



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 06:49 AM UTC

PDB ID : 4WF9 / pdb_00004wf9
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with telithromycin
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on : 2014-09-14
Resolution : 3.43 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

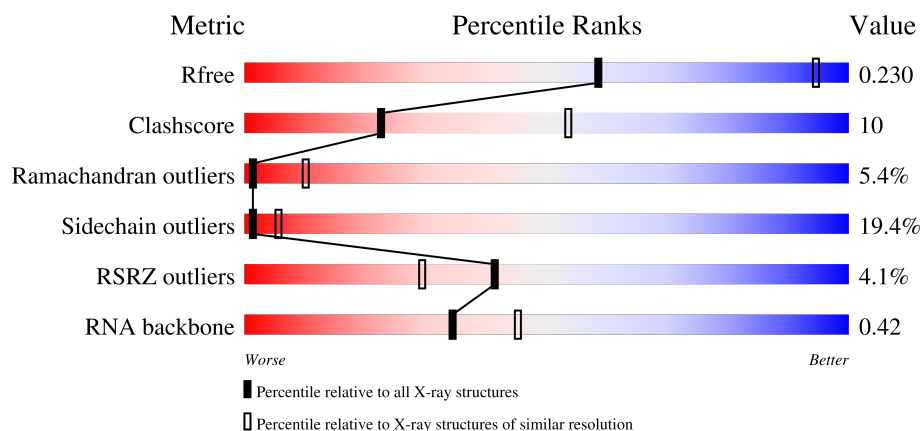
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

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	X	2923	
2	Y	114	
3	A	277	

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Mol	Chain	Length	Quality of chain
4	B	220	
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	V	69	
23	W	59	
24	Z	58	
25	2	45	
26	3	66	

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
27	TEL	X	3001	X	-	-	-
28	MPD	X	3005	-	-	X	-
29	MG	X	3229	-	-	-	X
32	EOH	X	3367	-	-	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 81033 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	X	2712	Total	C	N	O	P	0	0	0
			58145	25958	10650	18825	2712			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	269	Total	C	N	O	S	0	0	0
			1640	995	319	321	5			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1566	980	291	290	5			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	200	Total	C	N	O	S	0	0	0
			1314	812	250	250	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	160	Total	C	N	O	S	0	0	0
			823	498	160	164	1			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			930	575	173	181	1			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1105	691	205	206	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			877	542	166	165	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			830	503	164	162	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1054	673	196	181	4			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			900	554	174	171	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	0	0	0
			667	405	134	128			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O			
			834	526	167	141	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S		
			929	584	188	153	4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S		
			756	481	138	136	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S		
			856	534	161	158	3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S		
			600	375	107	116	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	101	Total	C	N	O	S		
			609	373	111	124	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S		
			1082	680	192	208	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			541	336	101	104			

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	63	Total	C	N	O	0	0	0
			416	256	75	85			

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Z	45	Total	C	N	O	S	0	0	0
			352	215	73	60	4			

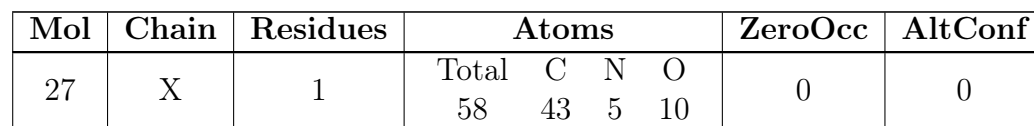
- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	60	Total	C	N	O	S	0	0	0
			390	239	77	72	2			

- Molecule 27 is TELITHROMYCIN (CCD ID: TEL) (formula: C₄₃H₆₅N₅O₁₀).



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- The chemical structure of 2-methylpentane-2,4-diol (MPD) is shown. The molecule consists of a five-carbon chain. The second carbon (C2) is bonded to a methyl group (CM) and a hydroxyl group (OH, labeled O2). The fourth carbon (C4) is bonded to a hydroxyl group (OH, labeled O4) and a methyl group (C5). The third carbon (C3) is bonded to the second and fourth carbons. The labels C1, C2, C3, C4(S), and C5 are in green. The labels OH and O2 are in red. The label CM is in green. The label MPD is in black at the top.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	X	136	Total	Mg	0	0
			136	136		
29	Y	4	Total	Mg	0	0
			4	4		
29	A	1	Total	Mg	0	0
			1	1		
29	B	1	Total	Mg	0	0
			1	1		
29	C	3	Total	Mg	0	0
			3	3		
29	G	1	Total	Mg	0	0
			1	1		
29	O	1	Total	Mg	0	0
			1	1		
29	R	1	Total	Mg	0	0
			1	1		
29	T	1	Total	Mg	0	0
			1	1		

- Molecule 30 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

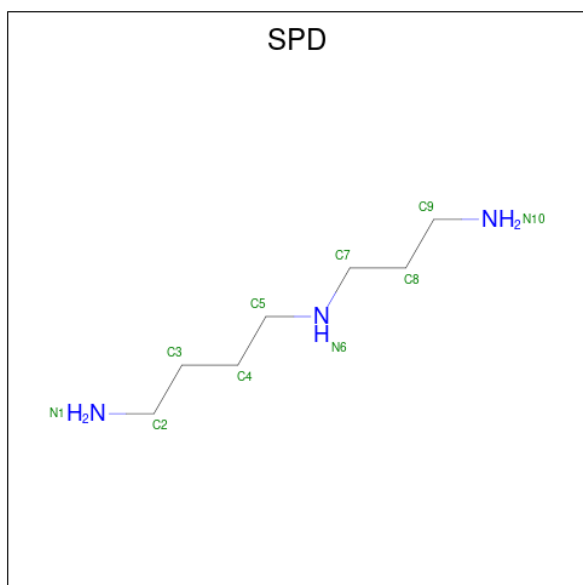
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	221	Total	Mn	0	0
			221	221		
30	Y	6	Total	Mn	0	0
			6	6		
30	I	2	Total	Mn	0	0
			2	2		

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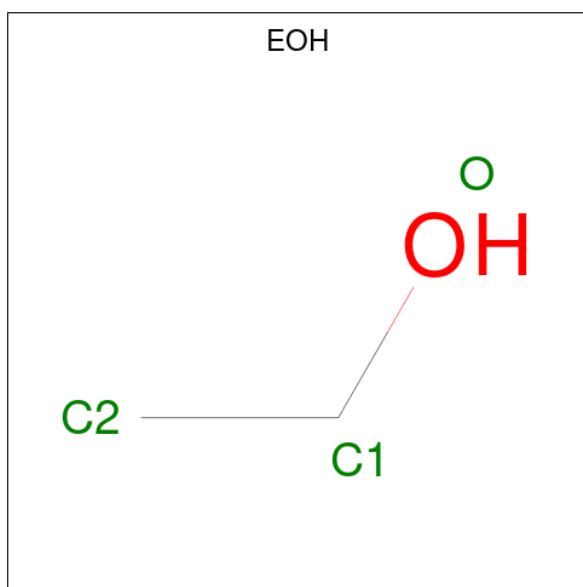
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	1	Total	Mn	0	0
			1	1		
30	M	1	Total	Mn	0	0
			1	1		

- Molecule 31 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



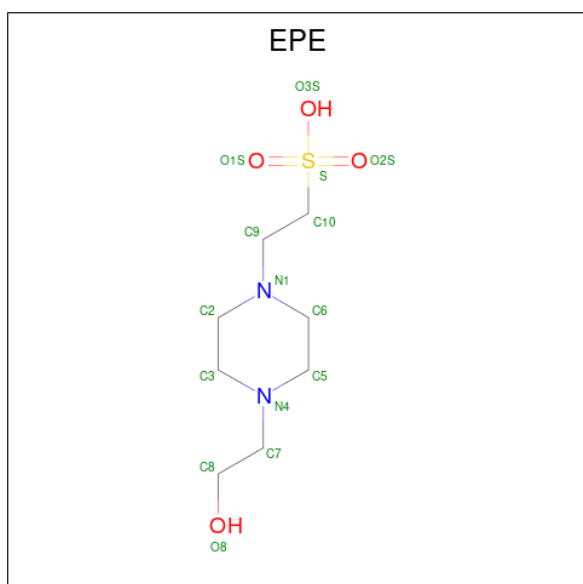
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	S	1	Total	C	N	0	0
			10	7	3		

- Molecule 32 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			3	2	1		
32	X	1	Total	C	O	0	0
			3	2	1		
32	X	1	Total	C	O	0	0
			3	2	1		

- Molecule 33 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

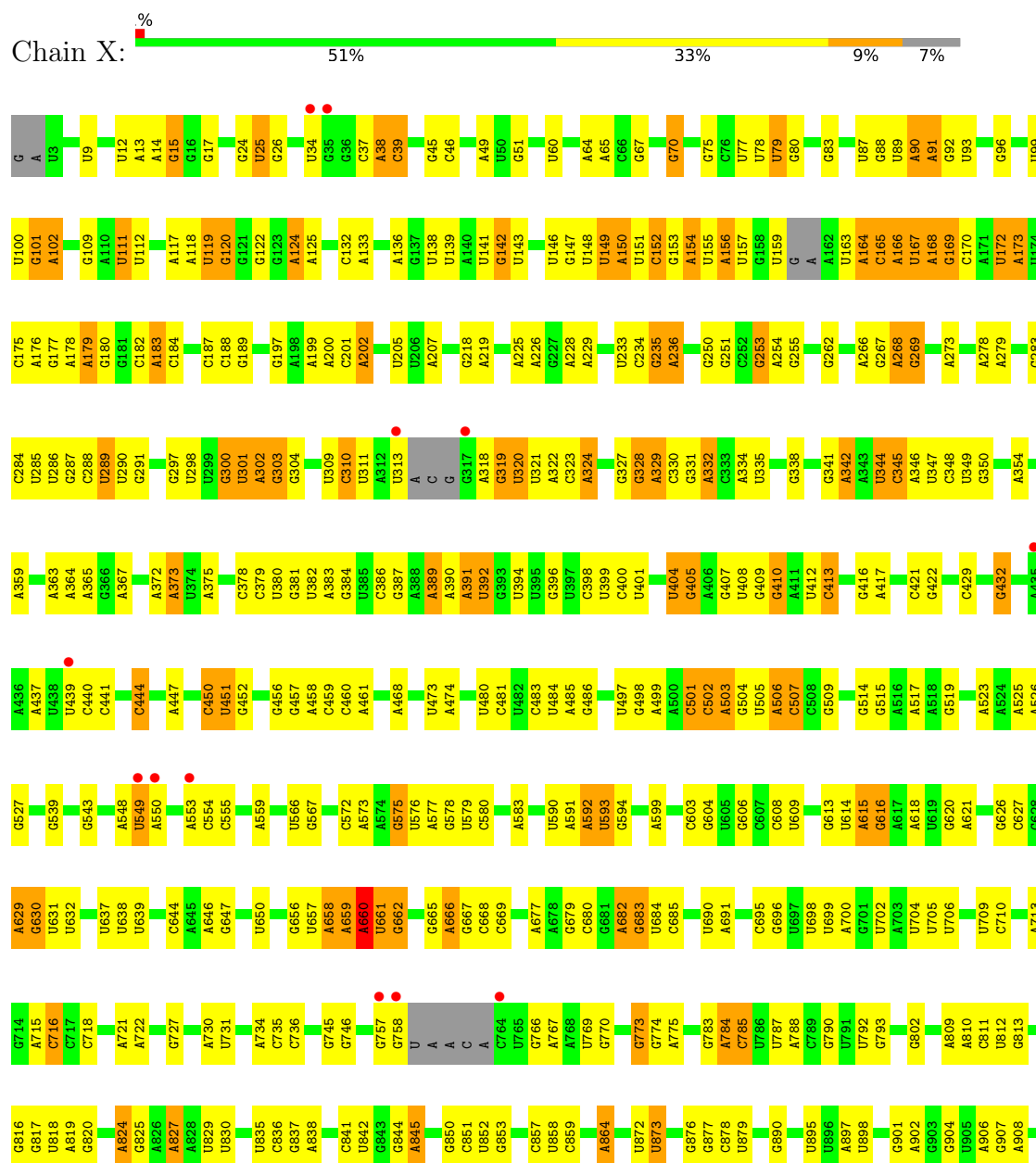


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

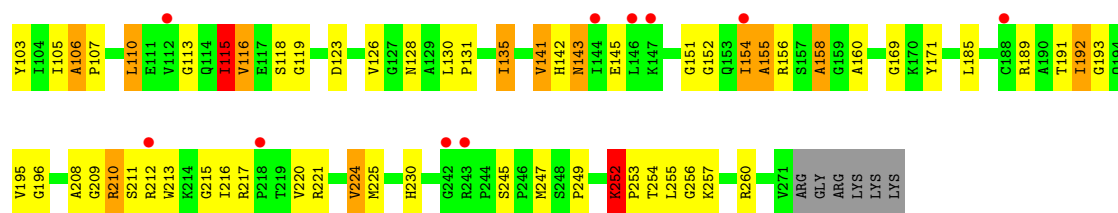
3 Residue-property plots

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.

