74,74	0
32	MG	0	8006	1/1	0.80	0.17	33,33,33,33	0
36	SR	0	8908	1/1	0.81	0.29	175,175,175,175	0
36	SR	0	8922	1/1	0.81	0.27	156,156,156,156	0
34	NA	0	8565	1/1	0.81	1.90	100,100,100,100	0
32	MG	0	8062	1/1	0.82	0.28	61,61,61,61	0
32	MG	0	8092	1/1	0.82	0.10	80,80,80,80	0
36	SR	A	8930	1/1	0.82	0.26	169,169,169,169	0
34	NA	0	8536	1/1	0.82	0.07	65,65,65,65	0
32	MG	K	8054	1/1	0.82	0.21	47,47,47,47	0
32	MG	0	8069	1/1	0.82	0.19	49,49,49,49	0
34	NA	0	8515	1/1	0.82	0.15	50,50,50,50	0
34	NA	0	8550	1/1	0.82	0.49	59,59,59,59	0
36	SR	0	8968	1/1	0.83	0.06	165,165,165,165	0
36	SR	0	8920	1/1	0.83	0.59	185,185,185,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	S	8961	1/1	0.83	0.12	145,145,145,145	0
37	WIN	0	9101	39/39	0.83	0.33	125,127,128,129	0
34	NA	0	8501	1/1	0.84	0.18	54,54,54,54	0
36	SR	0	9002	1/1	0.84	0.15	183,183,183,183	0
36	SR	0	8969	1/1	0.84	0.14	173,173,173,173	0
36	SR	0	8943	1/1	0.84	0.10	95,95,95,95	0
32	MG	0	8052	1/1	0.84	0.06	58,58,58,58	0
32	MG	0	8037	1/1	0.84	0.16	80,80,80,80	0
32	MG	0	8027	1/1	0.85	0.17	47,47,47,47	0
36	SR	0	8986	1/1	0.85	0.48	200,200,200,200	0
36	SR	0	8901	1/1	0.85	0.14	96,96,96,96	0
36	SR	0	8934	1/1	0.85	0.32	166,166,166,166	0
34	NA	0	8535	1/1	0.85	0.38	63,63,63,63	0
34	NA	J	8538	1/1	0.85	0.21	67,67,67,67	0
34	NA	0	8571	1/1	0.85	0.31	98,98,98,98	0
34	NA	0	8561	1/1	0.86	0.65	90,90,90,90	0
36	SR	0	8937	1/1	0.86	0.33	125,125,125,125	0
32	MG	0	8039	1/1	0.86	0.22	63,63,63,63	0
36	SR	0	8909	1/1	0.86	0.17	99,99,99,99	0
34	NA	Q	8540	1/1	0.87	0.13	58,58,58,58	0
34	NA	R	8532	1/1	0.87	0.11	59,59,59,59	0
32	MG	0	8066	1/1	0.87	0.34	88,88,88,88	0
34	NA	0	8558	1/1	0.87	0.50	63,63,63,63	0
36	SR	0	8989	1/1	0.87	0.17	185,185,185,185	0
34	NA	0	8568	1/1	0.87	0.22	57,57,57,57	0
34	NA	0	8553	1/1	0.87	0.42	69,69,69,69	0
32	MG	0	8063	1/1	0.87	0.22	80,80,80,80	0
36	SR	0	8954	1/1	0.87	0.11	109,109,109,109	0
34	NA	0	8511	1/1	0.87	0.22	67,67,67,67	0
32	MG	0	8080	1/1	0.87	0.29	87,87,87,87	0
36	SR	0	8981	1/1	0.87	0.21	158,158,158,158	0
36	SR	0	8962	1/1	0.88	0.17	180,180,180,180	0
