



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2023 – 11:50 AM EDT

PDB ID : 3DLL
Title : The oxazolidinone antibiotics perturb the ribosomal peptidyl-transferase center and effect tRNA positioning
Authors : Wilson, D.N.; Schlutzen, F.; Harms, J.M.; Starosta, A.L.; Connell, S.R.; Fucini, P.
Deposited on : 2008-06-27
Resolution : 3.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

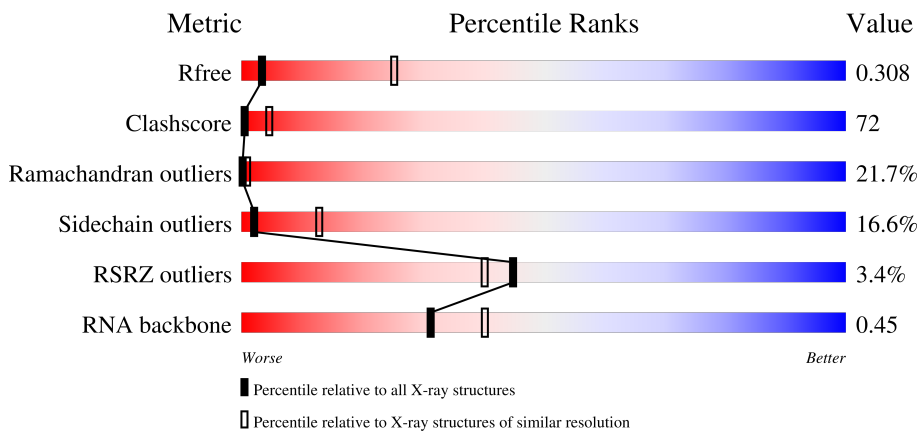
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



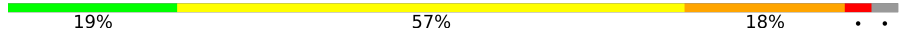


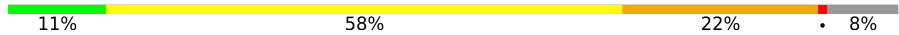


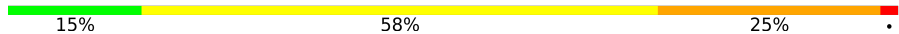
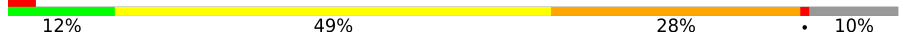
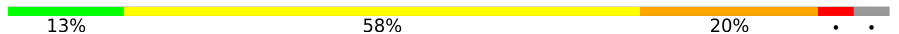
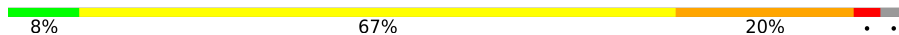
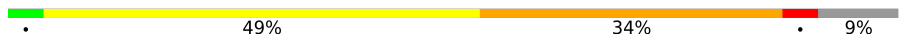

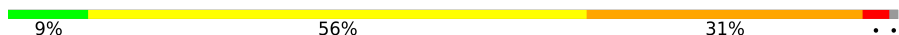
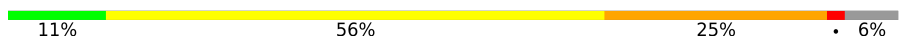
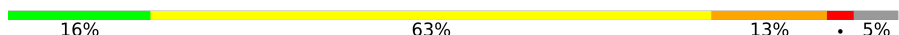







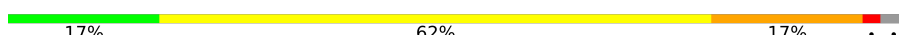


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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	2880	
2	Z	123	
3	A	274	

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Mol	Chain	Length	Quality of chain
4	B	211	
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	142	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Y	60	
27	1	55	
28	2	47	

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Mol	Chain	Length	Quality of chain
29	3	66	<p>74% 92% 5%</p>
30	4	37	<p>8% 5% 78% 16%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	ZLD	X	2911	-	-	X	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 83657 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 rRNA-23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2686	57651	25718	10642	18606	2685	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Z	122	2598	1161	476	840	121	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	218	1637	1017	326	292	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	205	1539	965	295	271	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	197	1506	935	287	282	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	177	1400	892	247	254	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	171	1286	812	237	236	1	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	F	70	504	314	90	97	3	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	G	142	1114	704	209	198	3	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	H	134	997	614	198	180	5	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	I	141	1067	655	216	196	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	J	136	1090	696	202	185	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP Q9RXJ5

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	K	113	878	541	178	157	2	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	L	104	779	476	161	142		0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	M	108	871	543	172	156		0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	N	117	978	608	210	159	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	O	94	741	465	139	137		0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	P	127	1014	639	199	174	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	Q	93	726	458	136	130	2	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	R	110	825	513	160	151	1	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	S	175	1345	849	236	254	6	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	T	84	625	393	122	109	1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
23	U	72	552	341	116	95	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	V	66	533	327	107	96	3	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	W	55	424	264	82	76	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	Y	58	457	281	94	77	5	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C 53 53	0	0	53

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

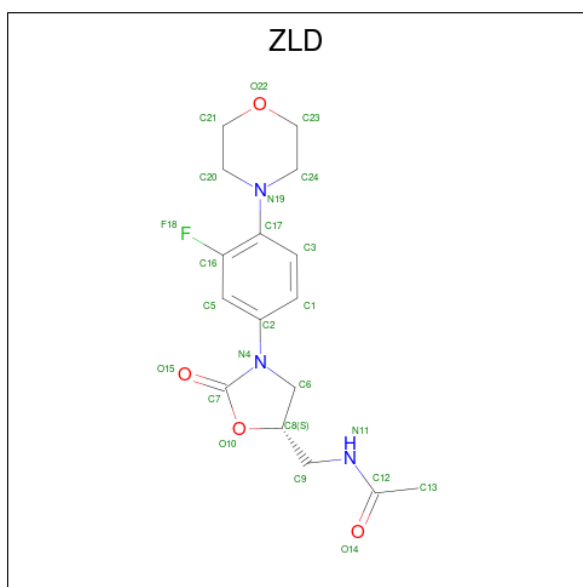
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	30	Total Mg 30 30	0	0
31	Z	4	Total Mg 4 4	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is N-[[[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl]acetamide (three-letter code: ZLD) (formula: C₁₆H₂₀FN₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	X	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

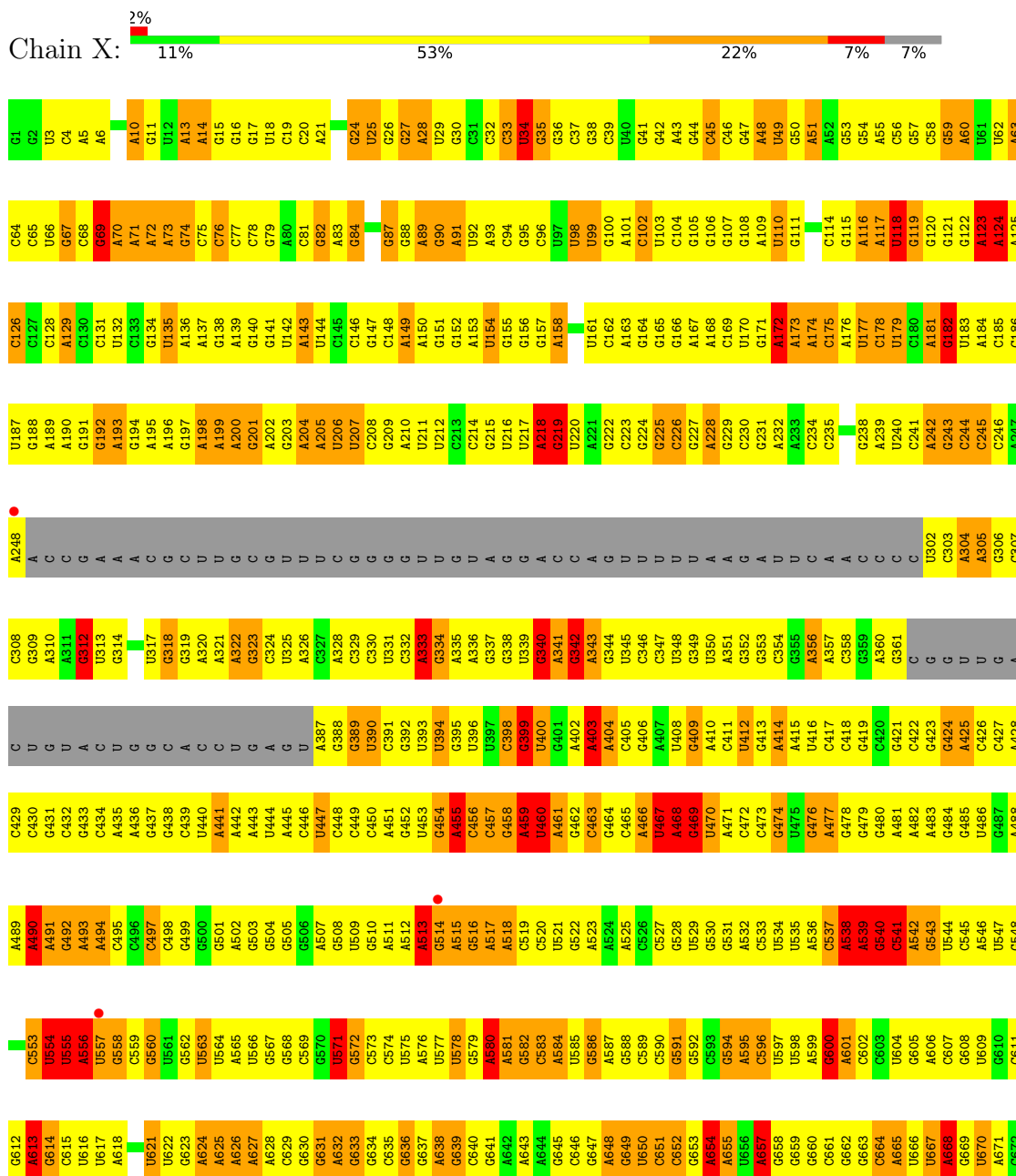
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

