



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:27 AM UTC

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

This is a 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 types of validation reports are described at

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

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

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

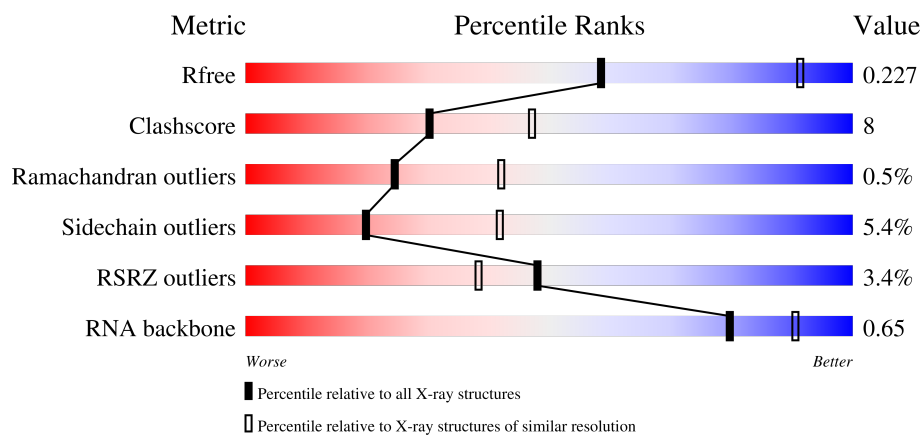
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	2923	
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
34	NA	0	8522	-	-	-	X
34	NA	0	8559	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	0	1	Total	C	O	0	0
			39	28	11		

- Molecule 38 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 39 is water.

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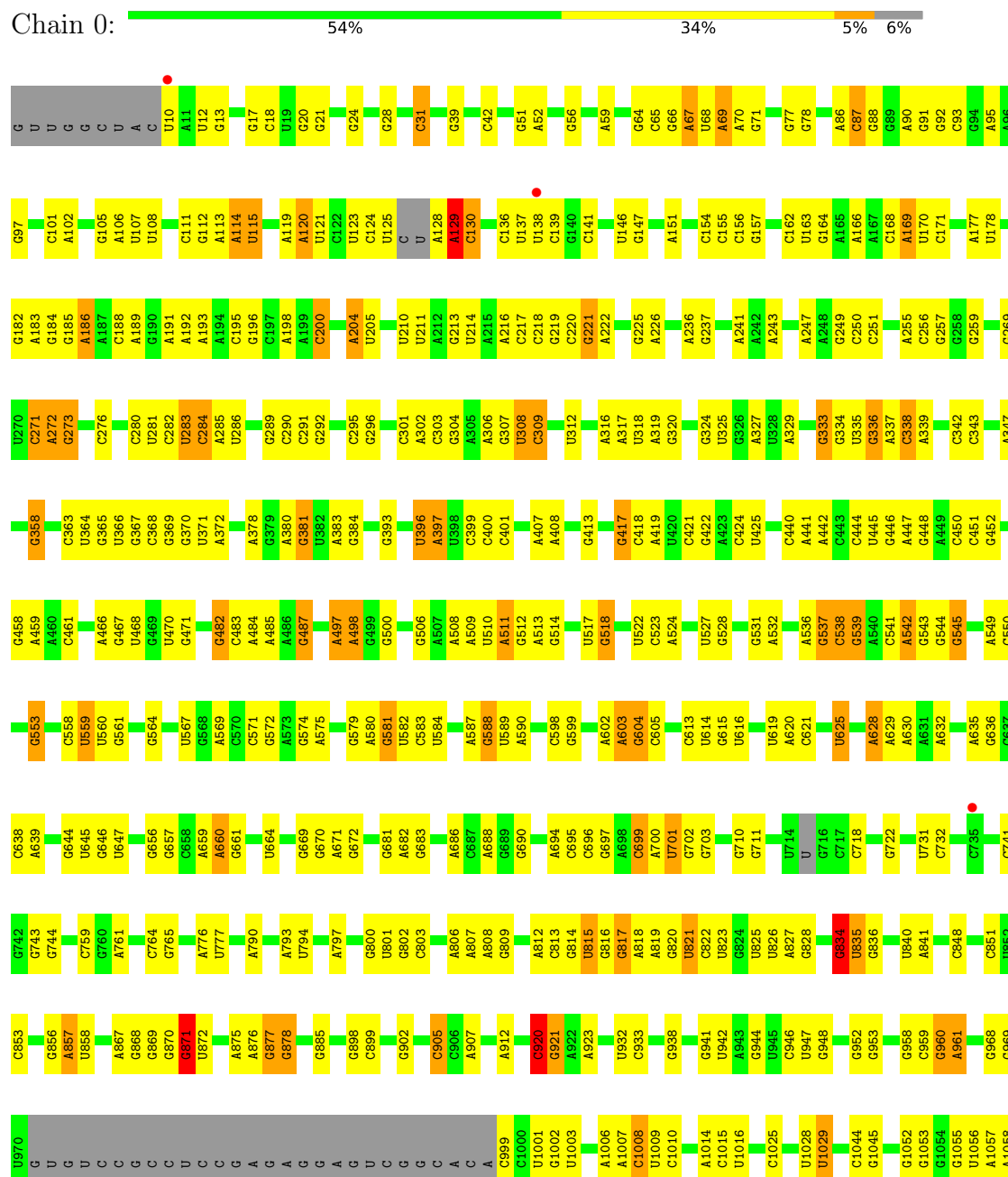
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	20	Total 20	O 20	0	0
39	Y	94	Total 94	O 94	0	0
39	Z	28	Total 28	O 28	0	0
39	1	52	Total 52	O 52	0	0
39	2	39	Total 39	O 39	0	0
39	3	66	Total 66	O 66	0	0
39	9	149	Total 149	O 149	0	0

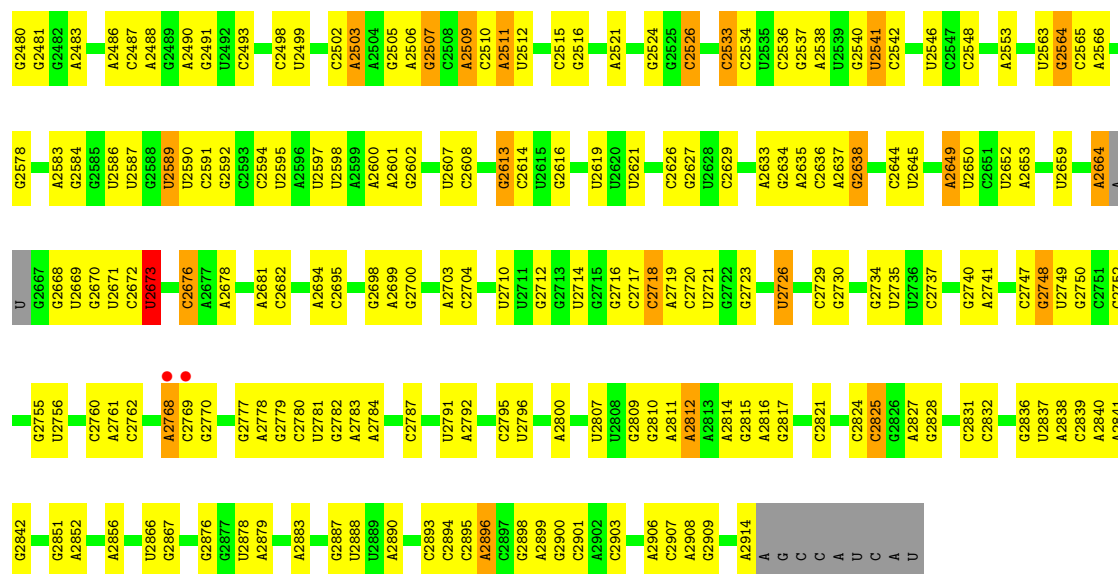
3 Residue-property plots ⓘ

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.

