



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 02:18 PM UTC

PDB ID : 3G4S / pdb_00003g4s
Title : Co-crystal structure of Tiamulin bound to the large ribosomal subunit
Authors : Gurel, G.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2009-02-04
Resolution : 3.20 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

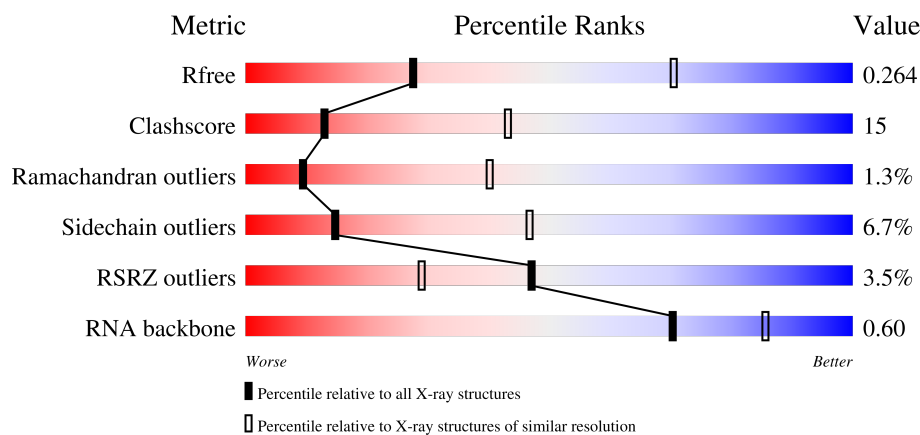
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	33% 54% 7% 6%
2	A	237	2% 78% 20% .
3	B	337	2% 75% 23% .
4	C	246	2% 79% 18% .

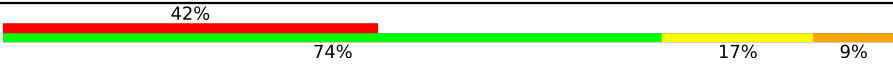
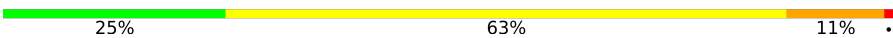
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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	172	
7	F	119	
8	G	348	
9	H	177	
10	I	70	
11	J	142	
12	K	132	
13	L	165	
14	M	194	
15	N	186	
16	O	115	
17	P	143	
18	Q	95	
19	R	150	
20	S	81	
21	T	119	
22	U	53	
23	V	65	
24	W	154	
25	X	82	
26	Y	142	
27	Z	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
36	SR	0	8997	-	-	-	X
36	SR	L	8969	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99167 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 L10.

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	84	Total	Mg	0	0
			84	84		
32	A	2	Total	Mg	0	0
			2	2		
32	B	1	Total	Mg	0	0
			1	1		
32	C	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	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	1	Total K 1 1	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	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	2	Total Na 2 2	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	10	Total Cl 10 10	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	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
35	O	1	Total Cl 1 1	0	0

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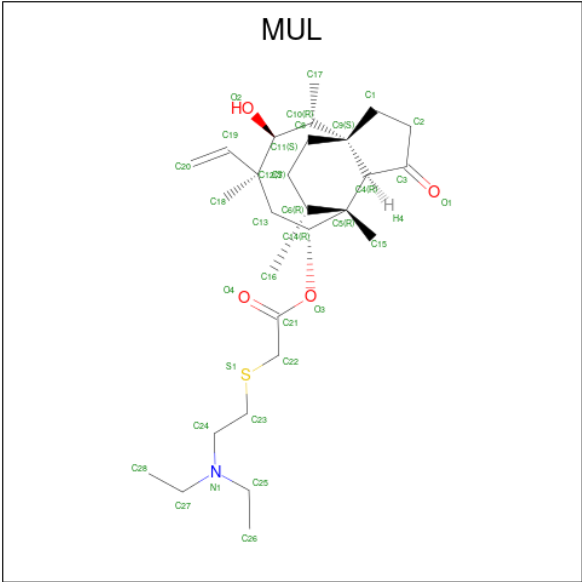
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	91	Total 91	Sr 91	0	0
36	A	3	Total 3	Sr 3	0	0
36	B	2	Total 2	Sr 2	0	0
36	F	1	Total 1	Sr 1	0	0
36	H	1	Total 1	Sr 1	0	0
36	J	1	Total 1	Sr 1	0	0
36	L	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	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	9	2	Total 2	Sr 2	0	0

- Molecule 37 is TIAMULIN (CCD ID: MUL) (formula: C₂₈H₄₇NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	0	1	Total	C	N	O	S	0	0
			34	28	1	4	1		

- Molecule 38 is CADMIUM ION (CCD ID: 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	5940	Total	O	0	0
			5940	5940		
39	A	125	Total	O	0	0
			125	125		
39	B	140	Total	O	0	0
			140	140		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	C	158	Total 158	O 158	0	0
39	D	45	Total 45	O 45	0	0
39	E	42	Total 42	O 42	0	0
39	F	26	Total 26	O 26	0	0
39	G	18	Total 18	O 18	0	0
39	H	70	Total 70	O 70	0	0
39	I	4	Total 4	O 4	0	0
39	J	47	Total 47	O 47	0	0
39	K	58	Total 58	O 58	0	0
39	L	94	Total 94	O 94	0	0
39	M	132	Total 132	O 132	0	0
39	N	55	Total 55	O 55	0	0
39	O	43	Total 43	O 43	0	0
39	P	59	Total 59	O 59	0	0
39	Q	52	Total 52	O 52	0	0
39	R	80	Total 80	O 80	0	0
39	S	30	Total 30	O 30	0	0
39	T	30	Total 30	O 30	0	0
39	U	30	Total 30	O 30	0	0
39	V	11	Total 11	O 11	0	0
39	W	59	Total 59	O 59	0	0

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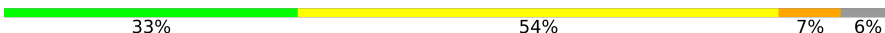
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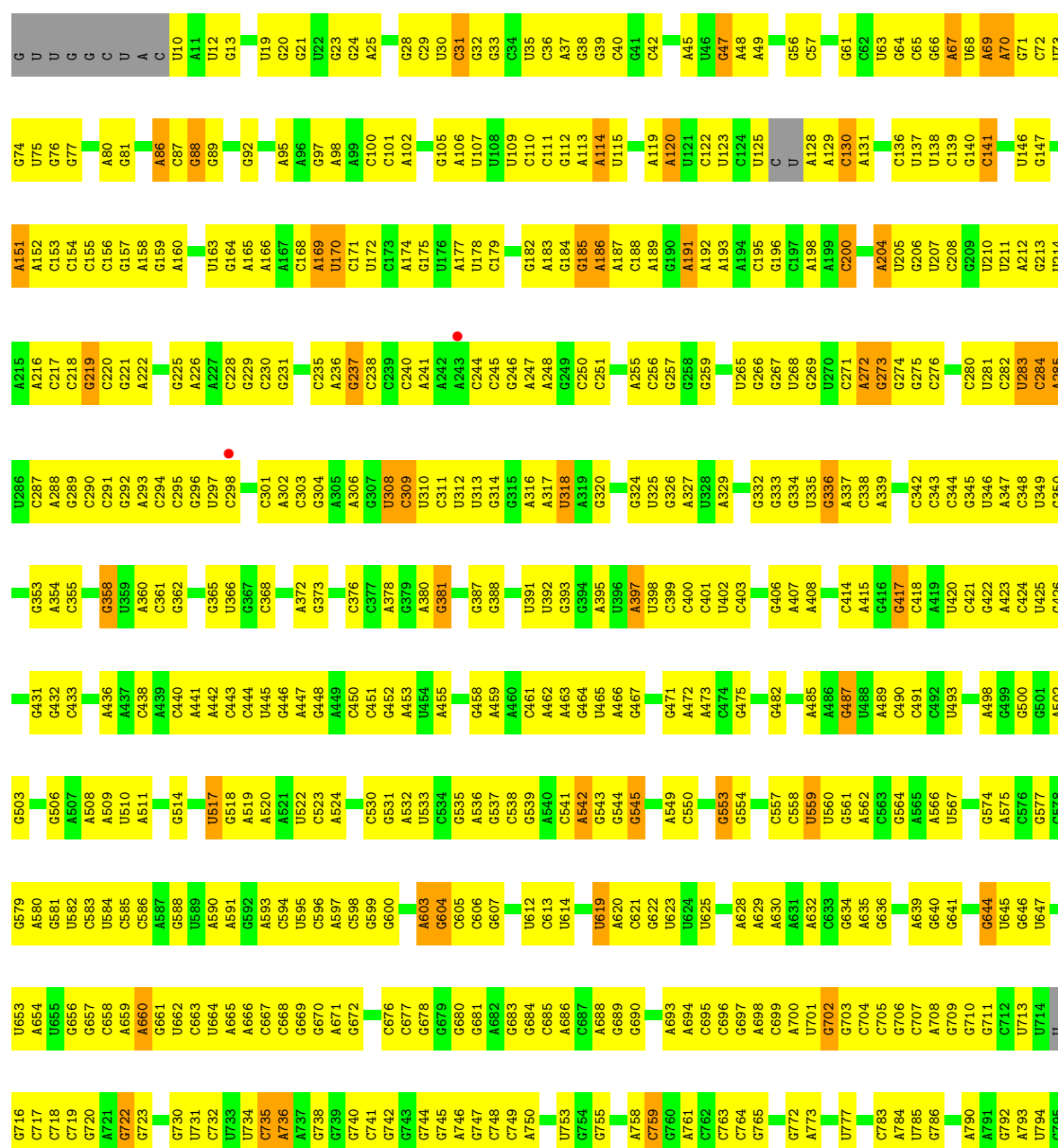
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	22	Total 22	O 22	0	0
39	Y	105	Total 105	O 105	0	0
39	Z	30	Total 30	O 30	0	0
39	1	55	Total 55	O 55	0	0
39	2	48	Total 48	O 48	0	0
39	3	62	Total 62	O 62	0	0
39	9	152	Total 152	O 152	0	0

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.