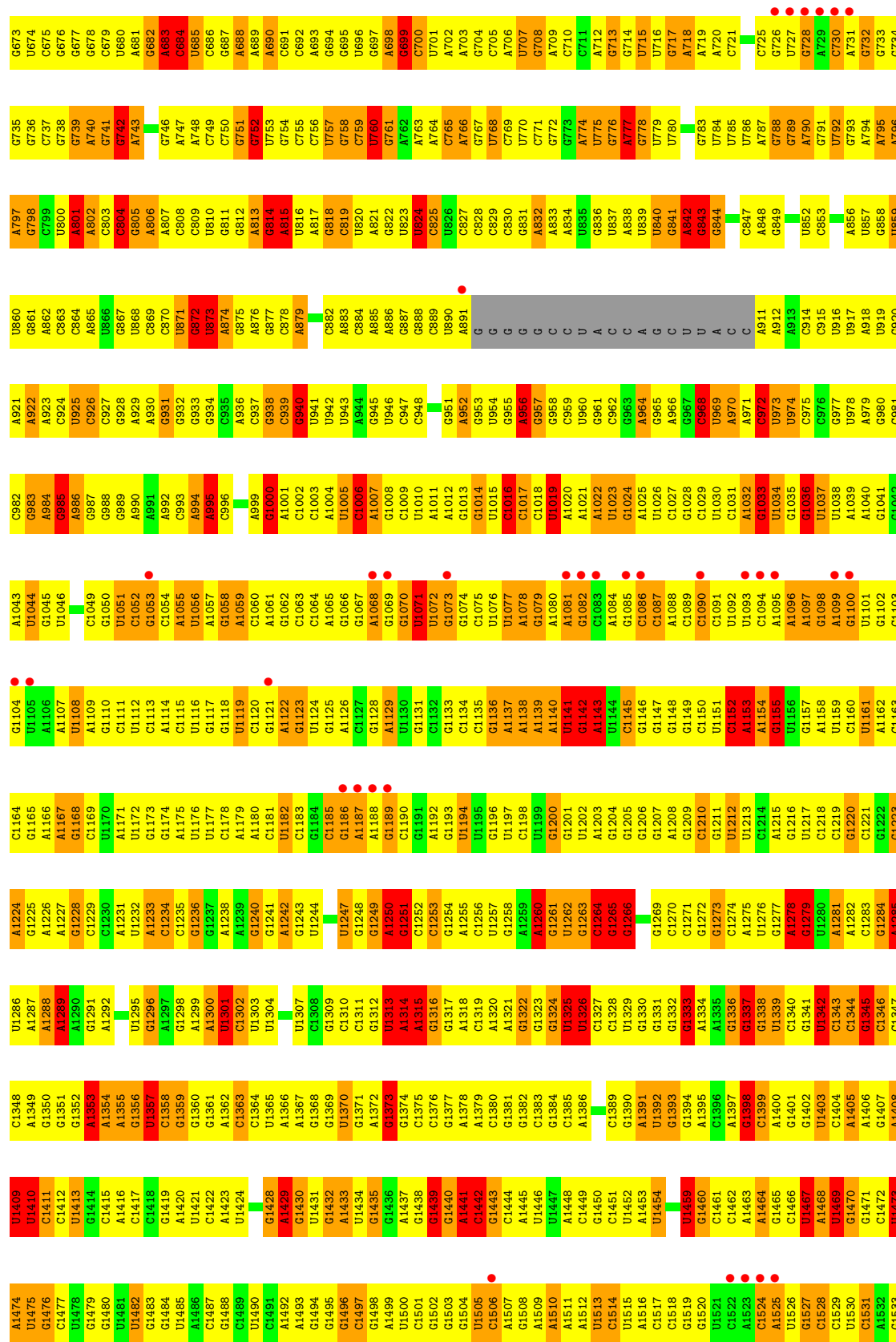
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	Y	1	Total	Zn	0	0
			1	1		
33	4	1	Total	Zn	0	0
			1	1		

3 Residue-property plots i

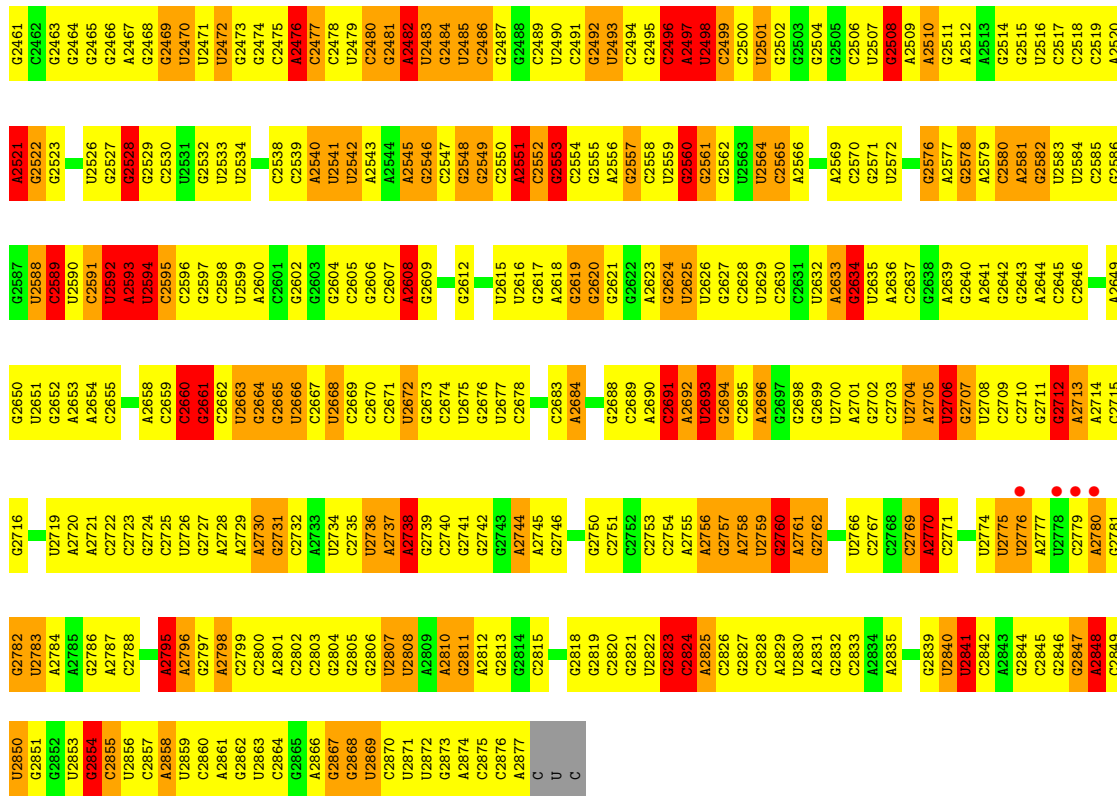
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: rRNA-23S ribosomal RNA