34	NA	0	8567	1/1	0.88	0.51	87,87,87,87	0
35	CL	0	8815	1/1	0.88	0.14	83,83,83,83	0
36	SR	0	8988	1/1	0.88	0.12	158,158,158,158	0
32	MG	0	8085	1/1	0.88	0.11	69,69,69,69	0
32	MG	A	8051	1/1	0.88	0.29	98,98,98,98	0
32	MG	0	8053	1/1	0.88	0.06	69,69,69,69	0
34	NA	0	8505	1/1	0.88	1.08	44,44,44,44	0
34	NA	0	8537	1/1	0.88	0.21	50,50,50,50	0
32	MG	0	8018	1/1	0.88	0.28	54,54,54,54	0
32	MG	0	8084	1/1	0.88	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	0	8916	1/1	0.88	0.10	129,129,129,129	0
36	SR	0	8902	1/1	0.89	0.17	70,70,70,70	0
32	MG	0	8002	1/1	0.89	0.18	26,26,26,26	0
34	NA	0	8562	1/1	0.89	0.62	82,82,82,82	0
36	SR	A	8929	1/1	0.89	0.10	142,142,142,142	0
36	SR	0	8971	1/1	0.89	0.06	185,185,185,185	0
32	MG	0	8047	1/1	0.89	0.39	71,71,71,71	0
34	NA	0	8544	1/1	0.89	0.19	73,73,73,73	0
34	NA	0	8509	1/1	0.89	0.28	77,77,77,77	0
34	NA	0	8533	1/1	0.89	0.15	72,72,72,72	0
33	K	0	8402	1/1	0.89	0.45	90,90,90,90	0
34	NA	0	8514	1/1	0.89	0.71	54,54,54,54	0
34	NA	0	8573	1/1	0.89	0.12	87,87,87,87	0
32	MG	0	8082	1/1	0.90	0.31	81,81,81,81	0
34	NA	0	8507	1/1	0.90	0.17	46,46,46,46	0
34	NA	0	8520	1/1	0.90	0.10	55,55,55,55	0
36	SR	0	8990	1/1	0.90	0.11	116,116,116,116	0
36	SR	0	8975	1/1	0.90	0.07	154,154,154,154	0
34	NA	0	8530	1/1	0.90	0.30	60,60,60,60	0
36	SR	0	8914	1/1	0.91	0.30	127,127,127,127	0
34	NA	0	8508	1/1	0.91	0.20	63,63,63,63	0
32	MG	0	8020	1/1	0.91	0.16	57,57,57,57	0
32	MG	0	8059	1/1	0.91	0.12	52,52,52,52	0
34	NA	0	8512	1/1	0.91	0.30	48,48,48,48	0
32	MG	T	8057	1/1	0.91	0.04	72,72,72,72	0
36	SR	0	8923	1/1	0.91	0.15	112,112,112,112	0
32	MG	0	8013	1/1	0.92	0.06	30,30,30,30	0
32	MG	0	8043	1/1	0.92	0.16	58,58,58,58	0
34	NA	0	8541	1/1	0.92	0.34	70,70,70,70	0
32	MG	0	8068	1/1	0.92	0.10	67,67,67,67	0
36	SR	1	8952	1/1	0.92	0.16	93,93,93,93	0
32	MG	2	8060	1/1	0.92	0.10	65,65,65,65	0
32	MG	0	8079	1/1	0.92	0.29	67,67,67,67	0
36	SR	0	8957	1/1	0.92	0.20	200,200,200,200	0
36	SR	0	8931	1/1	0.92	0.09	136,136,136,136	0
38	CD	Z	8703	1/1	0.92	0.06	172,172,172,172	0
32	MG	0	8078	1/1	0.93	0.29	54,54,54,54	0