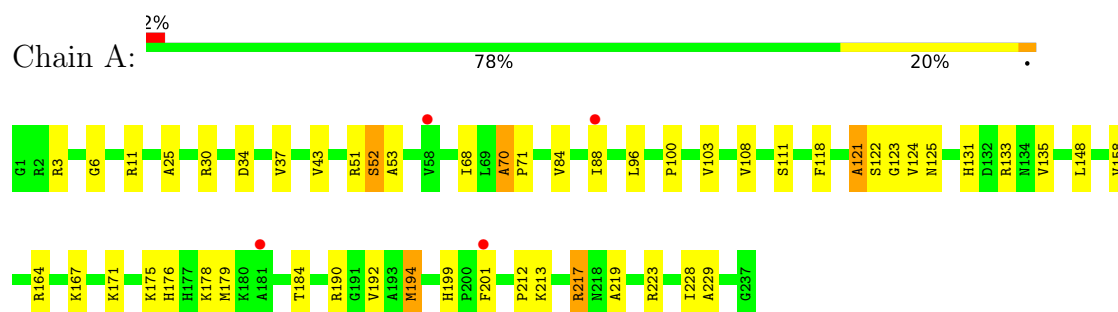
• Molecule 1: 23S ribosomal RNA

Chain 0: 

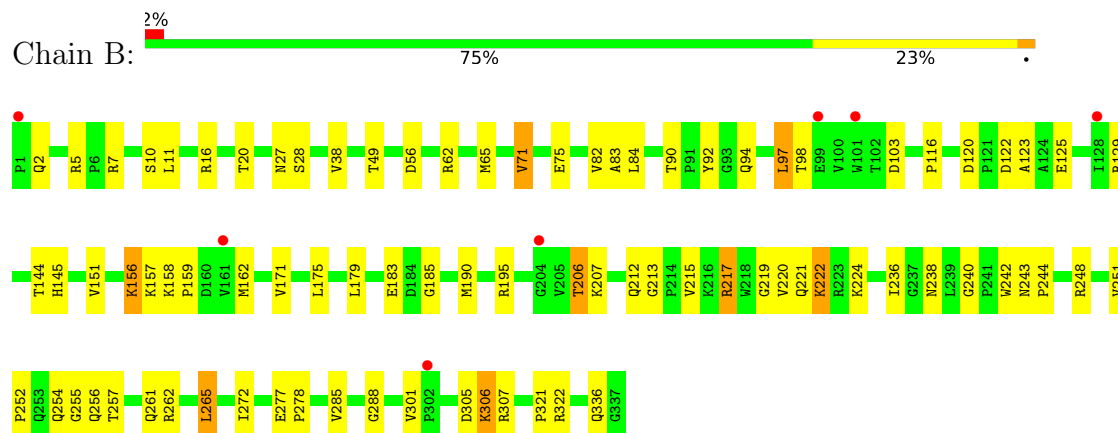


G1812	G1745	C1674	G1602	C1517	G1444	U1368	U1298	U1218	C1156	A1082	A1005	G941	A796
G1813	A1746	C1675	A1603	A1518	G1445	A1369	G1299	U1219	C1157	C1083	A1006	U942	
A1814	U1747	G1676	G1604		U1446	A1372	G1300	G1158	G1158	C1085	A1007	A943	U801
C1816	U1748	U1677	G1605	C1521	U1447			G1159	G1160	C1086	U1008	G944	G802
	U1749	C1678	A1606	G1523	A1448	A1375	C1303	G1161	A1161	C1087	U1009	U945	A806
C1818	G1752	C1679	G1607	U1524	G1449	G1376	C1304	G1162	A1162	A1088	C1010	U947	A807
G1819	G1753	G1680	G1608	G1525	C1450	C1377	U1306	G1163	G1163	U1096	C1011	G946	A808
A1820	A1754	A1682	C1609	G1526	C1451	G1378	A1307	A1231	U1164	A1097	A1012		A809
A1821	A1755	G1683	G1611	A1527	G1452	A1379	A1308	A1232	G1165	A1098	A1013	A951	G878
A1822	G1756	A1684	G1612	A1528	G1453	A1379	U1309	A1233	A1166	G1099	A1014	G952	C810
G1823	U1757	A1685	C1613	A1529	U1454	U1383	U1310	U1234	G1167	G1099	C1015	G953	A812
C1824	U1758	C1686	G1614	U1531	C1455	U1384	G1311		C1168	G1100	U1016	U954	A813
U1825	A1759	C1687	A1615		U1457		G1312	C1238	U1169	U1101		A955	G814
G1826	G1760	G1688	A1616	G1535	A1458	G1387	A1313	G1239	U1170	C1102	C1023	U883	U815
G1827	U1761	A1689	C1617	C1536	A1459	U1388	A1314	G1239	A1171	C1103	G1024	G956	G816
G1828	C1762		G1618		G1460	G1389	G1315	A1242	G1172	A1098	C1025	A957	G817
A1829	C1763	C1692	G1619	U1544	U1461	A1390	G1316	C1243	A1173	G1105	U1026	G958	G818
C1830	C1764		G1620	C1545	C1462	G1391		U1244	A1174	A1106	G1027	G960	A819
U1831	G1765	G1695	G1621	G1546	U1463	A1392		C1245	G1175		U1028	A961	G820
G1832	U1766	U1696	G1622	A1547	C1464		G1323	A1246		U1109	U1029	C962	U821
C1833	A1767	G1697	C1623	U1548	A1465	C1396	G1324			G1110	U1030	G963	U822
C1834	C1768	U1698	G1624	C1549	A1465	C1397	C1326			G1111	G1031	G964	U823
U1835	C1769		U1625		U1473	G1398	G1327	U1249	C1179	G1113	A1032		G824
	U1770	A1701	A1626	C1554	G1474	A1399	A1328	C1250	U1180		U1041		U825
	U1771	U1702	G1627	G1555	G1475	C1400		C1251	A1181	A1114		G968	U826
U1838	U1772	G1703		G1556	C1476	G1401	G1331	A1252	C1182	U1115	C1044	G969	
A1839	G1773	G1704	A1630	G1557	C1477		C1332	C1183	C1183	U1116	G1045	U970	G834
A1840	U1774	C1705	A1631	G1558	U1478	A1407	U1333	C1254	C1184	A1117	G1046	G	U835
C1841	A1775	G1706	A1632	A1559	U1478	U1408	C1334	A1255	U1185	A1118	G1046	G	G836
	U1776	G1707	C1633	U	C1483	G1409	C1335	G1257	C1187	G1119	U1047	G	U837
G1844	G1777		G1634	U1561	C1484			G1258	U1187	U1120		U	C838
A1845	A1778	A1710	U1635		A1485	U1412	U1338	A1259	A1188	G1121	C1051	C	C839
A1847	A1779	A1711	G1636	G1567	A1486	G1415	G1339	G1260	A1189		G1052	C	C906
G1848	G1780				A1487	G1416		C1262	A1190	U1124	G1053	G	A907
G1849		C1714	U1639	C1570	U1488		C1342	C1262	A1191	U1125	G1054	C	U840
U1850	C1715	G1571	C1640	G1572	A1492	U1419	C1343	G1268	A1193	U1126	G1055	C	C842
G1851	A1716	C1572	A1641	A1573	A1493	C1420	G1344	G1269	A1194	C1127	U1056	U	A843
A1852		U1722	C1642	C1574		G1421	U1347		G1195	U1128	A1057	C	
C1853	G1785	G1723	C1643	C1575	A1496	U1422	G1348	C1273	A1199	G1131	C1058	C	A846
G1854	C1787	U1724	U1644	C1575	G1497	C1423	U1350	A1274	G1069	U1130	C1060	A	C847
G1855	U1788	C1725	U1645		G1498	A1424	G1351	U1276	C1201	A1132	C1061	G	C848
C1856	G1789		G1646	C1585			U1356	U1277	G1202	U1133			U850
A1857	C1790	G1728	G1647	G1586	A1501	A1427	A1356	G1283	U1206	G1138	A1070	U	G856
A1858	U1791		G1648	U1587	U1502	C1428	A1357	G1284	A1207	U1139	G1071	C	A857
	U1792	A1729	G1649	G1588	U1503	U1436	U1358		C1208	U1140	G1072	G	U852
C1861	C1793	G1730	U1504	G1589	U1504	U1429	U1359	A1287	C1209	U1141	A1067	G	C853
C1862	G1794	C1731	A1505	G1590	U1505	G1430	G1354	U1278	G1203	U1136	C1068	A	G854
		A1732	A1656	A1591	U1506	U1433	A1355	U1205	U1205	G1137	C1069	G	U855
A1866	A1797	C1733	A1657	G1592	U1507	G1434	A1356	G1283	U1206	G1138	A1070	U	G856
G1867	G1798	C1734	A1661	G1593	C1507	A1434	A1357	G1284	A1207	U1139	G1071	C	A857
G1868	U1799	C1735	C1662	U1594	U1508	U1436	U1358		C1208	U1141	G1072	G	U858
	G1800	A1736	A1664	G1595	U1509	A1437	C1360	C1289	G1210	U1141	A1073	C	C859
G1873			A1665	U1596	G1510	U1438	U1362	U1206	G1212	G1075	A	C	U860
	C1803	G1739	G1665	A1597	G1512	C1439	U1363	U1293	C1213	U1149	G1076	A	G862
G1877	A1804	U1740	C1666	U1598	C1513	U1440	G1364	A1294	G1214	A1150	G1077	C	G863
G1878	G1805	U1741	A1667	A1599	C1514	G1441	C1365	A1296	G1215	G1151	A1078		U864
U1879	G1806	A1742	U1668	G1600	A1514	A1442	C1366	G1216	A1216	A1152	C1080	G	G865
C1880	U1807	G1743	U1673	G1601	U1516	G1443	A1367	U1297	G1217	C1153	U1001	G	U866
A1881		G1744									A1081	G1002	A857