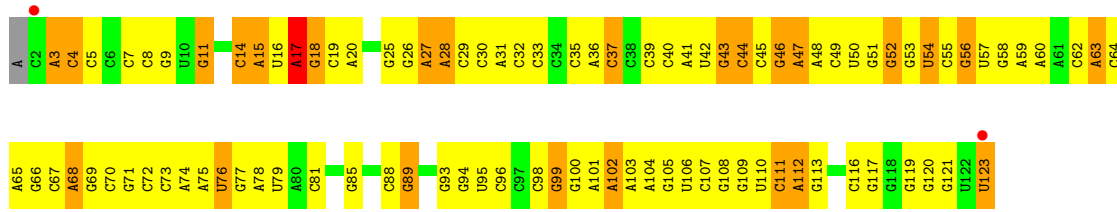




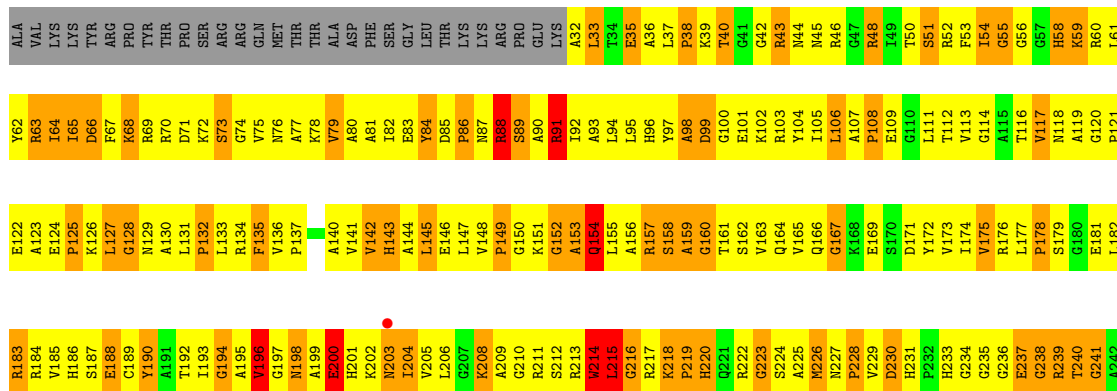
A2401	A2339	U2275	U2212	G	G2029	G1969	G1847	A1785	C1725	G1660	A1594
U2402	C2340	C2276	G2213	A	U2030	G1970	U1848	C1786	C1726	C1661	A1596
C2403	G2341	A2404	G2214	G	A2031	C1971	G1849	U1787	C1727	C1662	A1597
A2404	U2342	C2281	G2215	A	G2032	A1972	G1850	C1788	G1728	C1663	A1598
A2405	C2343	G2282	G2216	G	C2033	C1973	U1789	U1789	C1729	C1664	A1599
C2406	G2344	G2283	U2217	U	A2034	U1974	G1851	G1790	G1665	U1600	G1541
G2407	A2345	U2284	G2218	A	G2035	G1975	G1854	C1791	C1731	G1602	G1542
G2408	C2346	U2285	U2219	C	A2036	A1976	G1855	C1792	C1732	A1603	G1543
A2409	C2347	G2286	A2220	G	A2037	C1977	U1856	C1793	U1733	G1668	A1604
U2410	A2348	C2287	G2221	A	C2038	U1978	G1857	A1794	U1734	A1669	A1605
A2411	G2349	U2288	U2222	U	G2039	C1979	G1858	C1795	G1735	G1670	G1545
A2412	G2350	A2289	U2223	C	A2040	A1980	G1859	A1795	G1736	A1671	G1546
A2413	G2351	U2290	U2224	C	A2041	A1981	A1859	A1796	G1737	A1672	U1547
A2414	G2352	U2291	G2225	U	A2042	C1982	A1860	A1797	G1738	A1673	U1548
G2415	G2353	A2292	A2226	G	A2043	G1983	G1861	C1798	U1738	C1674	C1549
U2416	G2354	C2293	G2227	G	G2044	A1984	U1862	C1799	C1675	U1551	C1550
U2417	A2355	U2294	G2228	G	A2045	G1985	G1864	A1799	U1676	C1613	G1552
A2418	A2356	U2295	U2229	G	C2046	G1986	C1865	A1800	U1679	C1614	G1553
C2419	A2357	G2296	C2170	A	C2047	G1987	G1866	C1801	G1742	C1615	C1554
C2420	U2358	U2298	C2171	G	C2048	A1988	A1867	A1806	C1743	C1616	A1555
C2421	U2359	A2299	U2172	C	C2049	C1989	A1868	A1807	C1744	A1681	A1556
C2422	G2360	G2300	G2173	C	G2050	U1990	A1869	C1808	C1745	A1682	U1618
G2423	C2361	A2301	U2051	U	U2051	C1991	U1870	G1809	G1747	G1683	A1619
G2424	G2362	C2302	A2175	C	G2052	G1992	G1871	U1810	C1621	C1620	G1557
G2425	A2363	C2303	U2176	G	G2053	G1993	A1872	A1811	G1748	G1684	G1558
G2426	C2364	G2304	U2177	G	A2054	U1994	A1873	U1812	A1750	G1685	A1560
A2427	U2365	C2305	U2178	A	A2055	G1995	G1874	U1813	A1751	C1687	A1561
U2428	C2366	A2306	G2179	A	C2056	A1996	U1875	A1814	C1625	G1562	G1562
A2429	A2367	G2307	U2180	A	U2057	A1997	C1876	G1815	A1626	A1625	A1625
A2430	C2368	C2308	A2181	C	U2058	A1998	C1877	G1816	G1627	G1626	U1564
C2431	U2369	G2309	A2182	C	U2059	U1999	C1878	U1817	G1627	G1627	G1565
A2432	G2370	G2310	G2183	U	A2060	U2000	G1879	G1818	C1756	C1628	G1566
A2433	A2371	U2311	C2184	G	C2061	G2001	G1880	U1819	C1757	A1629	A1567
G2434	C2372	G2312	U2185	G	U2064	A2002	U1881	G1820	C1758	A1630	A1568
C2435	C2373	G2313	G2186	C	A2003	A2003	U1882	A1821	U1697	A1632	A1569
U2436	U2249	A2187	A2187	U	U2067	U2005	A1883	C1822	G1759	C1633	C1570
G2437	G2250	A2188	A2188	U	U2067	U2006	A1884	G1823	G1761	A1634	C1572
A2438	U2251	A2189	A2189	U	C2068	G2006	C1885	C1824	C1762	G1635	G1573
U2439	A2252	A2190	A2190	U	U2069	G2007	G1886	C1825	G1763	C1703	A1574
C2440	G2253	A2191	U2192	U	G2070	C2008	G1887	U1826	A1764	G1704	C1575
U2441	G2254	U2192	C2193	G	G2071	U2009	C1888	U1827	C1765	U1575	G1576
C2442	G2255	C2193	G2193	G	C2072	G2010	G	C1828	C1766	C1641	G1577
C2443	G2256	A2194	A2194	U	A2073	U2011	C	C1829	G1767	G1642	U1578
C2444	A2257	C2195	C2195	U	U2074	A2012	C	C1830	C1768	G1579	G1579
C2445	G2258	U2196	U2196	C	U2075	A2013	C	G1831	U1769	C1580	C1580
C2446	G2261	U2197	G2200	G	G2076	A2014	G	G1832	U1770	G1644	C1581
G2447	C2262	U2198	G2201	G	G2077	A2015	A	U1833	A1771	U1645	A1582
A2448	C2263	G2200	G2202	U	A2078	C2016	A	G1834	C1772	G1646	A1583
G2449	C2264	G2201	G2203	G	A2079	U2017	C	C1835	C1773	U1647	G1584
A2450	A2265	G2202	G2204	A	U2080	G2018	U	C1836	A1774	C1648	A1585
U2451	A2266	G2203	G2205	G	U2081	C2019	U	G1837	A1775	A1650	A1586
U2452	A2267	A2204	C2206	G	G2082	G2020	A	U1838	A1776	U1645	A1587
C2453	G2268	C2205	G2208	C	G2083	G2021	A	U1839	A1777	G1652	A1588
C2454	G2269	C2206	U2085	C	G2084	C2022	A	A1840	U1778	C1653	G1589
A2455	U2270	G2207	U2086	A	U2085	G2023	A	G1841	C1779	A1654	G1590
U2456	U2271	U2208	U2087	C	U2086	U2024	G	G1842	G1780	G1720	U1591
A2457	A2272	G2209	U2088	G	U2087	A2025	G	U1843	C1781	U1656	U1592
U2458	C2273	C2210	C2089	G	U2088	C2026	U	C1844	A1782	A1657	A1593
C2459	U2337	G2211	C2090	G	U2090	C2027	C	U1845	G1783	U1723	C1594
G2460	C2374	U2211	G2208	U		C2028	C	A1846	C1784	G1659	A1595

