



wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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

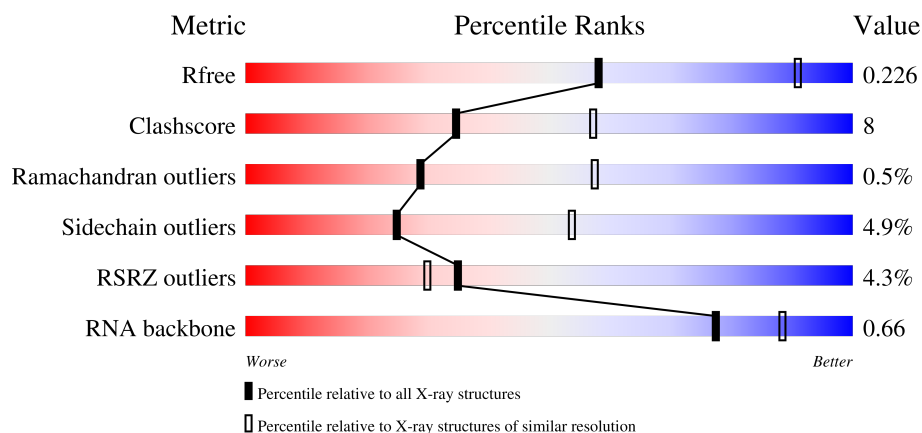
1 Overall quality at a glance

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	
2	A	237	
3	B	337	
4	C	246	

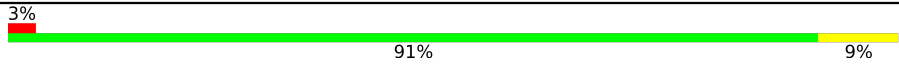

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	172	
7	F	119	
8	G	348	
9	H	177	
10	I	70	
11	J	142	
12	K	132	
13	L	165	
14	M	194	
15	N	186	
16	O	115	
17	P	143	
18	Q	95	
19	R	150	
20	S	81	
21	T	119	
22	U	53	
23	V	65	
24	W	154	
25	X	82	
26	Y	142	
27	Z	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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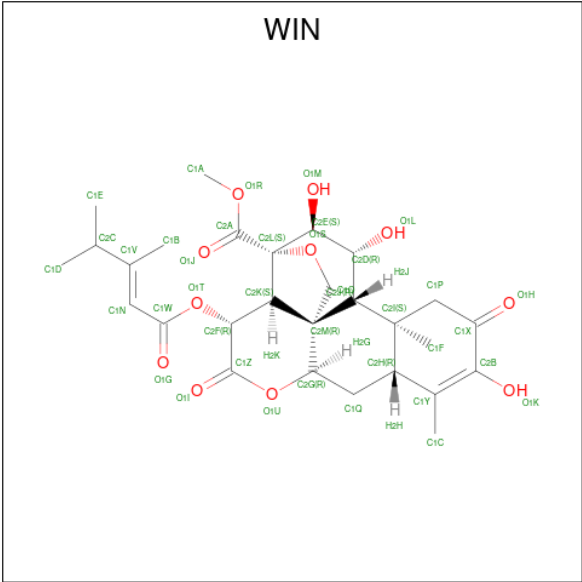
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0

- 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-{[(2 E)-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
37	0	1	Total	C	O	0	0
			39	28	11		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 39 is water.