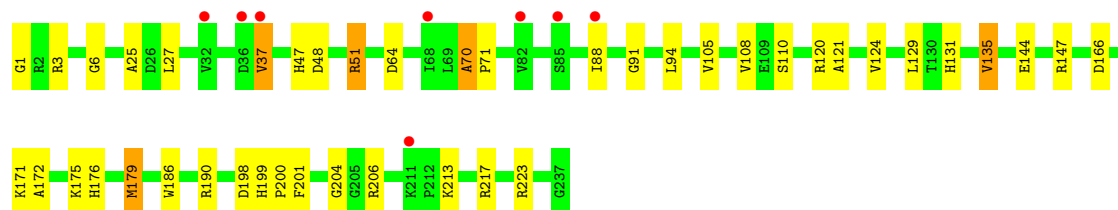
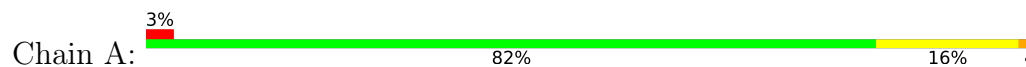
• Molecule 1: 23S ribosomal RNA



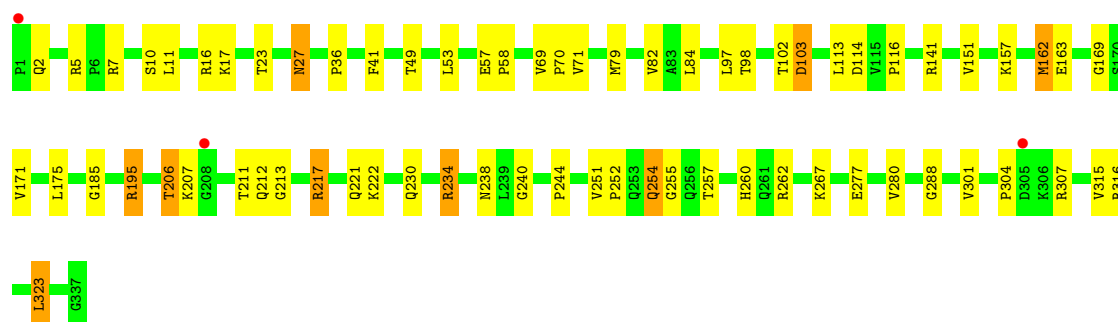
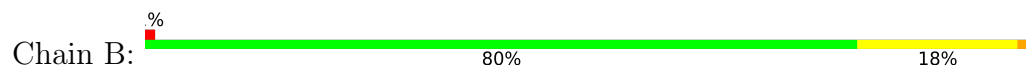
U2373	G2566	U2133	U2032	A1941	G1819	A1733	G1634	C1537	A1424	C1334	U1234	G1160	G1059
G2374	G2257	G2134	G2033	A1942	G1820	C1734	U1635	U1544	A1427	C1342	U1237	A1161	C1060
A2375	A2258	A2135	U2034	C1943	A1829	C1735	G1636	C1545	C1343	C1343	C1238	G1163	G1063
C2376	U2265	G2136	A2039	G1947	G1834	A1736	A1637	G1546	U1434	A1352	G1239	U1164	U1066
G2379	A2266	C	C2040	G1948	U1835	A1742	A1642	G1556	A1435	C1353	A1243	G1165	A1067
A2380	C2267	A	G2041	G1951	U1836	A1749	C1643	G1557	C1436	C1357	C1245	G1167	G1071
C2381	C2268	U	U2042	U	U1838	G1752	U1645	C1558	C1439	C1360	U1244	U1169	A1072
A2382	C2269	C	G2045	A	A1839	A1759	U1646	U	U1440	C1361	G1246	A1170	G1073
G2385	G2270	G	G2046	A	A1840	G1760	U1652	U1561	A1442	U1362	U1249	G1171	G1074
U2387	C2271	C	C2047	C	G1844	A1755	A1653	C1562	A1443	G1363	C1250	G1172	G1075
C2388	U2272	C	G2050	A	A1845	G1756	U1654	C1566	G1444	G1364	C1251	A1173	G1076
U2389	C2281	A	A2054	U	U1846	A1760	G1655	G1567	G1445	C1365	G1257	G1174	G1077
C2392	U2282	C	G2064	A	G1848	G1762	A1657	U1569	U1447	C1366	C1258	G1175	A1078
G2401	A2291	U	U2064	C	G1849	C1763	A1658	G1570	G1463	G1370	U1259	C1176	A1081
A2402	A2300	G	G2070	C	G1855	C1766	U1664	A1571	U1464	U1371	A1260	U1180	C1084
C2411	A2301	G	C2071	U1964	C1856	U1766	G1665	A1572	C1465	A1372	A1261	C1181	G1087
G2412	A2302	A	G2072	C1965	A1857	A1767	C1666	A1573	U1457	C1375	C1268	C1183	A1088
A2413	G2073	A	U1966	U1967	A1858	C1768	A1667	G1576	U1463	G1376	C1269	U1185	A1097
A2414	A2074	G	U1967	U1968	G1861	C1769	U1668	U1577	U1464	G1377	C1273	C1186	A1098
A2415	C2308	C	A1968	A1969	C1864	U1770	U1677	U1587	C1474	A1381	A1278	G1187	G1099
G2416	G2316	U	G2080	G1970	U1867	G1773	A1678	G1588	C1474	G1382	U1279	C1189	G1100
C2417	C2317	A	A2081	C1971	G1868	A1778	C1680	G1589	C1477	U1383	C1289	C1190	C1104
U2418	U2320	C	G2082	A1972	G1873	A1779	A1682	G1593	U1478	G1384	A1290	C1192	C1105
G2420	A2321	C	A2083	G1974	G1877	U1783	A1683	C1594	A1482	G1385	A1291	A1193	A1106
C2421	C2322	U	C2087	A1978	G1878	U1784	A1684	C1595	C1483	G1386	A1294	G1197	U1109
U2422	U2325	G	C2088	G1979	U1879	G1789	A1685	G1596	G1484	G1387	C1295	U1110	G1110
G2426	C2326	U	G2089	U1980	G1880	C1787	C1686	A1597	C1485	G1391	G1299	C1201	U1115
U2435	G2338	G	G2091	A1981	A1881	U1788	G1687	A1598	C1495	A1392	G1299	A1202	U1116
U2436	A	C	G2092	U1982	C1882	G1789	G1688	A1603	C1496	A1393	G1300	G1203	A1117
A2437	C	A	G2093	C1983	U1883	G1790	C1692	G1604	C1497	C1394	G1306	C1204	A1118
G2438	G	G	G2094	A1984	G1886	U1791	U1702	G1605	U1500	C1395	U1307	U1205	G1119
C2439	A2096	U	A2096	G1985	A1886	G1795	A1702	A1606	U1503	C1396	A1308	U1206	U1120
C2443	G2344	A	A2100	U1996	U1903	G1796	A1706	A1607	U1504	G1398	G1308	C1207	G1121
U2444	C2345	C	A2101	C2002	A1904	A1797	G1706	C1613	A1504	A1399	G1311	U1130	U1130
U2445	C2347	G	G2102	U2003	U1909	C1798	G1707	G1614	U1505	A1406	G1312	G1131	G1131
G2446	C2348	A	A2103	U2004	A1910	G1799	A1710	A1615	U1506	A1407	A1312	G1211	A1150
C2462	C2353	U	C2104	G2005	G1919	G1800	G1714	A1616	U1507	U1408	A1313	G1212	A1151
G2465	A2354	G	C2105	C2006	A1919	C1803	C1715	C1617	A1515	G1409	G1315	C1213	G1154
A2466	C2361	A	C2106	U2007	A1920	A1804	C1716	G1622	U1516	G1410	G1316	U1214	G1155
A2467	A2362	C	G2110	U2008	A1921	G1805	A1716	G1623	U1524	A1413	A1321	A1215	U1149
A2468	A2364	C	G2111	A2011	A1922	A1811	U1722	C1624	G1525	A1414	G1322	G1216	U1150
G2472	G2365	G	C2114	U2012	C1928	G1812	G1723	U1625	A1526	G1415	G1322	U1218	G1151
U2473	A2366	C	U2115	G2013	G1929	U1813	U1724	A1626	A1527	C1328	G1328	U1219	U1151
A2474	C2367	C	U2116	U2016	G1937	G1814	C1725	G1627	U1528	U1419	A1330	U1220	A1154
C2475	A2368	U	C2121	U2017	U1938	A1815	G1730	A1631	G1529	C1420	A1331	C1229	G1155
C2476	A2369	A	C2122	A2022	U1939	U1816	C1731	A1632	G1536	U1421	G1332	U1230	G1158
	A2372	G			C1940	C1818	A1732	C1633		C1423	U1333		G1159