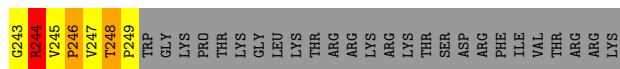


• Molecule 2: rRNA-5S ribosomal RNA

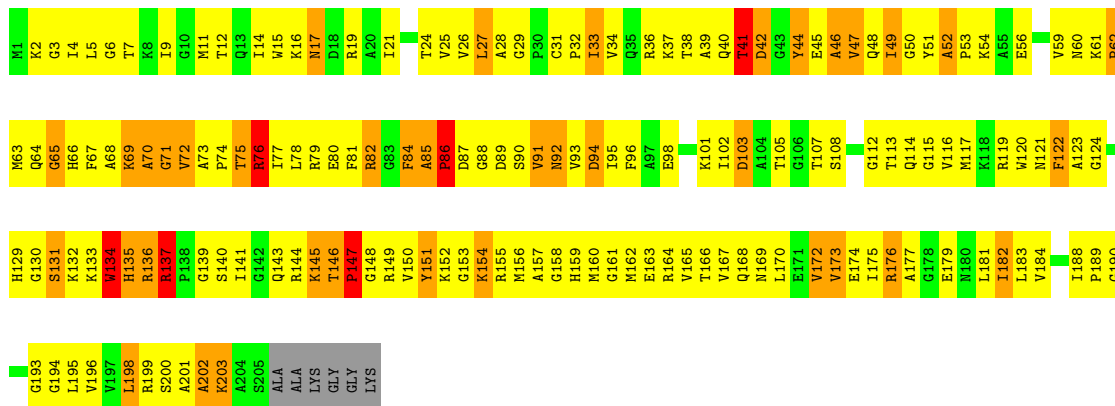


• Molecule 3: 50S ribosomal protein L2

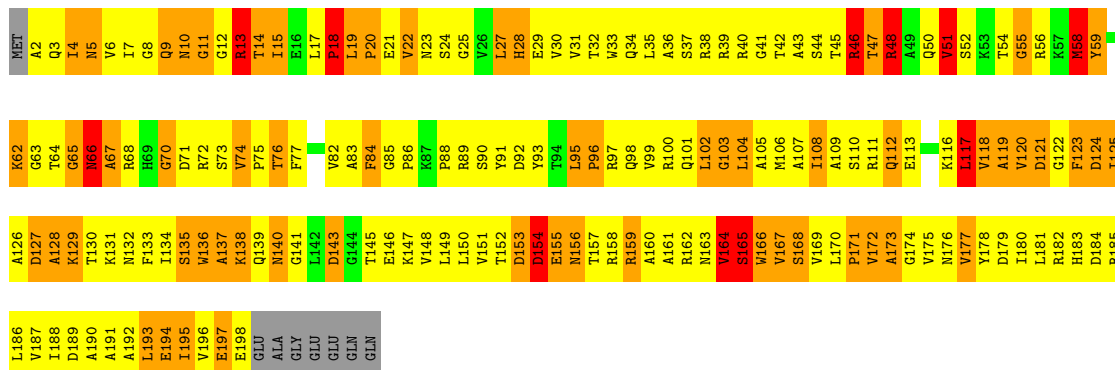
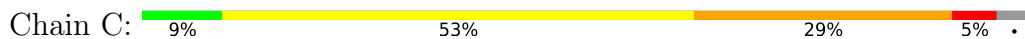




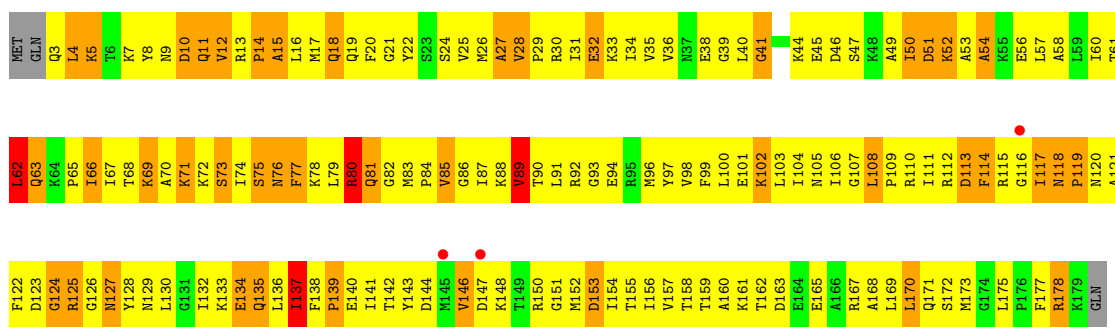
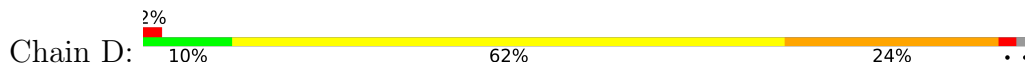
• Molecule 4: 50S ribosomal protein L3



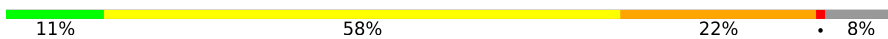
• Molecule 5: 50S ribosomal protein L4

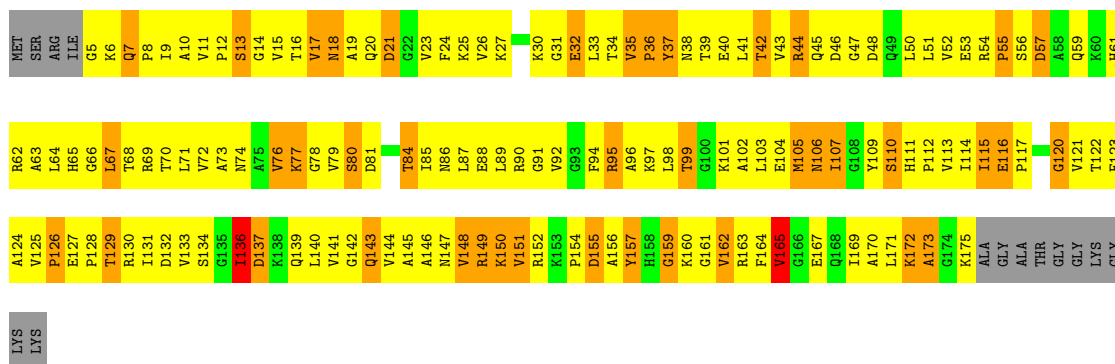


• Molecule 6: 50S ribosomal protein L5




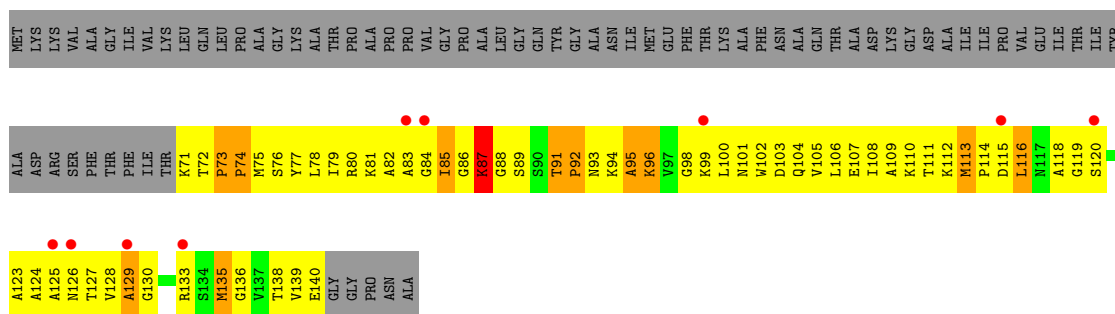
• Molecule 7: 50S ribosomal protein L6

Chain E: 



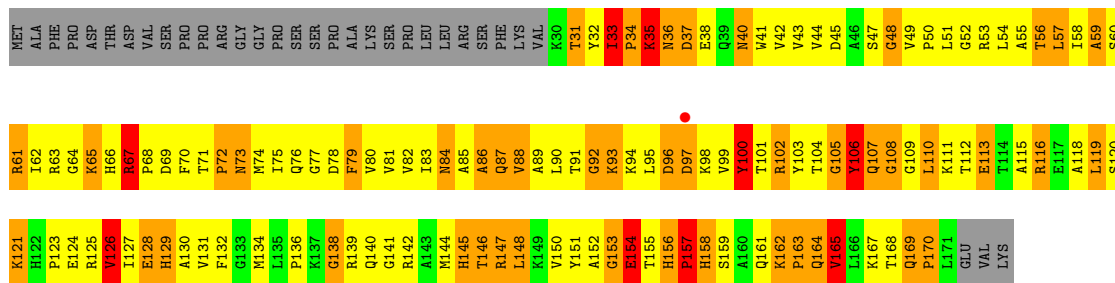
• Molecule 8: 50S ribosomal protein L11

Chain F: 




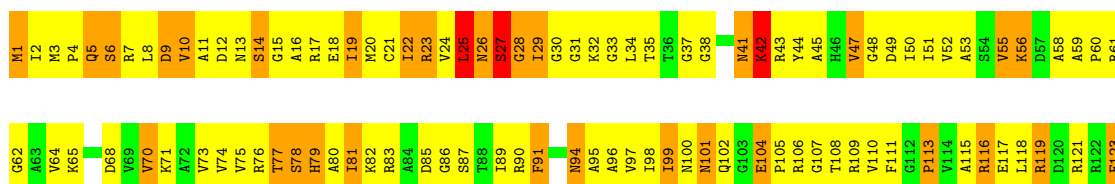
• Molecule 9: 50S ribosomal protein L13

Chain G: 



• Molecule 10: 50S ribosomal protein L14

Chain H: 



M124
K125
I126
V127
S128
L129
A130
P131
E132
V133
L134

- Molecule 11: 50S ribosomal protein L15

Chain I: 3%
12% 49% 28% 10%

MET LYS LEU H4 H5 L6 K7 P8 T9 P10 G11 G12 S12 R13 K14 D15 L16 K17 R18 V19 G20 R21 R22 G23 G24 G25 G26 D27 K28 R29 T29 A30 G31 R32 R33 G34 R35 K36 G37 Q37 K38 S39 R40 R41 N102 G42 G43 G44 R45 G46 G47 A48 F49 F49 E50 G51 G52 G53 S54 S54 R55 L56 L57 L58 A58 R59 L60

P61 K62 R63 G64 F65 N66 N67 V68 G69 T70 T71 T72 E73 K76 L77 S78 Q79 L80 Q81 D82 L83 E84 E84 D85 T86 T87 F88 D89 R90 R90 D91 T92 L93 R94 E94 Y96 R97 L98 V99 R100 R101 N103 G102 N103 R104 R105 V106 K107 L108 L109 A110 S111 G112 E113 I114 S115 R116 L117 V118 T119 V120 L121