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

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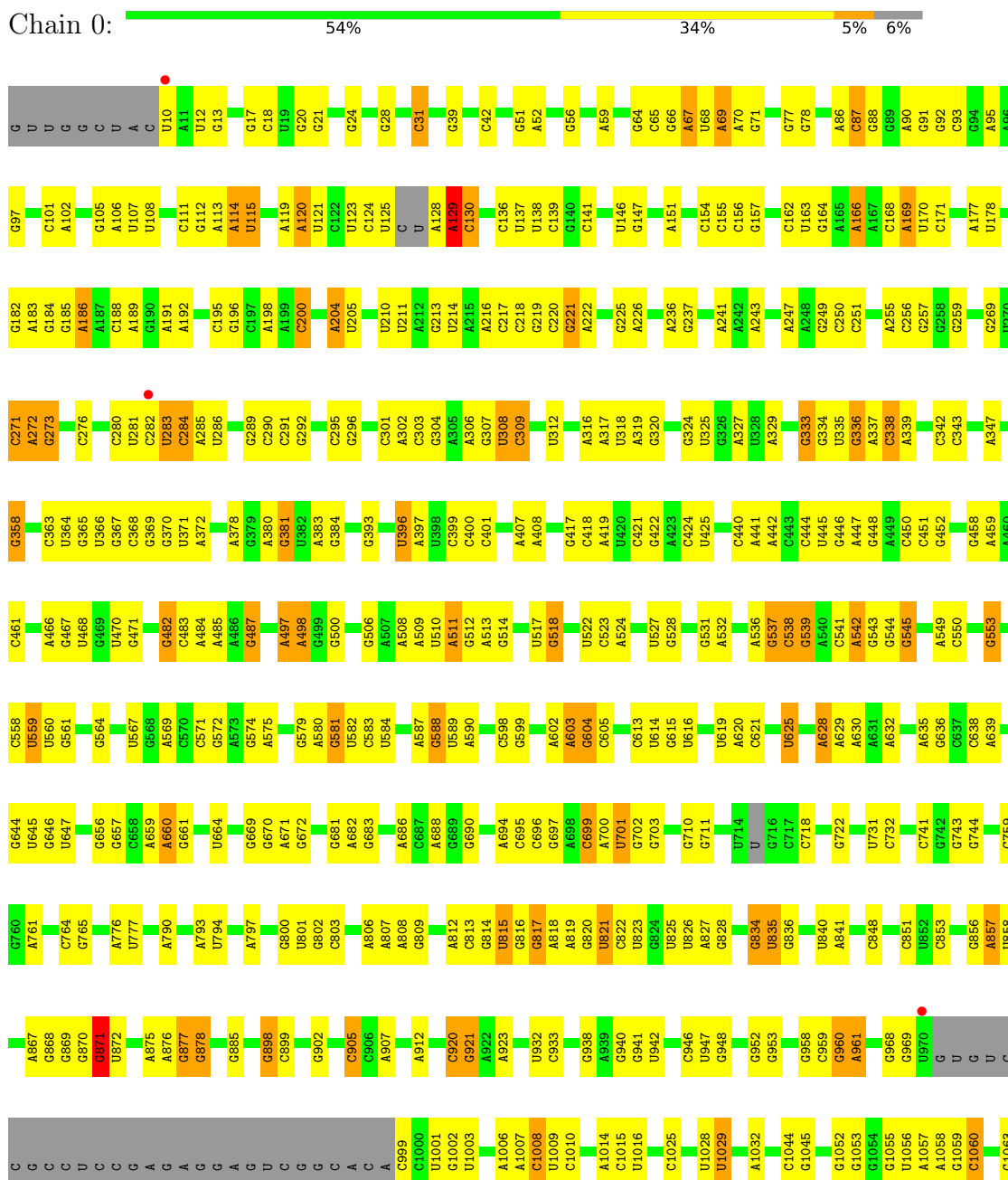
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	20	Total 20	O 20	0	0
39	Y	94	Total 94	O 94	0	0
39	Z	28	Total 28	O 28	0	0
39	1	52	Total 52	O 52	0	0
39	2	39	Total 39	O 39	0	0
39	3	66	Total 66	O 66	0	0
39	9	149	Total 149	O 149	0	0

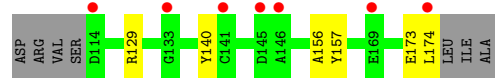
3 Residue-property plots

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.

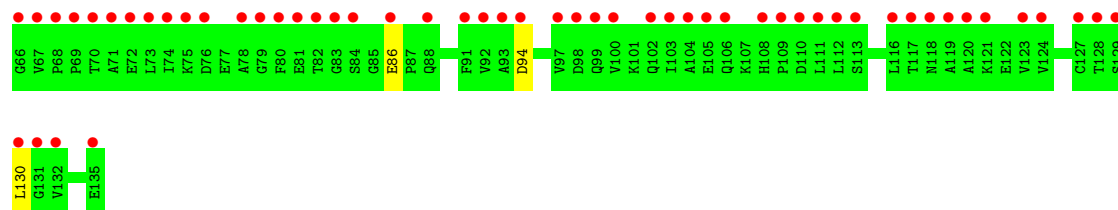
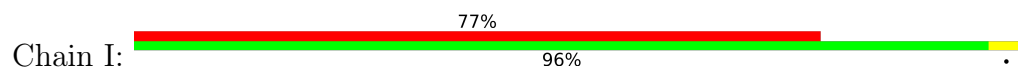
• Molecule 1: 23S ribosomal RNA



