



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:37 PM UTC

PDB ID : 7A0R / pdb_00007a0r
Title : 50S Deinococcus radiodurans ribosome bounded with mycinamicin I
Authors : Breiner, E.; Eyal, Z.; Matzov, D.; Halfon, Y.; Cimicata, G.; Rozenberg, H.;
Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2020-08-10
Resolution : 3.30 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

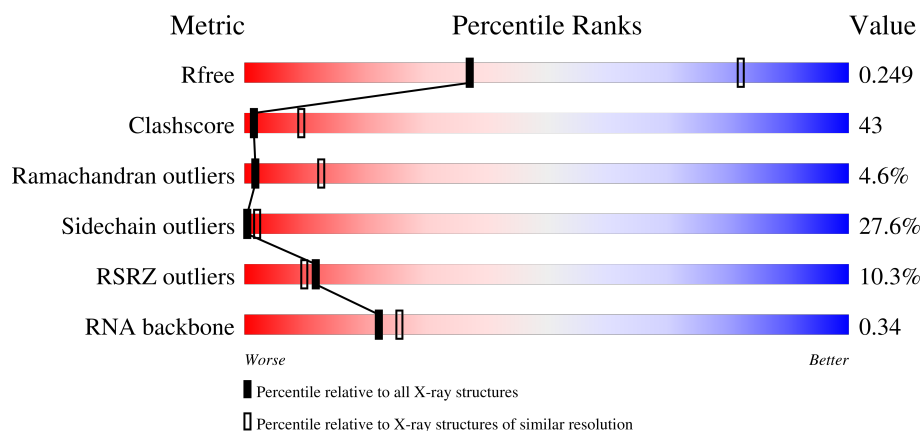
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	2877	3% 21% 49% 24% 5%
2	Y	120	% 19% 59% 22%
3	A	271	20% 41% 42% 16% .
4	B	206	6% 43% 40% 17%

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Mol	Chain	Length	Quality of chain
5	C	197	
6	D	177	
7	E	171	
8	G	143	
9	H	134	
10	I	137	
11	J	136	
12	K	116	
13	L	104	
14	M	113	
15	N	117	
16	O	98	
17	P	128	
18	Q	93	
19	R	110	
20	S	175	
21	T	74	
22	U	74	
23	V	61	
24	W	55	
25	Z	58	
26	1	49	
27	2	47	
28	3	63	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	2902	-	-	-	X
30	MG	X	2918	-	-	-	X
30	MG	X	2942	-	-	-	X
30	MG	X	2951	-	-	-	X
30	MG	X	2971	-	-	-	X
30	MG	X	2999	-	-	-	X
30	MG	X	3022	-	-	-	X
30	MG	X	3057	-	-	-	X
30	MG	X	3071	-	-	-	X
30	MG	X	3072	-	-	-	X
30	MG	X	3094	-	-	-	X
30	MG	X	3113	-	-	-	X
30	MG	X	3141	-	-	-	X
30	MG	X	3162	-	-	-	X
30	MG	X	3175	-	-	-	X
30	MG	X	3177	-	-	-	X
30	MG	X	3187	-	-	-	X
30	MG	X	3191	-	-	-	X
30	MG	X	3208	-	-	-	X
30	MG	Y	204	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 84973 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 RNA (2730-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2730	Total	C	N	O	P	0	0	0
			58592	26137	10810	18916	2729			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073

- Molecule 2 is a RNA chain called RNA (120-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	271	Total	C	N	O	S	0	0	0
			1976	1234	382	358	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	206	Total	C	N	O	S	0	0	0
			1529	959	290	272	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1486	924	282	278	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1353	865	234	248	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1270	803	234	232	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	143	Total	C	N	O	S	0	0	0
			1106	697	205	201	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			991	611	195	180	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	137	Total	C	N	O	S	0	0	0
			970	594	191	184	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1064	675	197	185	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	116	Total	C	N	O	S	0	0	0
			900	554	183	160	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			772	470	161	141			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	113	Total	C	N	O	S	0	0	0
			885	554	171	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	117	Total	C	N	O	S	0	0	0
			972	605	207	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	98	Total	C	N	O	S	0	0	0
			733	460	134	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	128	Total	C	N	O	S	0	0	0
			1006	634	195	175	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	6	ALA	GLN	conflict	UNP Q9RXJ7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			712	451	131	128	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			813	507	154	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1309	823	227	253	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	74	Total	C	N	O	S	0	0	0
			543	344	102	96	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	74	Total	C	N	O		0	0	0
			537	338	101	98				

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	61	Total	C	N	O	S	0	0	0
			490	301	100	87	2			

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

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

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	1	49	Total	C	N	O	0	0	0
			303	187	54	62			

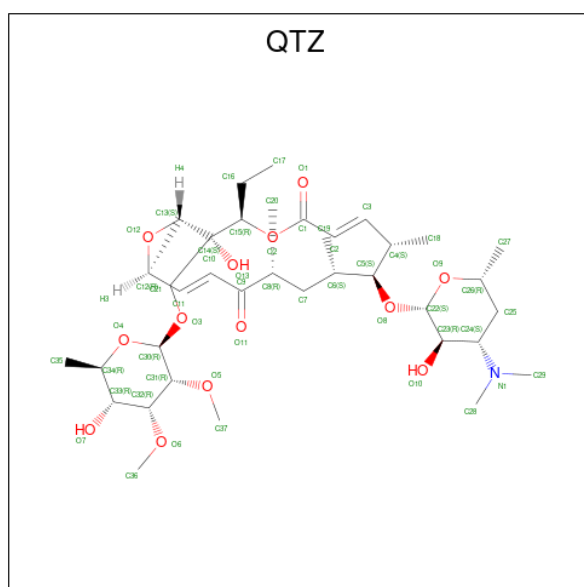
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			376	224	88	62	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	63	Total	C	N	O	S	0	0	0
			447	278	92	75	2			

- Molecule 29 is mycinamicin II (CCD ID: QTZ) (formula: $C_{37}H_{61}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	X	1	Total	C	N	O	3	0
			51	37	1	13		

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	320	Total	Mg	0	0
			320	320		