V122 D123 A124 A125 A129 I130 K131 A132 V133 E134 A135 A136 G137 G138 R139 V140 V141 L142 F143 E144 VAL THR GLN GLN ASP ASP ALA ALA LYS ALA GLU

- Molecule 12: 50S ribosomal protein L16

Chain J: 13% 58% 20%

MET MET LEU LEU PRO K6 K7 T8 R9 R11 R12 Q13 F14 R15 G16 R17 R18 R19 G20 G21 A22 K23 G24 G25 D26 Y27 Y33 G34 L35 L36 A37 K38 E39 P40 R41 W42 L43 K44 S45 N46 Q47 L48 E49 A50 C51 R52 L53 V54 M55 K56 R57 H58 F59 R60 R61

G62 G63 K64 L65 Y66 R67 R68 I69 F70 P71 D72 K73 P74 V75 T76 K77 R78 P79 A80 E81 T82 R83 K86 K88 G89 A90 Y91 E92 Y93 Y94 Y95 S96 Y97 V98 A97 K99 P100 G101 R102 W103 M104 F105 E106 V107 A108 G109 V110 T111 E112 Q113 E114 A115 K116 E117 A118 F119 R120 L121 A122

G123 H124 K125 L126 P127 I128 Q129 K131 M132 V133 K134 R135 E136 Y137 Y138 E140 A141 GLN

- Molecule 13: 50S ribosomal protein L17

Chain K: 8% 67% 20%

MET ARG H3 G4 K5 A6 G7 R8 R9 L10 M11 R12 M13 S14 S15 R16 R17 V18 W18 A19 L20 A21 R22 A23 A24 A25 T26 R27 L28 L29 R30 R31 G32 G33 R34 R35 Q36 T36 R37 L38 T39 R40 R41 R42 R43 G44 L44 R45 V108 P46 F47 M10 M10 E49 O50 L51 L52 T53 T54 A55 A55 K56 G57 D58 D59 L60

H61 S62 R63 R64 V66 A67 Q68 I70 D73 D74 V75 V76 R77 R78 W79 R80 R81 R82 W83 A84 P85 K86 Y87 R90 P91 G92 G93 Y94 R95 R96 R97 L98 R99 V100 G101 T102 R103 R104 G105 D106 G107 V108 T109 M10 A111 L112 L113 E114 L115 VAL


- Molecule 14: 50S ribosomal protein L18

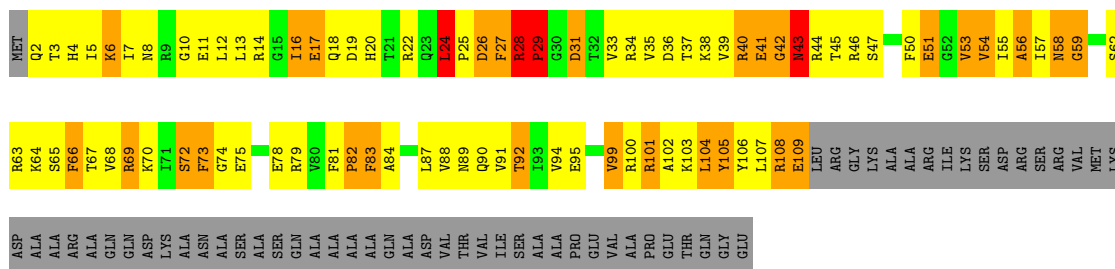
Chain L: 49% 34% 9%

MET ALA THR ALA THR THR LLE R8 R9 R10 L11 R12 T13 R14 R15 V17 R18 T19 T20 T21 R22 A23 A24 A25 G26 R26 L27 R28 L29 S30 S31 Y32 Y33 R33 S34 S35 K36 H37 L38 Y39 A40 Q41 I42 I43 D44 D45 S46 R47 C48 T50 T50 L51 A52 A53 A54 S55 S55 A57 A58 L59 R60


S61 G62 N63 R64 T65 D66 T67 A68 A69 V70 V71 G72 K73 A74 A75 A76 A77 A78 A79 A80 E81 R82 G83 G84 T84 K85 Q86 R87 W88 F89 D90 R91 G92 S93 Y94 K95 Y96 H97 G98 R99 V100 K101 A102 L103 A104 D105 A106 R107 R108 E109 G110 G111 LEU ASP PHE

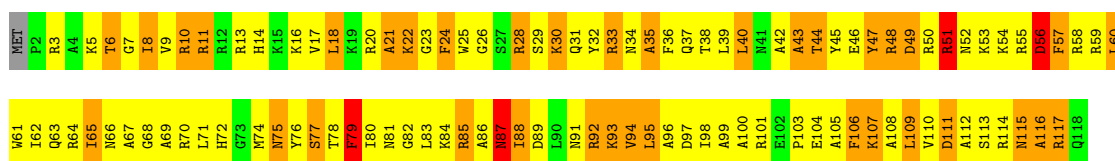
- Molecule 15: 50S ribosomal protein L19

Chain M: 




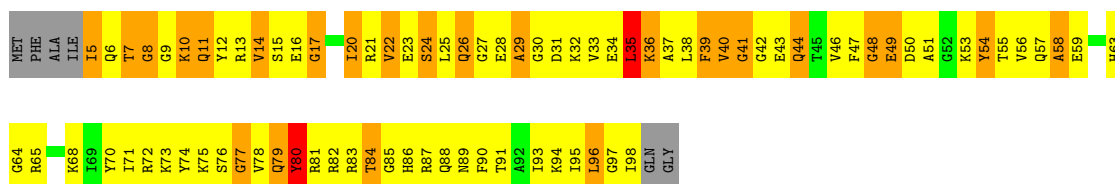
• Molecule 16: 50S ribosomal protein L20

Chain N: 



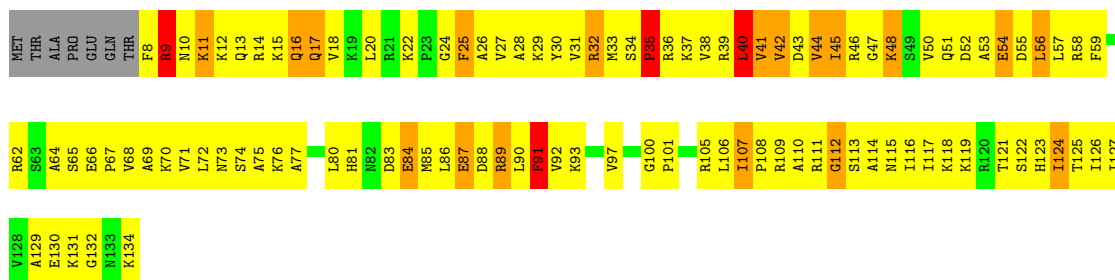
• Molecule 17: 50S ribosomal protein L21

Chain O: 



• Molecule 18: 50S ribosomal protein L22

Chain P: 



• Molecule 19: 50S ribosomal protein L23

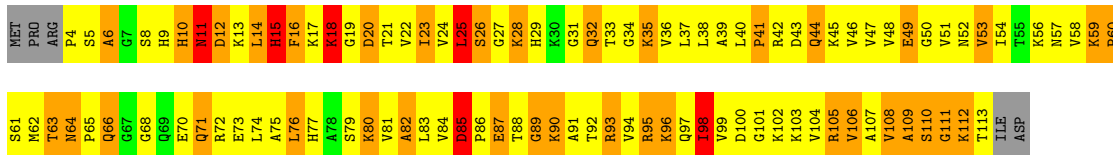
Chain Q: 





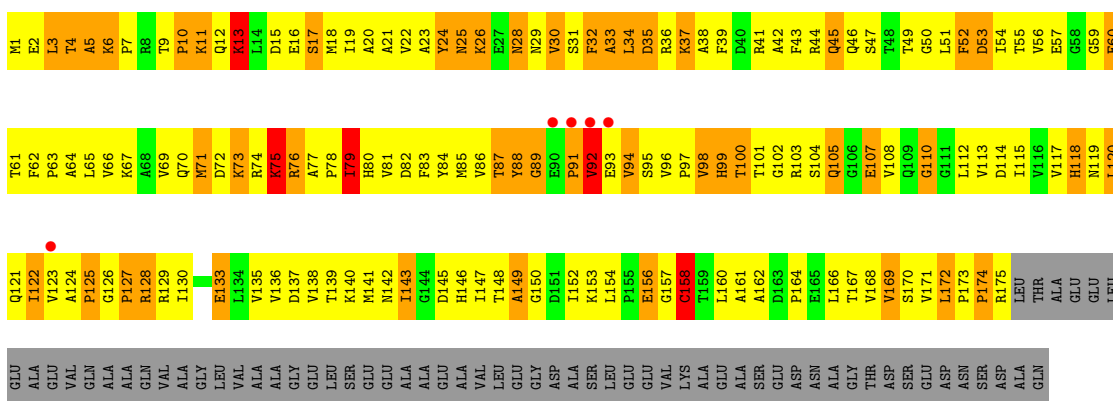
- Molecule 20: 50S ribosomal protein L24