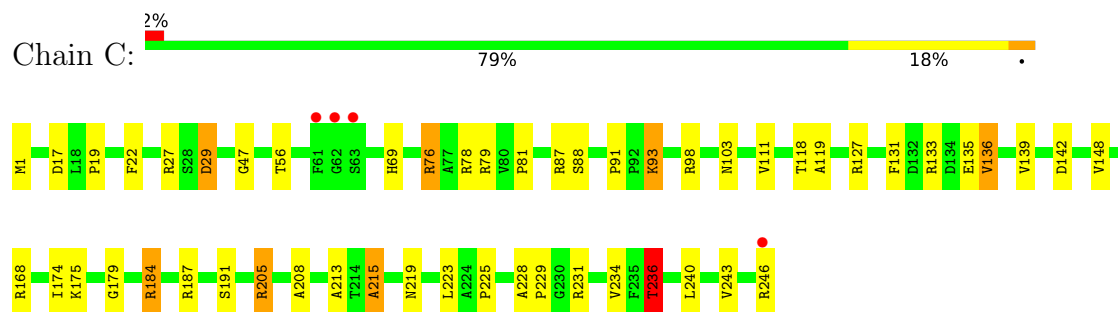
- Molecule 2: 50S ribosomal protein L2P



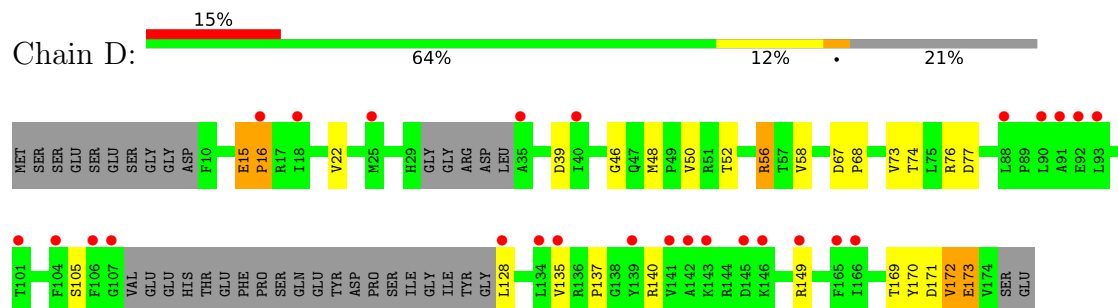
• Molecule 3: 50S ribosomal protein L3P



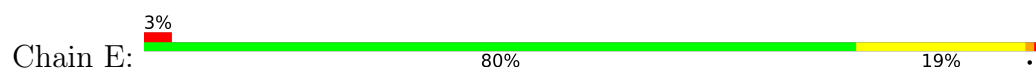
• Molecule 4: 50S ribosomal protein L4P

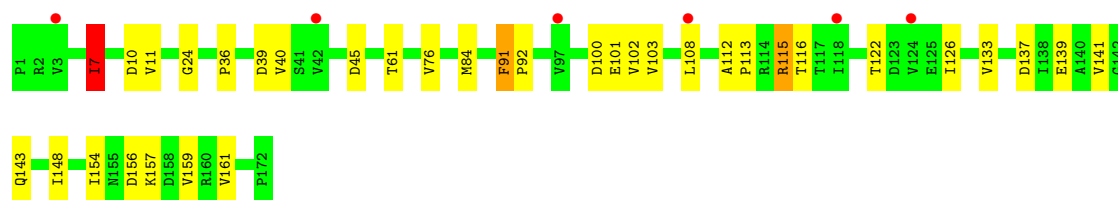


• Molecule 5: 50S ribosomal protein L5P

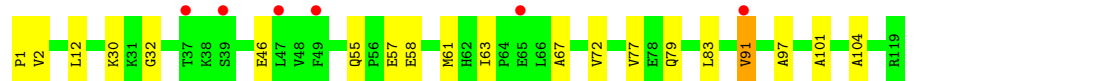
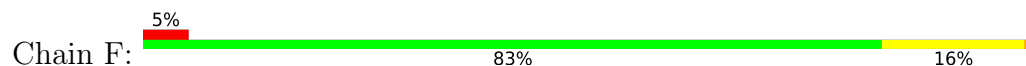


• Molecule 6: 50S ribosomal protein L6P

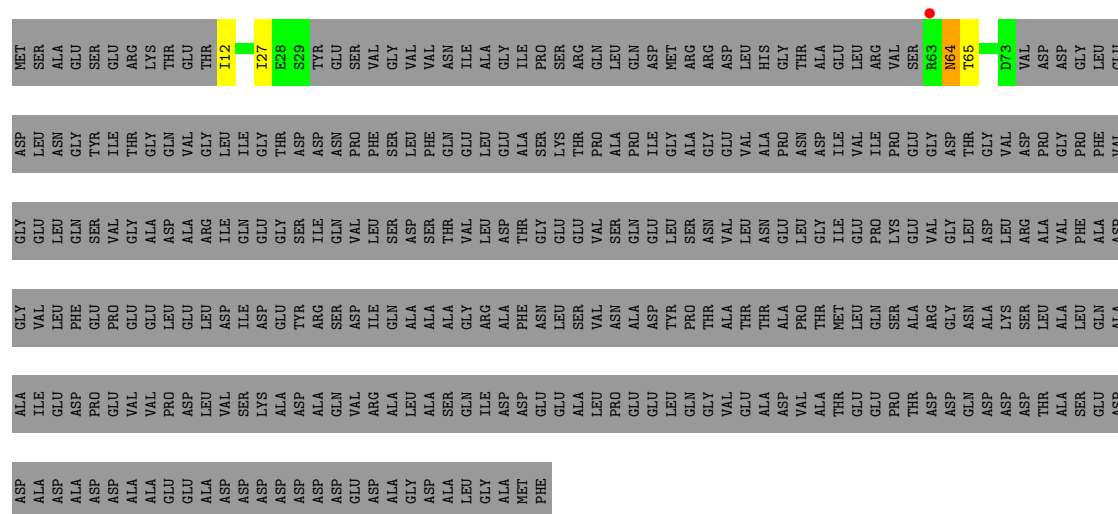




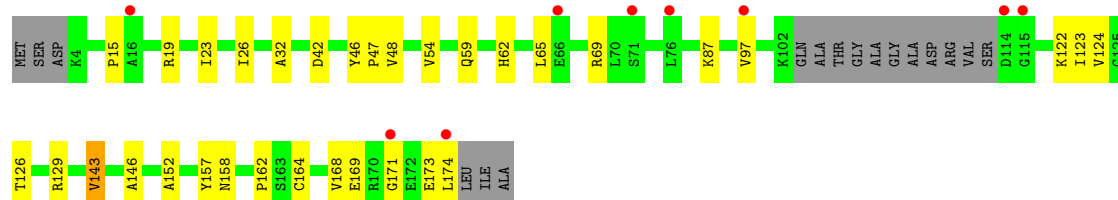
• Molecule 7: 50S ribosomal protein L7Ae



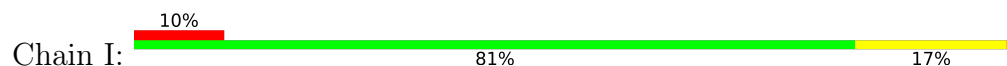
• Molecule 8: 50S ribosomal protein L10

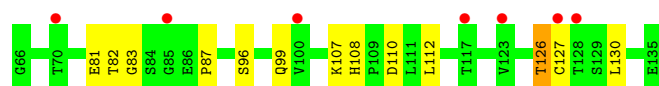


• Molecule 9: 50S ribosomal protein L10e

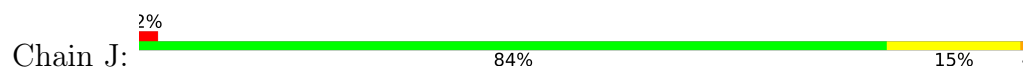


• Molecule 10: 50S ribosomal protein L11P

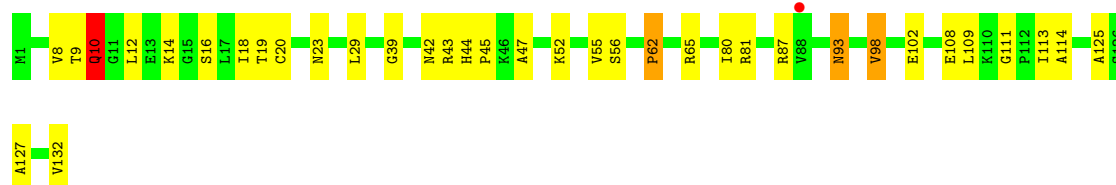




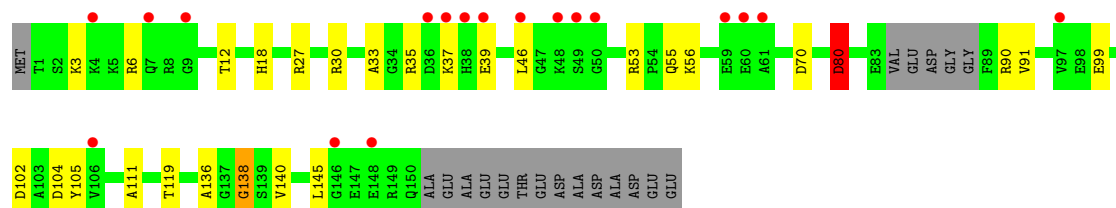
- Molecule 11: 50S ribosomal protein L13P



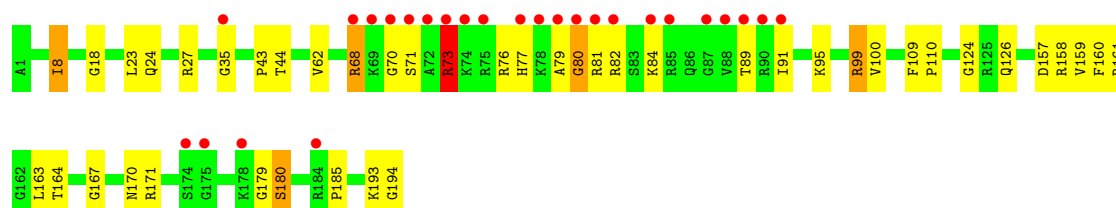
- Molecule 12: 50S ribosomal protein L14P



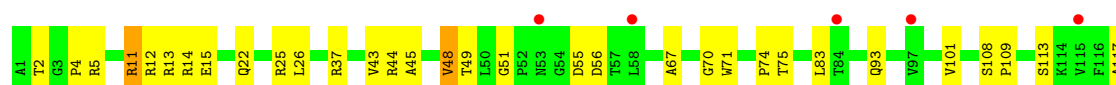
- Molecule 13: 50S ribosomal protein L15P