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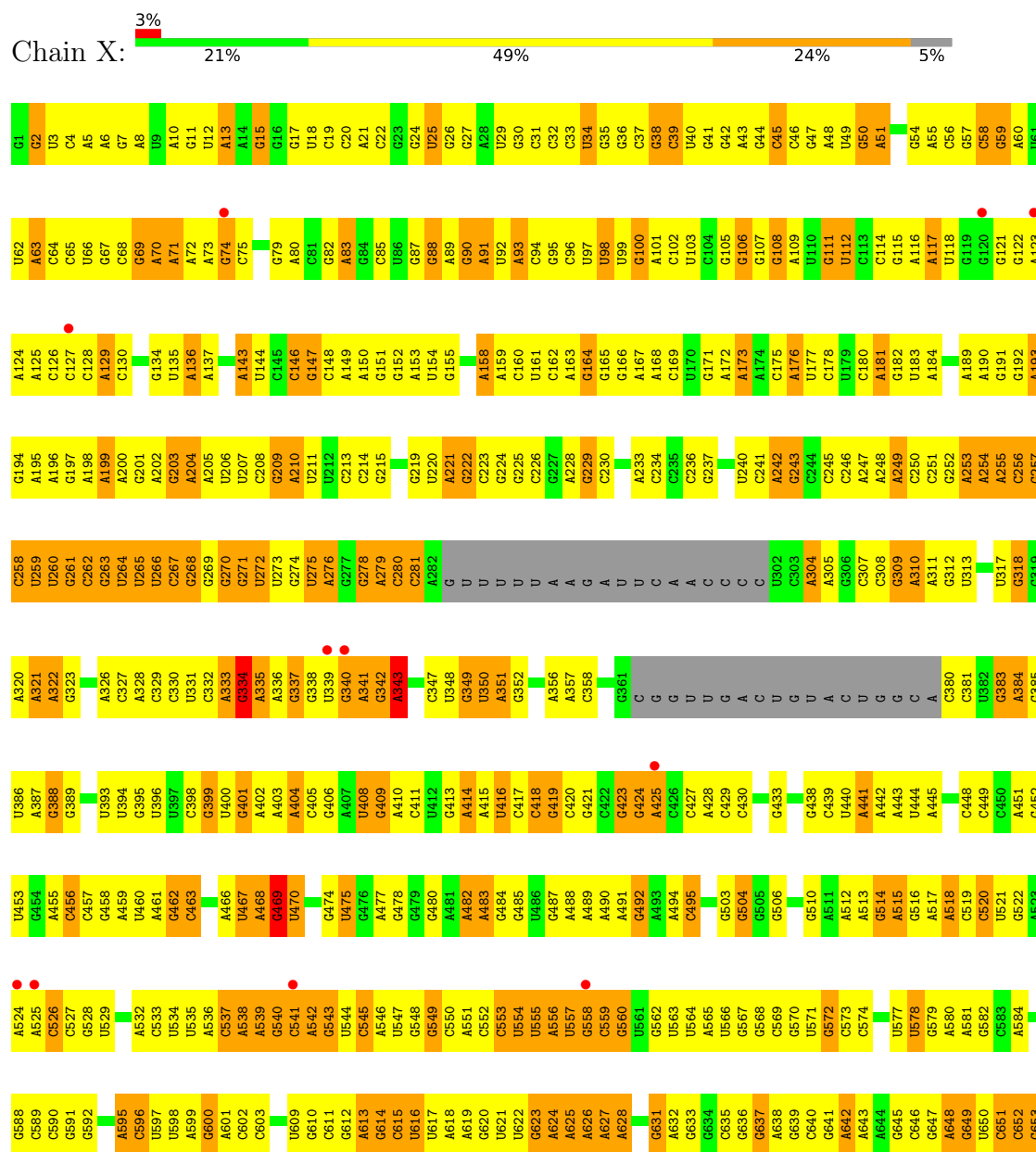
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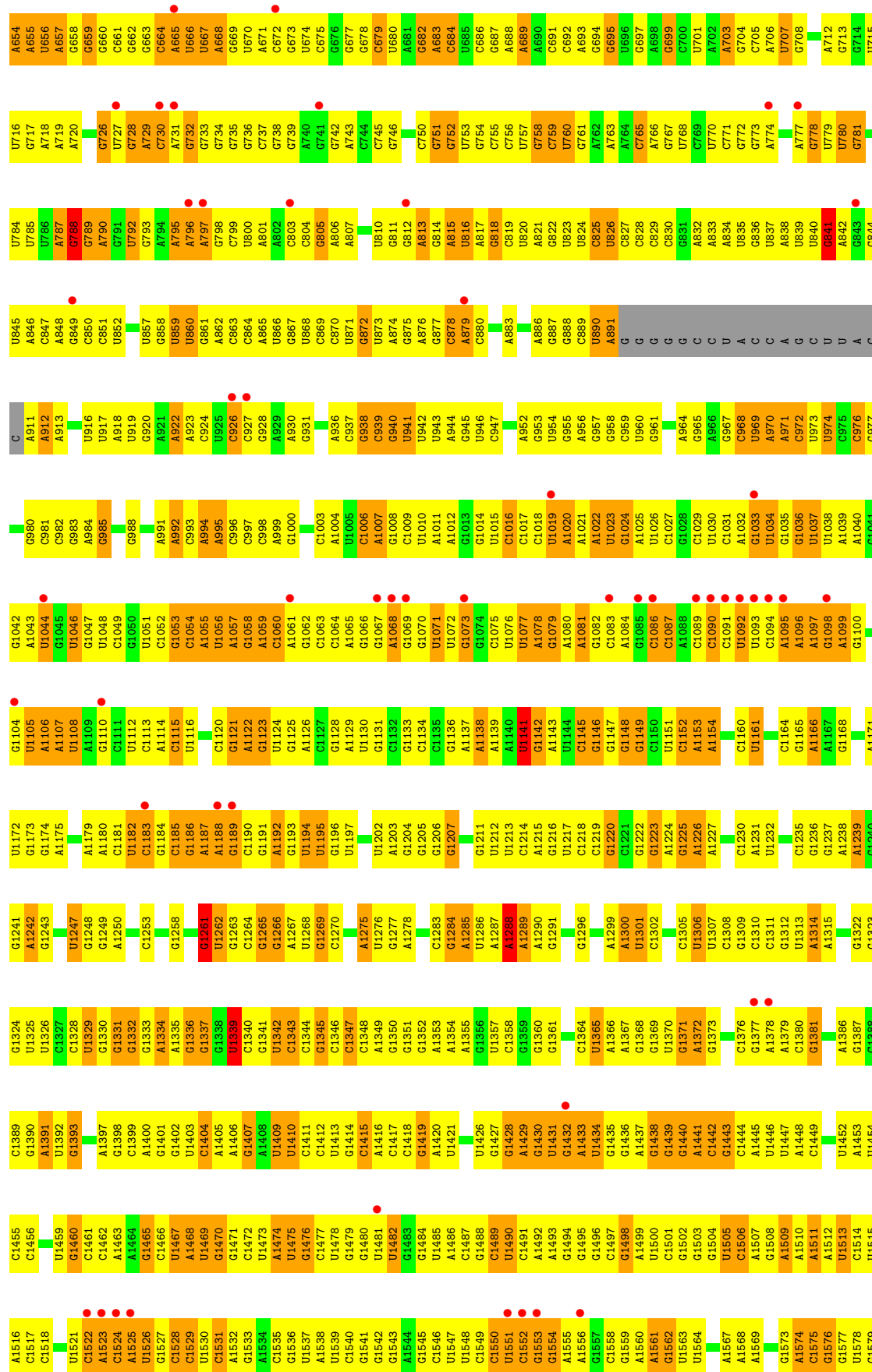
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	Y	16	Total 16	Mg 16	0	0
30	A	3	Total 3	Mg 3	0	0
30	I	1	Total 1	Mg 1	0	0
30	J	2	Total 2	Mg 2	0	0
30	K	1	Total 1	Mg 1	0	0
30	O	1	Total 1	Mg 1	0	0
30	2	1	Total 1	Mg 1	0	0

3 Residue-property plots

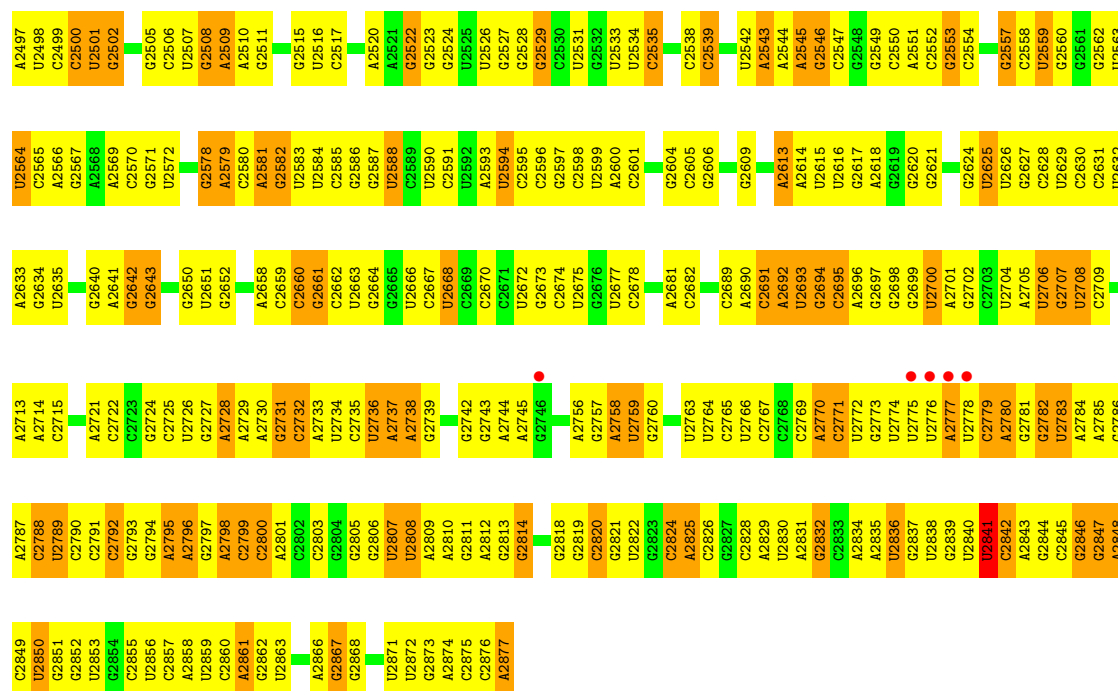
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA (2730-MER)