Chain R: 5% 53% 32% 5%



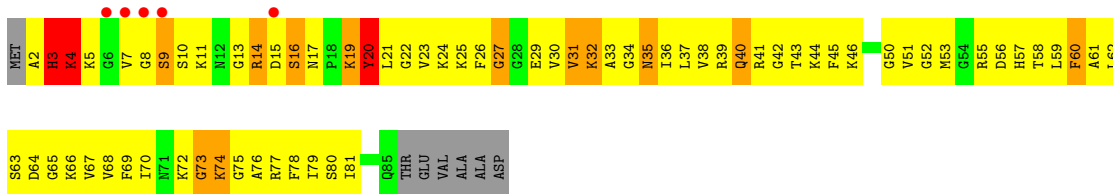
- Molecule 21: 50S ribosomal protein L25

Chain S: 2% 9% 43% 20% 26%



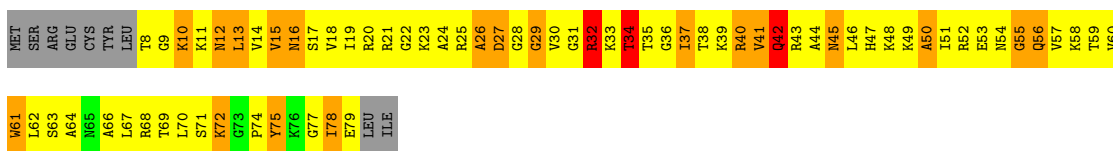
- Molecule 22: 50S ribosomal protein L27

Chain T: 5% 14% 62% 13% 8%



- Molecule 23: 50S ribosomal protein L28

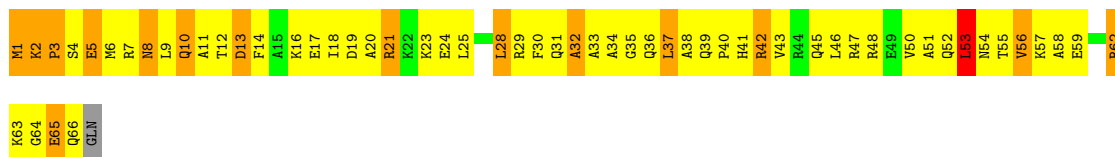
Chain U: 58% 23% 11%



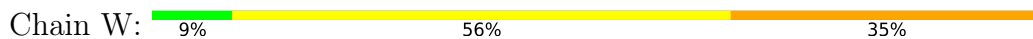
- Molecule 24: 50S ribosomal protein L29

Chain V: 12% 63% 22%





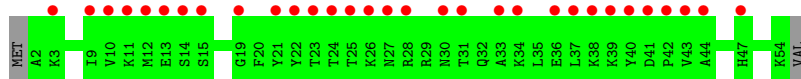
• Molecule 25: 50S ribosomal protein L30



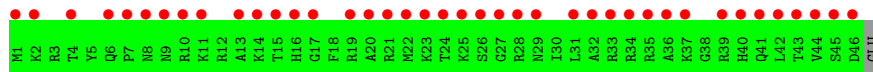
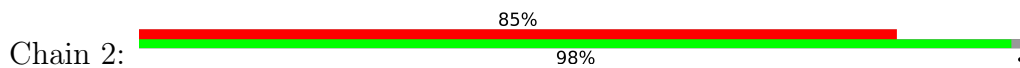
• Molecule 26: 50S ribosomal protein L32



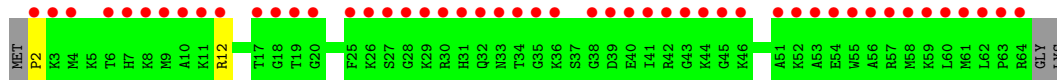
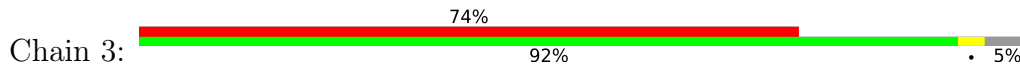
• Molecule 27: 50S ribosomal protein L33



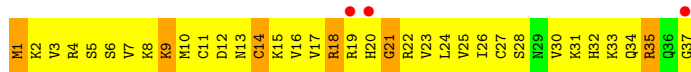
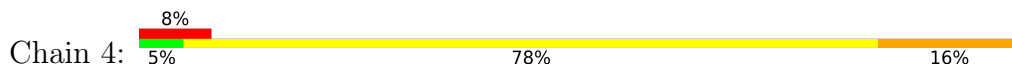
• Molecule 28: 50S ribosomal protein L34



• Molecule 29: 50S ribosomal protein L35



• Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.70Å 410.00Å 695.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 30.06 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.98-3.50) 85.7 (30.06-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.31Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.280 0.268 , 0.308	Depositor DCC
R_{free} test set	15358 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	83657	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ZLD

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	0.83	19/64561 (0.0%)	0.93	192/100708 (0.2%)
2	Z	0.56	0/2904	0.78	0/4525
3	A	0.62	0/1669	0.95	1/2254 (0.0%)
4	B	0.76	0/1567	0.99	1/2105 (0.0%)
5	C	0.62	0/1529	0.92	1/2070 (0.0%)
6	D	0.50	0/1419	0.79	0/1903
7	E	0.49	0/1308	0.80	0/1771
8	F	0.51	0/510	0.82	0/688
9	G	0.62	0/1138	0.95	2/1539 (0.1%)
10	H	0.75	0/1007	0.99	2/1352 (0.1%)
11	I	0.66	1/1081 (0.1%)	0.98	0/1448
12	J	0.68	1/1113 (0.1%)	0.87	0/1486
13	K	0.90	0/886	1.07	1/1188 (0.1%)
14	L	0.53	0/785	0.84	0/1048
15	M	0.76	0/884	1.24	5/1186 (0.4%)
16	N	0.64	0/994	0.84	0/1323
17	O	0.60	0/750	0.92	1/1000 (0.1%)
18	P	0.76	0/1027	0.99	1/1373 (0.1%)
19	Q	0.62	0/737	0.93	2/988 (0.2%)
20	R	0.53	0/835	0.91	3/1121 (0.3%)
21	S	0.51	0/1370	0.82	0/1862
22	T	0.59	0/633	0.89	0/838
23	U	0.57	0/556	0.92	0/741
24	V	0.51	0/537	0.82	0/714
25	W	0.54	0/426	0.86	0/568
26	Y	0.71	0/469	1.01	0/629
30	4	0.48	0/298	0.77	0/390
All	All	0.78	21/90993 (0.0%)	0.92	212/136818 (0.2%)

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	X	0	228
2	Z	0	4
9	G	0	1
17	O	0	1
All	All	0	234

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2594	U	P-OP2	17.32	1.78	1.49
1	X	2594	U	P-OP1	-13.28	1.26	1.49
1	X	2592	U	P-OP2	-12.20	1.28	1.49
1	X	28	A	C5-C6	-6.98	1.34	1.41
1	X	1333	G	N9-C4	-6.33	1.32	1.38

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	28	ARG	C-N-CD	-19.65	77.37	120.60
1	X	2594	U	O5'-P-OP2	-18.88	88.04	110.70
1	X	2592	U	O5'-P-OP2	-15.03	92.18	105.70
1	X	2592	U	N1-C1'-C2'	14.74	133.17	114.00
1	X	2592	U	C1'-O4'-C4'	-12.24	100.11	109.90

There are no chirality outliers.

5 of 234 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	10	A	Sidechain
1	X	24	G	Sidechain
1	X	25	U	Sidechain
1	X	34	U	Sidechain
1	X	98	U	Sidechain

5.2 Too-close contacts [\(i\)](#)

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	57651	0	29049	4430	0
2	Z	2598	0	1328	213	0
3	A	1637	0	1673	471	0
4	B	1539	0	1600	358	0
5	C	1506	0	1525	400	0
6	D	1400	0	1481	437	0
7	E	1286	0	1336	330	0
8	F	504	0	530	125	0
9	G	1114	0	1144	371	0
10	H	997	0	1046	213	1
11	I	1067	0	1103	324	0
12	J	1090	0	1125	259	0
13	K	878	0	930	165	1
14	L	779	0	820	275	0
15	M	871	0	894	204	0
16	N	978	0	1020	288	0
17	O	741	0	756	242	0
18	P	1014	0	1096	191	0
19	Q	726	0	753	197	0
20	R	825	0	881	271	0
21	S	1345	0	1372	323	0
22	T	625	0	655	144	0
23	U	552	0	604	192	0
24	V	533	0	558	133	0
25	W	424	0	470	103	0
26	Y	457	0	462	86	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	2	0
30	4	297	0	329	83	0
31	M	1	0	0	0	0
31	X	30	0	0	0	0
31	Z	4	0	0	0	0
32	X	24	0	19	22	0
33	4	1	0	0	0	0
33	Y	1	0	0	0	0
All	All	83657	0	54559	9938	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 72.