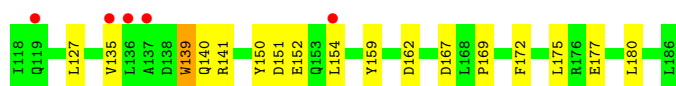


- Molecule 14: 50S ribosomal protein L15e

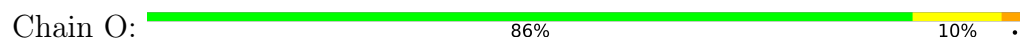


- Molecule 15: 50S ribosomal protein L18P

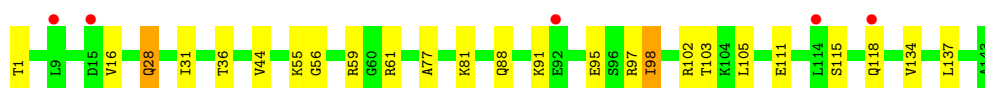
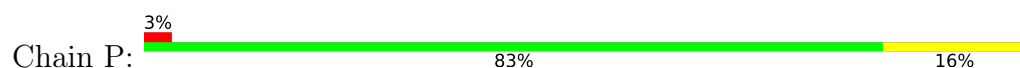




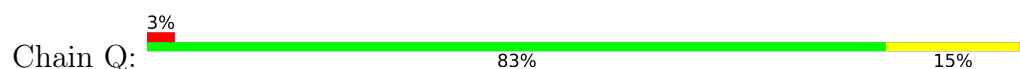
- Molecule 16: 50S ribosomal protein L18e



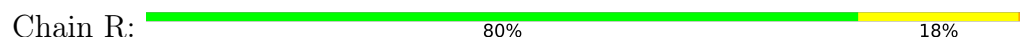
- Molecule 17: 50S ribosomal protein L19e



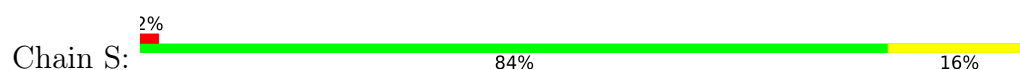
- Molecule 18: 50S ribosomal protein L21e



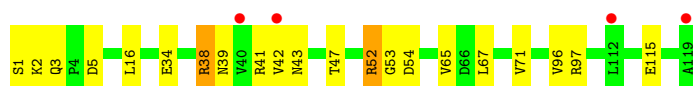
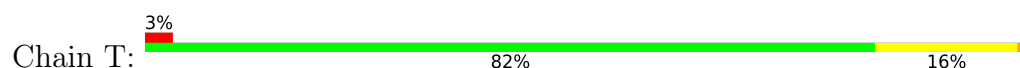
- Molecule 19: 50S ribosomal protein L22P



- Molecule 20: 50S ribosomal protein L23P

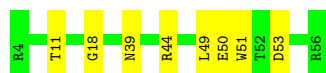


- Molecule 21: 50S ribosomal protein L24P



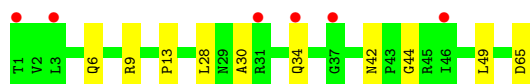
- Molecule 22: 50S ribosomal protein L24e

Chain U:  85% 15%



- Molecule 23: 50S ribosomal protein L29P

Chain V:  9% 85% 15%



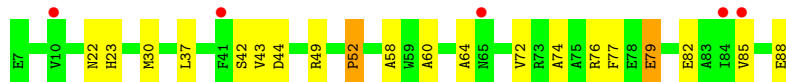
- Molecule 24: 50S ribosomal protein L30P

Chain W:  3% 75% 20% 5%



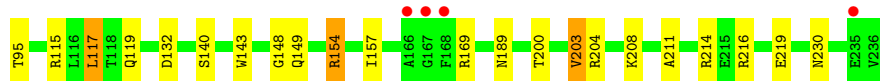
- Molecule 25: 50S ribosomal protein L31e

Chain X:  6% 76% 22%



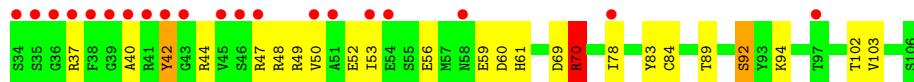
- Molecule 26: 50S ribosomal protein L32e

Chain Y:  3% 85% 13%



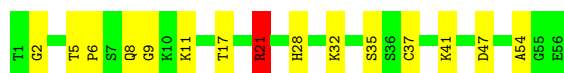
- Molecule 27: 50S ribosomal protein L37Ae

Chain Z:  27% 67% 29%

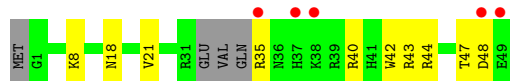


- Molecule 28: 50S ribosomal protein L37e

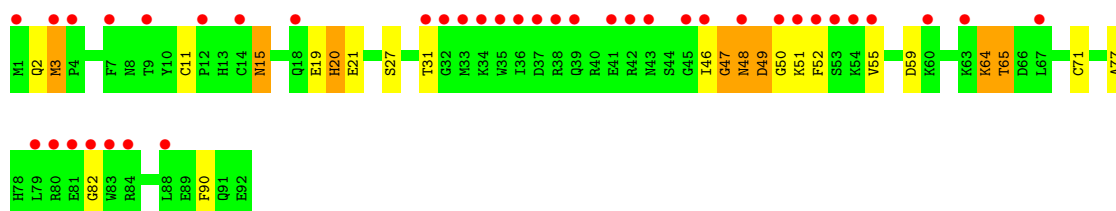
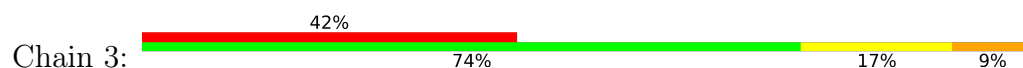
Chain 1:  73% 25%



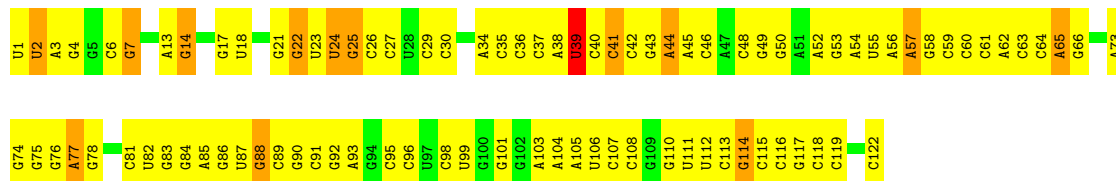
- Molecule 29: 50S ribosomal protein L39e



- 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	212.27Å 299.84Å 574.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.20 49.84 – 3.20	Depositor EDS
% Data completeness (in resolution range)	83.7 (49.84-3.20) 83.7 (49.84-3.20)	Depositor EDS
R_{merge}	0.18	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}	0.215 , 0.290 0.201 , 0.264	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 121.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	99167	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: PSU, MG, OMG, SR, UR3, 1MA, NA, MUL, K, OMU, CD, CL

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	0.43	0/65958	0.61	10/102869 (0.0%)
2	A	0.70	1/1787 (0.1%)	1.15	16/2408 (0.7%)
3	B	0.63	0/2690	1.14	16/3652 (0.4%)
4	C	0.65	0/1885	1.18	10/2552 (0.4%)
5	D	0.79	0/1111	1.18	9/1498 (0.6%)
6	E	0.69	1/1383 (0.1%)	1.03	4/1880 (0.2%)
7	F	0.71	1/901 (0.1%)	1.15	3/1224 (0.2%)
8	G	0.63	0/241	1.07	1/324 (0.3%)
9	H	0.65	0/1302	1.10	6/1743 (0.3%)
10	I	0.81	0/527	1.12	3/716 (0.4%)
11	J	0.64	0/1136	1.11	4/1530 (0.3%)
12	K	0.64	0/1004	1.10	5/1351 (0.4%)
13	L	0.65	0/1130	1.10	7/1509 (0.5%)
14	M	0.62	0/1583	1.12	11/2116 (0.5%)
15	N	0.68	0/1474	1.24	13/1999 (0.7%)
16	O	0.61	0/874	1.16	6/1181 (0.5%)
17	P	0.55	0/1148	1.10	7/1528 (0.5%)
18	Q	0.63	0/749	1.09	4/1005 (0.4%)
19	R	0.65	1/1173 (0.1%)	1.10	8/1578 (0.5%)
20	S	0.58	0/649	1.02	2/875 (0.2%)
21	T	0.56	0/958	1.13	7/1289 (0.5%)
22	U	0.67	0/418	1.16	2/562 (0.4%)
23	V	0.64	0/503	1.21	3/675 (0.4%)
24	W	0.68	1/1219 (0.1%)	1.20	10/1655 (0.6%)
25	X	0.69	0/665	1.22	6/895 (0.7%)
26	Y	0.62	0/1147	1.16	8/1536 (0.5%)
27	Z	0.80	0/585	1.23	6/781 (0.8%)
28	1	0.63	0/438	1.12	5/578 (0.9%)
29	2	0.55	0/401	1.03	1/529 (0.2%)
30	3	0.91	0/771	1.20	5/1024 (0.5%)
31	9	0.41	0/2904	0.57	1/4526 (0.0%)
All	All	0.51	5/98714 (0.0%)	0.79	199/147588 (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	25
24	W	0	1
All	All	0	26

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	63	ILE	CA-CB	7.77	1.58	1.54
24	W	153	MET	SD-CE	-6.01	1.64	1.79
19	R	109	MET	SD-CE	-5.77	1.65	1.79
6	E	7	ILE	CA-CB	5.21	1.60	1.54
2	A	194	MET	SD-CE	-5.07	1.66	1.79

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	170	TYR	N-CA-C	10.22	125.34	113.38
21	T	52	ARG	N-CA-C	9.15	125.14	113.88
16	O	7	LEU	N-CA-C	-8.65	101.56	112.90
16	O	43	VAL	N-CA-C	8.55	120.80	108.48
9	H	124	VAL	N-CA-C	8.54	118.81	111.90