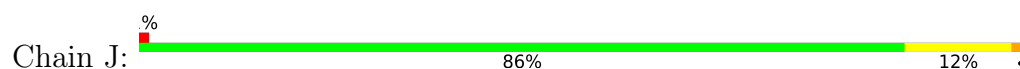
U2265	G2379	U2039	G1947	C1834	U1741	A1641	G1546	A1434	A1352	C1238	G1066
A2266	A2380	C2040	G1948	U1835	A1742	A1642	G1556	U1435	A1353	G1239	A1067
C2267	C2268	G2041	G1951	U1836	U1749	C1643	C1557	C1436	A1242	A1071	
G2269	G2270	C2042	U1838	A1839	U1752	U1644	C1558	C1439	U1243	G1072	
G2271	G2272	G2045	A1840	U1840	G1752	U1645	U1559	C1440	U1244	U1170	
U2277	U2278	G2046	C	A	C		U	G1441	C1245	A1073	
U2279	U2280	C2047	A	U1844	A1755	C1652	U1561	A1442	A1246	G1074	
C2281	C2282	G2050	U	U1845	G1756	A1653	C1562	G1443	C1360	G1075	
U2282	U2283	C2054	U	U1846	G1759	G1654	C1566	G1444	U1249	G1076	
A2291	A2292	G2054	G	U1847	A1759	A1655	G1566	G1445	C1250	G1077	
A2300	A2301	U2064	A	G1848	G1760	A1657	G1567	U1446	C1365	A1078	
A2302	A2303	C2070	C	G1849	U1761	A1658	U1569	U1447	C1366	A1081	
A2308	A2309	G2070	C	G1855	C1762	A1664	C1570	G1453	C1257	A1088	
C2310	C2311	C2071	U1964	C1856	C1763	G1665	A1572	A1454	G1258	C1084	
G2312	G2313	G2072	C1965	A1857	U1766	G1666	A1573	U1455	G1259	G1087	
C2314	C2315	G2073	U1966	A1858	C1767	A1667	A1574	C1456	C1260	A1088	
C2316	C2317	A2074	U1967	C1861	C1768	U1668	G1576	U1457	G1268	A1097	
U2320	U2321	G2079	A1968	C1862	C1769	U1677	U1577	U1463	G1269	A1098	
A2322	A2323	G2080	U1970	C1864	U1770	A1678	U1578	C1464	C1273	G1099	
C2324	C2325	A2081	G1971	G1868	G1773	C1679	G1588	C1474	U1278	G1100	
G2326	G2327	G2082	U1972	U1873	A1778	C1680	G1589	C1477	U1279	C1104	
U2328	U2329	C2087	A1973	G1877	A1779	G1681	G1592	C1478	C1289	C1105	
A2330	A2331	G2088	G1974	U1878	U1783	A1682	C1593	U1478	G1290	A1106	
C2332	C2333	A2089	U1975	G1879	A1784	G1683	C1594	A1482	A1291	G1097	
G2334	G2335	G2090	U1980	U1880	C1787	A1684	G1595	C1483	G1386	A1088	
A2336	A2337	C2091	U1981	C1880	U1788	C1686	U1596	G1484	C1387	A1097	
C2338	C2339	G2092	U1982	A1881	U1789	G1687	A1597	A1485	G1391	A1098	
A2340	A2341	U2093	U1992	C1882	C1790	C1688	A1598	C1495	A1392	A1099	
C2342	C2343	G2094	U1993	U1883	U1791	C1692	A1603	A1496	G1393	U1115	
G2344	G2345	A2095	G1994	A1886	G1795	A1701	G1604	G1497	G1394	U1116	
A2346	A2347	C2096	U1995	U1903	A1796	U1702	G1605	U1500	C1395	A1117	
C2348	C2349	G2097	U1996	A1904	A1797	G1706	A1607	U1503	G1396	A1118	
A2350	A2351	U2002	C2002	U1909	C1798	G1707	C1613	A1504	A1295	U1120	
C2352	C2353	U2003	U2003	A1910	G1799	G1707	G1614	U1505	G1300	G1121	
G2354	G2355	G2004	U2004	A1911	G1800	A1710	A1615	U1506	U1306	U1130	
A2356	A2357	C2105	C2006	A1919	C1803	C1714	A1616	A1515	A1307	G1131	
C2358	C2359	G2106	A2007	C1920	G1804	A1715	C1617	U1516	A1308	A1132	
A2360	A2361	U2110	U2008	A1921	G1805	A1716	G1622	U1524	G1309	A1133	
C2362	C2363	G2111	A2011	A1922	A1811	C1717	C1623	G1525	G1311	G1137	
G2364	G2365	C2114	U2012	C1928	G1812	U1722	A1624	A1526	G1312	U1149	
A2366	A2367	U2115	G2013	G1929	U1813	U1724	U1625	A1527	A1321	A1150	
C2368	C2369	G2116	U2016	U1937	G1814	C1725	G1627	U1528	G1322	G1151	
A2370	A2371	C2121	U2017	G1938	A1815	G1730	A1631	G1529	A1328	A1154	
C2372	C2373	U2122	A2022	U1939	U1817	A1732	A1632	C1421	G1329	G1155	
U2374	U2375	G2133	U2032	U1940	C1818	A1733	C1633	U1422	C1331	G1158	
A2376	A2377	C2134	U2033	A1941	G1819	A1734	G1634	U1423	U1332	G1159	
C2378	C2379	G2135	U2034	A1942	G1820	C1735	U1635	A1424	C1334	G1160	
G2380	G2381	U2136	G2034	C1943	A1829	A1736	A1637	A1427	C1342	A1161	
A2382	A2383	C2136	G2136						C1343	U1164	