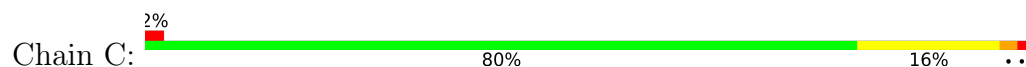
• Molecule 2: 50S ribosomal protein L2P

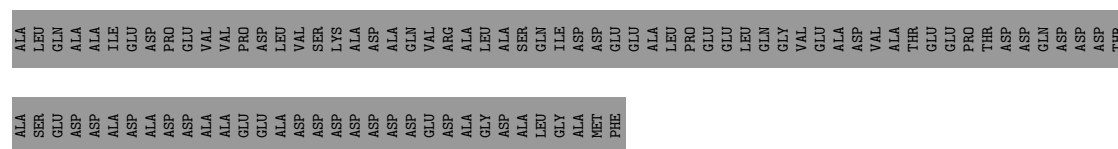


• Molecule 3: 50S ribosomal protein L3P

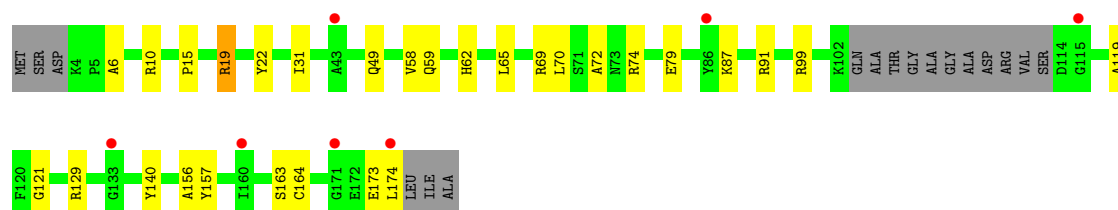


• Molecule 4: 50S ribosomal protein L4P

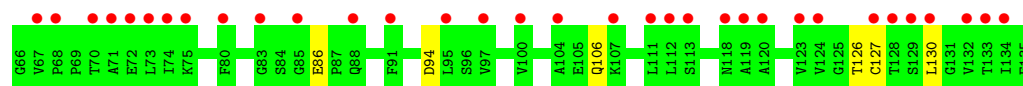




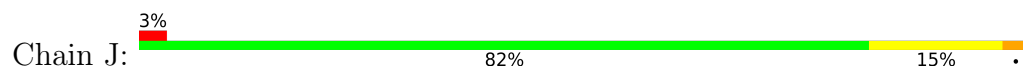
• Molecule 9: 50S ribosomal protein L10e



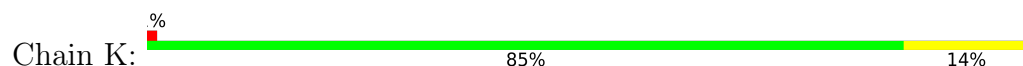
• Molecule 10: 50S ribosomal protein L11P



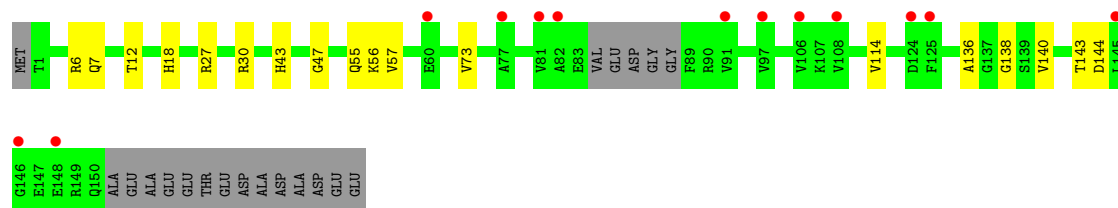
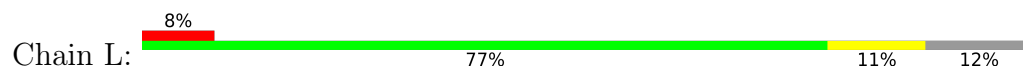
• Molecule 11: 50S ribosomal protein L13P



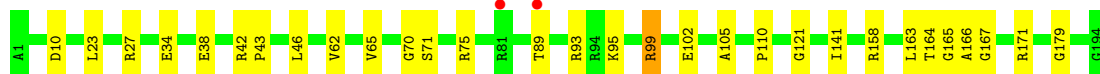
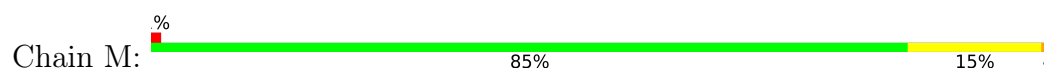
• Molecule 12: 50S ribosomal protein L14P



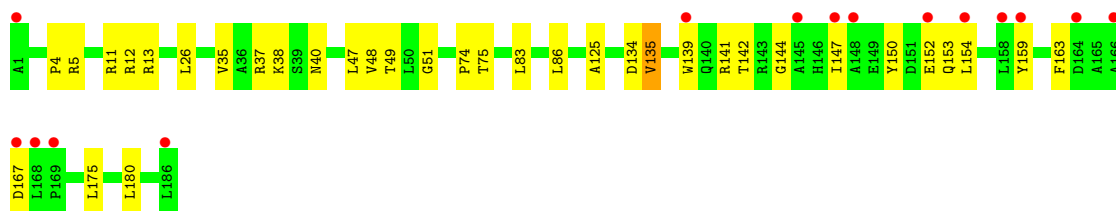
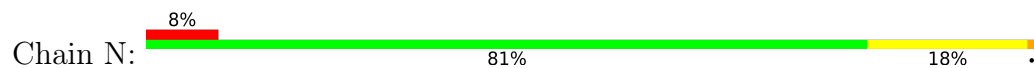
• Molecule 13: 50S ribosomal protein L15P



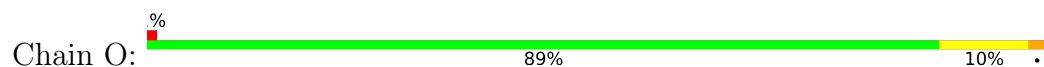
• Molecule 14: 50S ribosomal protein L15e



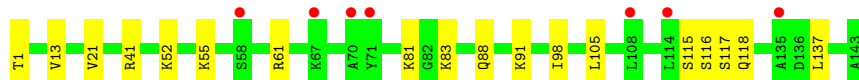
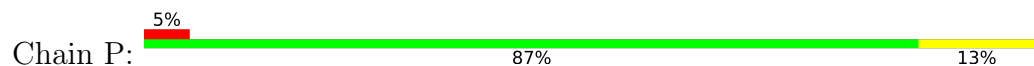
• Molecule 15: 50S ribosomal protein L18P



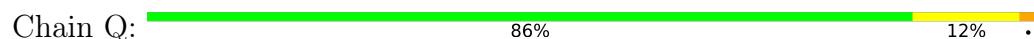
• Molecule 16: 50S ribosomal protein L18e



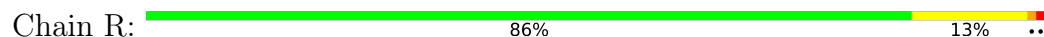
• Molecule 17: 50S ribosomal protein L19e



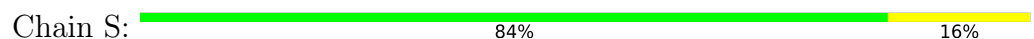
• Molecule 18: 50S ribosomal protein L21e



• Molecule 19: 50S ribosomal protein L22P

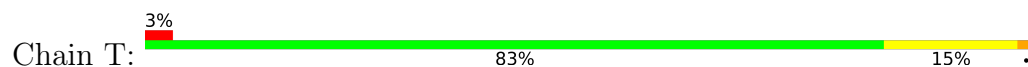


• Molecule 20: 50S ribosomal protein L23P

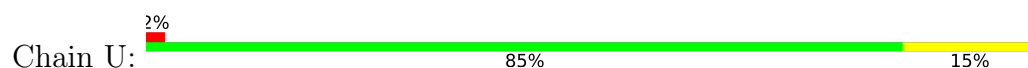




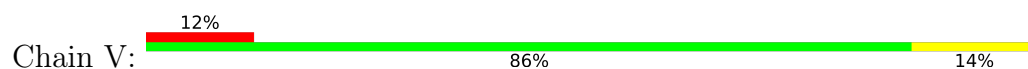
- Molecule 21: 50S ribosomal protein L24P



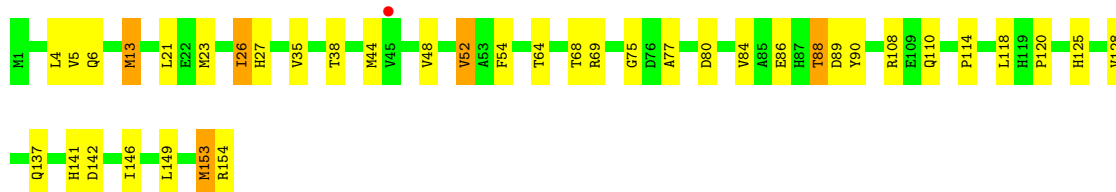
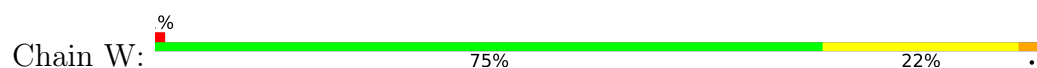
- Molecule 22: 50S ribosomal protein L24e