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	436	A	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain
1	0	49	A	Sidechain
1	0	493	U	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	1926	0
2	A	1754	0	1766	27	0
3	B	2625	0	2533	40	0
4	C	1860	0	1813	31	0
5	D	1094	0	1085	12	0
6	E	1358	0	1266	13	0
7	F	890	0	843	7	0
8	G	240	0	231	1	0
9	H	1282	0	1292	12	0
10	I	520	0	500	6	0
11	J	1120	0	1098	17	0
12	K	994	0	1027	20	0
13	L	1118	0	1076	13	0
14	M	1559	0	1573	32	0
15	N	1445	0	1401	20	0
16	O	865	0	873	9	0
17	P	1137	0	1123	17	0
18	Q	735	0	729	9	0
19	R	1150	0	1122	16	0
20	S	642	0	605	6	0
21	T	950	0	924	13	0
22	U	411	0	368	3	0
23	V	500	0	511	3	0
24	W	1196	0	1137	24	0
25	X	655	0	653	7	0
26	Y	1131	0	1133	10	0
27	Z	574	0	535	16	0
28	1	431	0	426	8	0
29	2	396	0	413	6	0
30	3	755	0	732	16	0
31	9	2599	0	1325	112	0
32	0	84	0	0	0	0
32	2	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	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	1	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	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	2	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	L	1	0	0	0	0
35	M	1	0	0	1	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	91	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	2	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	34	0	47	17	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	5940	0	0	277	0
39	1	55	0	0	0	0
39	2	48	0	0	1	0
39	3	62	0	0	1	0
39	9	152	0	0	12	0
39	A	125	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B	140	0	0	2	0
39	C	158	0	0	3	0
39	D	45	0	0	1	0
39	E	42	0	0	0	0
39	F	26	0	0	2	0
39	G	18	0	0	0	0
39	H	70	0	0	1	0
39	I	4	0	0	0	0
39	J	47	0	0	1	0
39	K	58	0	0	0	0
39	L	94	0	0	4	0
39	M	132	0	0	1	0
39	N	55	0	0	1	0
39	O	43	0	0	1	0
39	P	59	0	0	0	0
39	Q	52	0	0	0	0
39	R	80	0	0	0	0
39	S	30	0	0	1	0
39	T	30	0	0	0	0
39	U	30	0	0	1	0
39	V	11	0	0	0	0
39	W	59	0	0	0	0
39	X	22	0	0	0	0
39	Y	105	0	0	1	0
39	Z	30	0	0	2	0
All	All	99167	0	59972	2245	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 15.

The worst 5 of 2245 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:H8	1:0:871:G:H5'	1.00	1.13
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.13
1:0:2121:G:H4'	30:3:47:GLY:HA2	1.29	1.12
1:0:2717:C:H2'	1:0:2718:C:H5''	1.27	1.12
1:0:871:G:H5'	1:0:871:G:C8	1.88	1.08

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%)	210 (89%)	20 (8%)	5 (2%)	5	31
3	B	335/337 (99%)	305 (91%)	27 (8%)	3 (1%)	14	47
4	C	244/246 (99%)	223 (91%)	18 (7%)	3 (1%)	10	42
5	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	5	29
6	E	170/172 (99%)	157 (92%)	12 (7%)	1 (1%)	21	56
7	F	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	3	20
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	145 (93%)	10 (6%)	1 (1%)	21	56
10	I	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	8	37
11	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	9	39
12	K	130/132 (98%)	116 (89%)	13 (10%)	1 (1%)	16	50
13	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	18	52
14	M	192/194 (99%)	180 (94%)	7 (4%)	5 (3%)	4	26
15	N	184/186 (99%)	165 (90%)	15 (8%)	4 (2%)	5	29
16	O	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
17	P	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	18	52
18	Q	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	5	29
19	R	148/150 (99%)	141 (95%)	6 (4%)	1 (1%)	18	52
20	S	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
21	T	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
22	U	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
23	V	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
24	W	152/154 (99%)	139 (91%)	13 (9%)	0	100	100
25	X	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	40
26	Y	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	18	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	4	25
28	1	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	6	33
29	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
30	3	90/92 (98%)	75 (83%)	11 (12%)	4 (4%)	2	15
All	All	3705/4172 (89%)	3381 (91%)	277 (8%)	47 (1%)	9	40

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	52	SER
3	B	306	LYS
7	F	61	MET
11	J	5	GLU
14	M	80	GLY

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%)	169 (94%)	10 (6%)	19	52
3	B	282/282 (100%)	256 (91%)	26 (9%)	8	33
4	C	193/193 (100%)	177 (92%)	16 (8%)	10	38
5	D	117/148 (79%)	110 (94%)	7 (6%)	17	50
6	E	152/152 (100%)	139 (91%)	13 (9%)	10	36
7	F	93/93 (100%)	89 (96%)	4 (4%)	26	59
8	G	27/282 (10%)	24 (89%)	3 (11%)	6	25
9	H	134/145 (92%)	122 (91%)	12 (9%)	9	34
10	I	58/58 (100%)	55 (95%)	3 (5%)	21	54
11	J	118/118 (100%)	113 (96%)	5 (4%)	26	60
12	K	106/106 (100%)	97 (92%)	9 (8%)	10	37
13	L	113/127 (89%)	105 (93%)	8 (7%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	158/158 (100%)	150 (95%)	8 (5%)	21	54
15	N	149/149 (100%)	133 (89%)	16 (11%)	6	27
16	O	93/93 (100%)	86 (92%)	7 (8%)	12	42
17	P	113/113 (100%)	110 (97%)	3 (3%)	39	68
18	Q	79/79 (100%)	76 (96%)	3 (4%)	29	62
19	R	117/117 (100%)	111 (95%)	6 (5%)	21	54
20	S	71/71 (100%)	69 (97%)	2 (3%)	38	68
21	T	105/105 (100%)	99 (94%)	6 (6%)	18	51
22	U	44/44 (100%)	42 (96%)	2 (4%)	24	58
23	V	51/51 (100%)	46 (90%)	5 (10%)	7	31
24	W	130/130 (100%)	124 (95%)	6 (5%)	24	58
25	X	66/66 (100%)	59 (89%)	7 (11%)	6	27
26	Y	120/120 (100%)	113 (94%)	7 (6%)	18	51
27	Z	60/60 (100%)	57 (95%)	3 (5%)	22	55
28	1	46/46 (100%)	45 (98%)	1 (2%)	45	71
29	2	42/46 (91%)	39 (93%)	3 (7%)	13	44
30	3	79/79 (100%)	72 (91%)	7 (9%)	9	34
All	All	3095/3410 (91%)	2887 (93%)	208 (7%)	15	47

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	L	145	LEU
16	O	43	VAL
29	2	21	VAL
14	M	89	THR
15	N	56	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
19	R	98	ASN
24	W	59	GLN
19	R	140	GLN
21	T	73	HIS

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Mol	Chain	Res	Type
25	X	36	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	266 (9%)	19 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	283 (9%)	20 (0%)

5 of 283 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	47	G
1	0	67	A
1	0	69	A
1	0	70	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2467	A
1	0	2761	A
31	9	65	A
1	0	2791	U
1	0	1080	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MA	0	628	34,1	21,25,26	0.76	1 (4%)	30,37,40	0.91	2 (6%)
1	PSU	0	2621	1	18,21,22	1.43	2 (11%)	21,30,33	1.35	3 (14%)
1	UR3	0	2619	1	19,22,23	0.52	0	26,32,35	0.69	1 (3%)
1	OMU	0	2587	1	19,22,23	0.37	0	25,31,34	0.40	0
1	OMG	0	2588	1	23,26,27	0.33	0	32,38,41	0.39	0

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.50	1.42	1.36
1	0	2621	PSU	C6-C5	2.74	1.38	1.35
1	0	628	1MA	C6-N6	2.54	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	3.41	120.48	118.17
1	0	2621	PSU	C6-N1-C2	-3.10	119.81	122.69
1	0	628	1MA	CM1-N1-C6	2.90	124.64	120.15
1	0	2621	PSU	O2-C2-N1	2.86	125.74	122.79
1	0	628	1MA	N1-C2-N3	2.78	129.29	126.00

There are no chirality outliers.

All (2) 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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2621	PSU	1	0
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 304 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	MUL	0	9101	-	36,36,36	1.49	5 (13%)	55,55,55	2.24	18 (32%)

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	MUL	0	9101	-	-	3/18/79/79	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	MUL	C12-C19	-5.48	1.39	1.52
37	0	9101	MUL	C5-C14	-3.04	1.53	1.56
37	0	9101	MUL	C10-C11	-2.66	1.53	1.56
37	0	9101	MUL	C12-C11	-2.51	1.53	1.55
37	0	9101	MUL	C9-C10	-2.24	1.53	1.56

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	MUL	C12-C13-C14	-6.04	112.28	120.20
37	0	9101	MUL	C13-C14-C5	-5.90	109.94	116.28
37	0	9101	MUL	O3-C21-C22	5.48	119.56	110.52
37	0	9101	MUL	C18-C12-C13	5.12	109.33	105.51
37	0	9101	MUL	C14-O3-C21	-3.97	110.79	118.03

There are no chirality outliers.

All (3) torsion outliers are listed below:

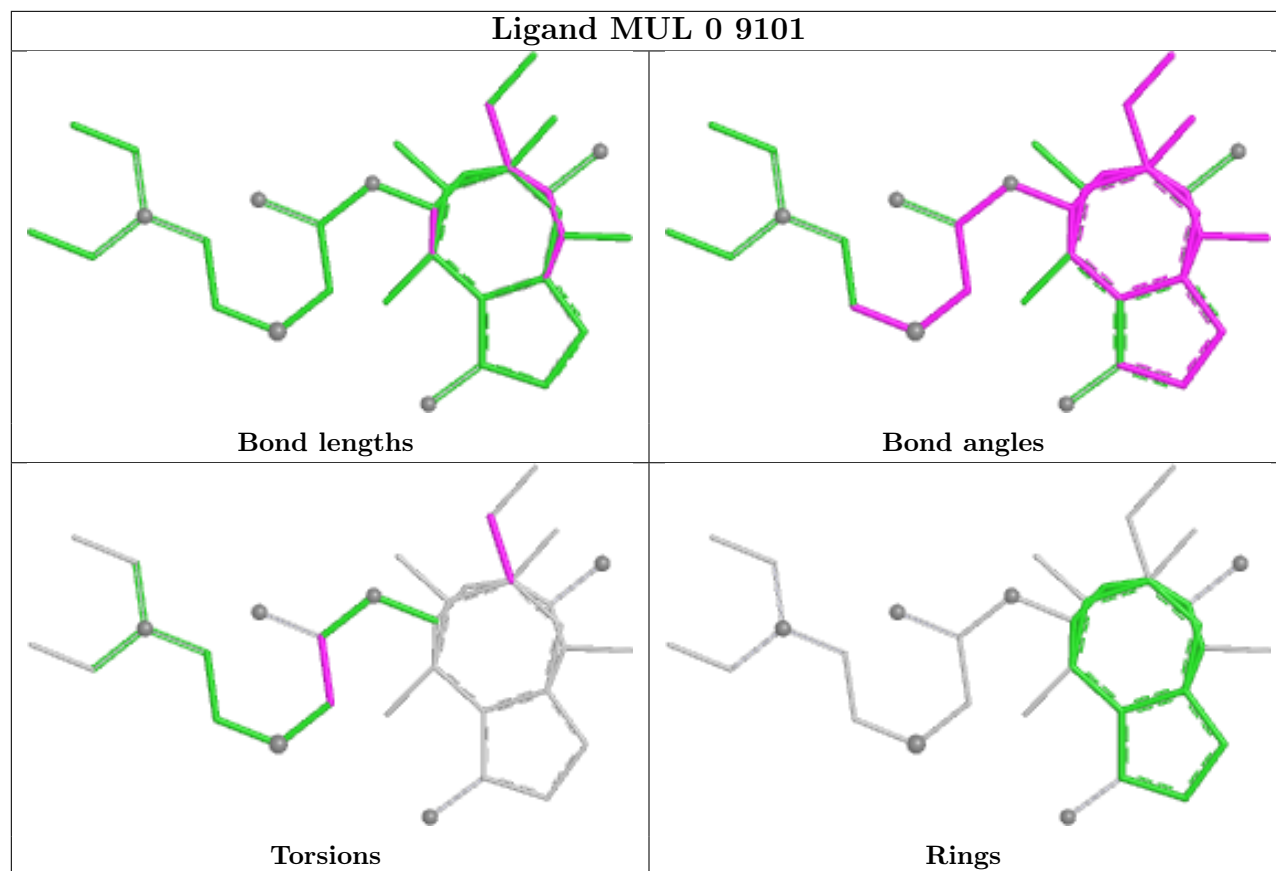
Mol	Chain	Res	Type	Atoms
37	0	9101	MUL	C13-C12-C19-C20
37	0	9101	MUL	O4-C21-C22-S1
37	0	9101	MUL	O3-C21-C22-S1

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	9101	MUL	17	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%)	-0.56	5 (0%) 91 85	29, 74, 140, 200	0
2	A	237/237 (100%)	0.20	4 (1%) 69 49	43, 97, 143, 167	0
3	B	337/337 (100%)	0.19	7 (2%) 63 43	40, 86, 129, 148	0
4	C	246/246 (100%)	0.04	4 (1%) 70 51	41, 72, 103, 112	0
5	D	140/177 (79%)	1.04	26 (18%) 3 3	118, 160, 184, 191	0
6	E	172/172 (100%)	0.30	6 (3%) 47 29	76, 104, 134, 146	0
7	F	119/119 (100%)	0.32	6 (5%) 34 22	74, 113, 153, 166	0
8	G	29/348 (8%)	0.48	1 (3%) 48 30	118, 140, 146, 150	0
9	H	160/177 (90%)	0.31	9 (5%) 30 19	77, 104, 146, 162	0
10	I	70/70 (100%)	1.11	7 (10%) 12 8	173, 199, 200, 200	0
11	J	142/142 (100%)	0.15	3 (2%) 63 43	55, 80, 104, 123	0
12	K	132/132 (100%)	0.09	1 (0%) 82 67	54, 79, 112, 118	0
13	L	145/165 (87%)	0.73	18 (12%) 8 6	62, 121, 171, 175	0
14	M	194/194 (100%)	0.55	26 (13%) 7 6	49, 70, 145, 160	0
15	N	186/186 (100%)	0.48	10 (5%) 31 20	82, 118, 178, 187	0
16	O	115/115 (100%)	0.22	0 100 100	66, 87, 105, 111	0
17	P	143/143 (100%)	0.37	5 (3%) 47 29	65, 88, 117, 124	0
18	Q	95/95 (100%)	0.25	3 (3%) 50 31	67, 87, 110, 117	0
19	R	150/150 (100%)	-0.12	0 100 100	47, 72, 103, 112	0
20	S	81/81 (100%)	0.26	2 (2%) 58 39	68, 93, 114, 130	0
21	T	119/119 (100%)	0.36	4 (3%) 48 30	69, 92, 136, 155	0
22	U	53/53 (100%)	0.16	0 100 100	94, 114, 136, 145	0
23	V	65/65 (100%)	0.49	6 (9%) 14 9	79, 112, 164, 170	0
24	W	154/154 (100%)	0.25	5 (3%) 50 31	56, 78, 110, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/82 (100%)	0.23	5 (6%) 27 17	63, 92, 125, 135	0
26	Y	142/142 (100%)	0.02	4 (2%) 55 35	45, 73, 109, 134	0
27	Z	73/73 (100%)	1.78	20 (27%) 1 1	149, 179, 191, 194	0
28	1	56/56 (100%)	-0.11	0 100 100	42, 53, 66, 76	0
29	2	46/50 (92%)	0.69	5 (10%) 10 7	48, 95, 145, 146	0
30	3	92/92 (100%)	2.23	39 (42%) 0 1	163, 185, 199, 200	0
31	9	122/122 (100%)	-0.32	0 100 100	66, 114, 143, 191	0
All	All	6646/7217 (92%)	-0.02	231 (3%) 47 29	29, 85, 168, 200	0

The worst 5 of 231 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	3	35	TRP	9.5
27	Z	35	SER	9.5
27	Z	40	ALA	9.3
14	M	80	GLY	9.2
30	3	38	ARG	8.8