36	SR	0	8939	1/1	0.93	0.07	145,145,145,145	0
35	CL	J	8801	1/1	0.93	0.09	82,82,82,82	0
36	SR	0	8919	1/1	0.93	0.08	179,179,179,179	0
34	NA	0	8516	1/1	0.93	0.15	37,37,37,37	0
32	MG	0	8034	1/1	0.93	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	0	8948	1/1	0.93	0.16	122,122,122,122	0
36	SR	F	9005	1/1	0.93	0.04	149,149,149,149	0
34	NA	0	8574	1/1	0.93	0.41	69,69,69,69	0
32	MG	0	8049	1/1	0.93	0.53	116,116,116,116	0
32	MG	0	8036	1/1	0.93	0.13	60,60,60,60	0
32	MG	0	8071	1/1	0.93	0.12	71,71,71,71	0
32	MG	0	8031	1/1	0.93	0.36	73,73,73,73	0
32	MG	0	8064	1/1	0.93	0.18	51,51,51,51	0
34	NA	0	8528	1/1	0.93	0.17	60,60,60,60	0
32	MG	0	8019	1/1	0.94	0.23	30,30,30,30	0
34	NA	0	8521	1/1	0.94	0.26	71,71,71,71	0
35	CL	A	8809	1/1	0.94	0.31	96,96,96,96	0
32	MG	0	8001	1/1	0.94	0.15	26,26,26,26	0
35	CL	L	8810	1/1	0.94	0.09	69,69,69,69	0
36	SR	0	8970	1/1	0.94	0.06	135,135,135,135	0
32	MG	0	8081	1/1	0.94	0.17	81,81,81,81	0
36	SR	0	8992	1/1	0.94	0.11	137,137,137,137	0
32	MG	0	8024	1/1	0.94	0.20	54,54,54,54	0
34	NA	0	8546	1/1	0.94	0.73	85,85,85,85	0
36	SR	0	8921	1/1	0.94	0.11	99,99,99,99	0
32	MG	0	8044	1/1	0.94	0.05	55,55,55,55	0
36	SR	0	8979	1/1	0.94	0.10	195,195,195,195	0
36	SR	0	8960	1/1	0.94	0.11	151,151,151,151	0
34	NA	0	8526	1/1	0.94	0.12	45,45,45,45	0
32	MG	0	8032	1/1	0.95	0.06	42,42,42,42	0
36	SR	0	9004	1/1	0.95	0.47	200,200,200,200	0
36	SR	0	8985	1/1	0.95	0.05	148,148,148,148	0
32	MG	0	8045	1/1	0.95	0.08	30,30,30,30	0
32	MG	0	8041	1/1	0.95	0.23	32,32,32,32	0
35	CL	0	8803	1/1	0.95	0.07	62,62,62,62	0
34	NA	0	8545	1/1	0.95	0.14	48,48,48,48	0
32	MG	9	8074	1/1	0.95	0.14	101,101,101,101	0
36	SR	0	8974	1/1	0.95	0.23	179,179,179,179	0
34	NA	0	8547	1/1	0.95	0.87	71,71,71,71	0
34	NA	0	8534	1/1	0.95	0.26	47,47,47,47	0
34	NA	0	8575	1/1	0.95	0.27	87,87,87,87	0
32	MG	0	8073	1/1	0.95	0.08	80,80,80,80	0
32	MG	0	8056	1/1	0.95	0.15	62,62,62,62	0
32	MG	0	8033	1/1	0.95	0.20	63,63,63,63	0
36	SR	0	8945	1/1	0.95	0.07	131,131,131,131	0
36	SR	0	8993	1/1	0.96	0.05	178,178,178,178	0