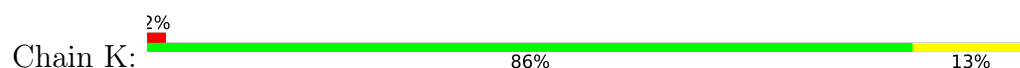
• Molecule 10: 50S ribosomal protein L11P



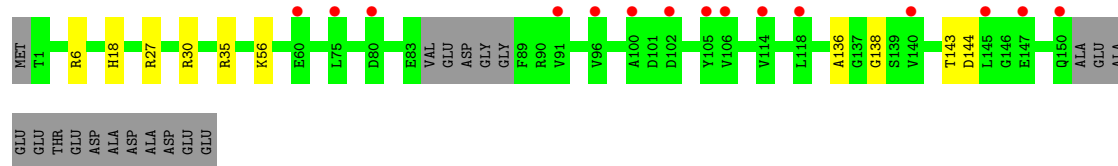
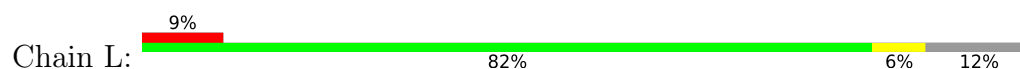
• Molecule 11: 50S ribosomal protein L13P



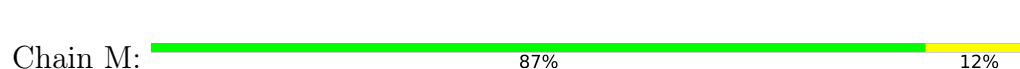
• Molecule 12: 50S ribosomal protein L14P



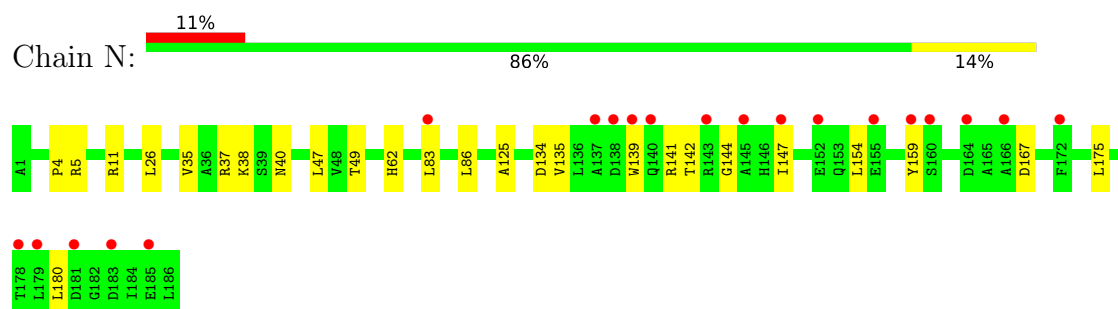
• Molecule 13: 50S ribosomal protein L15P