- Molecule 23: 50S ribosomal protein L29P



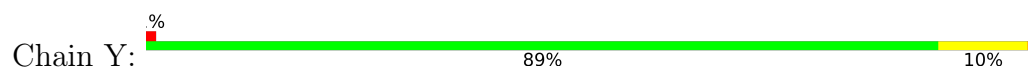
- Molecule 24: 50S ribosomal protein L30P



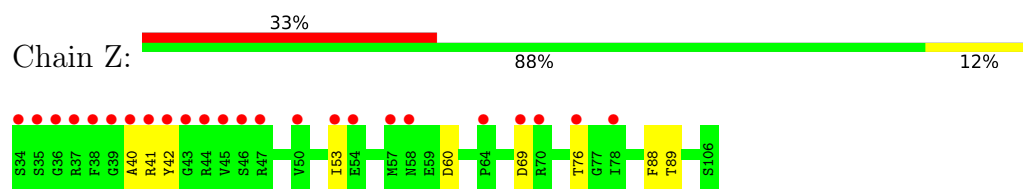
- Molecule 25: 50S ribosomal protein L31e



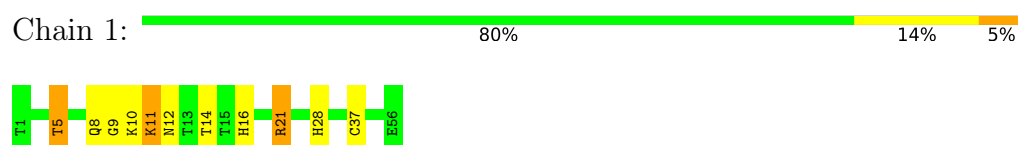
- Molecule 26: 50S ribosomal protein L32e



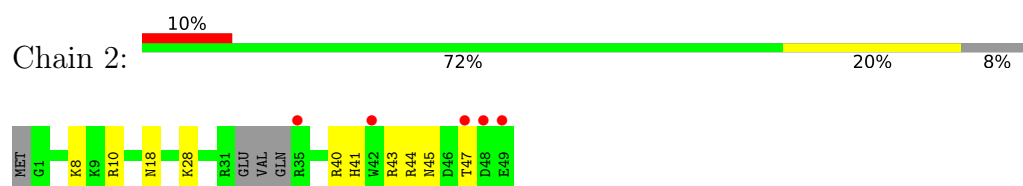
- Molecule 27: 50S ribosomal protein L37Ae



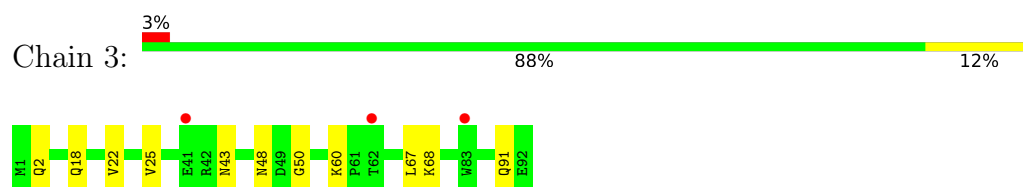
- Molecule 28: 50S ribosomal protein L37e



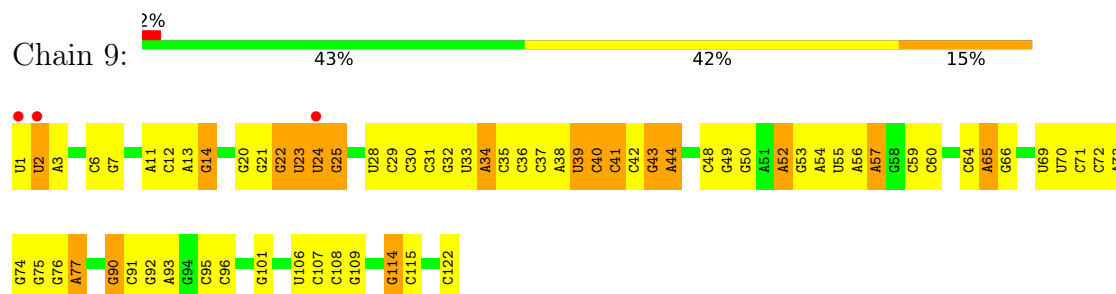
- Molecule 29: 50S ribosomal protein L39e



- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA



4 Data and refinement statistics

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

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

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

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

The worst 5 of 6 bond length outliers are listed below:

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

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	170	TYR	N-CA-C	9.79	124.81	112.86
21	T	52	ARG	N-CA-C	9.77	125.75	113.43
15	N	163	PHE	N-CA-C	-9.42	99.50	112.12
24	W	75	GLY	N-CA-C	9.01	121.18	112.08
9	H	10	ARG	N-CA-C	8.04	120.04	111.28

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1250 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H5'	1:0:871:G:H8	1.10	1.15
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12
1:0:871:G:H5'	1:0:871:G:C8	1.88	1.08
31:9:76:G:H3'	31:9:77:A:H5''	1.36	1.05
31:9:56:A:H2'	31:9:57:A:H5''	1.37	1.04

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%)	9	21
3	B	335/337 (99%)	307 (92%)	26 (8%)	2 (1%)	21	38
4	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	16	31
5	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	5	12
6	E	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
7	F	117/119 (98%)	109 (93%)	7 (6%)	1 (1%)	14	28
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	150 (96%)	5 (3%)	1 (1%)	21	38
10	I	68/70 (97%)	58 (85%)	10 (15%)	0	100	100
11	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
12	K	130/132 (98%)	125 (96%)	4 (3%)	1 (1%)	16	31
13	L	141/165 (86%)	127 (90%)	14 (10%)	0	100	100
14	M	192/194 (99%)	187 (97%)	4 (2%)	1 (0%)	24	42
15	N	184/186 (99%)	173 (94%)	8 (4%)	3 (2%)	7	17
16	O	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
17	P	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
18	Q	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	11	24
19	R	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
20	S	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
21	T	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	14	28
22	U	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
23	V	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
24	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
25	X	80/82 (98%)	77 (96%)	2 (2%)	1 (1%)	9	21
26	Y	140/142 (99%)	139 (99%)	1 (1%)	0	100	100

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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%)	24	42

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%)	167 (93%)	12 (7%)	15	31
3	B	282/282 (100%)	261 (93%)	21 (7%)	13	26
4	C	193/193 (100%)	176 (91%)	17 (9%)	9	20
5	D	117/148 (79%)	103 (88%)	14 (12%)	5	9
6	E	152/152 (100%)	145 (95%)	7 (5%)	24	48
7	F	93/93 (100%)	88 (95%)	5 (5%)	20	42
8	G	27/282 (10%)	27 (100%)	0	100	100
9	H	134/145 (92%)	129 (96%)	5 (4%)	30	55
10	I	58/58 (100%)	57 (98%)	1 (2%)	53	75
11	J	118/118 (100%)	110 (93%)	8 (7%)	14	30
12	K	106/106 (100%)	101 (95%)	5 (5%)	23	47
13	L	113/127 (89%)	110 (97%)	3 (3%)	39	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	158/158 (100%)	153 (97%)	5 (3%)	34	59
15	N	149/149 (100%)	139 (93%)	10 (7%)	15	31
16	O	93/93 (100%)	89 (96%)	4 (4%)	26	50
17	P	113/113 (100%)	108 (96%)	5 (4%)	25	49
18	Q	79/79 (100%)	76 (96%)	3 (4%)	29	54
19	R	117/117 (100%)	113 (97%)	4 (3%)	32	58
20	S	71/71 (100%)	69 (97%)	2 (3%)	38	62
21	T	105/105 (100%)	97 (92%)	8 (8%)	12	26
22	U	44/44 (100%)	44 (100%)	0	100	100
23	V	51/51 (100%)	49 (96%)	2 (4%)	28	54
24	W	130/130 (100%)	122 (94%)	8 (6%)	16	34
25	X	66/66 (100%)	56 (85%)	10 (15%)	3	5
26	Y	120/120 (100%)	116 (97%)	4 (3%)	33	58
27	Z	60/60 (100%)	59 (98%)	1 (2%)	53	75
28	1	46/46 (100%)	45 (98%)	1 (2%)	45	69
29	2	42/46 (91%)	41 (98%)	1 (2%)	43	67
30	3	79/79 (100%)	77 (98%)	2 (2%)	42	66
All	All	3095/3410 (91%)	2927 (95%)	168 (5%)	20	42