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	PSU	0	2621	20/21	0.94	0.08	59,63,65,66	0
1	OMU	0	2587	21/22	0.96	0.08	60,63,64,64	0
1	OMG	0	2588	24/25	0.96	0.07	50,54,58,60	0
1	UR3	0	2619	21/22	0.96	0.07	61,65,71,72	0
1	1MA	0	628	23/24	0.96	0.07	49,56,63,64	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	0.45	0.26	92,92,92,92	0
34	NA	0	8527	1/1	0.53	0.12	60,60,60,60	0
34	NA	0	8574	1/1	0.55	0.34	67,67,67,67	0
36	SR	0	8997	1/1	0.58	0.81	200,200,200,200	0
34	NA	0	8573	1/1	0.59	0.30	92,92,92,92	0
34	NA	0	8568	1/1	0.62	0.14	51,51,51,51	0
36	SR	9	9003	1/1	0.66	0.10	200,200,200,200	0
36	SR	J	8986	1/1	0.67	0.26	200,200,200,200	0
32	MG	0	8082	1/1	0.69	0.17	86,86,86,86	0
34	NA	0	8522	1/1	0.69	0.26	87,87,87,87	0
34	NA	0	8553	1/1	0.70	0.32	81,81,81,81	0
34	NA	0	8564	1/1	0.70	0.18	95,95,95,95	0
36	SR	0	8983	1/1	0.72	0.15	185,185,185,185	0
34	NA	0	8570	1/1	0.72	0.12	65,65,65,65	0
34	NA	0	8537	1/1	0.73	0.11	43,43,43,43	0
36	SR	0	9006	1/1	0.73	0.31	200,200,200,200	0
35	CL	J	8802	1/1	0.73	0.12	100,100,100,100	0
32	MG	B	8042	1/1	0.73	0.16	67,67,67,67	0
34	NA	0	8511	1/1	0.76	0.14	64,64,64,64	0
32	MG	0	8072	1/1	0.77	0.07	37,37,37,37	0
36	SR	0	8976	1/1	0.78	0.25	185,185,185,185	0
34	NA	9	8572	1/1	0.78	0.11	88,88,88,88	0
34	NA	0	8541	1/1	0.78	0.09	46,46,46,46	0
34	NA	0	8502	1/1	0.79	0.13	51,51,51,51	0
36	SR	0	8938	1/1	0.79	0.10	200,200,200,200	0
32	MG	0	8066	1/1	0.79	0.16	70,70,70,70	0
36	SR	L	8969	1/1	0.79	0.41	198,198,198,198	0
34	NA	0	8557	1/1	0.79	0.22	71,71,71,71	0
36	SR	0	8957	1/1	0.80	0.22	200,200,200,200	0
32	MG	0	8047	1/1	0.80	0.25	70,70,70,70	0
34	NA	0	8566	1/1	0.80	0.19	51,51,51,51	0
34	NA	R	8575	1/1	0.80	0.23	96,96,96,96	0
35	CL	0	8816	1/1	0.81	0.37	86,86,86,86	0
36	SR	0	8951	1/1	0.81	0.10	177,177,177,177	0
35	CL	0	8822	1/1	0.81	0.33	94,94,94,94	0
32	MG	0	8036	1/1	0.81	0.17	82,82,82,82	0
35	CL	N	8807	1/1	0.81	0.19	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8501	1/1	0.82	0.15	41,41,41,41	0
36	SR	B	8987	1/1	0.82	0.33	200,200,200,200	0
36	SR	0	8977	1/1	0.82	0.08	197,197,197,197	0
32	MG	9	8074	1/1	0.82	0.11	127,127,127,127	0
34	NA	0	8562	1/1	0.82	0.59	85,85,85,85	0
34	NA	0	8518	1/1	0.83	0.21	82,82,82,82	0
36	SR	0	8971	1/1	0.83	0.17	200,200,200,200	0
35	CL	3	8804	1/1	0.83	0.06	96,96,96,96	0
32	MG	0	8038	1/1	0.83	0.08	81,81,81,81	0
34	NA	0	8524	1/1	0.83	0.14	47,47,47,47	0
36	SR	0	8988	1/1	0.83	0.08	181,181,181,181	0
36	SR	0	8920	1/1	0.84	0.18	132,132,132,132	0
36	SR	0	8922	1/1	0.84	0.18	190,190,190,190	0
34	NA	0	8506	1/1	0.84	0.22	105,105,105,105	0
36	SR	0	8947	1/1	0.84	0.13	200,200,200,200	0
34	NA	0	8559	1/1	0.84	0.25	94,94,94,94	0
36	SR	0	9001	1/1	0.84	0.07	189,189,189,189	0
36	SR	0	8955	1/1	0.84	0.13	199,199,199,199	0
34	NA	0	8519	1/1	0.84	0.09	44,44,44,44	0
36	SR	0	8958	1/1	0.84	0.08	150,150,150,150	0
36	SR	0	8967	1/1	0.84	0.13	157,157,157,157	0
34	NA	0	8528	1/1	0.84	0.23	80,80,80,80	0
35	CL	A	8809	1/1	0.85	0.39	96,96,96,96	0
36	SR	0	8942	1/1	0.85	0.12	129,129,129,129	0
34	NA	0	8555	1/1	0.85	0.10	50,50,50,50	0
36	SR	9	8980	1/1	0.85	0.07	192,192,192,192	0
32	MG	0	8073	1/1	0.85	0.40	110,110,110,110	0
36	SR	0	9000	1/1	0.86	0.21	200,200,200,200	0
34	NA	R	8532	1/1	0.86	0.16	57,57,57,57	0
36	SR	0	8953	1/1	0.86	0.11	185,185,185,185	0
36	SR	A	8930	1/1	0.86	0.16	133,133,133,133	0
32	MG	0	8039	1/1	0.86	0.24	76,76,76,76	0
34	NA	9	8543	1/1	0.86	0.24	57,57,57,57	0
32	MG	0	8090	1/1	0.86	0.10	81,81,81,81	0
36	SR	0	8991	1/1	0.86	0.14	190,190,190,190	0
34	NA	Q	8540	1/1	0.86	0.12	92,92,92,92	0
34	NA	0	8571	1/1	0.87	0.14	89,89,89,89	0
36	SR	0	8916	1/1	0.87	0.11	129,129,129,129	0
36	SR	0	9007	1/1	0.87	0.34	180,180,180,180	0
36	SR	0	8959	1/1	0.87	0.11	194,194,194,194	0
32	MG	0	8037	1/1	0.87	0.33	84,84,84,84	0
36	SR	0	8994	1/1	0.87	0.42	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8995	1/1	0.87	0.11	128,128,128,128	0
36	SR	3	8999	1/1	0.87	0.18	160,160,160,160	0
35	CL	0	8805	1/1	0.87	0.24	97,97,97,97	0
34	NA	S	8510	1/1	0.87	0.12	69,69,69,69	0
34	NA	0	8523	1/1	0.88	0.12	58,58,58,58	0
34	NA	0	8569	1/1	0.88	0.23	72,72,72,72	0
36	SR	0	9004	1/1	0.88	0.14	200,200,200,200	0
34	NA	0	8544	1/1	0.88	0.12	68,68,68,68	0
32	MG	0	8040	1/1	0.88	0.22	100,100,100,100	0
35	CL	B	8819	1/1	0.88	0.27	68,68,68,68	0
32	MG	0	8085	1/1	0.89	0.24	83,83,83,83	0
34	NA	0	8509	1/1	0.89	0.16	66,66,66,66	0
34	NA	0	8545	1/1	0.89	0.11	40,40,40,40	0
36	SR	A	8993	1/1	0.89	0.06	177,177,177,177	0
35	CL	0	8815	1/1	0.89	0.10	90,90,90,90	0
34	NA	M	8539	1/1	0.89	0.10	34,34,34,34	0
34	NA	0	8530	1/1	0.89	0.20	49,49,49,49	0
34	NA	0	8533	1/1	0.89	0.26	68,68,68,68	0
34	NA	0	8556	1/1	0.89	0.17	95,95,95,95	0
32	MG	0	8063	1/1	0.89	0.18	67,67,67,67	0
34	NA	0	8520	1/1	0.90	0.24	57,57,57,57	0
32	MG	0	8031	1/1	0.90	0.09	71,71,71,71	0
32	MG	0	8029	1/1	0.90	0.17	54,54,54,54	0
36	SR	0	8924	1/1	0.90	0.12	138,138,138,138	0
36	SR	0	8962	1/1	0.90	0.11	155,155,155,155	0
36	SR	0	9002	1/1	0.90	0.09	188,188,188,188	0
36	SR	0	8964	1/1	0.90	0.08	149,149,149,149	0
36	SR	0	8927	1/1	0.90	0.10	172,172,172,172	0
36	SR	0	8933	1/1	0.90	0.10	122,122,122,122	0
36	SR	0	8975	1/1	0.90	0.07	158,158,158,158	0
32	MG	0	8044	1/1	0.90	0.08	49,49,49,49	0
32	MG	0	8068	1/1	0.90	0.07	49,49,49,49	0
36	SR	0	8978	1/1	0.90	0.07	130,130,130,130	0
35	CL	L	8810	1/1	0.90	0.11	86,86,86,86	0
36	SR	3	8932	1/1	0.90	0.19	149,149,149,149	0
35	CL	0	8811	1/1	0.90	0.19	99,99,99,99	0
36	SR	0	8989	1/1	0.90	0.17	196,196,196,196	0
32	MG	0	8089	1/1	0.90	0.10	72,72,72,72	0
34	NA	0	8561	1/1	0.91	0.25	73,73,73,73	0
32	MG	0	8092	1/1	0.91	0.06	53,53,53,53	0
36	SR	0	8919	1/1	0.91	0.18	194,194,194,194	0
32	MG	0	8064	1/1	0.91	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8979	1/1	0.91	0.07	200,200,200,200	0
34	NA	0	8548	1/1	0.91	0.21	52,52,52,52	0
34	NA	0	8531	1/1	0.91	0.23	42,42,42,42	0
36	SR	B	8950	1/1	0.91	0.13	151,151,151,151	0
32	MG	0	8077	1/1	0.91	0.16	47,47,47,47	0
36	SR	0	8960	1/1	0.91	0.07	174,174,174,174	0
34	NA	0	8535	1/1	0.91	0.20	45,45,45,45	0
34	NA	0	8526	1/1	0.91	0.05	52,52,52,52	0
32	MG	0	8055	1/1	0.91	0.10	67,67,67,67	0
36	SR	0	8998	1/1	0.91	0.35	169,169,169,169	0
36	SR	0	8944	1/1	0.91	0.09	171,171,171,171	0
38	CD	3	8704	1/1	0.91	0.39	176,176,176,176	0
32	MG	0	8080	1/1	0.92	0.08	98,98,98,98	0
32	MG	0	8034	1/1	0.92	0.11	43,43,43,43	0
34	NA	0	8547	1/1	0.92	0.27	81,81,81,81	0
36	SR	0	8974	1/1	0.92	0.15	191,191,191,191	0
32	MG	0	8043	1/1	0.92	0.08	55,55,55,55	0
34	NA	0	8550	1/1	0.92	0.24	98,98,98,98	0
34	NA	0	8551	1/1	0.92	0.20	81,81,81,81	0
34	NA	0	8505	1/1	0.92	0.27	56,56,56,56	0
34	NA	0	8554	1/1	0.92	0.24	71,71,71,71	0
32	MG	A	8051	1/1	0.92	0.11	90,90,90,90	0
32	MG	0	8087	1/1	0.92	0.19	20,20,20,20	0
35	CL	M	8818	1/1	0.92	0.10	73,73,73,73	0
32	MG	2	8060	1/1	0.92	0.05	56,56,56,56	0
34	NA	0	8558	1/1	0.92	0.21	50,50,50,50	0
34	NA	0	8514	1/1	0.92	0.39	61,61,61,61	0
34	NA	0	8560	1/1	0.92	0.12	64,64,64,64	0
34	NA	0	8542	1/1	0.92	0.26	51,51,51,51	0
34	NA	0	8563	1/1	0.93	0.30	74,74,74,74	0
34	NA	0	8529	1/1	0.93	0.11	49,49,49,49	0
36	SR	0	8954	1/1	0.93	0.06	122,122,122,122	0
35	CL	0	8814	1/1	0.93	0.42	67,67,67,67	0
36	SR	0	8928	1/1	0.93	0.08	164,164,164,164	0
36	SR	0	8982	1/1	0.93	0.14	200,200,200,200	0
34	NA	0	8508	1/1	0.93	0.18	70,70,70,70	0
36	SR	0	8936	1/1	0.93	0.07	109,109,109,109	0
34	NA	0	8521	1/1	0.93	0.05	34,34,34,34	0
36	SR	0	8939	1/1	0.93	0.11	145,145,145,145	0
36	SR	0	8941	1/1	0.93	0.09	143,143,143,143	0
34	NA	C	8503	1/1	0.93	0.08	39,39,39,39	0
36	SR	0	8996	1/1	0.93	0.11	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8968	1/1	0.93	0.07	181,181,181,181	0
32	MG	0	8059	1/1	0.93	0.08	40,40,40,40	0
35	CL	0	8803	1/1	0.93	0.08	66,66,66,66	0
36	SR	0	8915	1/1	0.94	0.06	125,125,125,125	0
34	NA	0	8536	1/1	0.94	0.11	72,72,72,72	0
36	SR	0	8917	1/1	0.94	0.09	121,121,121,121	0
32	MG	0	8071	1/1	0.94	0.30	50,50,50,50	0
36	SR	0	8973	1/1	0.94	0.06	134,134,134,134	0
36	SR	0	8945	1/1	0.94	0.08	111,111,111,111	0
36	SR	0	8946	1/1	0.94	0.08	138,138,138,138	0
32	MG	0	8081	1/1	0.94	0.18	104,104,104,104	0
36	SR	0	8949	1/1	0.94	0.07	120,120,120,120	0
32	MG	0	8033	1/1	0.94	0.12	56,56,56,56	0
32	MG	0	8032	1/1	0.94	0.06	64,64,64,64	0
36	SR	0	8926	1/1	0.94	0.07	145,145,145,145	0
34	NA	0	8517	1/1	0.94	0.08	30,30,30,30	0
36	SR	F	9005	1/1	0.94	0.09	154,154,154,154	0
36	SR	H	8972	1/1	0.94	0.12	157,157,157,157	0
36	SR	0	8984	1/1	0.94	0.05	139,139,139,139	0
32	MG	0	8049	1/1	0.94	0.06	61,61,61,61	0
36	SR	0	8931	1/1	0.94	0.06	123,123,123,123	0
34	NA	0	8567	1/1	0.94	0.09	58,58,58,58	0
36	SR	0	8992	1/1	0.94	0.11	149,149,149,149	0
35	CL	R	8806	1/1	0.94	0.06	62,62,62,62	0
38	CD	Z	8703	1/1	0.94	0.23	155,155,155,155	0
32	MG	T	8057	1/1	0.94	0.07	67,67,67,67	0
35	CL	O	8808	1/1	0.95	0.12	98,98,98,98	0
36	SR	0	8935	1/1	0.95	0.06	106,106,106,106	0
36	SR	0	8963	1/1	0.95	0.05	135,135,135,135	0
32	MG	0	8056	1/1	0.95	0.07	47,47,47,47	0
36	SR	0	8966	1/1	0.95	0.06	110,110,110,110	0
36	SR	0	8937	1/1	0.95	0.07	108,108,108,108	0
35	CL	0	8812	1/1	0.95	0.13	58,58,58,58	0
36	SR	0	8901	1/1	0.95	0.06	89,89,89,89	0
36	SR	0	8908	1/1	0.95	0.06	109,109,109,109	0
36	SR	0	8910	1/1	0.95	0.07	113,113,113,113	0
34	NA	J	8538	1/1	0.95	0.12	45,45,45,45	0
32	MG	0	8030	1/1	0.95	0.17	60,60,60,60	0
32	MG	Y	8086	1/1	0.95	0.05	55,55,55,55	0
32	MG	0	8061	1/1	0.95	0.10	42,42,42,42	0
32	MG	0	8017	1/1	0.95	0.08	29,29,29,29	0
33	K	0	8402	1/1	0.95	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8923	1/1	0.95	0.05	120,120,120,120	0
35	CL	J	8801	1/1	0.95	0.06	90,90,90,90	0
36	SR	0	8985	1/1	0.95	0.06	173,173,173,173	0
34	NA	0	8512	1/1	0.95	0.24	49,49,49,49	0
36	SR	0	8956	1/1	0.95	0.09	178,178,178,178	0
34	NA	0	8513	1/1	0.95	0.38	63,63,63,63	0
37	MUL	0	9101	34/34	0.95	0.14	85,87,104,104	0
32	MG	0	8010	1/1	0.95	0.06	35,35,35,35	0
34	NA	0	8552	1/1	0.95	0.12	68,68,68,68	0
32	MG	0	8091	1/1	0.96	0.04	42,42,42,42	0
32	MG	0	8053	1/1	0.96	0.05	57,57,57,57	0
34	NA	0	8565	1/1	0.96	0.25	106,106,106,106	0
35	CL	0	8813	1/1	0.96	0.07	68,68,68,68	0
34	NA	0	8546	1/1	0.96	0.18	69,69,69,69	0
36	SR	R	8912	1/1	0.96	0.07	106,106,106,106	0
36	SR	1	8913	1/1	0.96	0.05	97,97,97,97	0
36	SR	1	8952	1/1	0.96	0.05	81,81,81,81	0
36	SR	0	8925	1/1	0.96	0.04	105,105,105,105	0
32	MG	0	8079	1/1	0.96	0.10	63,63,63,63	0
34	NA	0	8516	1/1	0.96	0.18	26,26,26,26	0
36	SR	A	8929	1/1	0.96	0.16	157,157,157,157	0
36	SR	0	8965	1/1	0.96	0.07	135,135,135,135	0
32	MG	0	8020	1/1	0.96	0.11	52,52,52,52	0
36	SR	0	8981	1/1	0.96	0.10	151,151,151,151	0
34	NA	0	8549	1/1	0.97	0.23	83,83,83,83	0
35	CL	Y	8820	1/1	0.97	0.05	59,59,59,59	0
32	MG	0	8015	1/1	0.97	0.04	25,25,25,25	0
32	MG	0	8067	1/1	0.97	0.13	42,42,42,42	0
36	SR	0	8907	1/1	0.97	0.06	63,63,63,63	0
34	NA	0	8515	1/1	0.97	0.04	45,45,45,45	0
36	SR	0	8970	1/1	0.97	0.06	150,150,150,150	0
36	SR	0	8940	1/1	0.97	0.09	117,117,117,117	0
36	SR	0	8909	1/1	0.97	0.04	89,89,89,89	0
32	MG	0	8048	1/1	0.97	0.08	38,38,38,38	0
36	SR	0	8943	1/1	0.97	0.09	99,99,99,99	0
36	SR	0	8914	1/1	0.97	0.10	130,130,130,130	0
32	MG	0	8069	1/1	0.97	0.09	68,68,68,68	0
34	NA	0	8534	1/1	0.97	0.13	45,45,45,45	0
32	MG	0	8027	1/1	0.97	0.04	30,30,30,30	0
36	SR	0	8948	1/1	0.97	0.05	104,104,104,104	0
35	CL	0	8817	1/1	0.97	0.07	63,63,63,63	0
32	MG	0	8062	1/1	0.97	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	S	8961	1/1	0.97	0.04	127,127,127,127	0
36	SR	0	8921	1/1	0.97	0.04	90,90,90,90	0
32	MG	0	8014	1/1	0.97	0.07	30,30,30,30	0
32	MG	0	8076	1/1	0.97	0.05	36,36,36,36	0
32	MG	0	8046	1/1	0.97	0.08	48,48,48,48	0
34	NA	0	8507	1/1	0.97	0.09	39,39,39,39	0
32	MG	0	8093	1/1	0.97	0.04	40,40,40,40	0
32	MG	0	8078	1/1	0.97	0.08	64,64,64,64	0
32	MG	0	8065	1/1	0.97	0.06	41,41,41,41	0
32	MG	K	8054	1/1	0.97	0.03	32,32,32,32	0
32	MG	0	8023	1/1	0.98	0.05	21,21,21,21	0
32	MG	0	8035	1/1	0.98	0.07	47,47,47,47	0
35	CL	J	8821	1/1	0.98	0.07	70,70,70,70	0
32	MG	0	8052	1/1	0.98	0.03	40,40,40,40	0
32	MG	0	8070	1/1	0.98	0.05	54,54,54,54	0
32	MG	0	8024	1/1	0.98	0.07	58,58,58,58	0
32	MG	0	8025	1/1	0.98	0.05	44,44,44,44	0
32	MG	0	8026	1/1	0.98	0.04	32,32,32,32	0
32	MG	A	8050	1/1	0.98	0.04	52,52,52,52	0
32	MG	0	8075	1/1	0.98	0.03	40,40,40,40	0
32	MG	0	8006	1/1	0.98	0.05	62,62,62,62	0
36	SR	0	8902	1/1	0.98	0.03	63,63,63,63	0
36	SR	0	8903	1/1	0.98	0.10	62,62,62,62	0
36	SR	0	8905	1/1	0.98	0.10	70,70,70,70	0
36	SR	0	8990	1/1	0.98	0.06	111,111,111,111	0
36	SR	0	8906	1/1	0.98	0.04	65,65,65,65	0
32	MG	0	8016	1/1	0.98	0.06	38,38,38,38	0
32	MG	0	8041	1/1	0.98	0.03	27,27,27,27	0
32	MG	0	8004	1/1	0.98	0.06	32,32,32,32	0
32	MG	0	8018	1/1	0.98	0.04	42,42,42,42	0
36	SR	0	8911	1/1	0.98	0.04	109,109,109,109	0
32	MG	0	8005	1/1	0.98	0.15	30,30,30,30	0
38	CD	O	8705	1/1	0.98	0.12	115,115,115,115	0
32	MG	0	8022	1/1	0.98	0.05	29,29,29,29	0
32	MG	0	8084	1/1	0.98	0.12	50,50,50,50	0
32	MG	C	8012	1/1	0.99	0.03	19,19,19,19	0
32	MG	0	8001	1/1	0.99	0.03	28,28,28,28	0
32	MG	0	8013	1/1	0.99	0.03	21,21,21,21	0
36	SR	0	8934	1/1	0.99	0.04	114,114,114,114	0
32	MG	0	8002	1/1	0.99	0.05	26,26,26,26	0
32	MG	0	8088	1/1	0.99	0.04	39,39,39,39	0
32	MG	0	8003	1/1	0.99	0.05	31,31,31,31	0