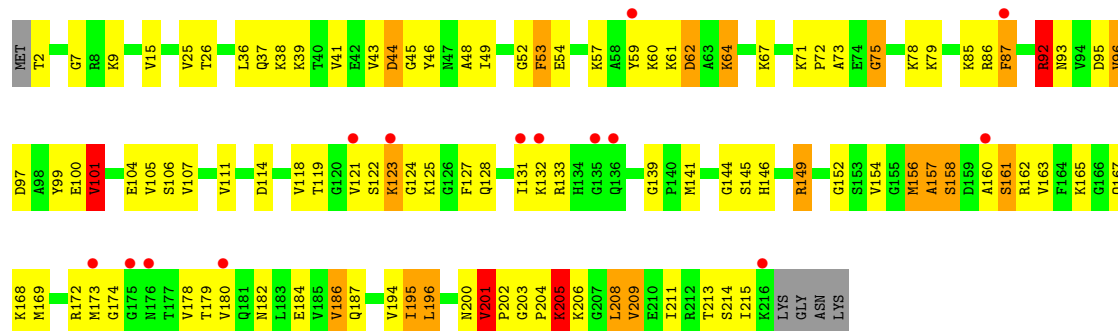
• Molecule 1: 23S ribosomal RNA



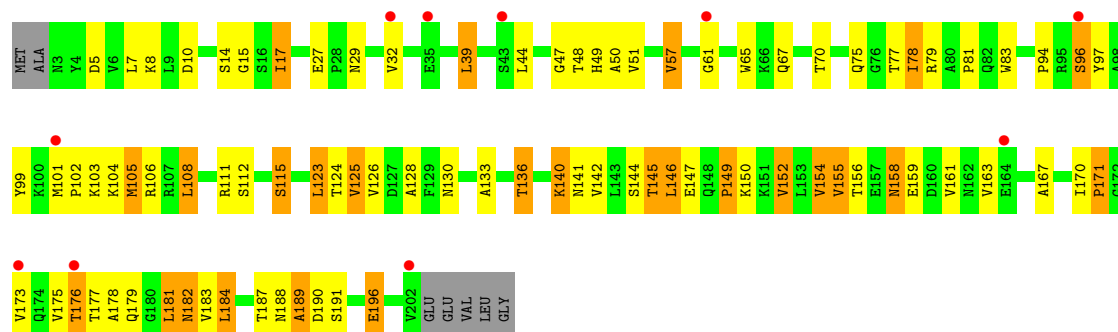
U2009	A1911	C1833	U1755	A1653	C	G1518	U	C1382	G1278	C1178	U	G	A911
C2017	A1912	G1834	U1756	A1654	A	U1519	U	G1383	C1279	C1179	G	G	C921
U2020	G1930	U	U1757	A1658	U	A	U	G1384	U1280	U1185	C	C	G922
C2023	G1931	A1836	U1758	A1659	G	G1521	A	G1385	U1281	U1186	U	U	A923
A2024	G1932	G1837	G1759	A1662	U	G1522	U1460	A1391	A1285	A1186	U	A	G924
G2025	G1933	G1838	G1760	A1669	C	C1523	G1461	G1392	G1286	A1195	A	A	G925
C2026	G1934	U1840	U1761	A1670	U	U1525	G1462	G1395	A1289	C1196	G	G	G926
G2037	G1935	G1841	U1762	A1675	C	G1526	U1463	G1398	G1290	C1197	A	A	G
A2040	C1936	U1842	G1766	U1674	U	G1527	U1464	G1399	G1291	A1199	A	A	C
U2043	U	U1843	G1767	G1675	U	U1528	U1465	G1400	A1292	C1206	C	C	C
C2044	A	U1844	G1768	A1676	C	A1530	G1466	G1401	G1294	A1200	A	A	C
U2047	U	U1845	C1770	A1592	G	U1531	G1468	A1402	G1294	G1206	G	G	U
G2048	C	A1848	A1771	G1593	U	U	G1469	A1405	G1300	G1207	C	C	U
A2050	U	G1849	G1772	U1594	A	A	G1470	G1406	U1301	G1208	C	C	U
C2051	U	A1773	A1773	C1595	G	G	A1471	G1408	G1302	A1034	U	U	C
U2052	A	U1774	U1774	G1596	C	C	C1472	U1409	U1209	A1037	A	A	C
G2053	A	G1855	G1775	U1597	A	A	G1473	U1410	U1210	C1038	C	C	C
A2054	C	U1856	A1776	U1598	A	A	C1474	U1411	U1211	C1039	U	U	C
C2055	G	C1857	G1780	G1601	U	U1539	U1475	G1412	U1212	A1040	A	A	C
U2056	U	G1882	C1781	U1602	A	U1540	U1476	G1413	C1213	C1049	C	C	U
G2057	C	U1883	G1789	U1603	C	G1541	A1477	G1414	C1214	C1055	U	U	U
A2058	U	G1884	G1790	C1604	U	C1542	A1478	G1415	G1309	A1056	A	A	C
C2059	A	U1885	G1791	A1605	G	G1543	U1482	U1416	A1310	A1057	A	A	C
U2060	C	G1886	C1792	G1606	A	G1544	A1483	G1417	A1311	U1066	C	C	C
G2061	G	U1887	G1793	A1607	U	U1545	U1486	G1418	A1312	A1064	C	C	C
A2062	U	G1888	C1794	G1612	U	A1546	C1487	G1419	A1313	A1065	U	U	C
C2063	C	U1889	U1795	G1613	A	C1547	U1488	U1420	A1314	G1066	A	A	C
U2064	U	A1890	A1796	U1614	U	G1550	A1489	A1421	C1332	C	C	C	C
G2065	A	G1891	A1800	G1615	A	U1551	G1490	A1422	A1333	G	G	G	C
A2066	C	U1892	U1806	A1616	U	A	C1491	C1423	G1234	U	U	U	C
C2067	U	G1893	U1807	A1617	A	U1552	G1492	A1424	U1238	A	A	A	C
U2068	C	U1894	U1808	U1623	U	G1553	G1493	G1425	A1241	U	U	U	C
A2069	U	G1895	U1809	C1624	A	G1554	G1494	G1426	A1242	A	A	A	C
C2070	C	U1896	G1815	U1625	U	G1555	G1495	G1429	G	C	C	C	C
U2071	U	U1897	C1816	C1626	U	U1556	G1496	A1430	C1144	U	U	U	C
A2072	C	U1898	A1817	G1627	A	U1557	A1497	U1431	U1145	C967	U	U	C
C2073	U	G1899	U1818	U1628	U	U1558	U1498	A1432	A968	A968	A	A	C
U2074	C	U1900	U1819	A1629	U	A1559	U1499	U1433	A969	U970	U	U	C
A2075	U	G1901	G1820	U1630	A	C1561	G1500	U1434	U1147	U971	C	C	C
C2076	C	U1902	G1821	G1631	U	U1562	G1501	C1435	C1148	A972	A	A	C
U2077	U	U1903	U1822	A1632	A	G1563	U1502	U1436	C1087	A973	C	C	C
A2078	C	G1904	C1823	U1635	U	G1564	U1503	C1437	C1088	U974	C	C	C
C2079	U	U1905	U1824	U1636	U	G1565	G1504	U1438	C1089	U975	U	U	C
U2080	C	G1906	G1825	U1637	A	G1566	C1505	U1439	A1090	A976	C	C	C
A2081	U	U1907	U1826	A1638	U	U1567	U1506	A1440	A1155	A977	A	A	C
C2082	C	U1908	U1827	U1639	U	U1568	U1507	U1441	G1156	A985	C	C	C
U2083	U	G1909	G1828	G1640	U	G1569	C1508	U1442	A1161	G986	U	U	C
A2084	C	U1910	U1829	U1643	U	U1570	G1509	A1443	U1097	U989	C	C	C
C2085	U	U1911	U1830	G1643	U	G1571	C1510	U1444	A1098	G990	A	A	C
U2086	C	G1912	A1831	G1650	U	U1572	U1511	U1445	G1169	G997	U	U	C
A2087	U	U1913	U1832	C1651	U	G1573	C1512	A1446	A1170	U	U	U	C
C2088	C	U1914	U1833	U1652	U	U1574	U1513	U1447	U1174	G	G	G	C
U2089	U	G1915	G1834	U1653	U	A1575	A1514	U1448	G1175	A	A	A	C
A2090	C	U1916	U1835	G1654	U	U1576	U1515	U1449	U1176	U	U	U	C
C2091	U	U1917	U1836	U1655	U	U1577	C1516	U1450	C1277	U	U	U	C
U2092	C	G1918	U1837	U1656	U	A1578	U1517	U1451	U	U	U	U	C
A2093	U	U1919	U1838	U1657	U	U1579	U1518	U1452	U	U	U	U	C
C2094	C	U1920	U1839	U1658	U	U1580	U1519	U1453	U	U	U	U	C
U2095	U	G1921	U1840	U1659	U	U1581	U1520	U1454	U	U	U	U	C
A2096	C	U1922	U1841	U1660	U	U1582	U1521	U1455	U	U	U	U	C
C2097	U	U1923	U1842	U1661	U	U1583	U1522	U1456	U	U	U	U	C
U2101	C	G1924	U1843	U1662	U	U1584	U1523	U1457	U	U	U	U	C
A2102	U	U1925	U1844	U1663	U	U1585	U1524	U1458	U	U	U	U	C
G2103	C	U1926	U1845	U1664	U	U1586	U1525	U1459	U	U	U	U	C
C2104	U	G1927	U1846	U1665	U	U1587	U1526	U1460	U	U	U	U	C
U2105	C	U1928	U1847	U1666	U	U1588	U1527	U1461	U	U	U	U	C
A2106	U	U1929	U1848	U1667	U	U1589	U1528	U1462	U	U	U	U	C
C2107	C	G1930	U1849	U1668	U	U1590	U1529	U1463	U	U	U	U	C
U2108	U	U1931	G1900	U1669	U	U1591	U1530	U1464	U	U	U	U	C
A2109	C	U1932	U1901	U1670	U	U1592	U1531	U1465	U	U	U	U	C
C2110	U	G1933	G1902	U1671	U	U1593	U1532	U1466	U	U	U	U	C
U2111	C	U1934	U1903	U1672	U	U1594	U1533	U1467	U	U	U	U	C
A2112	U	U1935	U1904	U1673	U	U1595	U1534	U1468	U	U	U	U	C
C2113	C	G1936	U1905	U1674	U	U1596	U1535	U1469	U	U	U	U	C
U2114	U	U1937	U1906	U1675	U	U1597	U1536	U1470	U	U	U	U	C
A2115	C	G1938	U1907	U1676	U	U1598	U1537	U1471	U	U	U	U	C
C2116	U	U1939	U1908	U1677	U	U1599	U1538	U1472	U	U	U	U	C
U2117	C	G1940	U1909	U1678	U	U1600	U1539	U1473	U	U	U	U	C
A2118	U	U1941	U1910	U1679	U	U1601	U1540	U1474	U	U	U	U	C
C2119	C	G1942	U1911	U1680	U	U1602	U1541	U1475	U	U	U	U	C
U2120	U	U1943	U1912	U1681	U	U1603	U1542	U1476	U	U	U	U	C
A2121	C	G1944	U1913	U1682	U	U1604	U1543	U1477	U	U	U	U	C
C2122	U	U1945	U1914	U1683	U	U1605	U1544	U1478	U	U	U	U	C
U2123	C	G1946	U1915	U1684	U	U1606	U1545	U1479	U	U	U	U	C
A2124	U	U1947	U1916	U1685	U	U1607	U1546	U1480	U	U	U	U	C
C2125	C	G1948	U1917	U1686	U	U1608	U1547	U1481	U	U	U	U	C
U2126	U	U1949	U1918	U1687	U	U1609	U1548	U1482	U	U	U	U	C
A2127	C	G1950	U1919	U1688	U	U1610	U1549	U1483	U	U	U	U	C
C2128	U	U1951	U1920	U1689	U	U1611	U1550	U1484	U	U	U	U	C
U2129	C	G1952	U1921	U1690	U	U1612	U1551	U1485	U	U	U	U	C
A2130	U	U1953	U1922	U1691	U	U1613	U1552	U1486	U	U	U	U	C
C2131	C	G1954	U1923	U1692	U	U1614	U1553	U1487	U	U	U	U	C
U2132	U	U1955	U1924	U1693	U	U1615	U1554	U1488	U	U	U	U	C
A2133	C	G1956	U1925	U1694	U	U1616	U1555	U1489	U	U	U	U	C
C2134	U	U1957	U1926	U1695	U	U1617	U1556	U1490	U	U	U	U	C
U2135	C	G1958	U1927	U1696	U	U1618	U1557	U1491	U	U	U	U	C
A2136	U	U1959	U1928	U1697	U	U1619	U1558	U1492	U	U	U	U	C
C2137	C	G1960	U1929	U1698	U	U1620	U1559	U1493	U	U	U	U	C
U2138	U	U1961	U1930	U1699	U	U1621	U1560	U1494	U	U	U	U	C
A2139	C	G1962	U1931	U1700	U	U1622	U1561	U1495	U	U	U	U	C
C2140	U	U1963	U1932	U1701	U	U1623	U1562	U1496	U	U	U	U	C
U2141	C	G1964	U1933	U1702	U	U1624	U1563	U1497	U	U	U	U	C
A2142	U	U1965	U1934	U1703	U	U1625	U1564	U1498	U	U	U	U	C
C2143	C	G1966	U1935	U1704	U	U1626	U1565	U1499	U	U	U	U	C
U2144	U	U1967	U1936	U1705	U	U1627	U1566	U1500	U	U	U	U	C
A2145	C	G1968	U1937	U1706	U	U1628	U1567	U1501	U	U	U	U	C
C2146	U	U1969	U1938	U1707	U	U1629	U1568	U1502	U	U	U	U	C
U2147	C	G1970	U1939	U1708	U	U1630	U1569	U1503	U	U	U	U	C