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	O	69	VAL
24	W	38	THR
17	P	52	LYS
20	S	81	ILE
25	X	43	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	40	HIS
23	V	60	GLN
19	R	94	ASN
20	S	21	GLN

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Mol	Chain	Res	Type
25	X	23	HIS

5.3.3 RNA ⓘ

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

5 of 258 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

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	OMU	0	2587	34,1	19,22,23	0.34	0	25,31,34	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	0	2621	1	18,21,22	1.59	2 (11%)	21,30,33	1.41	3 (14%)
1	OMG	0	2588	1	23,26,27	0.28	0	32,38,41	0.43	0
1	1MA	0	628	34,1	21,25,26	0.74	1 (4%)	30,37,40	0.84	2 (6%)
1	UR3	0	2619	1	19,22,23	0.50	0	26,32,35	0.68	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	34,1	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	1/9/27/28	0/3/3/3
1	1MA	0	628	34,1	-	2/7/25/26	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

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

The worst 5 of 6 bond angle outliers are listed below:

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

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	WIN	0	9101	-	40,43,43	1.93	9 (22%)	51,71,71	3.63	29 (56%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	WIN	0	9101	-	-	9/20/110/110	0/6/5/5

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	C1N-C1V	5.72	1.41	1.33
37	0	9101	WIN	C2M-C2G	5.40	1.61	1.53
37	0	9101	WIN	C2B-C1X	-4.24	1.40	1.46
37	0	9101	WIN	C1C-C1Y	3.69	1.56	1.50
37	0	9101	WIN	C1N-C1W	-2.98	1.39	1.46

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	9.00	125.14	111.46
37	0	9101	WIN	O1J-C2A-C2L	-6.63	111.90	123.67
37	0	9101	WIN	C1O-C2M-C2G	6.43	123.74	112.86
37	0	9101	WIN	C1P-C1X-C2B	6.30	126.51	117.19
37	0	9101	WIN	O1U-C1Z-O1I	6.17	127.45	118.52

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

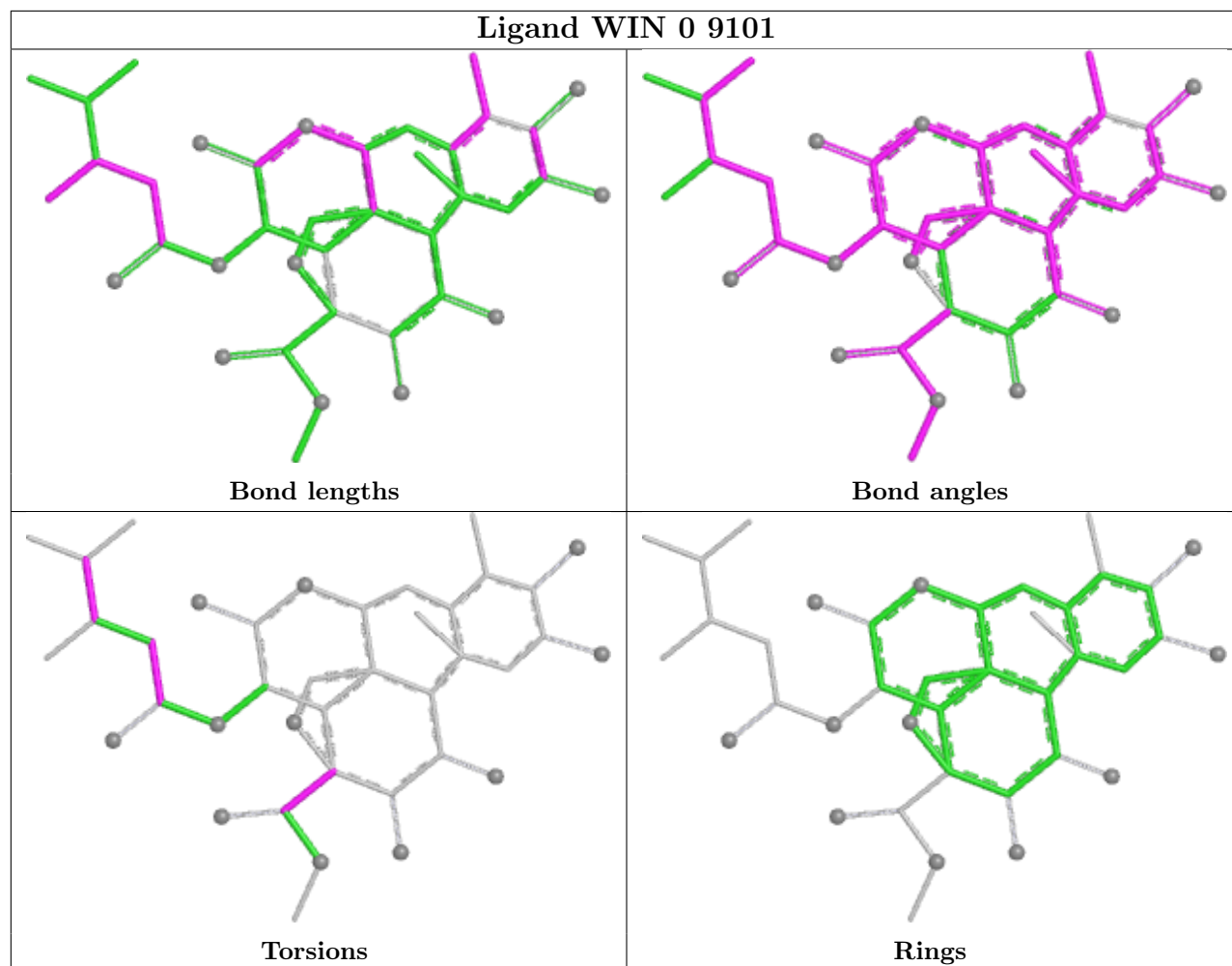
Mol	Chain	Res	Type	Atoms
37	0	9101	WIN	C1N-C1V-C2C-C1D
37	0	9101	WIN	C1N-C1V-C2C-C1E
37	0	9101	WIN	C1B-C1V-C2C-C1D
37	0	9101	WIN	O1J-C2A-C2L-O1S
37	0	9101	WIN	O1R-C2A-C2L-O1S

There are no ring outliers.

1 monomer is involved in 13 short contacts:

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

The worst 5 of 228 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	11.0
27	Z	46	SER	8.1
10	I	128	THR	7.5
27	Z	36	GLY	6.4
10	I	71	ALA	6.0