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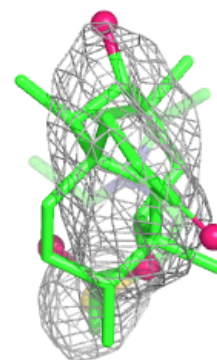
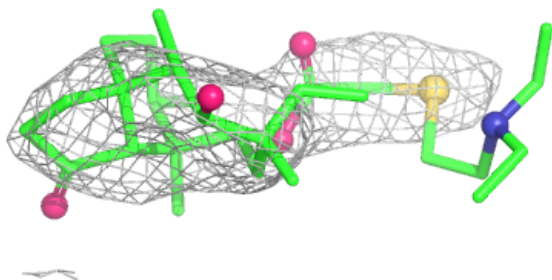
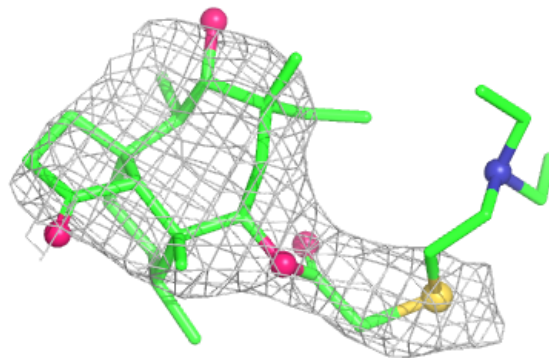
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8918	1/1	0.99	0.03	84,84,84,84	0
32	MG	0	8007	1/1	0.99	0.02	10,10,10,10	0
32	MG	0	8008	1/1	0.99	0.04	15,15,15,15	0
32	MG	0	8009	1/1	0.99	0.11	28,28,28,28	0
36	SR	0	8904	1/1	0.99	0.03	64,64,64,64	0
34	NA	0	8504	1/1	0.99	0.02	22,22,22,22	0
32	MG	0	8058	1/1	0.99	0.05	25,25,25,25	0
36	SR	0	9008	1/1	0.99	0.04	99,99,99,99	0
32	MG	0	8045	1/1	0.99	0.06	44,44,44,44	0
38	CD	U	8701	1/1	0.99	0.04	104,104,104,104	0
32	MG	0	8028	1/1	0.99	0.03	14,14,14,14	0
38	CD	1	8702	1/1	0.99	0.03	68,68,68,68	0
32	MG	0	8083	1/1	0.99	0.07	59,59,59,59	0
32	MG	0	8019	1/1	1.00	0.02	10,10,10,10	0
32	MG	0	8011	1/1	1.00	0.04	18,18,18,18	0
32	MG	0	8021	1/1	1.00	0.06	28,28,28,28	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.

Electron density around MUL 0 9101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.