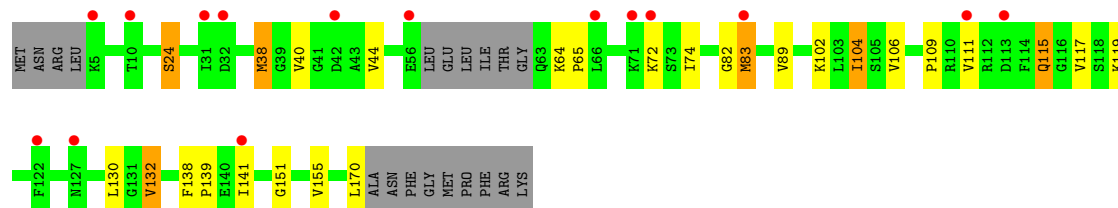
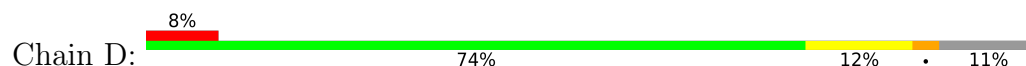
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

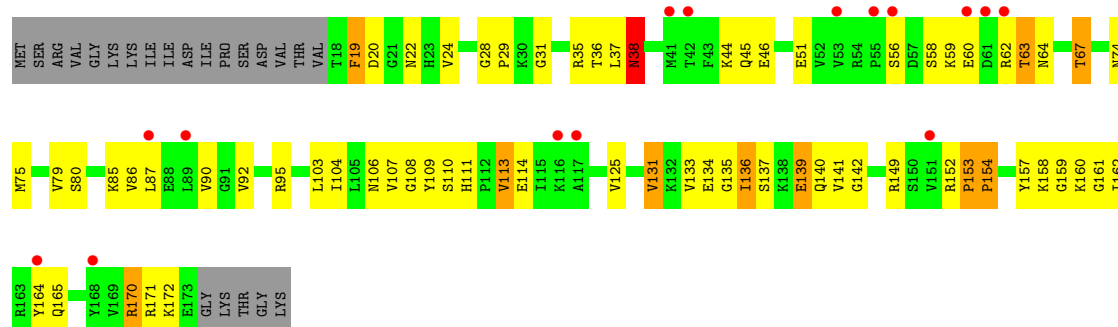


• Molecule 6: 50S ribosomal protein L5

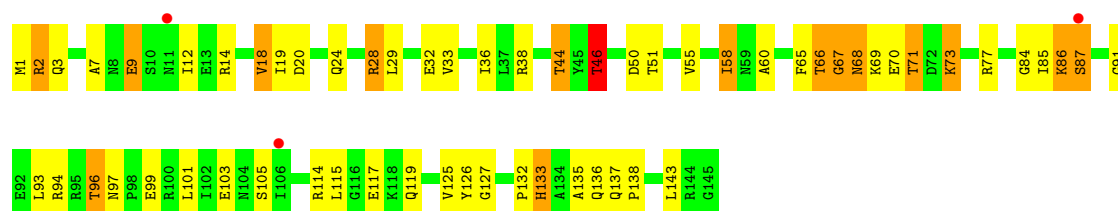


• Molecule 7: 50S ribosomal protein L6

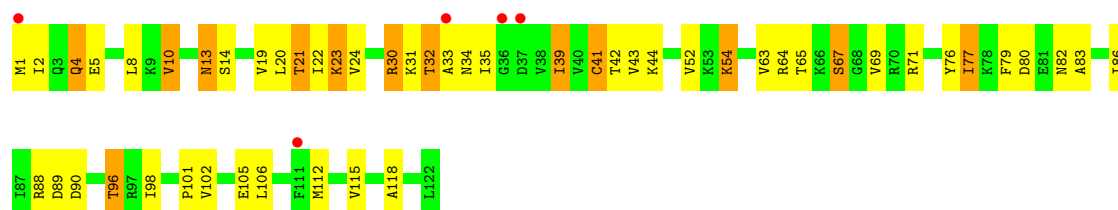




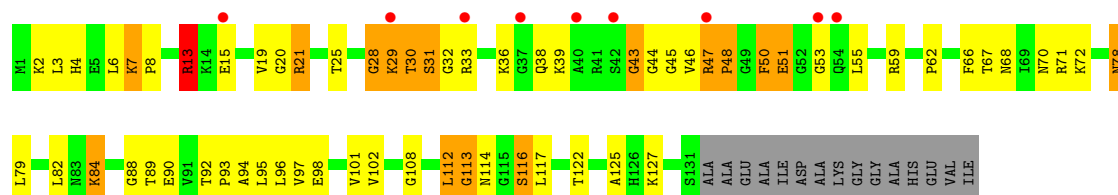
• Molecule 8: 50S ribosomal protein L13



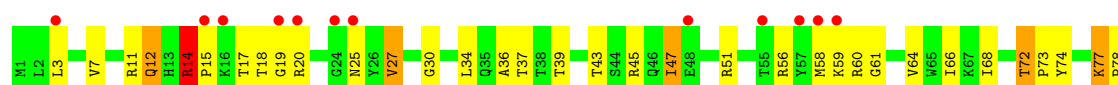
• Molecule 9: 50S ribosomal protein L14

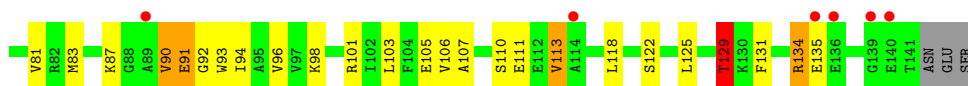


• Molecule 10: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L16

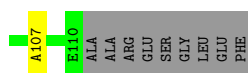




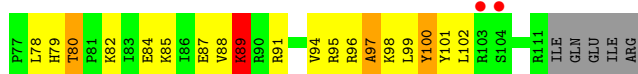
• Molecule 12: 50S ribosomal protein L17



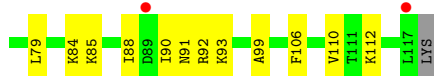
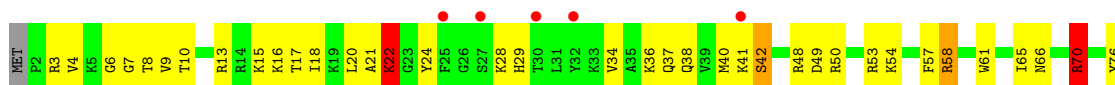
• Molecule 13: 50S ribosomal protein L18