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	OMG	0	2588	24/25	0.97	0.06	42,44,46,48	0
1	UR3	0	2619	21/22	0.97	0.07	45,48,51,54	0
1	1MA	0	628	23/24	0.98	0.06	34,36,38,39	0
1	OMU	0	2587	21/22	0.98	0.06	43,44,46,48	0
1	PSU	0	2621	20/21	0.98	0.06	30,35,50,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
34	NA	0	8525	1/1	0.22	0.39	93,93,93,93	0
34	NA	0	8573	1/1	0.58	0.23	87,87,87,87	0
34	NA	9	8572	1/1	0.59	0.26	117,117,117,117	0
36	SR	0	8983	1/1	0.59	0.23	199,199,199,199	0
32	MG	0	8090	1/1	0.62	0.31	121,121,121,121	0
34	NA	0	8557	1/1	0.63	0.36	74,74,74,74	0
34	NA	0	8559	1/1	0.64	0.53	95,95,95,95	0
34	NA	0	8571	1/1	0.66	0.32	98,98,98,98	0
34	NA	0	8556	1/1	0.66	0.39	68,68,68,68	0
36	SR	0	8996	1/1	0.66	0.23	200,200,200,200	0
36	SR	0	8991	1/1	0.69	0.21	195,195,195,195	0
32	MG	0	8063	1/1	0.70	0.29	80,80,80,80	0
32	MG	0	8049	1/1	0.71	0.30	116,116,116,116	0
34	NA	0	8511	1/1	0.72	0.17	67,67,67,67	0
36	SR	0	8977	1/1	0.74	0.08	197,197,197,197	0
34	NA	0	8548	1/1	0.74	0.34	67,67,67,67	0
34	NA	J	8538	1/1	0.75	0.20	67,67,67,67	0
34	NA	0	8522	1/1	0.75	0.84	108,108,108,108	0
34	NA	0	8509	1/1	0.77	0.35	77,77,77,77	0
34	NA	H	8518	1/1	0.77	0.27	95,95,95,95	0
36	SR	0	9006	1/1	0.77	0.35	200,200,200,200	0
36	SR	0	8959	1/1	0.78	0.09	181,181,181,181	0
34	NA	0	8554	1/1	0.78	0.16	70,70,70,70	0
36	SR	0	9000	1/1	0.78	0.22	200,200,200,200	0
36	SR	0	8920	1/1	0.78	0.24	185,185,185,185	0
36	SR	0	8933	1/1	0.79	0.18	143,143,143,143	0
36	SR	0	8997	1/1	0.79	0.28	200,200,200,200	0
36	SR	9	9003	1/1	0.79	0.14	187,187,187,187	0
36	SR	0	8917	1/1	0.80	0.20	151,151,151,151	0
36	SR	0	8944	1/1	0.80	0.19	178,178,178,178	0
36	SR	0	8947	1/1	0.80	0.24	200,200,200,200	0
36	SR	9	8978	1/1	0.80	0.15	169,169,169,169	0
36	SR	0	8927	1/1	0.80	0.16	167,167,167,167	0
36	SR	0	8993	1/1	0.81	0.14	178,178,178,178	0
34	NA	0	8533	1/1	0.81	0.31	72,72,72,72	0
32	MG	0	8072	1/1	0.81	0.18	82,82,82,82	0
32	MG	0	8091	1/1	0.81	0.12	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8982	1/1	0.81	0.31	200,200,200,200	0
36	SR	0	8934	1/1	0.81	0.24	166,166,166,166	0
36	SR	0	8919	1/1	0.81	0.16	179,179,179,179	0
34	NA	0	8501	1/1	0.82	0.14	54,54,54,54	0
32	MG	0	8080	1/1	0.82	0.08	87,87,87,87	0
36	SR	0	8956	1/1	0.82	0.11	187,187,187,187	0
36	SR	0	8989	1/1	0.82	0.23	185,185,185,185	0
34	NA	0	8524	1/1	0.82	0.22	73,73,73,73	0
36	SR	0	8971	1/1	0.82	0.15	185,185,185,185	0
34	NA	0	8506	1/1	0.83	0.12	76,76,76,76	0
34	NA	0	8535	1/1	0.83	0.23	63,63,63,63	0
36	SR	0	8941	1/1	0.83	0.17	131,131,131,131	0
32	MG	0	8092	1/1	0.83	0.12	80,80,80,80	0
32	MG	0	8031	1/1	0.83	0.13	73,73,73,73	0
34	NA	0	8561	1/1	0.84	0.53	90,90,90,90	0
36	SR	0	8942	1/1	0.84	0.17	144,144,144,144	0
36	SR	0	8922	1/1	0.84	0.18	156,156,156,156	0
34	NA	0	8536	1/1	0.84	0.12	65,65,65,65	0
36	SR	0	8984	1/1	0.84	0.13	143,143,143,143	0
32	MG	9	8074	1/1	0.84	0.25	101,101,101,101	0
36	SR	9	8980	1/1	0.84	0.09	175,175,175,175	0
32	MG	0	8071	1/1	0.84	0.31	71,71,71,71	0
36	SR	A	8930	1/1	0.85	0.21	169,169,169,169	0
36	SR	B	8987	1/1	0.85	0.41	200,200,200,200	0
36	SR	0	8976	1/1	0.85	0.17	200,200,200,200	0
36	SR	0	9002	1/1	0.85	0.16	183,183,183,183	0
34	NA	0	8562	1/1	0.85	0.51	82,82,82,82	0
36	SR	0	9001	1/1	0.86	0.11	184,184,184,184	0
36	SR	0	8986	1/1	0.86	0.27	200,200,200,200	0
36	SR	0	9004	1/1	0.86	0.22	200,200,200,200	0
34	NA	0	8564	1/1	0.86	0.23	95,95,95,95	0
36	SR	0	8951	1/1	0.86	0.07	149,149,149,149	0
36	SR	B	8950	1/1	0.86	0.16	119,119,119,119	0
36	SR	0	8955	1/1	0.86	0.23	198,198,198,198	0
34	NA	0	8574	1/1	0.86	0.38	69,69,69,69	0
33	K	0	8401	1/1	0.86	0.39	123,123,123,123	0
36	SR	0	8965	1/1	0.86	0.14	151,151,151,151	0
34	NA	0	8558	1/1	0.87	0.14	63,63,63,63	0
36	SR	0	8979	1/1	0.87	0.11	195,195,195,195	0
36	SR	0	8995	1/1	0.87	0.16	142,142,142,142	0
36	SR	0	8908	1/1	0.87	0.32	175,175,175,175	0
36	SR	0	8949	1/1	0.87	0.16	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8913	1/1	0.87	0.31	200,200,200,200	0
36	SR	0	8975	1/1	0.87	0.12	154,154,154,154	0
34	NA	0	8575	1/1	0.87	0.35	87,87,87,87	0
37	WIN	0	9101	39/39	0.87	0.27	125,127,128,129	0
34	NA	0	8560	1/1	0.88	0.23	97,97,97,97	0
36	SR	0	8957	1/1	0.88	0.20	200,200,200,200	0
34	NA	0	8507	1/1	0.88	0.14	46,46,46,46	0
36	SR	0	8964	1/1	0.88	0.10	139,139,139,139	0
34	NA	M	8539	1/1	0.88	0.20	53,53,53,53	0
36	SR	0	8967	1/1	0.88	0.12	147,147,147,147	0
34	NA	Q	8540	1/1	0.88	0.12	58,58,58,58	0
34	NA	R	8532	1/1	0.88	0.32	59,59,59,59	0
34	NA	0	8514	1/1	0.88	0.28	54,54,54,54	0
36	SR	0	8928	1/1	0.88	0.14	151,151,151,151	0
34	NA	0	8520	1/1	0.88	0.21	55,55,55,55	0
36	SR	0	8931	1/1	0.89	0.12	136,136,136,136	0
34	NA	0	8541	1/1	0.89	0.20	70,70,70,70	0
32	MG	0	8039	1/1	0.89	0.14	63,63,63,63	0
36	SR	0	8969	1/1	0.89	0.31	173,173,173,173	0
35	CL	A	8809	1/1	0.89	0.36	96,96,96,96	0
36	SR	0	8973	1/1	0.89	0.11	141,141,141,141	0
32	MG	0	8033	1/1	0.89	0.14	63,63,63,63	0
34	NA	0	8555	1/1	0.89	0.23	53,53,53,53	0
36	SR	0	8916	1/1	0.89	0.15	129,129,129,129	0
32	MG	0	8037	1/1	0.89	0.30	80,80,80,80	0
34	NA	0	8527	1/1	0.89	0.27	86,86,86,86	0
34	NA	0	8529	1/1	0.89	0.19	50,50,50,50	0
34	NA	0	8502	1/1	0.89	0.31	66,66,66,66	0
36	SR	F	9005	1/1	0.89	0.10	149,149,149,149	0
36	SR	3	8999	1/1	0.89	0.12	140,140,140,140	0
36	SR	0	8985	1/1	0.89	0.17	148,148,148,148	0
34	NA	0	8516	1/1	0.89	0.08	37,37,37,37	0
36	SR	0	8988	1/1	0.89	0.08	158,158,158,158	0
32	MG	A	8051	1/1	0.89	0.09	98,98,98,98	0
34	NA	0	8569	1/1	0.90	0.14	61,61,61,61	0
34	NA	0	8526	1/1	0.90	0.07	45,45,45,45	0
34	NA	0	8515	1/1	0.90	0.07	50,50,50,50	0
32	MG	0	8066	1/1	0.90	0.33	88,88,88,88	0
36	SR	0	8958	1/1	0.90	0.11	121,121,121,121	0