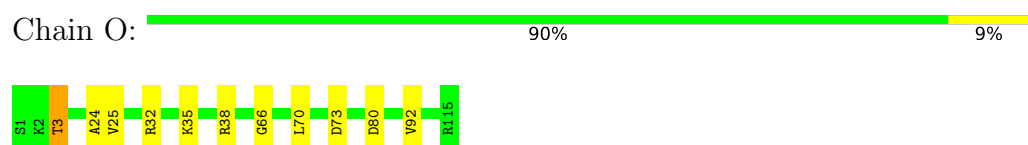
• Molecule 14: 50S ribosomal protein L15e



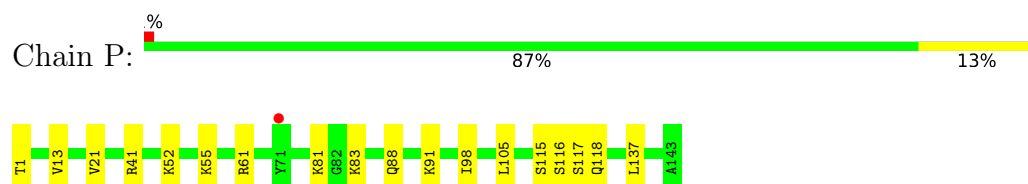
- Molecule 15: 50S ribosomal protein L18P



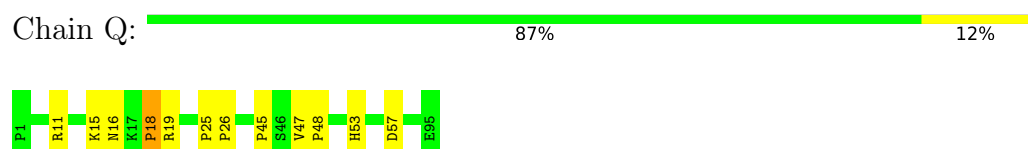
- Molecule 16: 50S ribosomal protein L18e



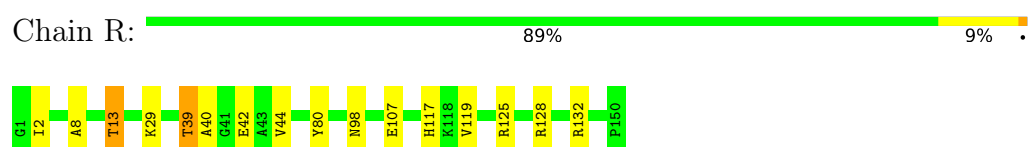
- Molecule 17: 50S ribosomal protein L19e



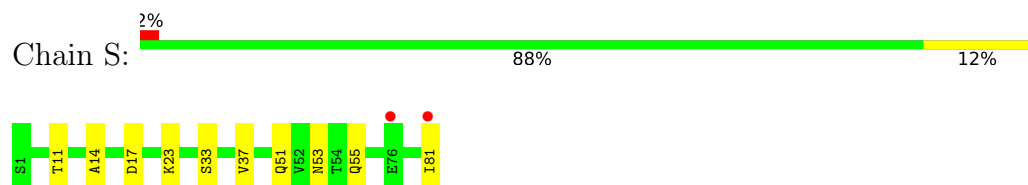
- Molecule 18: 50S ribosomal protein L21e



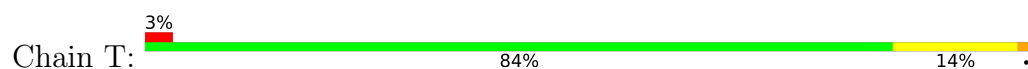
- Molecule 19: 50S ribosomal protein L22P