• Molecule 14: 50S ribosomal protein L19

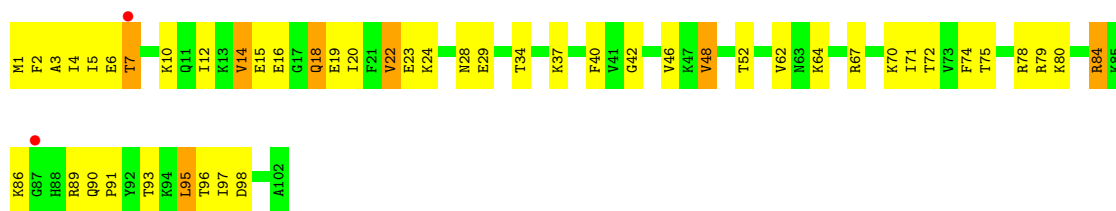


• Molecule 15: 50S ribosomal protein L20

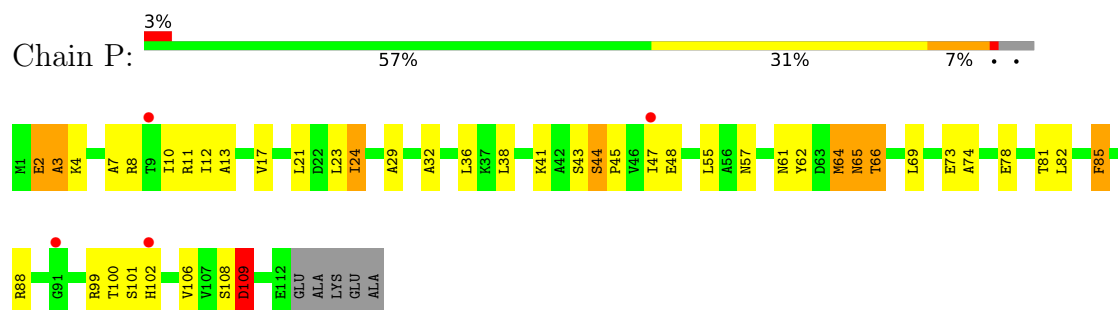


• Molecule 16: 50S ribosomal protein L21

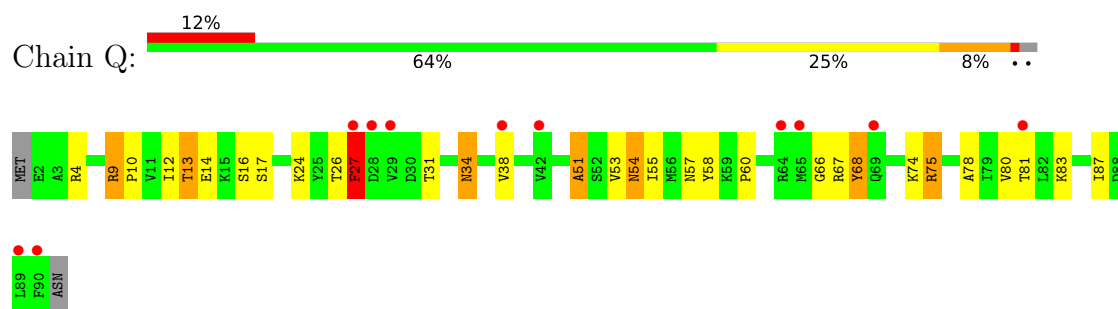




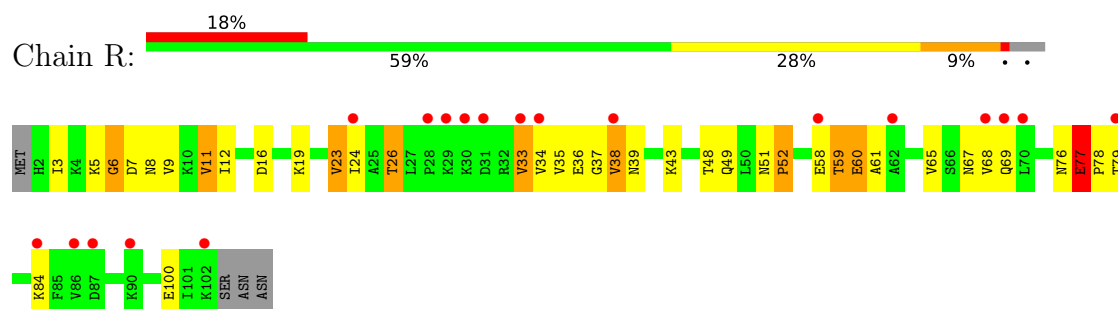
• Molecule 17: 50S ribosomal protein L22



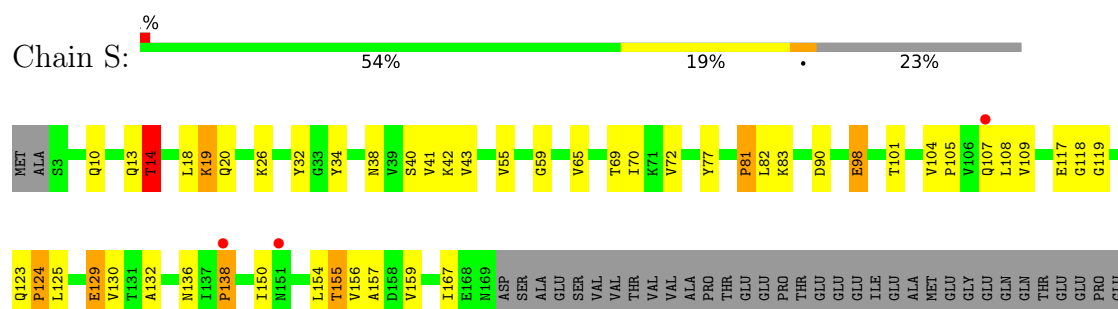
• Molecule 18: 50S ribosomal protein L23



• Molecule 19: 50S ribosomal protein L24



• Molecule 20: 50S ribosomal protein L25



VAL
VAL
GLY
GLY
SER
SER
LYS
GLU
ASP
GLU
LYS
LYS
THR
GLU

• Molecule 21: 50S ribosomal protein L27



MET LEU LYS LYS LEU LEU ASN ASN GLN PHE PHE ALA SER LYS LYS GLY VAL SER SER THR THR K19 D23 D24 S24 E25 E26 R44 K27 K28 R28 K32 K33 A34 S43 Y46 Y47 T51 K52 I53 G60 R61 G62 G63 D64 D65 T66 L67 F68 I71 D72 D83 K84 A93 GLU

• Molecule 22: 50S ribosomal protein L29



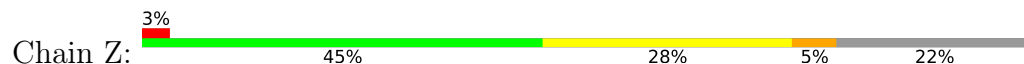
MET LYS ALA K4 E5 I6 T10 T11 E16 S20 R29 L32 L37 T40 I43 R44 T45 V46 R47 R48 T49 I50 A51 R52 T55 V56 I62 K66 ALA ASN GLN

• Molecule 23: 50S ribosomal protein L30



R1 L4 T7 V12 T13 G14 E17 T18 Q19 R20 K21 V23 L26 K29 K30 V36 N40 I43 R44 G45 Q46 V54 E57 E58 LYS

• Molecule 24: 50S ribosomal protein L32



MET A2 V3 P4 R7 T8 S9 K10 T11 R16 R17 T18 H19 F20 K21 I22 S23 V24 M27 T28 E29 C30 C33 E36 V37 K38 L39 S40 R41 R42 V43 C44 K45 R46 CYS GLY SER TYR ASN GLY GLU VAL ALA LYS

• Molecule 25: 50S ribosomal protein L34



MET V2 K3 R4 T5 P8 N9 K12 K15 V16 F19 R20 K21 S24 G28 V31 L32 R35 L43 S44 A45

• Molecule 26: 50S ribosomal protein L35



MET P2 A11 R12 R13 V14 K15 A18 Q21 R26 A27 F28 T29 A34 Q40 Q43 L49 V50 S53 D54 M55 V58 R59 Q60 L61 LEU ALA TYR LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	282.66Å 282.66Å 877.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.19 – 3.43 50.19 – 3.43	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.19-3.43) 97.4 (50.19-3.43)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.192 , 0.232 0.192 , 0.230	Depositor DCC
R_{free} test set	13519 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	81033	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% 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: EOH, EPE, MPD, SPD, MG, TEL, MN

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	X	0.30	0/65105	0.47	1/101500 (0.0%)
2	Y	0.27	0/2717	0.43	0/4232
3	A	0.56	0/1671	1.18	16/2304 (0.7%)
4	B	0.67	0/1589	1.19	7/2139 (0.3%)
5	C	0.65	1/1332 (0.1%)	1.18	13/1826 (0.7%)
6	D	0.40	0/826	1.17	8/1147 (0.7%)
7	E	0.80	1/941 (0.1%)	1.48	18/1302 (1.4%)
8	G	0.59	0/1127	1.11	9/1524 (0.6%)
9	H	0.51	0/884	0.99	0/1195
10	I	0.82	1/838 (0.1%)	1.37	12/1139 (1.1%)
11	J	0.59	0/1078	1.15	12/1457 (0.8%)
12	K	0.61	0/903	1.05	3/1209 (0.2%)
13	L	0.54	0/672	1.08	3/922 (0.3%)
14	M	0.58	0/846	1.14	2/1139 (0.2%)
15	N	0.61	0/941	1.00	2/1248 (0.2%)
16	O	0.56	0/766	1.05	1/1028 (0.1%)
17	P	0.66	0/864	1.08	4/1164 (0.3%)
18	Q	0.49	0/607	1.06	6/830 (0.7%)
19	R	0.64	1/614 (0.2%)	1.12	3/847 (0.4%)
20	S	0.56	1/1094 (0.1%)	1.01	3/1503 (0.2%)
21	T	0.59	0/547	1.01	2/733 (0.3%)
22	V	0.47	0/417	0.83	0/571
23	W	0.64	0/451	1.00	0/607
24	Z	0.61	0/358	0.94	0/478
25	2	0.53	0/366	1.00	1/480 (0.2%)
26	3	0.73	0/393	1.17	2/529 (0.4%)
All	All	0.39	5/87947 (0.0%)	0.66	128/133053 (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
3	A	0	1
5	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	51	GLU	CA-C	7.41	1.62	1.52
19	R	68	VAL	CA-CB	6.87	1.61	1.54
7	E	170	ARG	CA-C	5.92	1.60	1.52
20	S	14	THR	CA-CB	5.46	1.62	1.53
5	C	176	THR	CA-CB	5.38	1.60	1.53

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	153	PRO	CA-C-N	12.20	135.09	119.84
7	E	153	PRO	C-N-CA	12.20	135.09	119.84
4	B	144	GLY	N-CA-C	-10.96	98.20	111.35
8	G	97	ASN	CA-C-N	9.23	130.70	120.45
8	G	97	ASN	C-N-CA	9.23	130.70	120.45

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	115	ILE	Peptide
5	C	140	LYS	Peptide

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	X	58145	0	29245	737	1
2	Y	2430	0	1229	41	0
3	A	1640	0	1255	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1566	0	1559	70	0
5	C	1314	0	1146	45	0
6	D	823	0	433	8	0
7	E	930	0	688	34	0
8	G	1105	0	1064	34	0
9	H	877	0	882	35	0
10	I	830	0	703	33	0
11	J	1054	0	1040	32	0
12	K	900	0	924	38	0
13	L	667	0	507	20	0
14	M	834	0	850	31	0
15	N	929	0	988	35	0
16	O	756	0	754	31	0
17	P	856	0	909	35	0
18	Q	600	0	500	23	0
19	R	609	0	484	18	0
20	S	1082	0	919	17	0
21	T	541	0	518	12	0
22	V	416	0	348	6	0
23	W	449	0	490	8	0
24	Z	352	0	358	19	0
25	2	362	0	398	12	0
26	3	390	0	346	3	0
27	X	58	0	65	14	0
28	X	64	0	112	15	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	C	3	0	0	0	0
29	G	1	0	0	0	0
29	O	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	136	0	0	0	0
29	Y	4	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	X	221	0	0	0	0
30	Y	6	0	0	0	0
31	S	10	0	19	1	0
31	X	40	0	76	5	0
32	X	9	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	15	0	17	0	0
All	All	81033	0	48844	1302	1

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 10.