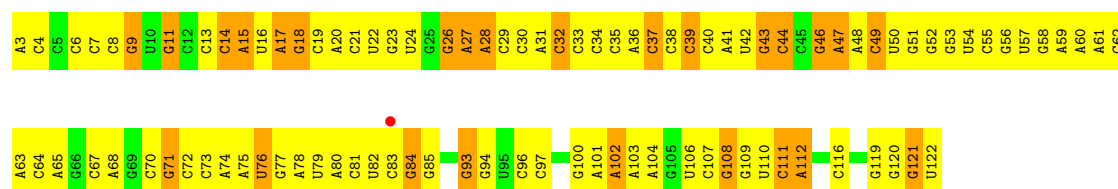




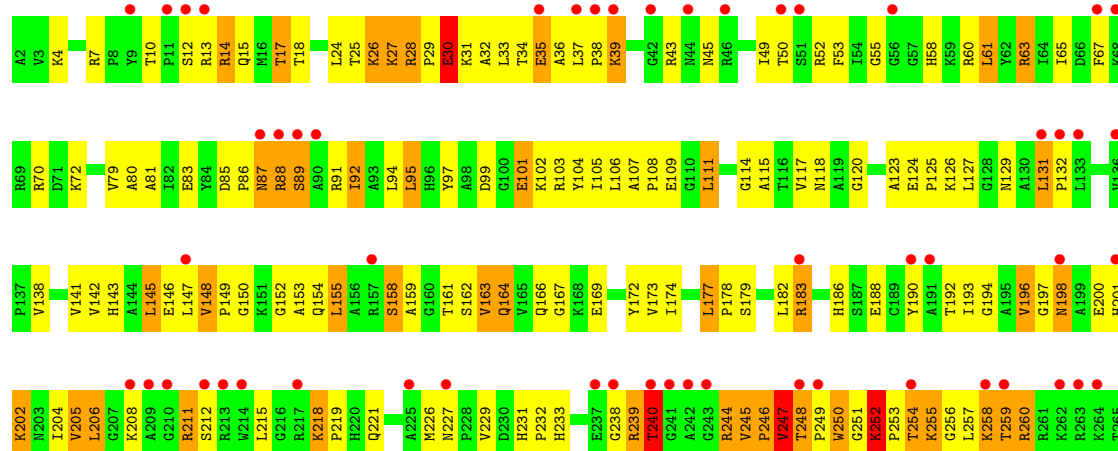
G2433	G2434	G2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	G2448	G2449	U2452	G2453	G2454	G2455	U2458	G2459	G2460	G2461	G2462	G2463	G2464	G2465	G2468	G2469	G2470	G2471	G2472	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2489	U2490	G2491	G2492	G2493	G2494	G2495	G2496					
G2370	A2306	A2307	A2308	C2372	C2373	C2374	G2375	G2379	U2380	C2382	U2385	G2386	U2387	U2388	G2389	A2390	A2391	G2392	G2393	G2394	G2395	G2396	A2397	U2398	G2399	G2400	G2401	U2402	G2403	G2404	A2405	G2406	G2407	G2408	A2409	G2410	A2411	A2412	A2413	A2414	G2415	U2416	G2417	A2418	G2419	G2420	G2421	G2422	G2423	G2424	G2425	G2426	A2427	U2428	A2429	G2430	G2431	G2432		
C2240	A2306	U2241	C2242	C2243	C2244	C2245	A2246	A2247	U2251	A2252	A2253	C2254	G2255	G2256	A2257	G2258	G2259	G2260	G2261	G2262	G2263	C2264	A2265	A2266	G2267	G2268	G2269	G2270	G2271	A2272	G2273	G2274	G2275	G2276	A2280	G2281	G2282	G2283	U2284	U2285	G2286	G2287	A2288	A2289	G2290	U2291	G2292	G2293	U2294	U2298	A2299	G2300	G2301	G2302	G2303	G2304	G2305			
U2176	U2176	U2177	U2178	C2179	U2180	A2181	C2184	U2185	U2186	A2187	A2188	A2189	A2190	U2191	U2192	C2195	U2196	U2197	U2198	C2199	G2200	G2201	G2202	G2203	A2204	G2205	G2206	G2207	U2208	G2209	G2210	U2211	U2212	C2215	G2216	G2217	G2218	U2219	A2220	G2221	U2222	U2223	U2224	G2225	A2226	C2227	U2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	U2236	C2237				
G2052	G2052	C2053	A2054	C2055	U2056	C2056	U2057	U2058	U2059	U2060	U2061	U2062	A2063	U2064	U2065	U2066	U2067	U2068	U2069	G2070	G2071	C2072	A2073	U2074	U2075	G2076	G2077	G2078	A2079	U2080	U2081	G2082	G2083	G2084	G2085	U2088	C2089	U2090	C	U	G	C	A	G	A	U	A	C	A	U	G	A2165	U2170	U2171	U2172	G2173	G2174	A2175		
U1922	U1922	U1923	C1924	C1925	U1926	U1927	G1928	G1933	U1934	A1935	A1936	G1937	U1938	U1939	U1943	A1948	A1949	A2012	A2013	A2014	G1951	A1952	A1953	A1954	G1955	G1958	U1959	A1960	A1961	G1962	G1963	A1964	U1965	C1966	U1967	G1968	G1969	G1970	C1971	G1972	C1973	U1974	U1975	U1976	C1977	U1978	C1979	A1980	U1981	C1982	G1985	G1986	G1987	A1988	C1989					
U1856	U1856	C1857	C1858	A1859	A1860	G1861	C1862	U1863	U1864	C1865	G1866	A1867	A1868	A1869	U1870	A1871	A1872	A1873	U1881	G1882	A1883	A1884	C1885	G1886	C1887	C1888	G1889	G1890	C1891	C	U	A	G1963	C1964	U1965	C1966	U1967	G1968	G1969	G1970	C1971	G1972	C1973	U1974	U1975	U1976	C1977	U1978	C1979	A1980	U1981	C1982	G1985	G1986	G1987	A1988	C1989			
C1786	U1787	C1788	U1789	G1790	G1791	C1792	U1793	A1794	C1795	A1796	A1799	A1800	C1801	A1802	G1803	U1804	G1805	G1806	A1807	C1808	A1809	U1810	U1811	U1812	A1813	G1814	G1815	G1816	U1817	G1818	U1819	G1820	A1821	G1822	G1823	C1824	C1825	U1826	U1827	C1830	G1831	G1832	U1833	G1834	C1835	C1836	G1837	G1838	A1839	U1840	G1841	G1842	U1843	G1850	A1851	C				
G1721	G1722	U1723	C1726	G1727	A1728	C1729	G1730	C1731	U1732	U1733	C1734	G1735	G1736	G1737	U1738	G1741	G1742	C1743	G1744	G1745	A1746	G1747	U1748	G1749	A1753	G1754	G1755	C1758	U1759	G1760	G1761	C1762	G1763	A1764	C1765	U1766	G1767	U1768	U1769	U1770	A1771	C1772	C1773	A1774	U1775	A1776	A1777	U1778	C1779	A1780	A1781	G1782	G1783	A1784	A1785					
C1653	A1654	U1655	A1656	G1657	A1658	G1659	C1660	C1661	G1662	C1663	G1664	C1665	G1666	A1667	G1668	A1669	C1670	C1673	C1674	C1675	U1679	U1680	A1681	G1682	G1683	G1684	A1685	A1686	C1687	U1688	U1689	G1690	C1691	C1692	A1693	A1694	U1695	C1696	U1697	C1698	A1699	C1700	U1705	A1706	A1707	C1708	U1709	U1710	G1713	G1642	U1645	G1646	U1647	A1714	A1715	G1716	A1717	U1650	A1718	C
C1580	C1581	A1582	A1583	G1584	A1585	G1586	A1587	A1588	U1592	C1593	U1594	A1595	A1596	A1597	C1598	G1599	U1600	U1601	G1602	A1603	A1604	A1605	C1606	A1607	U1608	G1609	A1610	U1611	U1612	C1615	C1616	A1617	C1623	A1624	A1625	A1626	C1627	C1628	U1629	A1630	A1631	A1632	A1633	G1634	G1635	G1642	U1645	G1646	U1647	A1714	A1715	G1716	A1717	U1650	A1718	C				

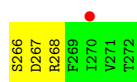


• Molecule 2: RNA (120-MER)