34	NA	0	8519	1/1	0.90	0.12	50,50,50,50	0
32	MG	0	8089	1/1	0.90	0.08	64,64,64,64	0
36	SR	0	8924	1/1	0.90	0.17	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8056	1/1	0.90	0.17	62,62,62,62	0
34	NA	0	8537	1/1	0.90	0.09	50,50,50,50	0
32	MG	0	8035	1/1	0.90	0.22	70,70,70,70	0
34	NA	0	8547	1/1	0.90	0.24	71,71,71,71	0
36	SR	0	9007	1/1	0.90	0.43	199,199,199,199	0
36	SR	A	8929	1/1	0.90	0.20	142,142,142,142	0
34	NA	S	8510	1/1	0.90	0.10	50,50,50,50	0
36	SR	0	8937	1/1	0.90	0.12	125,125,125,125	0
36	SR	0	8938	1/1	0.90	0.11	191,191,191,191	0
36	SR	0	8939	1/1	0.90	0.11	145,145,145,145	0
34	NA	0	8563	1/1	0.90	0.27	82,82,82,82	0
35	CL	0	8815	1/1	0.90	0.14	83,83,83,83	0
32	MG	0	8073	1/1	0.90	0.30	80,80,80,80	0
35	CL	J	8802	1/1	0.90	0.11	79,79,79,79	0
34	NA	0	8566	1/1	0.90	0.14	59,59,59,59	0
34	NA	0	8570	1/1	0.91	0.20	59,59,59,59	0
34	NA	0	8531	1/1	0.91	0.23	50,50,50,50	0
34	NA	0	8551	1/1	0.91	0.18	60,60,60,60	0
33	K	0	8402	1/1	0.91	0.17	90,90,90,90	0
36	SR	0	8945	1/1	0.91	0.14	131,131,131,131	0
36	SR	0	8998	1/1	0.91	0.18	175,175,175,175	0
36	SR	S	8961	1/1	0.91	0.11	145,145,145,145	0
34	NA	9	8543	1/1	0.91	0.26	57,57,57,57	0
34	NA	0	8534	1/1	0.91	0.16	47,47,47,47	0
36	SR	0	8936	1/1	0.91	0.11	108,108,108,108	0
34	NA	0	8568	1/1	0.91	0.17	57,57,57,57	0
32	MG	9	8040	1/1	0.91	0.15	97,97,97,97	0
36	SR	0	8901	1/1	0.92	0.09	96,96,96,96	0
32	MG	Y	8086	1/1	0.92	0.06	55,55,55,55	0
34	NA	0	8521	1/1	0.92	0.07	71,71,71,71	0
36	SR	0	8943	1/1	0.92	0.11	95,95,95,95	0
36	SR	0	8914	1/1	0.92	0.19	127,127,127,127	0
32	MG	0	8082	1/1	0.92	0.14	81,81,81,81	0
36	SR	0	9008	1/1	0.92	0.11	111,111,111,111	0
32	MG	T	8057	1/1	0.92	0.17	72,72,72,72	0
36	SR	0	8968	1/1	0.92	0.12	165,165,165,165	0
36	SR	0	8948	1/1	0.92	0.12	122,122,122,122	0
36	SR	0	8970	1/1	0.92	0.11	135,135,135,135	0
36	SR	0	8992	1/1	0.92	0.21	137,137,137,137	0
34	NA	0	8550	1/1	0.92	0.24	59,59,59,59	0
36	SR	0	8994	1/1	0.92	0.31	199,199,199,199	0
35	CL	J	8801	1/1	0.92	0.11	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8974	1/1	0.92	0.21	179,179,179,179	0
36	SR	0	8954	1/1	0.92	0.08	109,109,109,109	0
34	NA	0	8530	1/1	0.92	0.17	60,60,60,60	0
34	NA	0	8528	1/1	0.93	0.09	60,60,60,60	0
36	SR	0	8915	1/1	0.93	0.11	136,136,136,136	0
34	NA	0	8567	1/1	0.93	0.32	87,87,87,87	0
36	SR	0	8960	1/1	0.93	0.08	151,151,151,151	0
36	SR	0	8946	1/1	0.93	0.10	129,129,129,129	0
36	SR	0	8981	1/1	0.93	0.19	158,158,158,158	0
32	MG	2	8060	1/1	0.93	0.14	65,65,65,65	0
34	NA	0	8552	1/1	0.93	0.15	80,80,80,80	0
32	MG	0	8038	1/1	0.93	0.07	70,70,70,70	0
32	MG	0	8064	1/1	0.93	0.09	51,51,51,51	0
34	NA	0	8512	1/1	0.93	0.23	48,48,48,48	0
36	SR	0	8926	1/1	0.93	0.12	142,142,142,142	0
32	MG	0	8017	1/1	0.93	0.07	34,34,34,34	0
32	MG	0	8078	1/1	0.94	0.11	54,54,54,54	0
35	CL	3	8804	1/1	0.94	0.08	76,76,76,76	0
32	MG	0	8044	1/1	0.94	0.04	55,55,55,55	0
34	NA	0	8549	1/1	0.94	0.34	60,60,60,60	0
36	SR	0	8910	1/1	0.94	0.13	106,106,106,106	0
32	MG	0	8001	1/1	0.94	0.05	26,26,26,26	0
32	MG	0	8069	1/1	0.94	0.08	49,49,49,49	0
36	SR	0	8972	1/1	0.94	0.18	164,164,164,164	0
32	MG	B	8042	1/1	0.94	0.19	62,62,62,62	0
34	NA	0	8542	1/1	0.94	0.33	62,62,62,62	0
35	CL	0	8805	1/1	0.94	0.09	76,76,76,76	0
36	SR	1	8952	1/1	0.94	0.08	93,93,93,93	0
34	NA	0	8544	1/1	0.94	0.20	73,73,73,73	0
34	NA	C	8503	1/1	0.94	0.10	46,46,46,46	0
34	NA	0	8545	1/1	0.94	0.14	48,48,48,48	0
36	SR	0	8923	1/1	0.94	0.09	112,112,112,112	0
36	SR	0	8963	1/1	0.94	0.05	133,133,133,133	0
36	SR	0	8909	1/1	0.95	0.09	99,99,99,99	0
36	SR	0	8966	1/1	0.95	0.08	120,120,120,120	0
32	MG	0	8068	1/1	0.95	0.11	67,67,67,67	0
34	NA	0	8517	1/1	0.95	0.06	36,36,36,36	0
32	MG	0	8083	1/1	0.95	0.10	74,74,74,74	0
32	MG	0	8085	1/1	0.95	0.19	69,69,69,69	0
32	MG	0	8036	1/1	0.95	0.12	60,60,60,60	0
32	MG	0	8070	1/1	0.95	0.15	64,64,64,64	0
32	MG	0	8053	1/1	0.95	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8546	1/1	0.95	0.13	85,85,85,85	0
36	SR	0	8921	1/1	0.95	0.07	99,99,99,99	0
34	NA	0	8505	1/1	0.95	0.37	44,44,44,44	0
32	MG	0	8029	1/1	0.95	0.21	69,69,69,69	0
36	SR	0	8953	1/1	0.95	0.10	164,164,164,164	0
35	CL	0	8814	1/1	0.95	0.11	66,66,66,66	0
32	MG	0	8093	1/1	0.95	0.05	45,45,45,45	0
35	CL	0	8816	1/1	0.95	0.14	75,75,75,75	0
32	MG	0	8008	1/1	0.95	0.10	32,32,32,32	0
32	MG	0	8075	1/1	0.95	0.09	58,58,58,58	0
32	MG	0	8002	1/1	0.95	0.06	26,26,26,26	0
34	NA	0	8513	1/1	0.95	0.21	56,56,56,56	0
36	SR	0	8962	1/1	0.95	0.15	180,180,180,180	0
36	SR	0	8990	1/1	0.95	0.10	116,116,116,116	0
32	MG	0	8024	1/1	0.95	0.07	54,54,54,54	0
32	MG	0	8081	1/1	0.95	0.21	81,81,81,81	0
38	CD	Z	8703	1/1	0.95	0.10	172,172,172,172	0
36	SR	0	8918	1/1	0.96	0.09	94,94,94,94	0
32	MG	0	8061	1/1	0.96	0.09	36,36,36,36	0
32	MG	0	8062	1/1	0.96	0.12	61,61,61,61	0
32	MG	0	8032	1/1	0.96	0.05	42,42,42,42	0
35	CL	0	8813	1/1	0.96	0.06	54,54,54,54	0
34	NA	0	8523	1/1	0.96	0.12	65,65,65,65	0
32	MG	0	8011	1/1	0.96	0.10	30,30,30,30	0
32	MG	0	8084	1/1	0.96	0.09	36,36,36,36	0
35	CL	0	8822	1/1	0.96	0.25	86,86,86,86	0
32	MG	0	8065	1/1	0.96	0.07	41,41,41,41	0
35	CL	B	8819	1/1	0.96	0.09	57,57,57,57	0
32	MG	0	8034	1/1	0.96	0.05	47,47,47,47	0
32	MG	0	8045	1/1	0.96	0.06	30,30,30,30	0
35	CL	J	8821	1/1	0.96	0.08	78,78,78,78	0
35	CL	K	8812	1/1	0.96	0.13	57,57,57,57	0
35	CL	L	8810	1/1	0.96	0.14	69,69,69,69	0
35	CL	O	8808	1/1	0.96	0.13	79,79,79,79	0
36	SR	0	8940	1/1	0.96	0.06	94,94,94,94	0
35	CL	Y	8820	1/1	0.96	0.07	46,46,46,46	0
32	MG	0	8009	1/1	0.96	0.23	42,42,42,42	0
34	NA	0	8553	1/1	0.96	0.12	69,69,69,69	0
32	MG	0	8050	1/1	0.96	0.15	74,74,74,74	0
32	MG	0	8052	1/1	0.96	0.07	58,58,58,58	0
32	MG	0	8030	1/1	0.96	0.19	79,79,79,79	0
36	SR	3	8932	1/1	0.96	0.05	94,94,94,94	0