The worst 5 of 1302 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:X:2649:U:O2'	1:X:2845:G:N2	1.98	0.96
1:X:2231:C:HO2'	1:X:2232:A:H8	1.10	0.93
1:X:1886:A:N6	1:X:1910:G:O2'	2.06	0.89
1:X:721:A:H8	1:X:2096:G:H21	1.15	0.87
2:Y:18:G:H1	2:Y:61:U:H3	1.20	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:136:A:OP1	1:X:1453:G:N2[12_554]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	267/277 (96%)	211 (79%)	34 (13%)	22 (8%)	0	4
4	B	213/220 (97%)	179 (84%)	18 (8%)	16 (8%)	1	5
5	C	198/207 (96%)	166 (84%)	20 (10%)	12 (6%)	1	8
6	D	156/179 (87%)	114 (73%)	30 (19%)	12 (8%)	1	5
7	E	154/178 (86%)	112 (73%)	29 (19%)	13 (8%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	G	143/145 (99%)	126 (88%)	13 (9%)	4 (3%)	4	19
9	H	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
10	I	129/146 (88%)	89 (69%)	25 (19%)	15 (12%)	0	2
11	J	139/144 (96%)	119 (86%)	15 (11%)	5 (4%)	2	16
12	K	117/122 (96%)	99 (85%)	13 (11%)	5 (4%)	2	13
13	L	107/119 (90%)	88 (82%)	10 (9%)	9 (8%)	0	4
14	M	108/116 (93%)	94 (87%)	9 (8%)	5 (5%)	2	12
15	N	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	6	26
16	O	100/102 (98%)	90 (90%)	9 (9%)	1 (1%)	12	39
17	P	110/117 (94%)	104 (94%)	6 (6%)	0	100	100
18	Q	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	11	37
19	R	99/105 (94%)	72 (73%)	21 (21%)	6 (6%)	1	8
20	S	165/217 (76%)	129 (78%)	19 (12%)	17 (10%)	0	3
21	T	73/94 (78%)	66 (90%)	6 (8%)	1 (1%)	9	31
22	V	61/69 (88%)	57 (93%)	1 (2%)	3 (5%)	1	11
23	W	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	6	26
24	Z	43/58 (74%)	40 (93%)	3 (7%)	0	100	100
25	2	42/45 (93%)	39 (93%)	3 (7%)	0	100	100
26	3	58/66 (88%)	47 (81%)	6 (10%)	5 (9%)	0	4
All	All	2859/3116 (92%)	2383 (83%)	321 (11%)	155 (5%)	1	10

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	126	VAL
3	A	141	VAL
3	A	154	ILE

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	
3	A	109/224 (49%)	98 (90%)	11 (10%)	7	25
4	B	156/177 (88%)	122 (78%)	34 (22%)	1	3
5	C	103/169 (61%)	77 (75%)	26 (25%)	0	1
6	D	14/158 (9%)	12 (86%)	2 (14%)	3	13
7	E	56/155 (36%)	41 (73%)	15 (27%)	0	1
8	G	110/123 (89%)	89 (81%)	21 (19%)	1	6
9	H	89/100 (89%)	72 (81%)	17 (19%)	1	6
10	I	61/112 (54%)	43 (70%)	18 (30%)	0	1
11	J	99/119 (83%)	83 (84%)	16 (16%)	2	10
12	K	89/102 (87%)	68 (76%)	21 (24%)	1	2
13	L	36/95 (38%)	29 (81%)	7 (19%)	1	5
14	M	82/102 (80%)	61 (74%)	21 (26%)	0	1
15	N	92/98 (94%)	80 (87%)	12 (13%)	4	16
16	O	72/86 (84%)	58 (81%)	14 (19%)	1	5
17	P	90/94 (96%)	78 (87%)	12 (13%)	4	15
18	Q	46/82 (56%)	38 (83%)	8 (17%)	2	8
19	R	43/90 (48%)	28 (65%)	15 (35%)	0	1
20	S	84/190 (44%)	72 (86%)	12 (14%)	3	13
21	T	50/75 (67%)	43 (86%)	7 (14%)	3	13
22	V	33/62 (53%)	25 (76%)	8 (24%)	1	2
23	W	52/53 (98%)	41 (79%)	11 (21%)	1	4
24	Z	39/51 (76%)	34 (87%)	5 (13%)	4	16
25	2	37/40 (92%)	32 (86%)	5 (14%)	4	15
26	3	30/57 (53%)	24 (80%)	6 (20%)	1	5
All	All	1672/2614 (64%)	1348 (81%)	324 (19%)	1	5

5 of 324 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	O	75	THR
21	T	51	THR
17	P	43	SER

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Mol	Chain	Res	Type
19	R	33	VAL
23	W	21	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
10	I	114	ASN
15	N	38	GLN
25	2	7	GLN
20	S	58	ASN
23	W	5	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2693/2923 (92%)	625 (23%)	28 (1%)
2	Y	113/114 (99%)	16 (14%)	0
All	All	2806/3037 (92%)	641 (22%)	28 (0%)

5 of 641 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	9	U
1	X	14	A
1	X	15	G
1	X	25	U
1	X	34	U

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1490	G
1	X	2474	G
1	X	1568	U
1	X	1952	C
1	X	1521	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 398 ligands modelled in this entry, 380 are monoatomic - leaving 18 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	$\# Z > 2$
31	SPD	X	3362	-	9,9,9	0.18	0	8,8,8	0.23	0
32	EOH	X	3366	-	2,2,2	0.59	0	1,1,1	0.63	0
28	MPD	X	3009	-	7,7,7	0.44	0	9,10,10	0.27	0
31	SPD	X	3365	-	9,9,9	0.30	0	8,8,8	0.48	0
32	EOH	X	3367	-	2,2,2	0.49	0	1,1,1	0.76	0
31	SPD	X	3363	-	9,9,9	0.16	0	8,8,8	0.19	0
31	SPD	X	3364	-	9,9,9	0.23	0	8,8,8	0.32	0
28	MPD	X	3003	-	7,7,7	0.52	0	9,10,10	0.28	0
27	TEL	X	3001	-	60,62,62	0.57	1 (1%)	78,92,92	1.69	12 (15%)
28	MPD	X	3007	-	7,7,7	0.51	0	9,10,10	0.14	0
28	MPD	X	3002	-	7,7,7	0.67	0	9,10,10	0.49	0
28	MPD	X	3006	-	7,7,7	0.66	0	9,10,10	0.54	0
33	EPE	L	201	-	15,15,15	0.79	1 (6%)	19,20,20	0.48	0
28	MPD	X	3005	-	7,7,7	0.83	0	9,10,10	1.14	0
28	MPD	X	3008	-	7,7,7	0.75	0	9,10,10	0.31	0
31	SPD	S	301	-	9,9,9	0.18	0	8,8,8	0.44	0
32	EOH	X	3368	-	2,2,2	0.54	0	1,1,1	0.67	0
28	MPD	X	3004	-	7,7,7	0.50	0	9,10,10	0.24	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
31	SPD	X	3362	-	-	3/7/7/7	-
28	MPD	X	3009	-	-	5/5/5/5	-
31	SPD	X	3365	-	-	5/7/7/7	-
31	SPD	X	3363	-	-	2/7/7/7	-
31	SPD	X	3364	-	-	4/7/7/7	-
28	MPD	X	3003	-	-	2/5/5/5	-
27	TEL	X	3001	-	1/1/19/19	29/73/108/108	0/4/5/5
28	MPD	X	3007	-	-	0/5/5/5	-
28	MPD	X	3002	-	-	1/5/5/5	-
28	MPD	X	3006	-	-	1/5/5/5	-
33	EPE	L	201	-	-	3/9/19/19	0/1/1/1
28	MPD	X	3005	-	-	5/5/5/5	-
28	MPD	X	3008	-	-	3/5/5/5	-
31	SPD	S	301	-	-	2/7/7/7	-
28	MPD	X	3004	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	3001	TEL	C21-C26	3.15	1.57	1.52
33	L	201	EPE	C10-S	-2.85	1.73	1.77

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	3001	TEL	O5-C2-C4	-6.85	90.45	105.63
27	X	3001	TEL	O5-C2-C3	-5.62	97.55	103.28
27	X	3001	TEL	O32-C28-C24	4.40	114.97	105.71
27	X	3001	TEL	C2-O5-C10	-4.07	105.67	109.23
27	X	3001	TEL	O29-C26-C21	-3.35	114.52	120.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	X	3001	TEL	C21

5 of 67 torsion outliers are listed below:

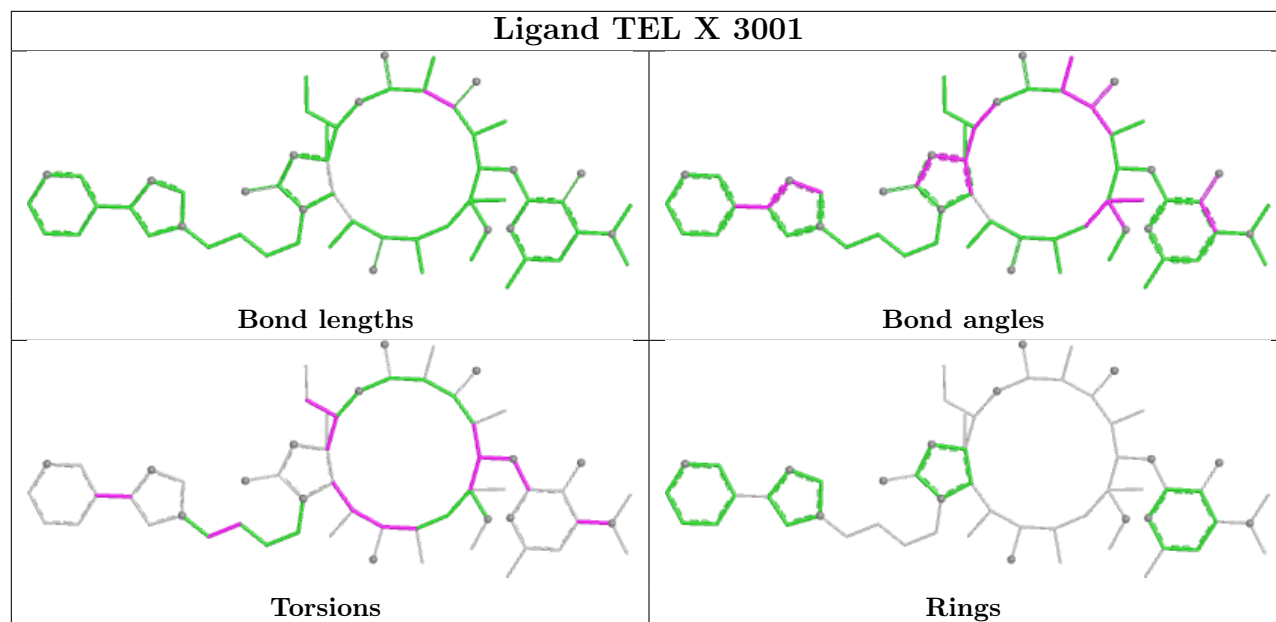
Mol	Chain	Res	Type	Atoms
27	X	3001	TEL	C1-C2-C4-O9
27	X	3001	TEL	O5-C2-C4-O9
27	X	3001	TEL	C2-C3-C7-C13
27	X	3001	TEL	N6-C3-C7-C13
27	X	3001	TEL	O18-C13-C19-C23

There are no ring outliers.

11 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	X	3009	MPD	1	0
31	X	3365	SPD	4	0
31	X	3364	SPD	1	0
28	X	3003	MPD	3	0
27	X	3001	TEL	14	0
28	X	3007	MPD	2	0
28	X	3002	MPD	1	0
28	X	3006	MPD	1	0
28	X	3005	MPD	6	0
28	X	3008	MPD	1	0
31	S	301	SPD	1	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	X	2712/2923 (92%)	-0.65	43 (1%) 70 57	27, 74, 174, 288	0
2	Y	114/114 (100%)	-0.82	1 (0%) 81 69	48, 98, 151, 203	0
3	A	269/277 (97%)	0.56	24 (8%) 15 14	56, 101, 146, 177	0
4	B	215/220 (97%)	0.03	14 (6%) 25 19	34, 49, 101, 155	0
5	C	200/207 (96%)	0.04	10 (5%) 34 25	40, 65, 112, 165	0
6	D	160/179 (89%)	0.44	15 (9%) 14 13	88, 155, 209, 263	0
7	E	156/178 (87%)	0.45	15 (9%) 13 13	71, 131, 190, 205	0
8	G	145/145 (100%)	-0.12	3 (2%) 63 48	36, 51, 83, 115	0
9	H	122/122 (100%)	-0.19	5 (4%) 41 29	57, 75, 116, 154	0
10	I	131/146 (89%)	0.56	9 (6%) 23 18	22, 78, 139, 210	0
11	J	141/144 (97%)	0.54	18 (12%) 7 9	43, 73, 162, 258	0
12	K	119/122 (97%)	0.01	3 (2%) 58 43	31, 57, 129, 169	0
13	L	109/119 (91%)	0.17	8 (7%) 21 18	55, 96, 149, 205	0
14	M	110/116 (94%)	0.06	5 (4%) 38 28	46, 69, 127, 189	0
15	N	116/118 (98%)	0.18	7 (6%) 27 21	18, 45, 80, 106	0
16	O	102/102 (100%)	-0.23	2 (1%) 65 50	23, 60, 93, 179	0
17	P	112/117 (95%)	-0.00	4 (3%) 46 33	37, 50, 116, 177	0
18	Q	89/91 (97%)	0.55	11 (12%) 8 9	63, 93, 138, 173	0
19	R	101/105 (96%)	0.95	19 (18%) 3 4	54, 98, 196, 218	0
20	S	167/217 (76%)	0.00	3 (1%) 67 53	48, 83, 170, 292	0
21	T	75/94 (79%)	0.28	4 (5%) 32 24	44, 65, 106, 134	0
22	V	63/69 (91%)	0.22	3 (4%) 35 26	82, 107, 145, 185	0
23	W	58/59 (98%)	-0.34	2 (3%) 48 35	26, 52, 98, 195	0
24	Z	45/58 (77%)	0.39	2 (4%) 39 28	29, 60, 157, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	44/45 (97%)	0.29	1 (2%) 61 46	59, 67, 97, 140	0
26	3	60/66 (90%)	0.50	6 (10%) 12 12	35, 57, 91, 96	0
All	All	5735/6153 (93%)	-0.21	237 (4%) 41 29	18, 75, 168, 292	0