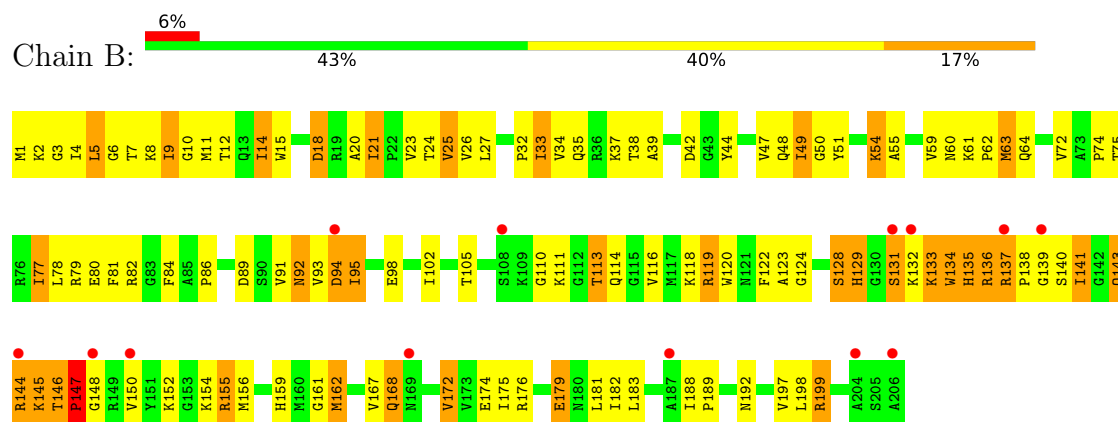


• Molecule 3: 50S ribosomal protein L2

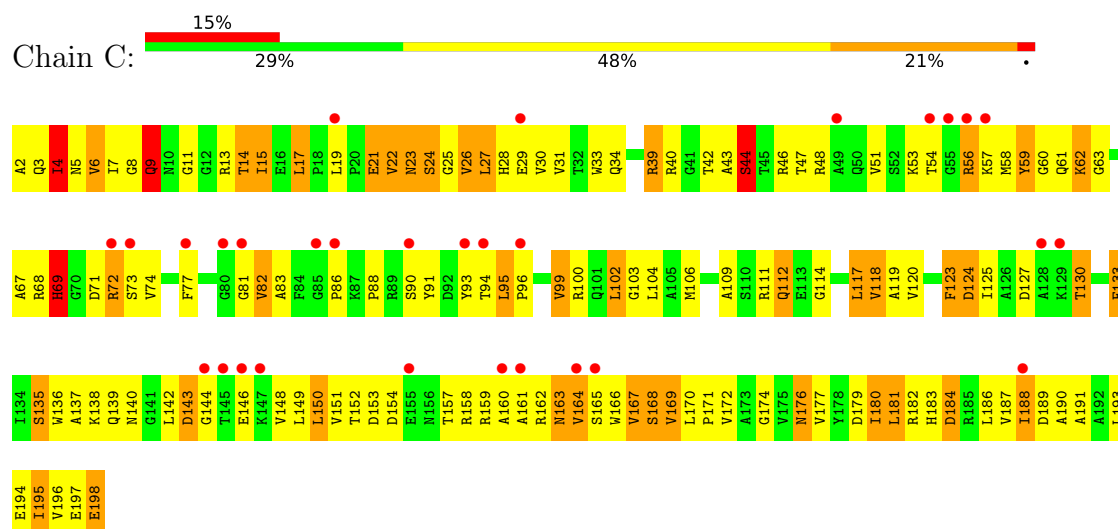




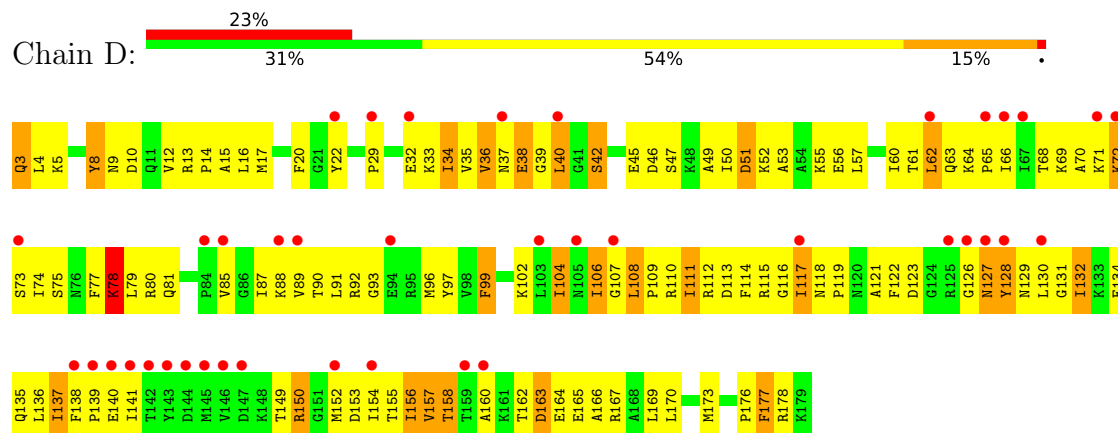
• Molecule 4: 50S ribosomal protein L3



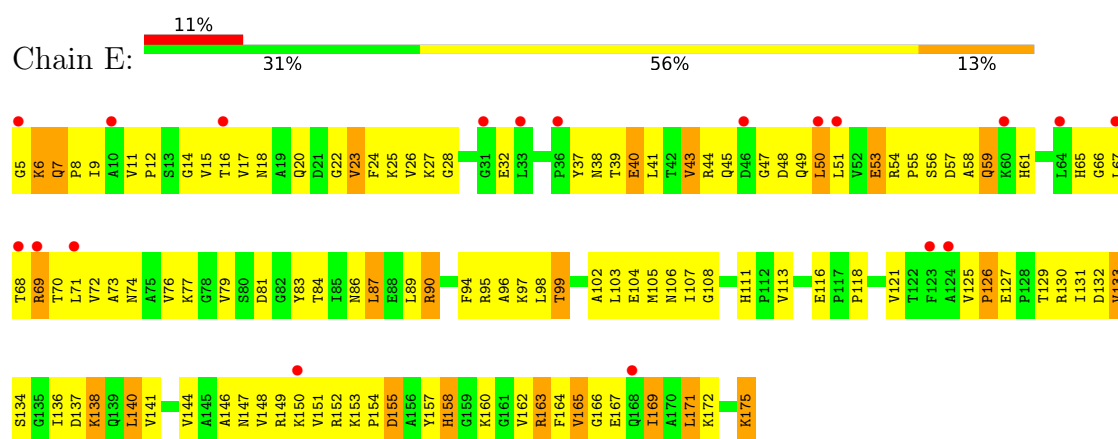
• Molecule 5: 50S ribosomal protein L4



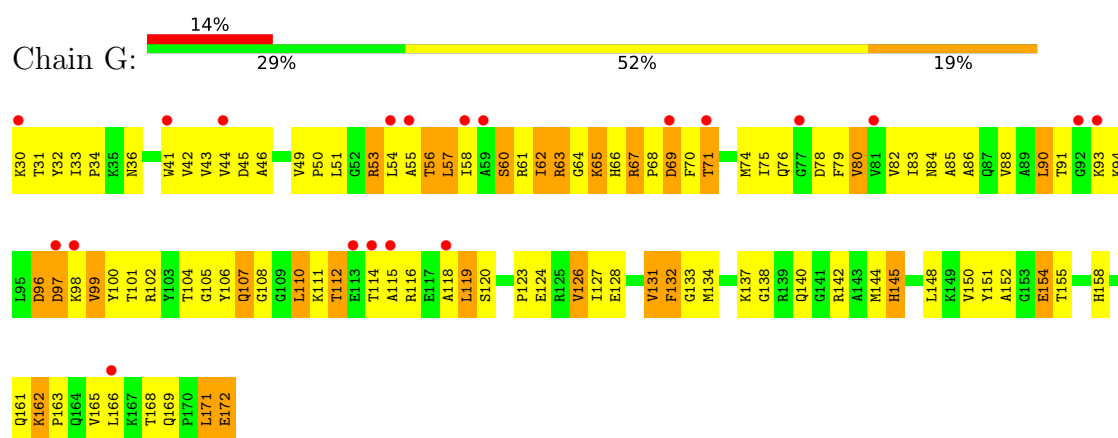
• Molecule 6: 50S ribosomal protein L5



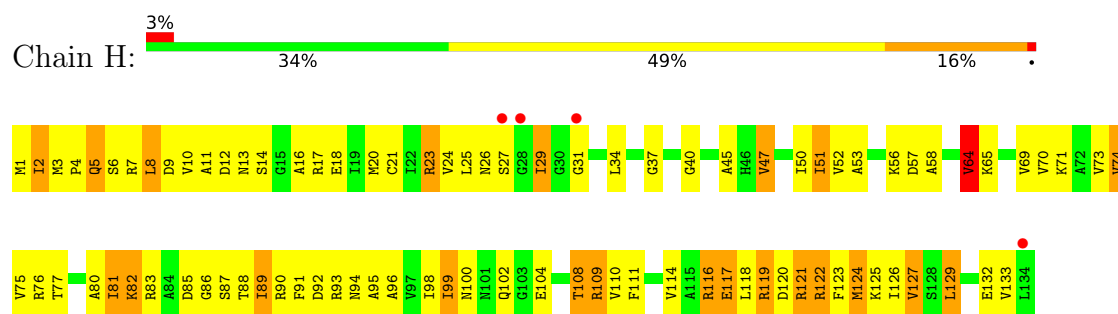
• Molecule 7: 50S ribosomal protein L6



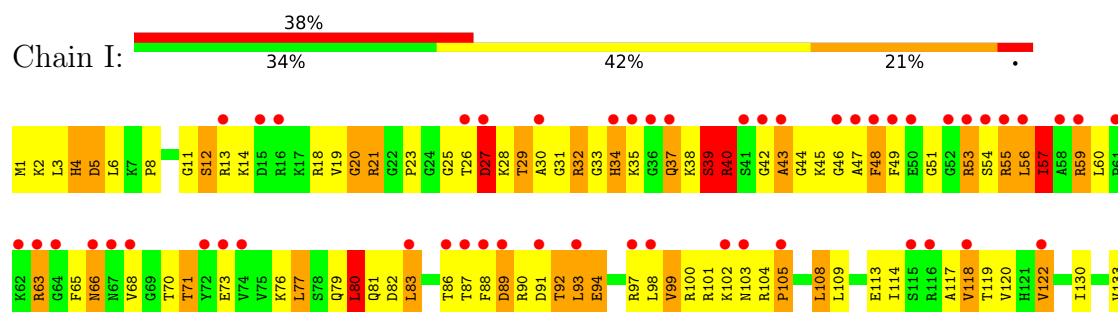
• Molecule 8: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L14

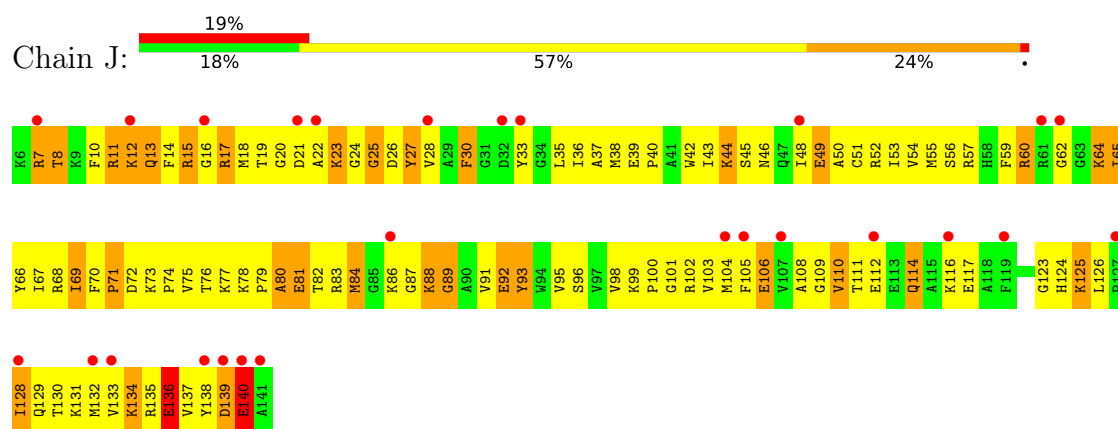


• Molecule 10: 50S ribosomal protein L15

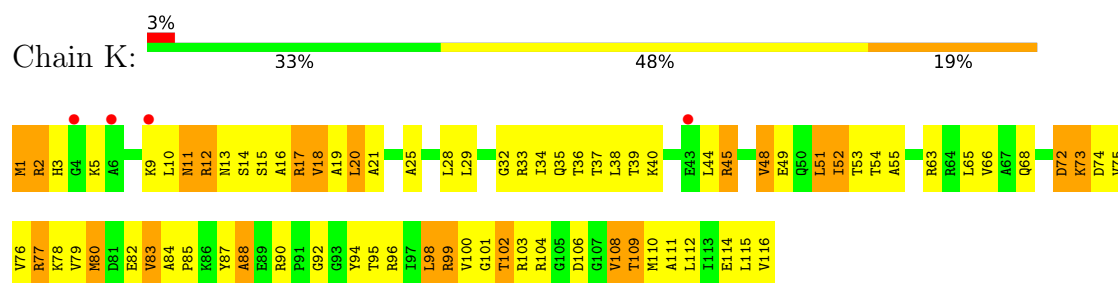




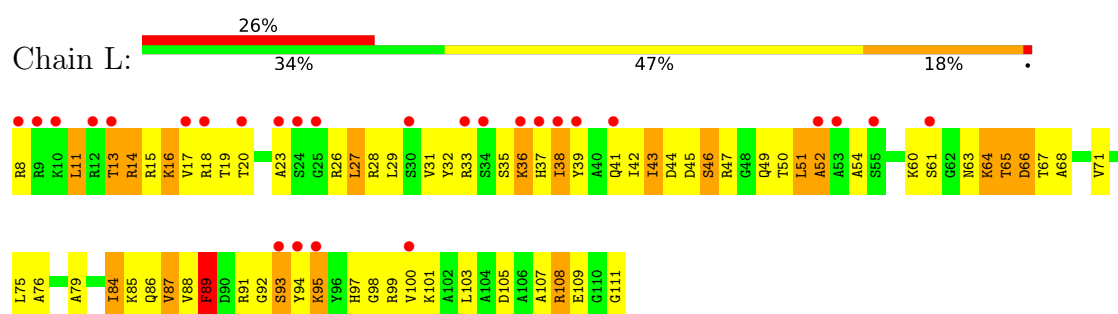
• Molecule 11: 50S ribosomal protein L16