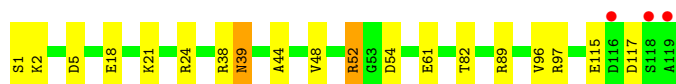


- Molecule 20: 50S ribosomal protein L23P



- Molecule 21: 50S ribosomal protein L24P

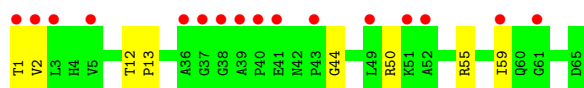
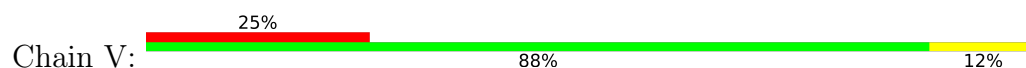




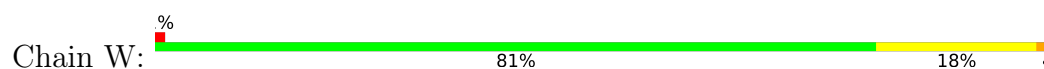
- Molecule 22: 50S ribosomal protein L24e



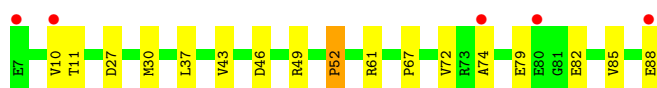
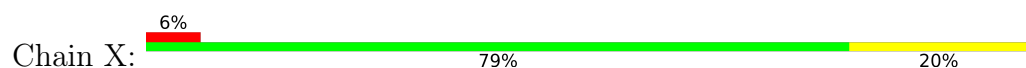
- Molecule 23: 50S ribosomal protein L29P



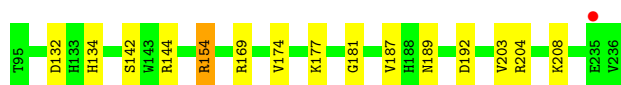
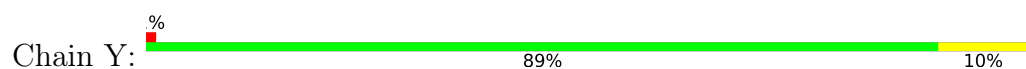
- Molecule 24: 50S ribosomal protein L30P



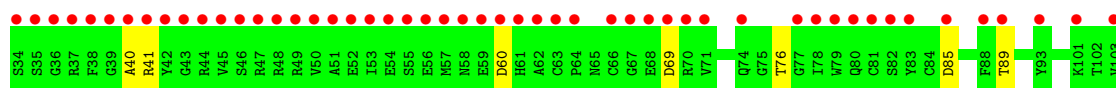
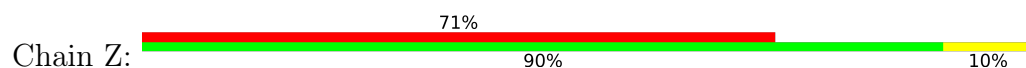
- Molecule 25: 50S ribosomal protein L31e




- Molecule 26: 50S ribosomal protein L32e



- Molecule 27: 50S ribosomal protein L37Ae




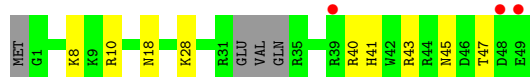
- Molecule 28: 50S ribosomal protein L37e

Chain 1:  80% 20%




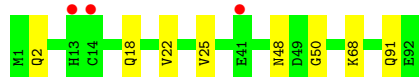
- Molecule 29: 50S ribosomal protein L39e

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

The worst 5 of 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

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	221	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	471	G	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
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

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

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

The worst 5 of 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

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

5.3.2 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	T	5	ASP
26	Y	174	VAL
21	T	82	THR
24	W	125	HIS
30	3	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
28	1	16	HIS
29	2	16	ASN
30	3	48	ASN
13	L	41	HIS

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Mol	Chain	Res	Type
13	L	18	HIS

5.3.3 RNA ⓘ

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%)

5 of 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

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1377	C
1	0	1684	A
1	0	2761	A
1	0	1667	A
1	0	1979	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	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