The worst 5 of 237 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	R	31	ASP	8.9
6	D	83	MET	7.3
3	A	38	PRO	7.2
19	R	28	PRO	6.8
3	A	94	VAL	6.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
31	SPD	X	3364	10/10	0.44	0.33	80,80,80,80	0
32	EOH	X	3367	3/3	0.52	0.48	77,77,77,77	0
29	MG	X	3031	1/1	0.53	0.15	45,45,45,45	0
29	MG	X	3341	1/1	0.54	0.20	92,92,92,92	0
32	EOH	X	3368	3/3	0.58	0.37	55,55,55,55	0
29	MG	X	3191	1/1	0.60	0.26	79,79,79,79	0
30	MN	X	3200	1/1	0.61	0.15	161,161,161,161	0
29	MG	X	3229	1/1	0.67	0.43	62,62,62,62	0
29	MG	X	3313	1/1	0.68	0.29	67,67,67,67	0
29	MG	X	3360	1/1	0.69	0.32	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	C	301	1/1	0.69	0.07	31,31,31,31	0
28	MPD	X	3002	8/8	0.70	0.23	44,44,44,44	0
29	MG	X	3354	1/1	0.70	0.24	59,59,59,59	0
30	MN	X	3151	1/1	0.71	0.33	135,135,135,135	0
29	MG	X	3010	1/1	0.72	0.28	84,84,84,84	0
29	MG	X	3337	1/1	0.73	0.24	69,69,69,69	0
29	MG	X	3282	1/1	0.73	0.26	43,43,43,43	0
29	MG	X	3011	1/1	0.75	0.22	50,50,50,50	0
29	MG	X	3230	1/1	0.75	0.24	71,71,71,71	0
29	MG	X	3352	1/1	0.76	0.22	66,66,66,66	0
29	MG	X	3273	1/1	0.76	0.20	78,78,78,78	0
30	MN	Y	210	1/1	0.76	0.14	176,176,176,176	0
29	MG	X	3260	1/1	0.77	0.27	64,64,64,64	0
28	MPD	X	3003	8/8	0.77	0.32	64,64,64,64	0
30	MN	X	3140	1/1	0.77	0.15	127,127,127,127	0
29	MG	X	3014	1/1	0.78	0.21	26,26,26,26	1
29	MG	X	3296	1/1	0.78	0.21	56,56,56,56	0
30	MN	X	3038	1/1	0.78	0.22	151,151,151,151	0
29	MG	X	3228	1/1	0.78	0.31	62,62,62,62	0
29	MG	X	3322	1/1	0.78	0.14	67,67,67,67	0
29	MG	X	3339	1/1	0.79	0.22	66,66,66,66	0
29	MG	X	3335	1/1	0.79	0.29	81,81,81,81	0
29	MG	X	3327	1/1	0.80	0.17	48,48,48,48	0
29	MG	X	3315	1/1	0.80	0.31	60,60,60,60	0
31	SPD	S	301	10/10	0.80	0.27	67,67,67,67	0
28	MPD	X	3004	8/8	0.80	0.25	86,86,86,86	0
30	MN	X	3037	1/1	0.80	0.12	131,131,131,131	0
30	MN	X	3206	1/1	0.81	0.11	133,133,133,133	0
30	MN	X	3361	1/1	0.81	0.15	158,158,158,158	0
29	MG	X	3022	1/1	0.81	0.35	62,62,62,62	0
31	SPD	X	3363	10/10	0.81	0.42	75,75,75,75	0
29	MG	X	3303	1/1	0.82	0.65	63,63,63,63	0
29	MG	X	3340	1/1	0.82	0.11	55,55,55,55	0
28	MPD	X	3006	8/8	0.82	0.32	74,74,74,74	0
29	MG	X	3343	1/1	0.82	0.22	53,53,53,53	0
30	MN	X	3207	1/1	0.82	0.18	130,130,130,130	0
29	MG	X	3326	1/1	0.82	0.33	71,71,71,71	0
29	MG	X	3353	1/1	0.83	0.18	39,39,39,39	0
30	MN	X	3056	1/1	0.83	0.11	135,135,135,135	0
30	MN	Y	208	1/1	0.83	0.14	173,173,173,173	0
29	MG	X	3019	1/1	0.83	0.13	32,32,32,32	0
29	MG	X	3342	1/1	0.83	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3183	1/1	0.83	0.11	128,128,128,128	0
30	MN	X	3199	1/1	0.83	0.23	132,132,132,132	0
28	MPD	X	3009	8/8	0.83	0.46	99,99,99,99	0
28	MPD	X	3008	8/8	0.83	0.16	61,61,61,61	0
29	MG	X	3317	1/1	0.84	0.14	49,49,49,49	0
29	MG	X	3312	1/1	0.84	0.24	36,36,36,36	0
29	MG	X	3277	1/1	0.84	0.08	51,51,51,51	0
30	MN	X	3142	1/1	0.84	0.07	117,117,117,117	0
29	MG	X	3350	1/1	0.84	0.13	71,71,71,71	0
29	MG	X	3012	1/1	0.84	0.23	16,16,16,16	1
33	EPE	L	201	15/15	0.84	0.11	125,125,125,125	0
29	MG	X	3030	1/1	0.85	0.17	48,48,48,48	0
29	MG	X	3372	1/1	0.85	0.39	56,56,56,56	0
30	MN	X	3271	1/1	0.85	0.16	140,140,140,140	0
30	MN	Y	205	1/1	0.86	0.07	132,132,132,132	0
30	MN	X	3205	1/1	0.86	0.08	141,141,141,141	0
30	MN	X	3171	1/1	0.86	0.07	82,82,82,82	0
29	MG	X	3295	1/1	0.86	0.26	57,57,57,57	0
30	MN	X	3220	1/1	0.86	0.22	153,153,153,153	0
30	MN	X	3265	1/1	0.86	0.18	148,148,148,148	0
29	MG	X	3336	1/1	0.86	0.09	40,40,40,40	0
30	MN	X	3272	1/1	0.86	0.21	156,156,156,156	0
29	MG	X	3324	1/1	0.86	0.18	55,55,55,55	0
29	MG	X	3299	1/1	0.87	0.23	52,52,52,52	0
29	MG	X	3338	1/1	0.87	0.26	64,64,64,64	0
29	MG	X	3231	1/1	0.87	0.56	64,64,64,64	0
29	MG	X	3224	1/1	0.87	0.19	70,70,70,70	0
29	MG	X	3325	1/1	0.87	0.34	49,49,49,49	0
29	MG	T	101	1/1	0.87	0.20	44,44,44,44	0
29	MG	X	3025	1/1	0.87	0.18	16,16,16,16	1
29	MG	X	3314	1/1	0.87	0.17	55,55,55,55	0
30	MN	X	3041	1/1	0.87	0.16	127,127,127,127	0
29	MG	X	3276	1/1	0.87	0.20	51,51,51,51	0
29	MG	X	3316	1/1	0.87	0.07	38,38,38,38	0
30	MN	X	3267	1/1	0.87	0.19	140,140,140,140	0
30	MN	X	3266	1/1	0.88	0.17	147,147,147,147	0
29	MG	X	3333	1/1	0.88	0.05	45,45,45,45	0
30	MN	X	3180	1/1	0.88	0.14	121,121,121,121	0
29	MG	X	3285	1/1	0.88	0.21	56,56,56,56	0
29	MG	X	3319	1/1	0.88	0.22	53,53,53,53	0
29	MG	X	3294	1/1	0.88	0.16	32,32,32,32	0
29	MG	X	3013	1/1	0.88	0.28	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	3196	1/1	0.88	0.50	41,41,41,41	0
29	MG	X	3028	1/1	0.88	0.44	66,66,66,66	0
30	MN	X	3214	1/1	0.88	0.06	78,78,78,78	0
29	MG	X	3302	1/1	0.88	0.07	61,61,61,61	0
30	MN	X	3222	1/1	0.88	0.07	101,101,101,101	0
30	MN	X	3254	1/1	0.88	0.14	105,105,105,105	0
29	MG	A	301	1/1	0.88	0.27	45,45,45,45	0
30	MN	X	3046	1/1	0.89	0.10	97,97,97,97	0
30	MN	X	3218	1/1	0.89	0.08	128,128,128,128	0
30	MN	X	3055	1/1	0.89	0.26	121,121,121,121	0
29	MG	X	3306	1/1	0.89	0.27	66,66,66,66	0
30	MN	X	3247	1/1	0.89	0.07	104,104,104,104	0
30	MN	X	3058	1/1	0.89	0.16	113,113,113,113	0
30	MN	X	3131	1/1	0.89	0.15	109,109,109,109	0
29	MG	X	3026	1/1	0.89	0.14	41,41,41,41	0
29	MG	X	3225	1/1	0.89	0.05	56,56,56,56	0
30	MN	X	3144	1/1	0.89	0.14	127,127,127,127	0
30	MN	X	3146	1/1	0.89	0.10	124,124,124,124	0
30	MN	X	3329	1/1	0.89	0.08	95,95,95,95	0
29	MG	X	3235	1/1	0.89	0.19	62,62,62,62	0
30	MN	Y	204	1/1	0.89	0.07	146,146,146,146	0
29	MG	X	3251	1/1	0.89	0.23	59,59,59,59	0
29	MG	X	3252	1/1	0.89	0.23	45,45,45,45	0
29	MG	X	3253	1/1	0.89	0.22	65,65,65,65	0
29	MG	X	3258	1/1	0.89	0.34	73,73,73,73	0
29	MG	X	3321	1/1	0.89	0.23	74,74,74,74	0
27	TEL	X	3001	58/58	0.89	0.17	30,40,52,52	0
29	MG	X	3020	1/1	0.89	0.42	40,40,40,40	0
29	MG	X	3275	1/1	0.89	0.23	29,29,29,29	0
30	MN	X	3212	1/1	0.89	0.26	94,94,94,94	0
29	MG	C	302	1/1	0.90	0.17	44,44,44,44	0
30	MN	X	3182	1/1	0.90	0.10	117,117,117,117	0
29	MG	C	303	1/1	0.90	0.18	38,38,38,38	0
30	MN	X	3065	1/1	0.90	0.16	76,76,76,76	0
29	MG	X	3300	1/1	0.90	0.20	59,59,59,59	0
28	MPD	X	3007	8/8	0.90	0.14	70,70,70,70	0
29	MG	Y	203	1/1	0.90	0.23	19,19,19,19	0
30	MN	X	3039	1/1	0.90	0.27	107,107,107,107	0
29	MG	Y	209	1/1	0.90	0.21	59,59,59,59	0
30	MN	X	3150	1/1	0.90	0.19	123,123,123,123	0
29	MG	X	3334	1/1	0.90	0.18	64,64,64,64	0
30	MN	X	3163	1/1	0.90	0.12	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	M	201	1/1	0.90	0.10	105,105,105,105	0
29	MG	X	3318	1/1	0.90	0.17	47,47,47,47	0
30	MN	X	3237	1/1	0.90	0.17	87,87,87,87	0
31	SPD	X	3365	10/10	0.90	0.19	54,54,54,54	0
30	MN	X	3239	1/1	0.90	0.06	154,154,154,154	0
30	MN	X	3244	1/1	0.90	0.10	96,96,96,96	0
30	MN	X	3246	1/1	0.90	0.09	104,104,104,104	0
30	MN	X	3172	1/1	0.90	0.14	113,113,113,113	0
30	MN	X	3132	1/1	0.91	0.32	116,116,116,116	0
30	MN	X	3262	1/1	0.91	0.07	130,130,130,130	0
30	MN	X	3198	1/1	0.91	0.23	162,162,162,162	0
29	MG	X	3232	1/1	0.91	0.20	42,42,42,42	0
29	MG	X	3259	1/1	0.91	0.24	63,63,63,63	0
29	MG	X	3024	1/1	0.91	0.26	31,31,31,31	1
29	MG	X	3347	1/1	0.91	0.09	37,37,37,37	0
30	MN	X	3147	1/1	0.91	0.08	89,89,89,89	0
30	MN	X	3210	1/1	0.91	0.08	128,128,128,128	0
30	MN	X	3148	1/1	0.91	0.21	112,112,112,112	0
30	MN	X	3051	1/1	0.91	0.14	120,120,120,120	0
30	MN	X	3217	1/1	0.91	0.08	116,116,116,116	0
29	MG	X	3249	1/1	0.91	0.13	59,59,59,59	0
30	MN	J	201	1/1	0.91	0.11	103,103,103,103	0
29	MG	X	3274	1/1	0.91	0.25	44,44,44,44	0
31	SPD	X	3362	10/10	0.91	0.20	16,16,16,16	0
30	MN	X	3164	1/1	0.91	0.05	103,103,103,103	0
30	MN	X	3227	1/1	0.91	0.27	116,116,116,116	0
29	MG	X	3197	1/1	0.91	0.16	58,58,58,58	0
29	MG	X	3192	1/1	0.91	0.18	45,45,45,45	0
30	MN	X	3068	1/1	0.91	0.18	102,102,102,102	0
30	MN	X	3181	1/1	0.91	0.08	121,121,121,121	0
29	MG	X	3194	1/1	0.91	0.20	34,34,34,34	0
30	MN	X	3202	1/1	0.92	0.11	124,124,124,124	0
30	MN	X	3204	1/1	0.92	0.09	141,141,141,141	0