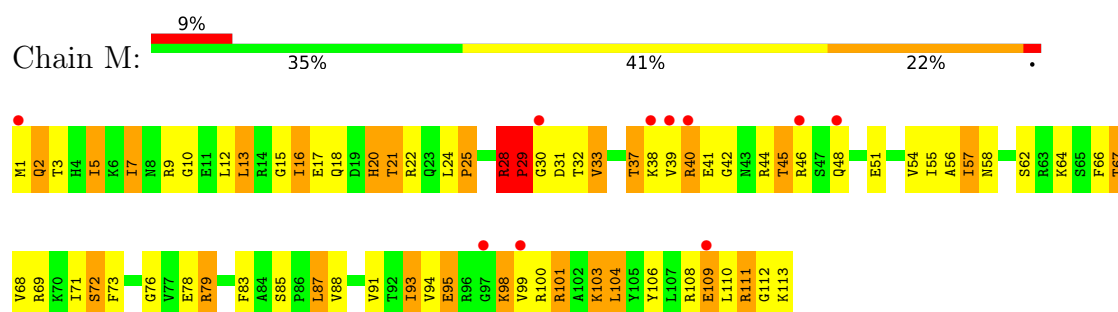
• Molecule 12: 50S ribosomal protein L17



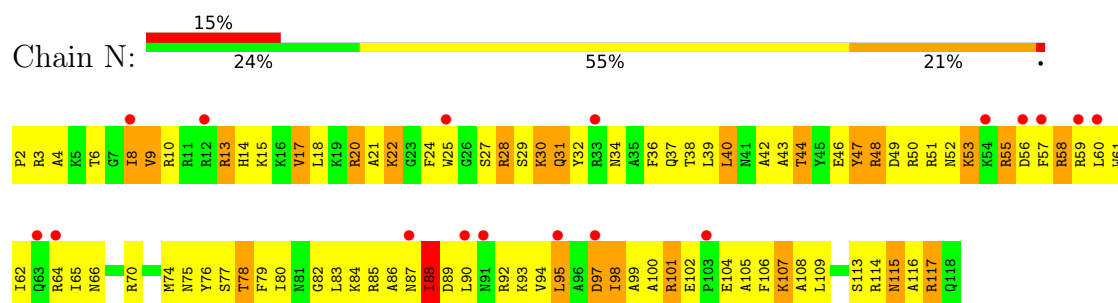
• Molecule 13: 50S ribosomal protein L18



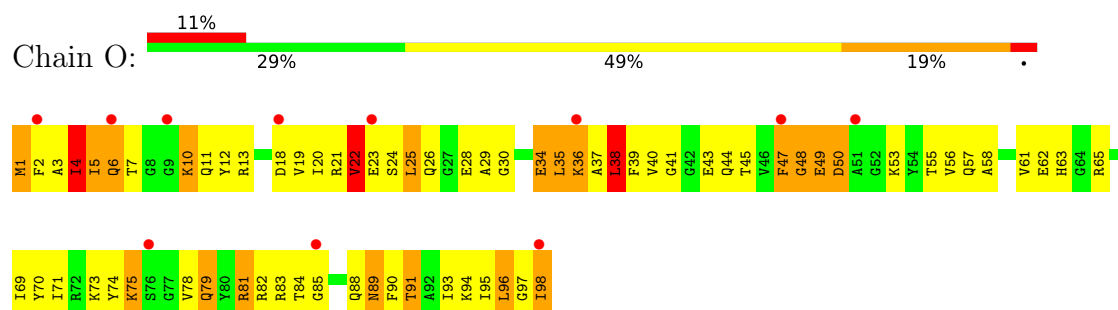
• Molecule 14: 50S ribosomal protein L19



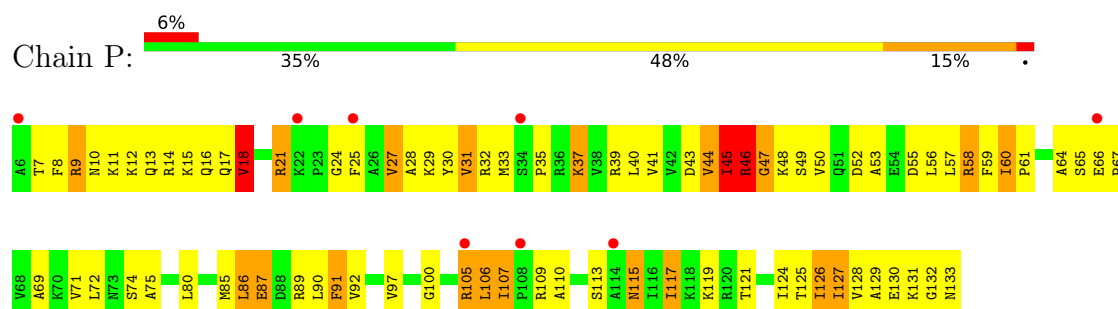
- Molecule 15: 50S ribosomal protein L20



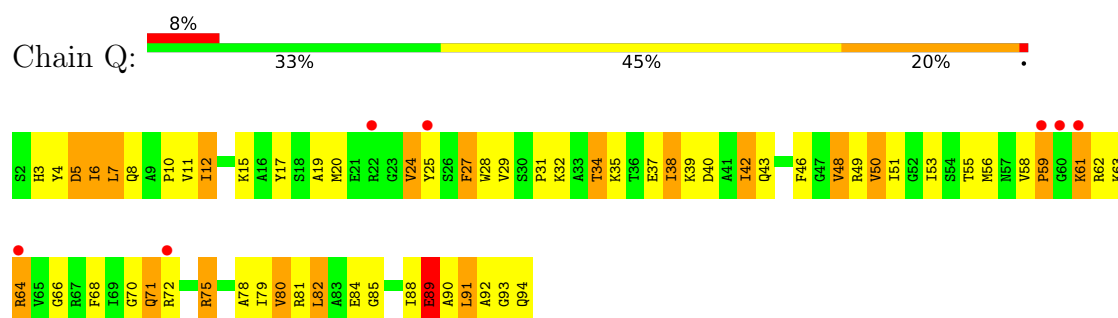
- Molecule 16: 50S ribosomal protein L21



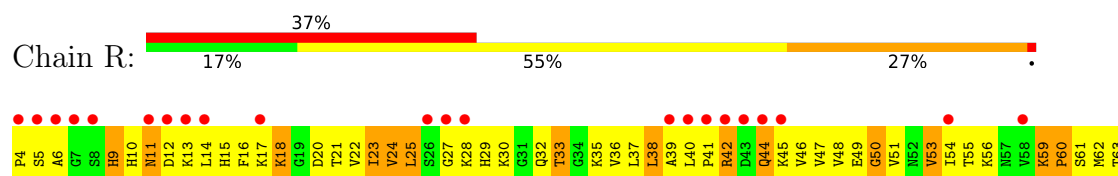
- Molecule 17: 50S ribosomal protein L22