The worst 5 of 9938 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:1281:A:H1'	1:X:2592:U:C5	1.68	1.26
1:X:2198:U:H3'	1:X:2199:C:C4'	1.66	1.24
1:X:2198:U:C3'	1:X:2199:C:H4'	1.68	1.23
1:X:1781:C:OP1	3:A:219:PRO:HB2	1.41	1.20
1:X:1281:A:C1'	1:X:2592:U:H5	1.55	1.20

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)
10:H:107:GLY:O	13:K:86:LYS:NZ[8_555]	2.03	0.17

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	216/274 (79%)	109 (50%)	52 (24%)	55 (26%)	0	0
4	B	203/211 (96%)	124 (61%)	47 (23%)	32 (16%)	0	2
5	C	195/205 (95%)	92 (47%)	46 (24%)	57 (29%)	0	0
6	D	175/180 (97%)	78 (45%)	54 (31%)	43 (25%)	0	0
7	E	169/185 (91%)	91 (54%)	42 (25%)	36 (21%)	0	1
8	F	68/144 (47%)	37 (54%)	21 (31%)	10 (15%)	0	3
9	G	140/174 (80%)	66 (47%)	32 (23%)	42 (30%)	0	0
10	H	132/134 (98%)	91 (69%)	26 (20%)	15 (11%)	0	6
11	I	139/156 (89%)	51 (37%)	50 (36%)	38 (27%)	0	0
12	J	134/142 (94%)	63 (47%)	46 (34%)	25 (19%)	0	2
13	K	111/116 (96%)	61 (55%)	31 (28%)	19 (17%)	0	2
14	L	102/114 (90%)	48 (47%)	25 (24%)	29 (28%)	0	0
15	M	106/166 (64%)	68 (64%)	17 (16%)	21 (20%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	115/118 (98%)	56 (49%)	30 (26%)	29 (25%)	0	0
17	O	92/100 (92%)	52 (56%)	19 (21%)	21 (23%)	0	1
18	P	125/134 (93%)	75 (60%)	35 (28%)	15 (12%)	0	5
19	Q	91/95 (96%)	44 (48%)	23 (25%)	24 (26%)	0	0
20	R	108/115 (94%)	63 (58%)	17 (16%)	28 (26%)	0	1
21	S	173/237 (73%)	97 (56%)	40 (23%)	36 (21%)	0	1
22	T	82/91 (90%)	51 (62%)	16 (20%)	15 (18%)	0	2
23	U	70/81 (86%)	39 (56%)	15 (21%)	16 (23%)	0	1
24	V	64/67 (96%)	32 (50%)	19 (30%)	13 (20%)	0	1
25	W	53/55 (96%)	22 (42%)	18 (34%)	13 (24%)	0	0
26	Y	56/60 (93%)	31 (55%)	17 (30%)	8 (14%)	0	3
30	4	35/37 (95%)	22 (63%)	11 (31%)	2 (6%)	1	16
All	All	2954/3391 (87%)	1563 (53%)	749 (25%)	642 (22%)	0	1

5 of 642 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	33	LEU
3	A	58	HIS
3	A	66	ASP
3	A	91	ARG
3	A	98	ALA

5.3.2 Protein sidechains [i](#)

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	164/215 (76%)	130 (79%)	34 (21%)	1	6
4	B	155/157 (99%)	132 (85%)	23 (15%)	3	17
5	C	157/163 (96%)	126 (80%)	31 (20%)	1	7
6	D	153/156 (98%)	139 (91%)	14 (9%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	136/144 (94%)	119 (88%)	17 (12%)	4	23
8	F	53/107 (50%)	48 (91%)	5 (9%)	8	35
9	G	118/146 (81%)	96 (81%)	22 (19%)	1	8
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	4
11	I	108/121 (89%)	91 (84%)	17 (16%)	2	15
12	J	110/116 (95%)	92 (84%)	18 (16%)	2	13
13	K	90/93 (97%)	71 (79%)	19 (21%)	1	5
14	L	74/82 (90%)	54 (73%)	20 (27%)	0	3
15	M	94/134 (70%)	81 (86%)	13 (14%)	3	20
16	N	96/97 (99%)	80 (83%)	16 (17%)	2	12
17	O	75/79 (95%)	69 (92%)	6 (8%)	12	41
18	P	109/115 (95%)	92 (84%)	17 (16%)	2	16
19	Q	75/76 (99%)	62 (83%)	13 (17%)	2	11
20	R	91/96 (95%)	70 (77%)	21 (23%)	1	4
21	S	149/192 (78%)	123 (83%)	26 (17%)	2	11
22	T	62/67 (92%)	53 (86%)	9 (14%)	3	18
23	U	57/66 (86%)	46 (81%)	11 (19%)	1	7
24	V	54/55 (98%)	45 (83%)	9 (17%)	2	12
25	W	48/48 (100%)	41 (85%)	7 (15%)	3	18
26	Y	51/53 (96%)	45 (88%)	6 (12%)	5	25
30	4	35/35 (100%)	30 (86%)	5 (14%)	3	19
All	All	2417/2716 (89%)	2015 (83%)	402 (17%)	2	13

5 of 402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	L	59	LEU
18	P	40	LEU
30	4	12	ASP
14	L	89	PHE
16	N	40	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
18	P	81	HIS
22	T	57	HIS
19	Q	73	ASN
21	S	45	GLN
24	V	36	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	678 (25%)	283 (10%)
2	Z	121/123 (98%)	24 (19%)	0
All	All	2801/3003 (93%)	702 (25%)	283 (10%)

5 of 702 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	13	A
1	X	14	A
1	X	27	G
1	X	34	U
1	X	35	G

5 of 283 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	2324	G
1	X	2418	A
1	X	2624	G
1	X	995	A
1	X	984	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 37 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
32	ZLD	X	2911	-	26,26,26	1.26	2 (7%)	36,36,36	3.05	8 (22%)

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
32	ZLD	X	2911	-	-	9/13/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2911	ZLD	O10-C7	3.48	1.40	1.35
32	X	2911	ZLD	C5-C16	2.11	1.41	1.37

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2911	ZLD	O10-C8-C9	9.66	117.90	109.33
32	X	2911	ZLD	C6-C8-C9	9.32	123.40	113.08
32	X	2911	ZLD	C2-N4-C7	-6.22	119.25	125.91
32	X	2911	ZLD	O15-C7-N4	4.94	132.83	128.91
32	X	2911	ZLD	O10-C7-N4	-4.77	106.55	109.83

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2911	ZLD	C5-C2-N4-C7

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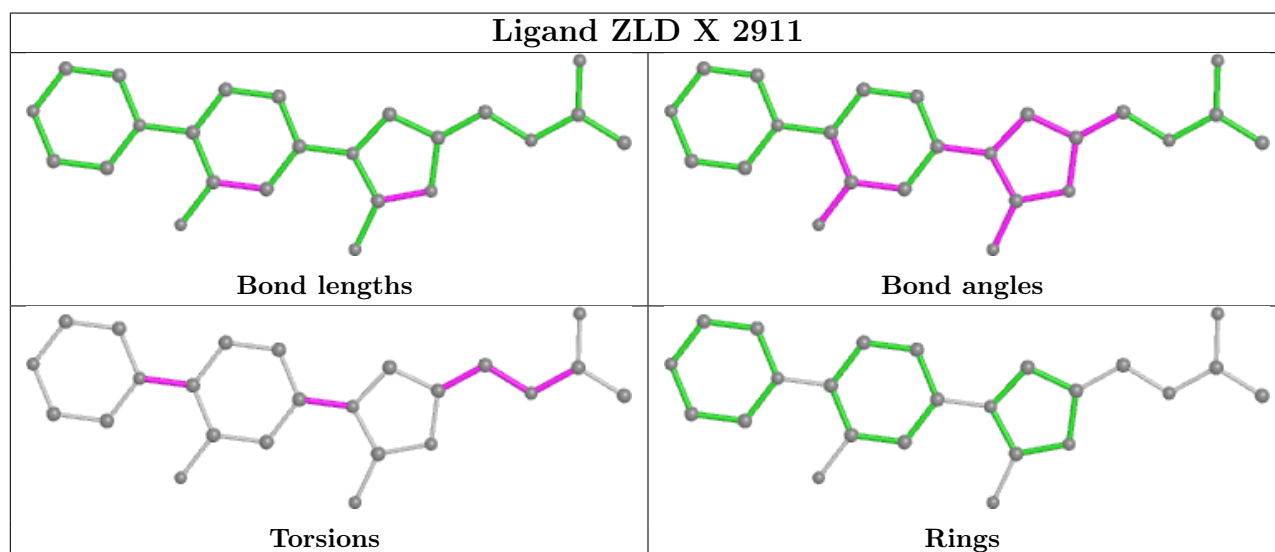
Mol	Chain	Res	Type	Atoms
32	X	2911	ZLD	C1-C2-N4-C7
32	X	2911	ZLD	C6-C8-C9-N11
32	X	2911	ZLD	O10-C8-C9-N11
32	X	2911	ZLD	C13-C12-N11-C9