36	SR	0	8940	1/1	0.96	0.10	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	0	8967	1/1	0.96	0.04	147,147,147,147	0
32	MG	0	8005	1/1	0.96	0.23	35,35,35,35	0
32	MG	0	8029	1/1	0.96	0.18	69,69,69,69	0
34	NA	0	8519	1/1	0.96	0.33	50,50,50,50	0
34	NA	9	8543	1/1	0.96	0.17	57,57,57,57	0
32	MG	0	8046	1/1	0.96	0.18	53,53,53,53	0
36	SR	0	8946	1/1	0.96	0.17	129,129,129,129	0
36	SR	0	8947	1/1	0.96	0.25	200,200,200,200	0
32	MG	0	8023	1/1	0.96	0.20	30,30,30,30	0
36	SR	0	9007	1/1	0.96	0.67	199,199,199,199	0
35	CL	0	8811	1/1	0.96	0.11	72,72,72,72	0
34	NA	0	8551	1/1	0.96	0.20	60,60,60,60	0
34	NA	0	8552	1/1	0.96	0.27	80,80,80,80	0
32	MG	0	8061	1/1	0.96	0.22	36,36,36,36	0
35	CL	J	8821	1/1	0.96	0.09	78,78,78,78	0
34	NA	0	8570	1/1	0.96	0.08	59,59,59,59	0
32	MG	0	8048	1/1	0.96	0.23	28,28,28,28	0
32	MG	0	8087	1/1	0.96	0.13	36,36,36,36	0
36	SR	3	8932	1/1	0.96	0.10	94,94,94,94	0
32	MG	0	8035	1/1	0.96	0.19	70,70,70,70	0
32	MG	0	8076	1/1	0.96	0.10	38,38,38,38	0
36	SR	0	8963	1/1	0.96	0.09	133,133,133,133	0
34	NA	0	8513	1/1	0.96	0.34	56,56,56,56	0
32	MG	0	8016	1/1	0.96	0.16	30,30,30,30	0
32	MG	Y	8086	1/1	0.97	0.10	55,55,55,55	0
35	CL	0	8814	1/1	0.97	0.09	66,66,66,66	0
32	MG	0	8007	1/1	0.97	0.19	40,40,40,40	0
35	CL	0	8822	1/1	0.97	0.35	86,86,86,86	0
32	MG	0	8065	1/1	0.97	0.07	41,41,41,41	0
34	NA	M	8539	1/1	0.97	0.29	53,53,53,53	0
32	MG	0	8093	1/1	0.97	0.07	45,45,45,45	0
32	MG	0	8014	1/1	0.97	0.20	33,33,33,33	0
35	CL	N	8807	1/1	0.97	0.18	72,72,72,72	0
35	CL	O	8808	1/1	0.97	0.20	79,79,79,79	0
34	NA	S	8510	1/1	0.97	0.15	50,50,50,50	0
32	MG	0	8025	1/1	0.97	0.10	37,37,37,37	0
36	SR	0	8926	1/1	0.97	0.12	142,142,142,142	0
36	SR	0	8927	1/1	0.97	0.11	167,167,167,167	0
36	SR	0	8973	1/1	0.97	0.11	141,141,141,141	0
34	NA	0	8517	1/1	0.97	0.11	36,36,36,36	0
36	SR	0	8904	1/1	0.97	0.21	64,64,64,64	0
32	MG	0	8058	1/1	0.97	0.07	23,23,23,23	0

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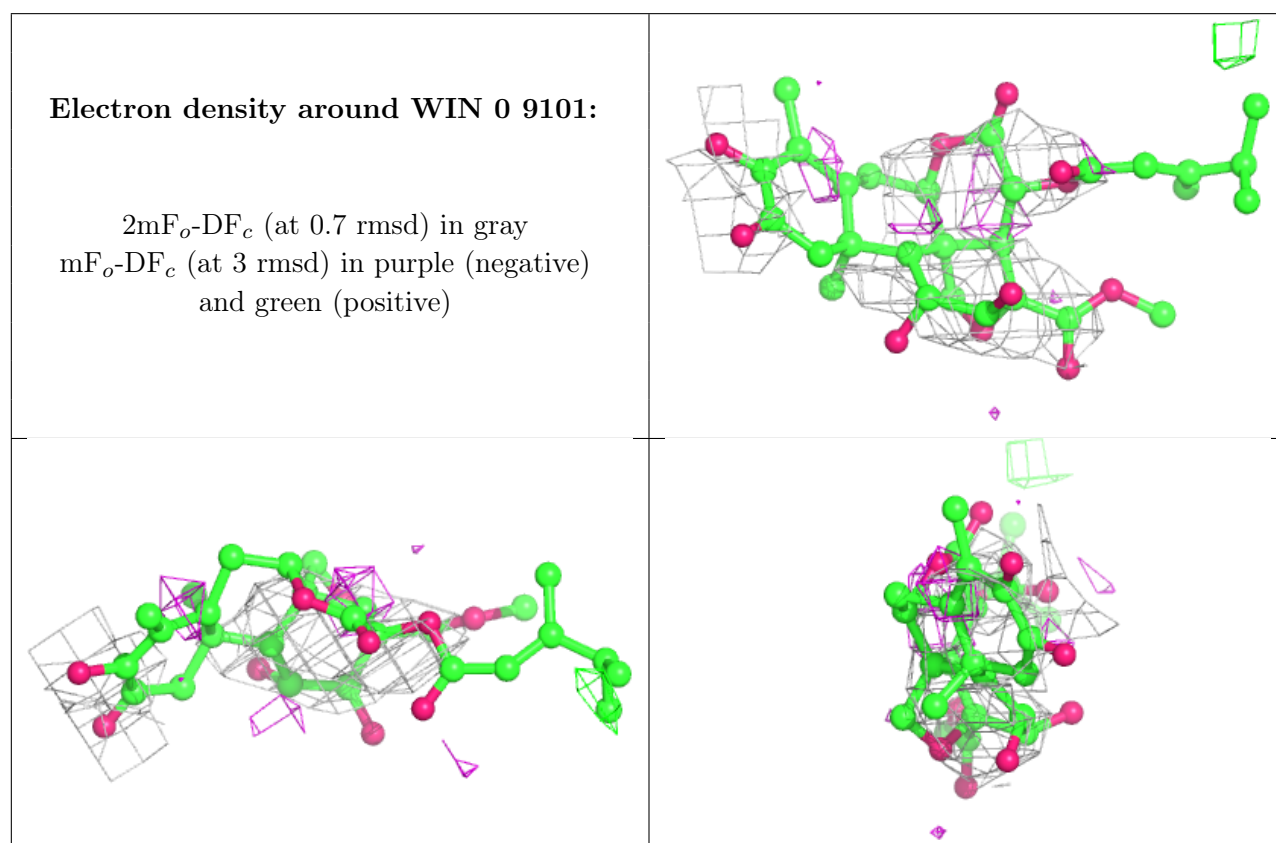
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	CL	0	8805	1/1	0.97	0.10	76,76,76,76	0
32	MG	0	8017	1/1	0.98	0.08	34,34,34,34	0