The worst 5 of 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

The worst 5 of 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

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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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

The worst 5 of 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

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

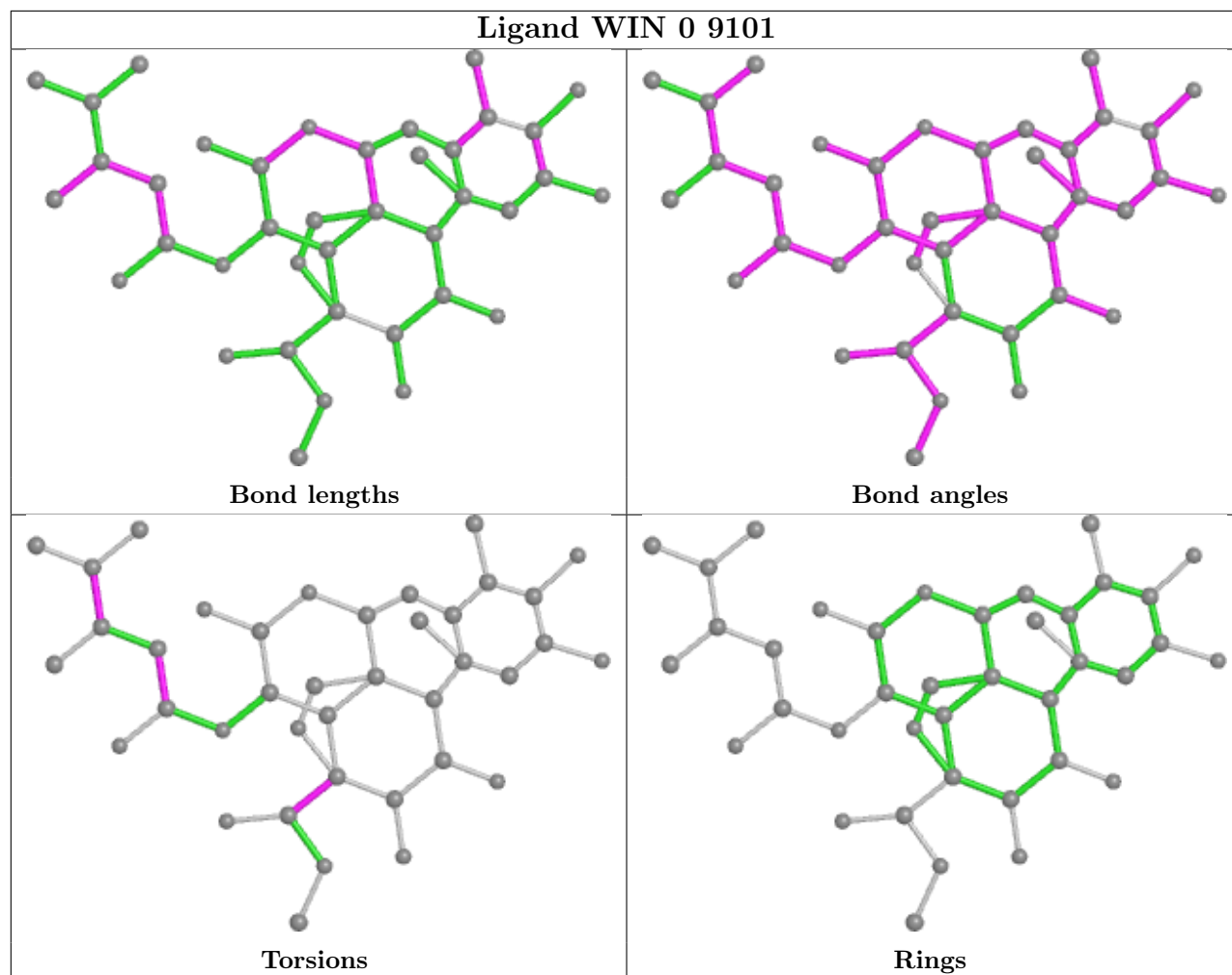
Mol	Chain	Res	Type	Atoms
37	0	9101	WIN	C1B-C1V-C2C-C1E
37	0	9101	WIN	O1J-C2A-C2L-O1S
37	0	9101	WIN	O1R-C2A-C2L-O1S
37	0	9101	WIN	C1V-C1N-C1W-O1T
37	0	9101	WIN	O1R-C2A-C2L-C2K