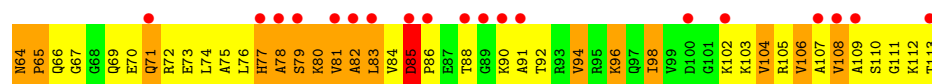


- Molecule 18: 50S ribosomal protein L23

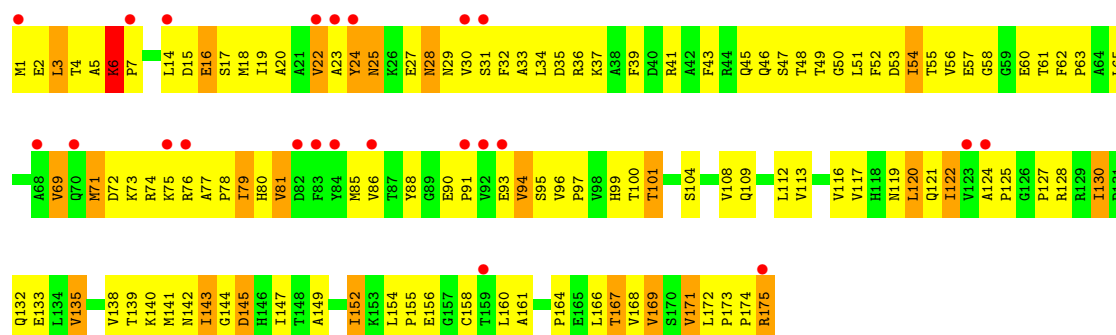


- Molecule 19: 50S ribosomal protein L24

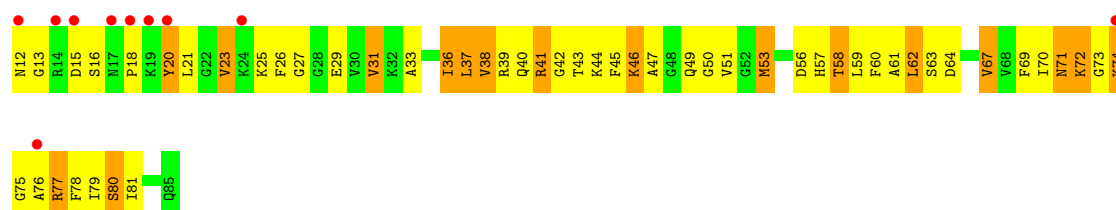




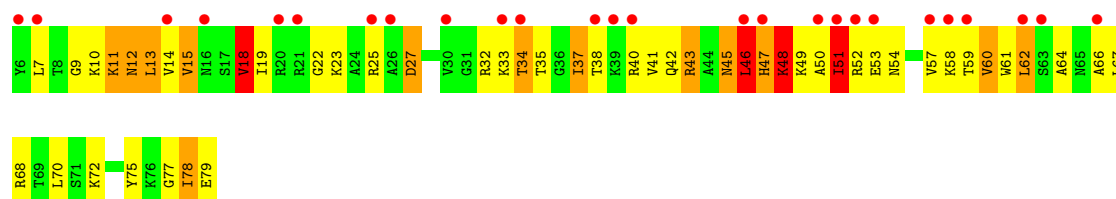
• Molecule 20: 50S ribosomal protein L25



• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L28

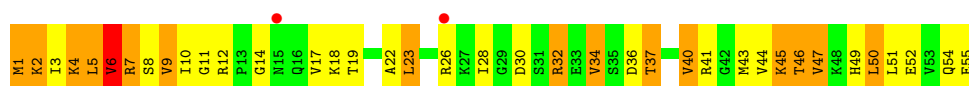


• Molecule 23: 50S ribosomal protein L29



• Molecule 24: 50S ribosomal protein L30

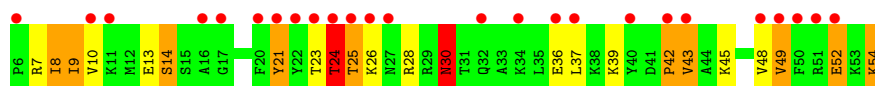




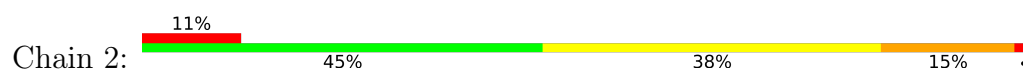
- Molecule 25: 50S ribosomal protein L32



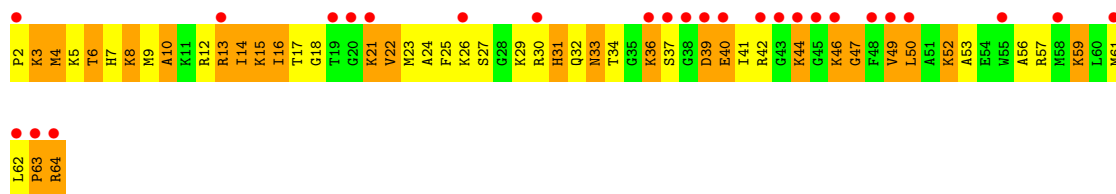
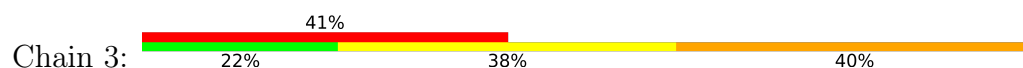
- Molecule 26: 50S ribosomal protein L33



- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.48Å 408.93Å 697.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 3.30 49.55 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.55-3.30) 98.3 (49.55-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.215 , 0.249 0.214 , 0.249	Depositor DCC
R_{free} test set	17957 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	98.1	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 88.1	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	84973	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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: QTZ, MG

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	0.45	0/65613	0.67	22/102349 (0.0%)
2	Y	0.31	0/2863	0.53	0/4461
3	A	0.40	0/2016	0.68	1/2735 (0.0%)
4	B	0.57	0/1556	0.82	0/2093
5	C	0.43	0/1509	0.72	0/2046
6	D	0.24	0/1372	0.44	0/1848
7	E	0.29	0/1292	0.51	0/1751
8	G	0.49	0/1130	0.77	1/1532 (0.1%)
9	H	0.59	0/1001	0.84	2/1345 (0.1%)
10	I	0.52	0/982	0.88	0/1326
11	J	0.44	0/1085	0.73	0/1453
12	K	0.67	0/908	0.88	0/1218
13	L	0.31	0/777	0.65	0/1037
14	M	0.66	0/898	0.94	2/1207 (0.2%)
15	N	0.51	0/988	0.81	0/1316
16	O	0.40	0/741	0.76	0/994
17	P	0.63	0/1019	0.80	0/1368
18	Q	0.42	0/723	0.71	0/971
19	R	0.40	0/823	0.67	0/1107
20	S	0.27	0/1333	0.50	0/1821
21	T	0.48	0/550	0.72	0/732
22	U	0.42	0/542	0.65	0/729
23	V	0.29	0/493	0.46	0/656
24	W	0.36	0/426	0.66	0/568
25	Z	0.62	0/469	0.87	0/629
26	1	0.36	0/305	0.68	0/420
27	2	0.46	0/379	0.82	0/500
28	3	0.51	0/451	0.78	0/596
All	All	0.45	0/92244	0.68	28/138808 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
4	B	0	2
5	C	0	2
8	G	0	2
9	H	0	1
10	I	0	5
11	J	0	2
14	M	0	1
17	P	0	1
19	R	0	1
22	U	0	2
28	3	0	1
All	All	0	21

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2018	G	N9-C1'-C2'	8.00	126.00	114.00
1	X	1975	G	C2'-C3'-O3'	7.70	121.04	109.50
1	X	841	G	N9-C1'-C2'	6.76	122.14	112.00
8	G	108	GLY	N-CA-C	-6.63	104.31	111.93
1	X	1288	A	N9-C1'-C2'	6.38	121.57	112.00

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	247	VAL	Peptide
4	B	129	HIS	Peptide
4	B	131	SER	Peptide
5	C	159	ARG	Peptide
5	C	164	VAL	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	58592	0	29522	2979	0
2	Y	2561	0	1306	156	0
3	A	1976	0	1957	265	0
4	B	1529	0	1578	172	0
5	C	1486	0	1488	290	0
6	D	1353	0	1388	231	0
7	E	1270	0	1310	155	0
8	G	1106	0	1108	144	0
9	H	991	0	1035	125	0
10	I	970	0	940	178	0
11	J	1064	0	1078	180	0
12	K	900	0	953	109	0
13	L	772	0	813	119	0
14	M	885	0	898	126	0
15	N	972	0	1009	127	0
16	O	733	0	725	108	0
17	P	1006	0	1073	123	0
18	Q	712	0	730	84	0
19	R	813	0	859	183	0
20	S	1309	0	1293	161	0
21	T	543	0	553	71	0
22	U	537	0	557	108	0
23	V	490	0	509	41	0
24	W	424	0	470	43	0
25	Z	457	0	464	84	0
26	1	303	0	238	37	0
27	2	376	0	396	46	0
28	3	447	0	465	116	0
29	X	51	0	0	2	0
30	2	1	0	0	0	0
30	A	3	0	0	0	0
30	I	1	0	0	0	0
30	J	2	0	0	0	0
30	K	1	0	0	0	0
30	O	1	0	0	0	0
30	X	320	0	0	0	0
30	Y	16	0	0	0	0
All	All	84973	0	54715	5953	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

The worst 5 of 5953 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)
8:G:42:VAL:CG1	8:G:166:LEU:HD13	1.32	1.51
8:G:42:VAL:CG1	8:G:166:LEU:CD1	1.88	1.48
8:G:42:VAL:HG11	8:G:166:LEU:CD1	1.56	1.26
8:G:61:ARG:NH1	8:G:166:LEU:HD21	1.49	1.23
1:X:1277:G:OP1	25:Z:19:ARG:NH2	1.73	1.20

There are no symmetry-related clashes.

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	269/271 (99%)	240 (89%)	21 (8%)	8 (3%)	3	20
4	B	204/206 (99%)	183 (90%)	13 (6%)	8 (4%)	2	16
5	C	195/197 (99%)	157 (80%)	28 (14%)	10 (5%)	1	11
6	D	175/177 (99%)	158 (90%)	12 (7%)	5 (3%)	3	21
7	E	169/171 (99%)	148 (88%)	16 (10%)	5 (3%)	3	20
8	G	141/143 (99%)	120 (85%)	18 (13%)	3 (2%)	5	26
9	H	132/134 (98%)	118 (89%)	11 (8%)	3 (2%)	5	25
10	I	135/137 (98%)	100 (74%)	20 (15%)	15 (11%)	0	2
11	J	134/136 (98%)	110 (82%)	14 (10%)	10 (8%)	1	6
12	K	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	6	29
13	L	102/104 (98%)	84 (82%)	11 (11%)	7 (7%)	1	7
14	M	111/113 (98%)	95 (86%)	12 (11%)	4 (4%)	2	17
15	N	115/117 (98%)	104 (90%)	7 (6%)	4 (4%)	3	18
16	O	96/98 (98%)	76 (79%)	12 (12%)	8 (8%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	P	126/128 (98%)	109 (86%)	13 (10%)	4 (3%)	3	19
18	Q	91/93 (98%)	79 (87%)	8 (9%)	4 (4%)	2	13
19	R	108/110 (98%)	82 (76%)	18 (17%)	8 (7%)	1	6
20	S	173/175 (99%)	154 (89%)	14 (8%)	5 (3%)	3	21
21	T	72/74 (97%)	66 (92%)	4 (6%)	2 (3%)	4	21
22	U	72/74 (97%)	52 (72%)	13 (18%)	7 (10%)	0	3
23	V	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
24	W	53/55 (96%)	50 (94%)	2 (4%)	1 (2%)	6	28
25	Z	56/58 (97%)	48 (86%)	6 (11%)	2 (4%)	2	17
26	1	47/49 (96%)	33 (70%)	10 (21%)	4 (8%)	0	4
27	2	45/47 (96%)	36 (80%)	4 (9%)	5 (11%)	0	2
28	3	61/63 (97%)	49 (80%)	6 (10%)	6 (10%)	0	3
All	All	3055/3107 (98%)	2612 (86%)	303 (10%)	140 (5%)	2	13