35	CL	Y	8820	1/1	0.98	0.05	46,46,46,46	0
32	MG	B	8042	1/1	0.98	0.13	62,62,62,62	0
36	SR	0	8935	1/1	0.98	0.09	93,93,93,93	0
36	SR	0	8936	1/1	0.98	0.07	108,108,108,108	0
32	MG	0	8011	1/1	0.98	0.24	30,30,30,30	0
32	MG	0	8070	1/1	0.98	0.28	64,64,64,64	0
34	NA	0	8569	1/1	0.98	0.16	61,61,61,61	0
32	MG	0	8012	1/1	0.98	0.20	26,26,26,26	0
32	MG	0	8003	1/1	0.98	0.15	35,35,35,35	0
35	CL	0	8813	1/1	0.98	0.02	54,54,54,54	0
32	MG	0	8021	1/1	0.98	0.10	43,43,43,43	0
32	MG	0	8088	1/1	0.98	0.18	46,46,46,46	0
35	CL	0	8816	1/1	0.98	0.22	75,75,75,75	0
35	CL	0	8817	1/1	0.98	0.05	68,68,68,68	0
32	MG	0	8008	1/1	0.98	0.16	32,32,32,32	0
32	MG	0	8015	1/1	0.98	0.14	33,33,33,33	0
35	CL	B	8819	1/1	0.98	0.10	57,57,57,57	0
32	MG	0	8077	1/1	0.98	0.06	43,43,43,43	0
36	SR	0	8953	1/1	0.98	0.19	164,164,164,164	0
35	CL	J	8802	1/1	0.98	0.07	79,79,79,79	0
32	MG	0	8010	1/1	0.98	0.11	34,34,34,34	0
36	SR	3	8999	1/1	0.98	0.10	140,140,140,140	0
35	CL	K	8812	1/1	0.98	0.11	57,57,57,57	0
36	SR	0	8925	1/1	0.98	0.11	95,95,95,95	0
32	MG	0	8067	1/1	0.98	0.26	34,34,34,34	0
35	CL	M	8818	1/1	0.98	0.04	49,49,49,49	0
38	CD	O	8705	1/1	0.98	0.06	105,105,105,105	0
34	NA	0	8564	1/1	0.98	0.65	95,95,95,95	0
32	MG	0	8028	1/1	0.99	0.25	30,30,30,30	0
36	SR	R	8912	1/1	0.99	0.19	93,93,93,93	0
32	MG	0	8009	1/1	0.99	0.35	42,42,42,42	0
32	MG	0	8022	1/1	0.99	0.17	37,37,37,37	0
32	MG	0	8055	1/1	0.99	0.20	49,49,49,49	0
36	SR	0	8905	1/1	0.99	0.26	73,73,73,73	0
36	SR	0	8918	1/1	0.99	0.14	94,94,94,94	0
36	SR	0	8906	1/1	0.99	0.23	67,67,67,67	0
32	MG	0	8083	1/1	0.99	0.27	74,74,74,74	0
32	MG	0	8026	1/1	0.99	0.13	55,55,55,55	0
32	MG	0	8004	1/1	0.99	0.17	29,29,29,29	0
36	SR	0	8911	1/1	0.99	0.08	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	CD	1	8702	1/1	0.99	0.14	72,72,72,72	0
38	CD	3	8704	1/1	0.99	0.06	94,94,94,94	0
38	CD	U	8701	1/1	1.00	0.12	71,71,71,71	0
35	CL	R	8806	1/1	1.00	0.10	55,55,55,55	0
36	SR	0	8907	1/1	1.00	0.14	62,62,62,62	0
36	SR	0	8903	1/1	1.00	0.21	66,66,66,66	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.