30	MN	X	3064	1/1	0.92	0.17	94,94,94,94	0
29	MG	X	3358	1/1	0.92	0.21	59,59,59,59	0
29	MG	X	3359	1/1	0.92	0.25	60,60,60,60	0
30	MN	X	3208	1/1	0.92	0.10	109,109,109,109	0
30	MN	X	3209	1/1	0.92	0.06	122,122,122,122	0
30	MN	X	3332	1/1	0.92	0.13	122,122,122,122	0
30	MN	X	3162	1/1	0.92	0.10	114,114,114,114	0
30	MN	X	3076	1/1	0.92	0.09	85,85,85,85	0
30	MN	X	3107	1/1	0.92	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3215	1/1	0.92	0.12	95,95,95,95	0
30	MN	X	3112	1/1	0.92	0.17	77,77,77,77	0
30	MN	X	3040	1/1	0.92	0.13	100,100,100,100	0
30	MN	X	3175	1/1	0.92	0.06	111,111,111,111	0
29	MG	X	3156	1/1	0.92	0.16	14,14,14,14	0
30	MN	X	3135	1/1	0.92	0.10	99,99,99,99	0
29	MG	X	3226	1/1	0.92	0.09	64,64,64,64	0
29	MG	R	201	1/1	0.92	0.05	24,24,24,24	0
30	MN	X	3184	1/1	0.92	0.07	99,99,99,99	0
29	MG	X	3281	1/1	0.92	0.14	21,21,21,21	0
30	MN	X	3033	1/1	0.92	0.10	106,106,106,106	0
29	MG	X	3349	1/1	0.92	0.31	74,74,74,74	0
30	MN	X	3248	1/1	0.93	0.08	115,115,115,115	0
29	MG	X	3308	1/1	0.93	0.20	44,44,44,44	0
30	MN	X	3042	1/1	0.93	0.12	161,161,161,161	0
30	MN	X	3264	1/1	0.93	0.17	103,103,103,103	0
30	MN	X	3203	1/1	0.93	0.10	78,78,78,78	0
30	MN	X	3145	1/1	0.93	0.07	122,122,122,122	0
29	MG	Y	207	1/1	0.93	0.28	51,51,51,51	0
30	MN	X	3269	1/1	0.93	0.17	134,134,134,134	0
29	MG	X	3293	1/1	0.93	0.16	32,32,32,32	0
29	MG	X	3344	1/1	0.93	0.10	67,67,67,67	0
29	MG	B	301	1/1	0.93	0.07	46,46,46,46	0
29	MG	X	3255	1/1	0.93	0.13	59,59,59,59	0
30	MN	X	3356	1/1	0.93	0.22	41,41,41,41	0
29	MG	X	3193	1/1	0.93	0.17	27,27,27,27	0
30	MN	X	3369	1/1	0.93	0.22	70,70,70,70	0
30	MN	Y	202	1/1	0.93	0.08	126,126,126,126	0
29	MG	X	3029	1/1	0.93	0.09	51,51,51,51	0
29	MG	X	3279	1/1	0.93	0.15	66,66,66,66	0
28	MPD	X	3005	8/8	0.93	0.17	20,20,20,20	0
30	MN	X	3101	1/1	0.93	0.12	83,83,83,83	0
30	MN	X	3173	1/1	0.93	0.11	72,72,72,72	0
29	MG	X	3301	1/1	0.93	0.06	30,30,30,30	0
30	MN	X	3035	1/1	0.93	0.14	149,149,149,149	0
30	MN	X	3120	1/1	0.93	0.08	98,98,98,98	0
30	MN	X	3122	1/1	0.93	0.08	71,71,71,71	0
29	MG	X	3233	1/1	0.93	0.29	57,57,57,57	0
30	MN	X	3243	1/1	0.93	0.15	107,107,107,107	0
29	MG	X	3234	1/1	0.93	0.20	34,34,34,34	0
29	MG	X	3291	1/1	0.93	0.15	26,26,26,26	0
29	MG	X	3307	1/1	0.93	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3139	1/1	0.94	0.14	121,121,121,121	0
29	MG	X	3348	1/1	0.94	0.25	46,46,46,46	0
29	MG	X	3223	1/1	0.94	0.10	42,42,42,42	0
30	MN	X	3143	1/1	0.94	0.06	85,85,85,85	0
30	MN	X	3071	1/1	0.94	0.14	77,77,77,77	0
29	MG	X	3305	1/1	0.94	0.31	60,60,60,60	0
30	MN	X	3091	1/1	0.94	0.11	78,78,78,78	0
30	MN	X	3092	1/1	0.94	0.22	103,103,103,103	0
30	MN	X	3098	1/1	0.94	0.17	94,94,94,94	0
30	MN	X	3331	1/1	0.94	0.20	119,119,119,119	0
30	MN	X	3100	1/1	0.94	0.08	57,57,57,57	0
29	MG	X	3278	1/1	0.94	0.32	63,63,63,63	0
30	MN	X	3102	1/1	0.94	0.12	100,100,100,100	0
30	MN	X	3032	1/1	0.94	0.18	122,122,122,122	0
30	MN	X	3373	1/1	0.94	0.06	44,44,44,44	0
30	MN	X	3108	1/1	0.94	0.14	70,70,70,70	0
30	MN	X	3165	1/1	0.94	0.10	83,83,83,83	0
30	MN	X	3170	1/1	0.94	0.10	70,70,70,70	0
29	MG	X	3323	1/1	0.94	0.14	48,48,48,48	0
30	MN	X	3115	1/1	0.94	0.12	65,65,65,65	0
30	MN	X	3119	1/1	0.94	0.09	87,87,87,87	0
29	MG	X	3021	1/1	0.94	0.10	56,56,56,56	0
30	MN	X	3178	1/1	0.94	0.13	98,98,98,98	0
30	MN	X	3036	1/1	0.94	0.10	96,96,96,96	0
29	MG	X	3017	1/1	0.94	0.23	46,46,46,46	0
30	MN	X	3059	1/1	0.94	0.14	111,111,111,111	0
29	MG	X	3157	1/1	0.94	0.24	61,61,61,61	0
30	MN	X	3138	1/1	0.94	0.06	91,91,91,91	0
30	MN	X	3185	1/1	0.94	0.08	112,112,112,112	0
30	MN	X	3188	1/1	0.94	0.07	54,54,54,54	0
30	MN	X	3116	1/1	0.95	0.20	70,70,70,70	0
30	MN	X	3070	1/1	0.95	0.13	74,74,74,74	0
29	MG	X	3023	1/1	0.95	0.06	26,26,26,26	1
30	MN	X	3270	1/1	0.95	0.09	120,120,120,120	0
30	MN	X	3167	1/1	0.95	0.18	110,110,110,110	0
29	MG	X	3016	1/1	0.95	0.38	12,12,12,12	1
30	MN	X	3077	1/1	0.95	0.13	62,62,62,62	0
30	MN	X	3330	1/1	0.95	0.04	83,83,83,83	0
30	MN	X	3080	1/1	0.95	0.08	55,55,55,55	0
30	MN	X	3134	1/1	0.95	0.14	90,90,90,90	0
30	MN	X	3355	1/1	0.95	0.15	68,68,68,68	0
30	MN	X	3044	1/1	0.95	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	3283	1/1	0.95	0.15	36,36,36,36	0
30	MN	X	3093	1/1	0.95	0.12	83,83,83,83	0
30	MN	X	3094	1/1	0.95	0.18	94,94,94,94	0
30	MN	X	3141	1/1	0.95	0.08	99,99,99,99	0
30	MN	X	3236	1/1	0.95	0.09	105,105,105,105	0
29	MG	X	3320	1/1	0.95	0.10	53,53,53,53	0
29	MG	X	3297	1/1	0.95	0.31	44,44,44,44	0
29	MG	X	3195	1/1	0.95	0.34	28,28,28,28	0
29	MG	X	3288	1/1	0.95	0.20	39,39,39,39	0
29	MG	X	3250	1/1	0.95	0.20	25,25,25,25	0
29	MG	X	3292	1/1	0.95	0.14	30,30,30,30	0
30	MN	X	3111	1/1	0.95	0.22	71,71,71,71	0
29	MG	X	3257	1/1	0.95	0.06	48,48,48,48	0
30	MN	X	3261	1/1	0.95	0.04	89,89,89,89	0
30	MN	X	3113	1/1	0.95	0.13	62,62,62,62	0
30	MN	X	3263	1/1	0.95	0.12	114,114,114,114	0
30	MN	X	3159	1/1	0.95	0.06	81,81,81,81	0
29	MG	X	3357	1/1	0.95	0.11	51,51,51,51	0
30	MN	X	3186	1/1	0.96	0.09	142,142,142,142	0
29	MG	X	3284	1/1	0.96	0.12	12,12,12,12	0
30	MN	X	3190	1/1	0.96	0.05	77,77,77,77	0
29	MG	X	3280	1/1	0.96	0.16	51,51,51,51	0
30	MN	X	3067	1/1	0.96	0.19	83,83,83,83	0
29	MG	X	3286	1/1	0.96	0.11	30,30,30,30	0
30	MN	X	3149	1/1	0.96	0.14	112,112,112,112	0
29	MG	X	3346	1/1	0.96	0.10	31,31,31,31	0
29	MG	X	3155	1/1	0.96	0.21	21,21,21,21	0
30	MN	X	3152	1/1	0.96	0.07	104,104,104,104	0
30	MN	X	3158	1/1	0.96	0.05	91,91,91,91	0
30	MN	X	3328	1/1	0.96	0.12	88,88,88,88	0
30	MN	X	3072	1/1	0.96	0.10	74,74,74,74	0
30	MN	X	3161	1/1	0.96	0.07	93,93,93,93	0
30	MN	X	3073	1/1	0.96	0.08	65,65,65,65	0
30	MN	X	3117	1/1	0.96	0.12	67,67,67,67	0
30	MN	X	3074	1/1	0.96	0.14	68,68,68,68	0
29	MG	G	201	1/1	0.96	0.13	31,31,31,31	0
30	MN	X	3166	1/1	0.96	0.07	72,72,72,72	0
30	MN	X	3216	1/1	0.96	0.09	78,78,78,78	0
29	MG	O	201	1/1	0.96	0.20	0,0,0,0	1
30	MN	Y	201	1/1	0.96	0.06	84,84,84,84	0
29	MG	X	3289	1/1	0.96	0.08	61,61,61,61	0
30	MN	X	3085	1/1	0.96	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3221	1/1	0.96	0.10	51,51,51,51	0
30	MN	X	3048	1/1	0.96	0.06	90,90,90,90	0
30	MN	X	3050	1/1	0.96	0.09	87,87,87,87	0
30	MN	I	202	1/1	0.96	0.17	100,100,100,100	0
30	MN	X	3137	1/1	0.96	0.10	103,103,103,103	0
30	MN	X	3177	1/1	0.96	0.07	89,89,89,89	0
30	MN	X	3238	1/1	0.96	0.11	126,126,126,126	0
29	MG	X	3298	1/1	0.96	0.21	41,41,41,41	0
29	MG	X	3015	1/1	0.96	0.17	48,48,48,48	0
30	MN	X	3095	1/1	0.96	0.25	87,87,87,87	0
29	MG	Y	206	1/1	0.96	0.05	45,45,45,45	0
32	EOH	X	3366	3/3	0.96	0.18	32,32,32,32	0
30	MN	X	3099	1/1	0.96	0.14	88,88,88,88	0
29	MG	X	3351	1/1	0.96	0.05	57,57,57,57	0
29	MG	X	3018	1/1	0.96	0.35	42,42,42,42	0
29	MG	X	3304	1/1	0.97	0.30	40,40,40,40	0
30	MN	X	3043	1/1	0.97	0.08	67,67,67,67	0
30	MN	X	3169	1/1	0.97	0.04	85,85,85,85	0
30	MN	X	3057	1/1	0.97	0.13	28,28,28,28	0
29	MG	X	3310	1/1	0.97	0.20	36,36,36,36	0
30	MN	X	3045	1/1	0.97	0.04	82,82,82,82	0
30	MN	X	3106	1/1	0.97	0.13	42,42,42,42	0
30	MN	X	3062	1/1	0.97	0.11	72,72,72,72	0
30	MN	X	3176	1/1	0.97	0.10	78,78,78,78	0
29	MG	X	3287	1/1	0.97	0.21	36,36,36,36	0
30	MN	X	3110	1/1	0.97	0.07	51,51,51,51	0
30	MN	X	3179	1/1	0.97	0.05	69,69,69,69	0
30	MN	X	3082	1/1	0.97	0.13	71,71,71,71	0
30	MN	X	3084	1/1	0.97	0.09	72,72,72,72	0
30	MN	X	3370	1/1	0.97	0.11	98,98,98,98	0
30	MN	X	3371	1/1	0.97	0.13	34,34,34,34	0
29	MG	X	3290	1/1	0.97	0.24	45,45,45,45	0
30	MN	X	3086	1/1	0.97	0.05	74,74,74,74	0
30	MN	X	3088	1/1	0.97	0.04	97,97,97,97	0
30	MN	X	3089	1/1	0.97	0.10	89,89,89,89	0
30	MN	X	3241	1/1	0.97	0.09	66,66,66,66	0
30	MN	X	3066	1/1	0.97	0.12	49,49,49,49	0
29	MG	X	3027	1/1	0.97	0.17	38,38,38,38	0
30	MN	I	201	1/1	0.97	0.09	71,71,71,71	0
30	MN	X	3245	1/1	0.97	0.10	98,98,98,98	0
30	MN	X	3189	1/1	0.97	0.12	43,43,43,43	0
30	MN	X	3154	1/1	0.97	0.15	47,47,47,47	0