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2911	ZLD	22	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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	2686/2880 (93%)	-0.47	52 (1%) 66 61	1, 35, 97, 115	0
2	Z	122/123 (99%)	0.00	2 (1%) 72 66	28, 74, 94, 101	0
3	A	218/274 (79%)	-0.53	1 (0%) 91 88	8, 44, 57, 63	0
4	B	205/211 (97%)	-0.89	0 100 100	1, 12, 35, 53	0
5	C	197/205 (96%)	-0.57	0 100 100	2, 45, 62, 78	0
6	D	177/180 (98%)	-0.13	3 (1%) 70 64	54, 65, 73, 76	0
7	E	171/185 (92%)	-0.50	0 100 100	38, 59, 72, 76	0
8	F	70/144 (48%)	0.69	9 (12%) 3 4	62, 71, 75, 76	0
9	G	142/174 (81%)	-0.65	1 (0%) 87 83	19, 37, 53, 57	0
10	H	134/134 (100%)	-0.91	0 100 100	1, 8, 30, 42	0
11	I	141/156 (90%)	-0.09	5 (3%) 44 39	10, 54, 69, 84	0
12	J	136/142 (95%)	-0.53	0 100 100	25, 44, 59, 66	0
13	K	113/116 (97%)	-0.91	0 100 100	1, 2, 13, 23	0
14	L	104/114 (91%)	-0.24	0 100 100	38, 54, 61, 67	0
15	M	108/166 (65%)	-0.96	0 100 100	1, 11, 40, 46	0
16	N	117/118 (99%)	-0.77	0 100 100	2, 32, 55, 64	0
17	O	94/100 (94%)	-0.69	0 100 100	13, 46, 63, 66	0
18	P	127/134 (94%)	-0.89	0 100 100	1, 10, 40, 57	0
19	Q	93/95 (97%)	-0.63	0 100 100	23, 36, 60, 63	0
20	R	110/115 (95%)	-0.56	0 100 100	32, 44, 66, 70	0
21	S	175/237 (73%)	-0.17	5 (2%) 51 45	53, 62, 72, 79	0
22	T	84/91 (92%)	-0.05	5 (5%) 21 19	23, 47, 66, 69	0
23	U	72/81 (88%)	-0.40	0 100 100	39, 52, 63, 64	0
24	V	66/67 (98%)	-0.77	0 100 100	34, 52, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
25	W	55/55 (100%)	-0.69	0	100	100	32, 41, 57, 66	0
26	Y	58/60 (96%)	-0.82	0	100	100	1, 7, 32, 34	0
27	1	53/55 (96%)	2.51	31 (58%)	0	0	33, 47, 62, 65	0
28	2	46/47 (97%)	3.37	40 (86%)	0	0	1, 12, 25, 35	0
29	3	63/66 (95%)	3.45	49 (77%)	0	0	23, 34, 43, 50	0
30	4	37/37 (100%)	0.52	3 (8%)	12	12	52, 65, 72, 73	0
All	All	5974/6562 (91%)	-0.39	206 (3%)	45	40	1, 41, 84, 115	0

The worst 5 of 206 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	34	THR	8.7
29	3	33	ASN	8.6
27	1	40	TYR	8.2
29	3	39	ASP	7.6
29	3	32	GLN	7.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

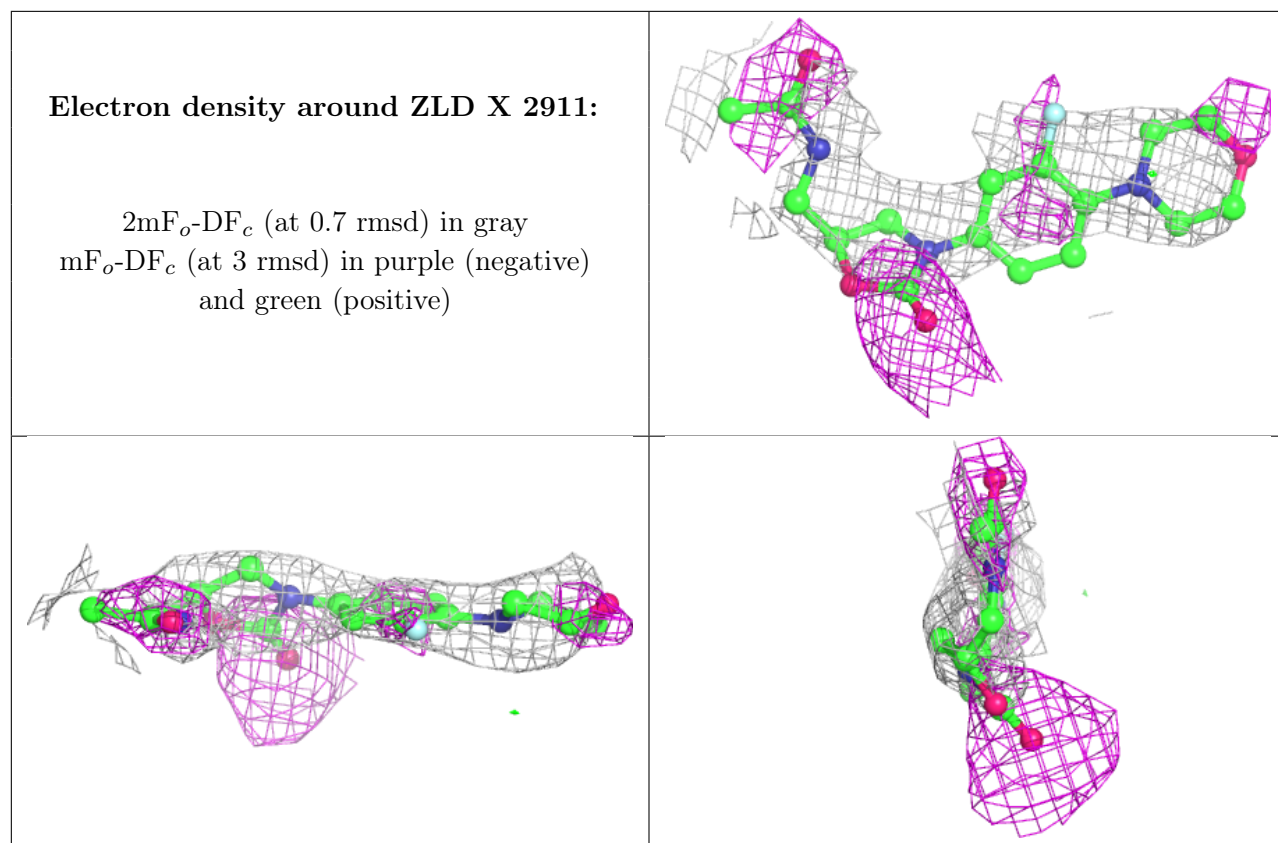
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	2885	1/1	0.89	0.20	45,45,45,45	0
31	MG	X	2897	1/1	0.90	0.26	1,1,1,1	0
31	MG	Z	124	1/1	0.90	0.20	11,11,11,11	0
32	ZLD	X	2911	24/24	0.90	0.47	28,31,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	2900	1/1	0.92	0.51	1,1,1,1	0
31	MG	X	2894	1/1	0.93	0.34	2,2,2,2	0
31	MG	X	2903	1/1	0.93	0.31	1,1,1,1	0
31	MG	X	2910	1/1	0.94	0.26	14,14,14,14	0
31	MG	X	2891	1/1	0.94	0.13	23,23,23,23	0
31	MG	X	2904	1/1	0.94	0.40	1,1,1,1	0
31	MG	X	2889	1/1	0.95	0.44	1,1,1,1	0
31	MG	X	2890	1/1	0.95	0.65	1,1,1,1	0
31	MG	X	2881	1/1	0.95	0.53	10,10,10,10	0
31	MG	Z	126	1/1	0.95	0.13	12,12,12,12	0
31	MG	X	2893	1/1	0.95	0.20	3,3,3,3	0
31	MG	X	2908	1/1	0.96	0.43	48,48,48,48	0
31	MG	X	2882	1/1	0.96	0.39	49,49,49,49	0
31	MG	X	2886	1/1	0.96	0.25	15,15,15,15	0
31	MG	X	2887	1/1	0.96	0.18	37,37,37,37	0
31	MG	X	2905	1/1	0.96	0.34	18,18,18,18	0
31	MG	X	2902	1/1	0.97	0.74	61,61,61,61	0
31	MG	X	2883	1/1	0.97	0.19	1,1,1,1	0
31	MG	X	2898	1/1	0.97	0.42	1,1,1,1	0
31	MG	X	2884	1/1	0.97	0.19	19,19,19,19	0
31	MG	Z	127	1/1	0.97	0.21	3,3,3,3	0
31	MG	X	2907	1/1	0.97	0.62	1,1,1,1	0
31	MG	X	2892	1/1	0.98	0.19	1,1,1,1	0
31	MG	Z	125	1/1	0.98	0.17	1,1,1,1	0
31	MG	X	2901	1/1	0.98	0.36	1,1,1,1	0
31	MG	X	2909	1/1	0.98	0.35	1,1,1,1	0
31	MG	M	167	1/1	0.98	0.56	1,1,1,1	0
31	MG	X	2895	1/1	0.98	0.31	1,1,1,1	0
33	ZN	Y	61	1/1	0.98	0.14	89,89,89,89	0
33	ZN	4	38	1/1	0.98	0.03	78,78,78,78	0
31	MG	X	2888	1/1	0.99	0.36	1,1,1,1	0
31	MG	X	2896	1/1	0.99	0.28	1,1,1,1	0
31	MG	X	2899	1/1	0.99	0.53	1,1,1,1	0
31	MG	X	2906	1/1	0.99	0.09	40,40,40,40	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.