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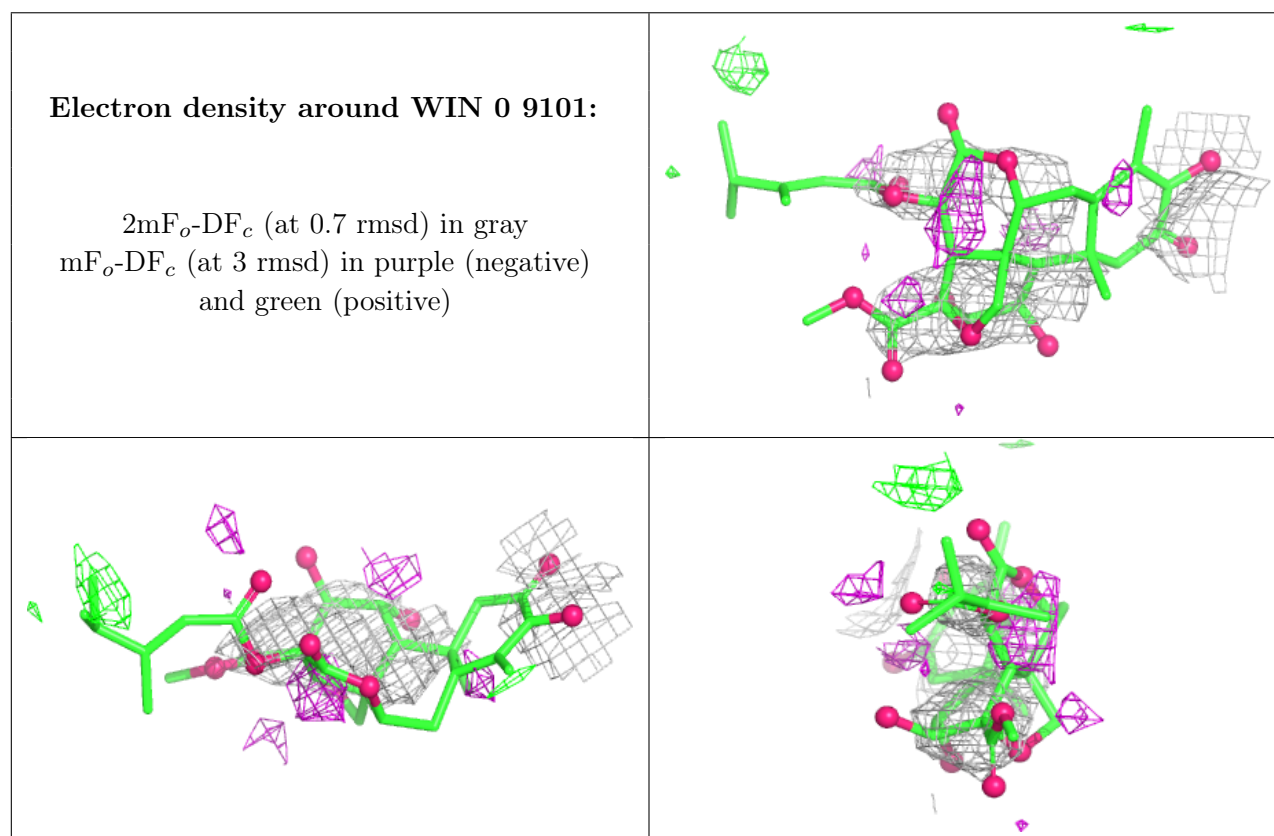
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8911	1/1	0.96	0.05	95,95,95,95	0
32	MG	0	8055	1/1	0.96	0.10	49,49,49,49	0
32	MG	0	8018	1/1	0.96	0.15	54,54,54,54	0
32	MG	0	8076	1/1	0.96	0.04	38,38,38,38	0
32	MG	0	8059	1/1	0.96	0.10	52,52,52,52	0
32	MG	0	8079	1/1	0.96	0.17	67,67,67,67	0
32	MG	0	8067	1/1	0.97	0.09	34,34,34,34	0
35	CL	N	8807	1/1	0.97	0.07	72,72,72,72	0
34	NA	0	8508	1/1	0.97	0.12	63,63,63,63	0
35	CL	0	8817	1/1	0.97	0.05	68,68,68,68	0
34	NA	0	8565	1/1	0.97	0.16	100,100,100,100	0
36	SR	0	8935	1/1	0.97	0.06	93,93,93,93	0
32	MG	0	8020	1/1	0.97	0.20	57,57,57,57	0
36	SR	0	8902	1/1	0.97	0.07	70,70,70,70	0
32	MG	0	8046	1/1	0.97	0.14	53,53,53,53	0
34	NA	0	8504	1/1	0.97	0.19	46,46,46,46	0
35	CL	0	8811	1/1	0.97	0.10	72,72,72,72	0
32	MG	0	8047	1/1	0.97	0.16	71,71,71,71	0
36	SR	0	8925	1/1	0.97	0.06	95,95,95,95	0
38	CD	O	8705	1/1	0.97	0.06	105,105,105,105	0
32	MG	0	8010	1/1	0.97	0.05	34,34,34,34	0
32	MG	0	8087	1/1	0.98	0.04	36,36,36,36	0
32	MG	0	8088	1/1	0.98	0.12	46,46,46,46	0
35	CL	M	8818	1/1	0.98	0.06	49,49,49,49	0
35	CL	0	8803	1/1	0.98	0.05	62,62,62,62	0
32	MG	0	8023	1/1	0.98	0.11	30,30,30,30	0
35	CL	R	8806	1/1	0.98	0.05	55,55,55,55	0
32	MG	0	8013	1/1	0.98	0.05	30,30,30,30	0
32	MG	0	8048	1/1	0.98	0.11	28,28,28,28	0
32	MG	0	8077	1/1	0.98	0.03	43,43,43,43	0
36	SR	R	8912	1/1	0.98	0.07	93,93,93,93	0
32	MG	0	8026	1/1	0.98	0.12	55,55,55,55	0
36	SR	0	8904	1/1	0.98	0.09	64,64,64,64	0
32	MG	0	8014	1/1	0.98	0.13	33,33,33,33	0
32	MG	0	8015	1/1	0.98	0.07	33,33,33,33	0
32	MG	K	8054	1/1	0.98	0.14	47,47,47,47	0
32	MG	0	8006	1/1	0.98	0.06	33,33,33,33	0
32	MG	0	8041	1/1	0.98	0.08	32,32,32,32	0
32	MG	0	8043	1/1	0.98	0.12	58,58,58,58	0
32	MG	0	8007	1/1	0.98	0.07	40,40,40,40	0
32	MG	0	8003	1/1	0.98	0.06	35,35,35,35	0
32	MG	0	8028	1/1	0.99	0.09	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8058	1/1	0.99	0.04	23,23,23,23	0
32	MG	0	8016	1/1	0.99	0.04	30,30,30,30	0
32	MG	0	8021	1/1	0.99	0.09	43,43,43,43	0
32	MG	0	8022	1/1	0.99	0.10	37,37,37,37	0
32	MG	0	8012	1/1	0.99	0.06	26,26,26,26	0
32	MG	0	8005	1/1	0.99	0.07	35,35,35,35	0
32	MG	0	8019	1/1	0.99	0.12	30,30,30,30	0
36	SR	0	8903	1/1	0.99	0.13	66,66,66,66	0
32	MG	0	8027	1/1	0.99	0.07	47,47,47,47	0
36	SR	0	8905	1/1	0.99	0.15	73,73,73,73	0
36	SR	0	8906	1/1	0.99	0.08	67,67,67,67	0
36	SR	0	8907	1/1	0.99	0.05	62,62,62,62	0
38	CD	3	8704	1/1	0.99	0.03	94,94,94,94	0
38	CD	U	8701	1/1	1.00	0.03	71,71,71,71	0
32	MG	0	8025	1/1	1.00	0.04	37,37,37,37	0
38	CD	1	8702	1/1	1.00	0.02	72,72,72,72	0
32	MG	0	8004	1/1	1.00	0.05	29,29,29,29	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.