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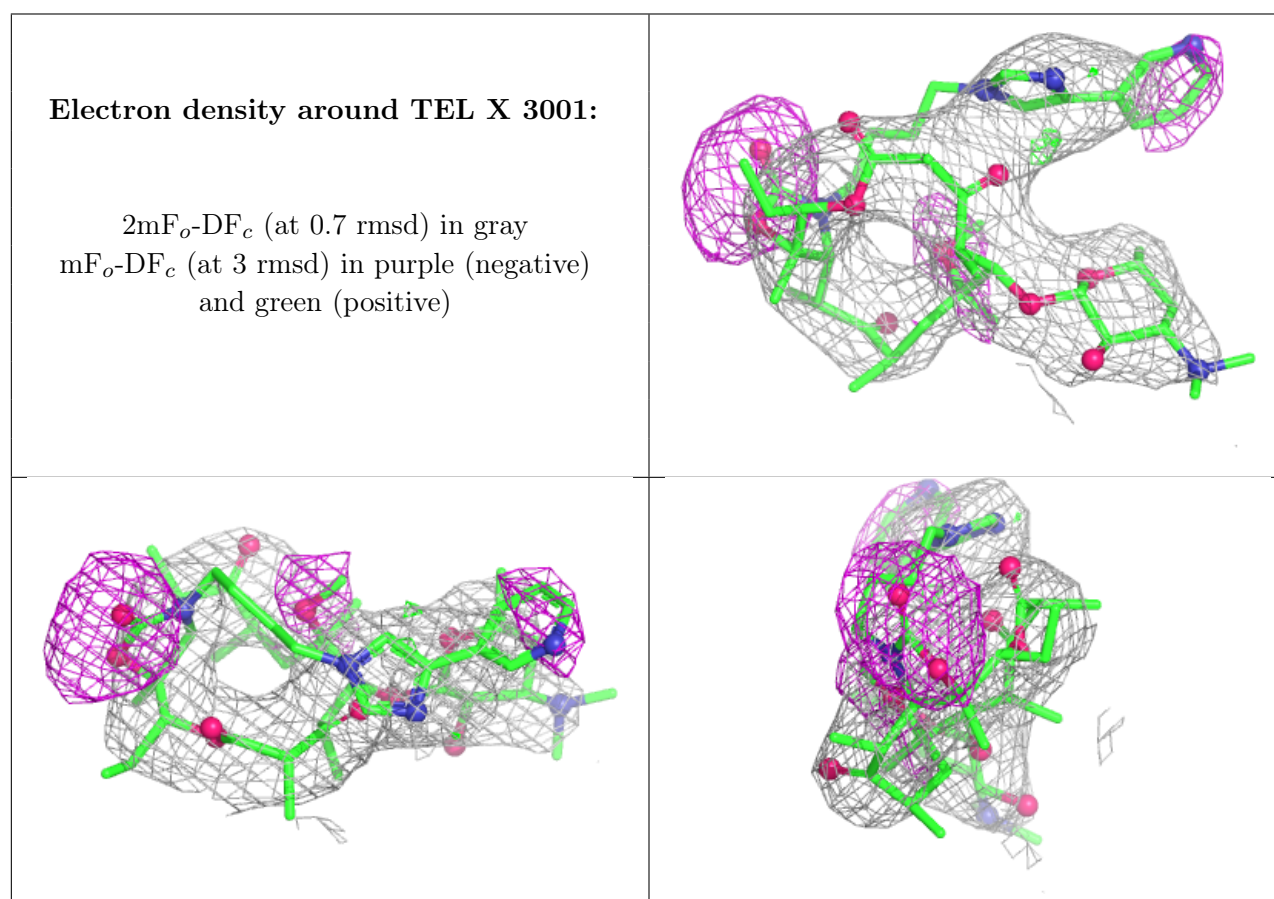
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3121	1/1	0.97	0.05	71,71,71,71	0
29	MG	X	3345	1/1	0.97	0.06	56,56,56,56	0
30	MN	X	3256	1/1	0.97	0.05	79,79,79,79	0
30	MN	X	3160	1/1	0.97	0.05	101,101,101,101	0
30	MN	X	3126	1/1	0.97	0.11	62,62,62,62	0
30	MN	X	3128	1/1	0.97	0.07	55,55,55,55	0
30	MN	X	3069	1/1	0.97	0.14	76,76,76,76	0
30	MN	X	3053	1/1	0.97	0.06	63,63,63,63	0
30	MN	X	3096	1/1	0.97	0.09	46,46,46,46	0
30	MN	X	3242	1/1	0.98	0.05	68,68,68,68	0
30	MN	X	3114	1/1	0.98	0.08	59,59,59,59	0
29	MG	X	3311	1/1	0.98	0.08	39,39,39,39	0
30	MN	X	3078	1/1	0.98	0.11	54,54,54,54	0
30	MN	X	3079	1/1	0.98	0.10	52,52,52,52	0
30	MN	X	3105	1/1	0.98	0.12	48,48,48,48	0
30	MN	X	3063	1/1	0.98	0.07	42,42,42,42	0
30	MN	X	3049	1/1	0.98	0.08	81,81,81,81	0
30	MN	X	3213	1/1	0.98	0.06	63,63,63,63	0
30	MN	X	3054	1/1	0.98	0.08	76,76,76,76	0
30	MN	X	3124	1/1	0.98	0.10	67,67,67,67	0
30	MN	X	3125	1/1	0.98	0.06	60,60,60,60	0
30	MN	X	3187	1/1	0.98	0.06	45,45,45,45	0
30	MN	X	3109	1/1	0.98	0.09	62,62,62,62	0
30	MN	X	3219	1/1	0.98	0.10	90,90,90,90	0
30	MN	X	3047	1/1	0.98	0.12	94,94,94,94	0
30	MN	X	3268	1/1	0.98	0.15	81,81,81,81	0
30	MN	X	3129	1/1	0.98	0.05	61,61,61,61	0
30	MN	X	3097	1/1	0.98	0.06	64,64,64,64	0
30	MN	X	3060	1/1	0.98	0.04	67,67,67,67	0
30	MN	X	3133	1/1	0.98	0.04	81,81,81,81	0
30	MN	X	3201	1/1	0.98	0.11	106,106,106,106	0
30	MN	X	3174	1/1	0.98	0.05	77,77,77,77	0
30	MN	X	3061	1/1	0.98	0.14	69,69,69,69	0
30	MN	X	3240	1/1	0.98	0.20	52,52,52,52	0
30	MN	X	3153	1/1	0.98	0.14	41,41,41,41	0
30	MN	X	3081	1/1	0.99	0.10	49,49,49,49	0
30	MN	X	3130	1/1	0.99	0.06	63,63,63,63	0
30	MN	X	3052	1/1	0.99	0.06	57,57,57,57	0
30	MN	X	3118	1/1	0.99	0.05	32,32,32,32	0
30	MN	X	3090	1/1	0.99	0.07	54,54,54,54	0
30	MN	X	3083	1/1	0.99	0.06	59,59,59,59	0
30	MN	X	3168	1/1	0.99	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3034	1/1	0.99	0.04	81,81,81,81	0
30	MN	X	3136	1/1	0.99	0.07	59,59,59,59	0
30	MN	X	3075	1/1	0.99	0.04	33,33,33,33	0
30	MN	X	3123	1/1	0.99	0.09	38,38,38,38	0
29	MG	X	3309	1/1	0.99	0.09	30,30,30,30	0
30	MN	X	3103	1/1	0.99	0.13	41,41,41,41	0
30	MN	X	3104	1/1	0.99	0.16	53,53,53,53	0
30	MN	X	3127	1/1	0.99	0.08	48,48,48,48	0
30	MN	X	3087	1/1	0.99	0.06	85,85,85,85	0
30	MN	X	3211	1/1	1.00	0.03	64,64,64,64	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 ⓘ

There are no such residues in this entry.