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	240	THR
3	A	244	ARG
4	B	94	ASP
4	B	136	ARG
5	C	44	SER

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	191/212 (90%)	142 (74%)	49 (26%)	0	2
4	B	152/155 (98%)	114 (75%)	38 (25%)	0	3
5	C	152/157 (97%)	104 (68%)	48 (32%)	0	1
6	D	141/153 (92%)	116 (82%)	25 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	132/136 (97%)	103 (78%)	29 (22%)	1	5
8	G	115/119 (97%)	86 (75%)	29 (25%)	0	3
9	H	102/103 (99%)	76 (74%)	26 (26%)	0	3
10	I	90/105 (86%)	61 (68%)	29 (32%)	0	1
11	J	105/110 (96%)	77 (73%)	28 (27%)	0	2
12	K	92/93 (99%)	66 (72%)	26 (28%)	0	2
13	L	73/74 (99%)	52 (71%)	21 (29%)	0	2
14	M	93/98 (95%)	64 (69%)	29 (31%)	0	1
15	N	95/96 (99%)	66 (70%)	29 (30%)	0	1
16	O	70/78 (90%)	47 (67%)	23 (33%)	0	1
17	P	107/109 (98%)	79 (74%)	28 (26%)	0	2
18	Q	72/75 (96%)	52 (72%)	20 (28%)	0	2
19	R	89/91 (98%)	61 (68%)	28 (32%)	0	1
20	S	141/149 (95%)	111 (79%)	30 (21%)	1	5
21	T	52/55 (94%)	31 (60%)	21 (40%)	0	0
22	U	52/59 (88%)	40 (77%)	12 (23%)	1	4
23	V	48/49 (98%)	39 (81%)	9 (19%)	1	7
24	W	48/48 (100%)	29 (60%)	19 (40%)	0	0
25	Z	51/51 (100%)	38 (74%)	13 (26%)	0	3
26	1	21/44 (48%)	7 (33%)	14 (67%)	0	0
27	2	37/40 (92%)	31 (84%)	6 (16%)	2	11
28	3	40/50 (80%)	18 (45%)	22 (55%)	0	0
All	All	2361/2509 (94%)	1710 (72%)	651 (28%)	0	2

5 of 651 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	Q	27	PHE
23	V	43	VAL
18	Q	91	LEU
18	Q	24	VAL
20	S	101	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	14	HIS
17	P	13	GLN
20	S	119	ASN
15	N	75	ASN
17	P	16	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2725/2877 (94%)	805 (29%)	104 (3%)
2	Y	119/120 (99%)	29 (24%)	1 (0%)
All	All	2844/2997 (94%)	834 (29%)	105 (3%)

5 of 834 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	13	A
1	X	15	G
1	X	25	U
1	X	34	U

5 of 105 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1474	A
1	X	1799	A
1	X	2807	U
1	X	1524	C
1	X	1634	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

Of 346 ligands modelled in this entry, 345 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	$\# Z > 2$
29	QTZ	X	2901	-	52,54,54	0.33	0	68,79,79	1.13	6 (8%)

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
29	QTZ	X	2901	-	-	16/57/103/103	0/3/4/4

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	QTZ	O12-C12-C11	3.30	123.38	115.43
29	X	2901	QTZ	C7-C8-C9	3.01	117.80	110.64
29	X	2901	QTZ	C5-C4-C3	2.96	118.89	109.46
29	X	2901	QTZ	C13-C12-C11	-2.39	115.58	122.45
29	X	2901	QTZ	C25-C24-N1	-2.20	109.40	115.59

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

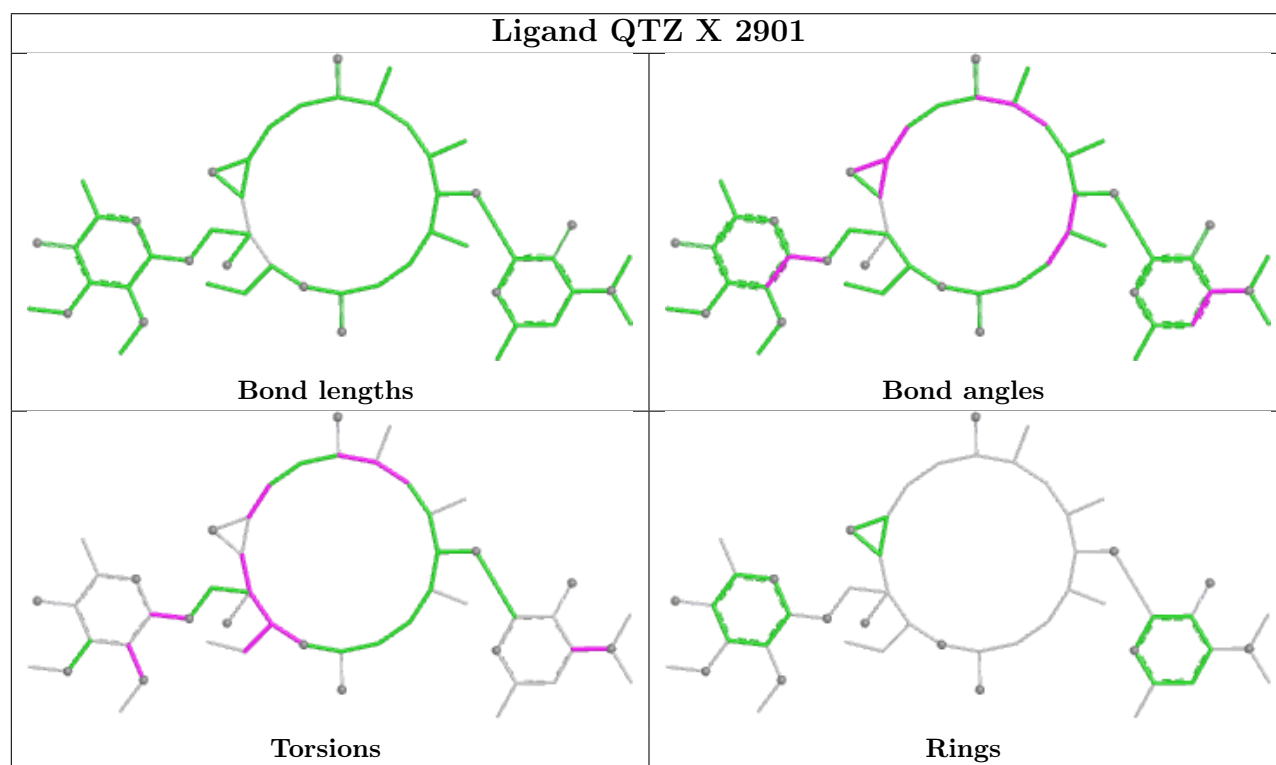
Mol	Chain	Res	Type	Atoms
29	X	2901	QTZ	C10-C11-C12-C13
29	X	2901	QTZ	C10-C11-C12-O12
29	X	2901	QTZ	C12-C13-C14-C21
29	X	2901	QTZ	C23-C24-N1-C29
29	X	2901	QTZ	C31-C30-O3-C21

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	2901	QTZ	2	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 ⓘ

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	2730/2877 (94%)	0.00	98 (3%)	46	31	60, 111, 218, 326	0
2	Y	120/120 (100%)	0.07	1 (0%)	82	68	119, 176, 204, 212	0
3	A	271/271 (100%)	1.13	55 (20%)	3	2	97, 129, 158, 168	0
4	B	206/206 (100%)	0.34	13 (6%)	26	17	71, 83, 105, 129	0
5	C	197/197 (100%)	0.81	30 (15%)	5	5	91, 137, 162, 205	0
6	D	177/177 (100%)	1.10	40 (22%)	2	2	190, 209, 236, 255	0
7	E	171/171 (100%)	0.68	19 (11%)	10	9	116, 158, 215, 221	0
8	G	143/143 (100%)	0.96	20 (13%)	6	5	82, 109, 128, 147	0
9	H	134/134 (100%)	0.25	4 (2%)	52	35	73, 83, 97, 108	0
10	I	137/137 (100%)	1.89	52 (37%)	1	1	94, 146, 163, 170	0
11	J	136/136 (100%)	0.84	26 (19%)	3	3	123, 142, 160, 166	0
12	K	116/116 (100%)	0.28	4 (3%)	48	32	60, 70, 80, 87	0
13	L	104/104 (100%)	1.28	27 (25%)	1	1	156, 174, 193, 206	0
14	M	113/113 (100%)	0.58	10 (8%)	15	12	71, 84, 129, 151	0
15	N	117/117 (100%)	0.66	17 (14%)	6	5	81, 107, 134, 147	0
16	O	98/98 (100%)	0.75	11 (11%)	10	9	95, 138, 176, 178	0
17	P	128/128 (100%)	0.48	8 (6%)	26	17	68, 81, 126, 158	0
18	Q	93/93 (100%)	0.69	7 (7%)	20	15	100, 123, 166, 170	0
19	R	110/110 (100%)	1.61	41 (37%)	1	1	105, 133, 180, 296	0
20	S	175/175 (100%)	0.75	23 (13%)	7	6	137, 177, 196, 209	0
21	T	74/74 (100%)	0.88	10 (13%)	7	6	126, 132, 152, 181	0
22	U	74/74 (100%)	1.78	26 (35%)	1	1	119, 143, 170, 178	0
23	V	61/61 (100%)	0.70	8 (13%)	7	6	130, 152, 208, 209	0
24	W	55/55 (100%)	0.38	2 (3%)	46	31	115, 132, 152, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	58/58 (100%)	0.65	6 (10%) 12 10	71, 82, 130, 133	0
26	1	49/49 (100%)	2.31	25 (51%) 0 0	145, 153, 184, 185	0
27	2	47/47 (100%)	1.06	5 (10%) 11 9	91, 98, 114, 116	0
28	3	63/63 (100%)	1.75	26 (41%) 0 0	114, 131, 156, 158	0
All	All	5957/6104 (97%)	0.47	614 (10%) 12 10	60, 123, 207, 326	0