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

The worst 5 of 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

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

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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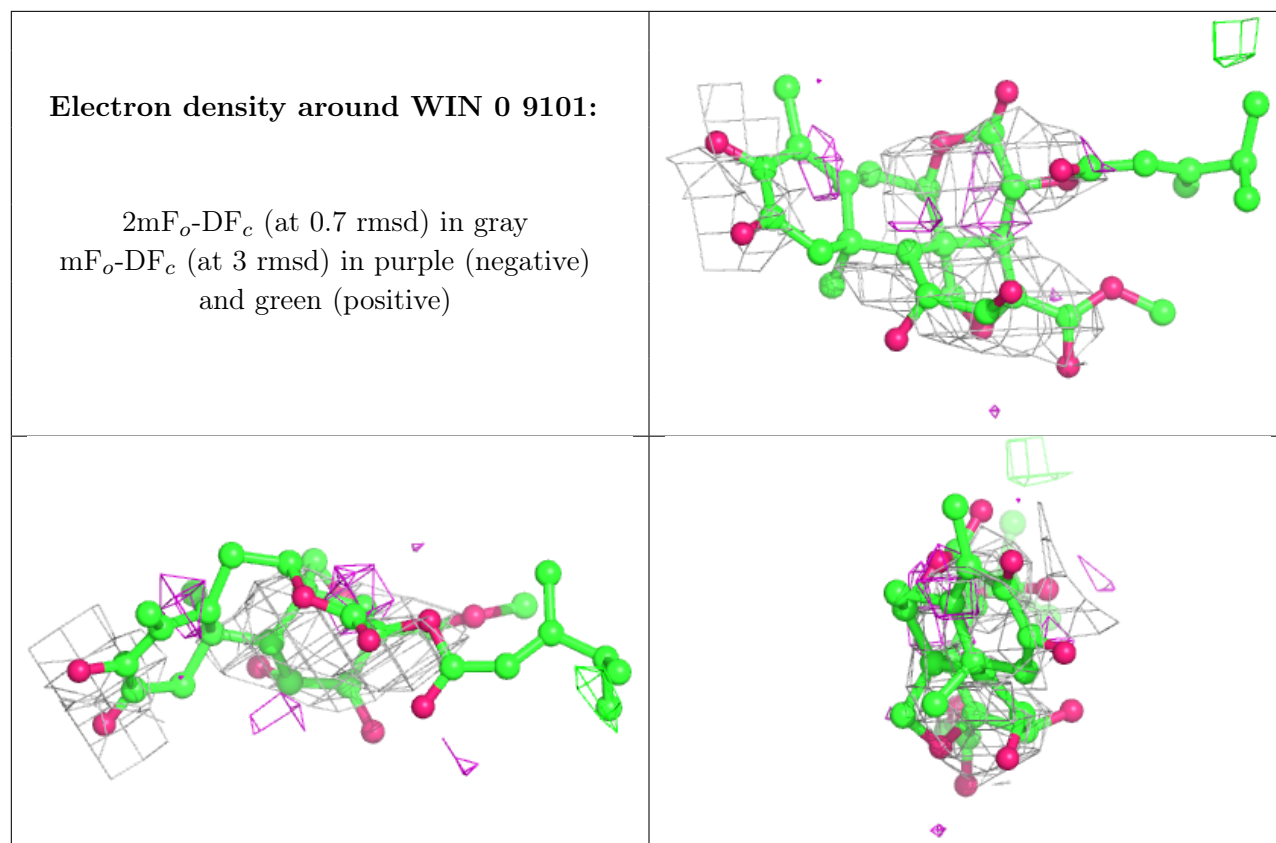
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8093	1/1	0.97	0.07	45,45,45,45	0
32	MG	0	8014	1/1	0.97	0.20	33,33,33,33	0
35	CL	N	8807	1/1	0.97	0.18	72,72,72,72	0
35	CL	O	8808	1/1	0.97	0.20	79,79,79,79	0
34	NA	S	8510	1/1	0.97	0.15	50,50,50,50	0
32	MG	0	8025	1/1	0.97	0.10	37,37,37,37	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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.