The worst 5 of 614 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	I	67	ASN	17.3
19	R	43	ASP	11.8
20	S	92	VAL	10.5
22	U	16	ASN	8.6
25	Z	2	ALA	8.6

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 oligosaccharides 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
30	MG	X	3162	1/1	0.11	0.40	166,166,166,166	0
30	MG	X	3177	1/1	0.13	0.59	156,156,156,156	0
30	MG	Y	208	1/1	0.46	0.28	158,158,158,158	0
30	MG	X	3057	1/1	0.47	0.50	120,120,120,120	0
30	MG	Y	206	1/1	0.50	0.34	120,120,120,120	0
30	MG	X	3094	1/1	0.52	0.46	104,104,104,104	0
30	MG	X	3191	1/1	0.52	0.41	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	Y	204	1/1	0.62	0.47	115,115,115,115	0
30	MG	Y	216	1/1	0.62	0.33	145,145,145,145	0
30	MG	X	3022	1/1	0.63	0.72	98,98,98,98	0
30	MG	X	2927	1/1	0.63	0.39	100,100,100,100	0
30	MG	X	2999	1/1	0.64	0.44	102,102,102,102	0
30	MG	X	3072	1/1	0.64	0.42	106,106,106,106	0
30	MG	X	3175	1/1	0.65	0.41	105,105,105,105	0
30	MG	Y	211	1/1	0.66	0.28	149,149,149,149	0
30	MG	X	2951	1/1	0.66	0.48	100,100,100,100	0
30	MG	X	2902	1/1	0.67	0.62	80,80,80,80	0
30	MG	X	3020	1/1	0.67	0.36	93,93,93,93	0
30	MG	X	3104	1/1	0.67	0.15	95,95,95,95	0
30	MG	X	3064	1/1	0.67	0.16	79,79,79,79	0
30	MG	X	3051	1/1	0.71	0.26	92,92,92,92	0
30	MG	X	3141	1/1	0.72	0.54	116,116,116,116	0
30	MG	X	3209	1/1	0.73	0.38	98,98,98,98	0
30	MG	X	3208	1/1	0.74	0.65	103,103,103,103	0
30	MG	Y	215	1/1	0.74	0.16	123,123,123,123	0
30	MG	Y	210	1/1	0.74	0.30	125,125,125,125	0
30	MG	X	2948	1/1	0.75	0.26	90,90,90,90	0
30	MG	X	3089	1/1	0.75	0.37	65,65,65,65	0
30	MG	X	2903	1/1	0.75	0.36	66,66,66,66	0
30	MG	X	3038	1/1	0.76	0.27	110,110,110,110	0
30	MG	X	2918	1/1	0.77	0.41	63,63,63,63	0
30	MG	X	2971	1/1	0.77	0.47	85,85,85,85	0
30	MG	X	3098	1/1	0.77	0.37	97,97,97,97	0
30	MG	X	3142	1/1	0.78	0.37	124,124,124,124	0
30	MG	X	3187	1/1	0.78	0.45	98,98,98,98	0
30	MG	X	2942	1/1	0.78	0.47	76,76,76,76	0
30	MG	X	3071	1/1	0.78	0.48	97,97,97,97	0
30	MG	X	3113	1/1	0.79	0.41	99,99,99,99	0
30	MG	X	2970	1/1	0.79	0.23	123,123,123,123	0
30	MG	X	3197	1/1	0.79	0.23	73,73,73,73	0
30	MG	X	2984	1/1	0.80	0.34	76,76,76,76	0
30	MG	X	3032	1/1	0.80	0.30	73,73,73,73	0
30	MG	X	2913	1/1	0.80	0.38	59,59,59,59	0
30	MG	X	3006	1/1	0.80	0.35	83,83,83,83	0
30	MG	X	2946	1/1	0.80	0.52	76,76,76,76	0
30	MG	X	2989	1/1	0.81	0.21	68,68,68,68	0
30	MG	X	3124	1/1	0.81	0.27	58,58,58,58	0
30	MG	X	3007	1/1	0.81	0.22	88,88,88,88	0
30	MG	X	2949	1/1	0.81	0.42	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3154	1/1	0.81	0.25	123,123,123,123	0
30	MG	A	302	1/1	0.81	0.68	79,79,79,79	0
30	MG	X	3189	1/1	0.82	0.44	132,132,132,132	0
30	MG	X	3169	1/1	0.82	0.14	64,64,64,64	0
30	MG	X	3173	1/1	0.82	0.10	80,80,80,80	0
30	MG	X	2947	1/1	0.82	0.33	64,64,64,64	0
30	MG	X	2982	1/1	0.82	0.34	93,93,93,93	0
30	MG	X	3212	1/1	0.82	0.20	69,69,69,69	0
30	MG	X	3112	1/1	0.82	0.22	84,84,84,84	0
30	MG	O	101	1/1	0.82	0.38	51,51,51,51	0
30	MG	X	2962	1/1	0.83	0.15	71,71,71,71	0
30	MG	X	2941	1/1	0.83	0.23	63,63,63,63	0
30	MG	X	3085	1/1	0.83	0.18	58,58,58,58	0
30	MG	X	3111	1/1	0.83	0.22	77,77,77,77	0
30	MG	X	3070	1/1	0.83	0.43	109,109,109,109	0
30	MG	Y	209	1/1	0.83	0.40	103,103,103,103	0
30	MG	X	3150	1/1	0.84	0.27	114,114,114,114	0
30	MG	X	3004	1/1	0.84	0.29	76,76,76,76	0
30	MG	X	2921	1/1	0.84	0.38	68,68,68,68	0
30	MG	X	3092	1/1	0.84	0.42	75,75,75,75	0
30	MG	X	2953	1/1	0.84	0.46	55,55,55,55	0
30	MG	Y	213	1/1	0.84	0.41	107,107,107,107	0
30	MG	X	2906	1/1	0.84	0.31	68,68,68,68	0
30	MG	X	3210	1/1	0.84	0.17	107,107,107,107	0
30	MG	X	3056	1/1	0.84	0.25	102,102,102,102	0
30	MG	X	3186	1/1	0.84	0.25	134,134,134,134	0
30	MG	Y	207	1/1	0.85	0.17	96,96,96,96	0
30	MG	X	3193	1/1	0.85	0.17	75,75,75,75	0
30	MG	X	3016	1/1	0.85	0.13	65,65,65,65	0
30	MG	X	3206	1/1	0.85	0.40	57,57,57,57	0
30	MG	X	2933	1/1	0.85	0.34	67,67,67,67	0
30	MG	X	3182	1/1	0.85	0.20	60,60,60,60	0
30	MG	X	3127	1/1	0.85	0.21	60,60,60,60	0
30	MG	X	3165	1/1	0.85	0.27	72,72,72,72	0
30	MG	X	3054	1/1	0.85	0.32	83,83,83,83	0
30	MG	X	3081	1/1	0.85	0.19	85,85,85,85	0
30	MG	X	3149	1/1	0.86	0.34	41,41,41,41	0
30	MG	X	3041	1/1	0.86	0.35	91,91,91,91	0
30	MG	X	2986	1/1	0.86	0.27	80,80,80,80	0
30	MG	X	3002	1/1	0.86	0.55	79,79,79,79	0
30	MG	X	3192	1/1	0.86	0.21	160,160,160,160	0
30	MG	X	3023	1/1	0.86	0.62	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2922	1/1	0.86	0.37	65,65,65,65	0
30	MG	X	3170	1/1	0.86	0.19	69,69,69,69	0
30	MG	X	3063	1/1	0.86	0.20	61,61,61,61	0
30	MG	X	3034	1/1	0.86	0.61	63,63,63,63	0
30	MG	X	3017	1/1	0.86	0.21	57,57,57,57	0
30	MG	X	3147	1/1	0.86	0.14	85,85,85,85	0
30	MG	2	101	1/1	0.86	0.40	77,77,77,77	0
30	MG	X	2967	1/1	0.87	0.29	84,84,84,84	0
30	MG	X	3078	1/1	0.87	0.24	85,85,85,85	0
30	MG	X	3080	1/1	0.87	0.19	91,91,91,91	0
30	MG	X	2996	1/1	0.87	0.26	59,59,59,59	0
30	MG	X	3026	1/1	0.87	0.16	78,78,78,78	0
30	MG	X	3172	1/1	0.87	0.32	63,63,63,63	0
30	MG	X	3198	1/1	0.87	0.20	72,72,72,72	0
30	MG	Y	212	1/1	0.87	0.13	164,164,164,164	0
30	MG	X	3202	1/1	0.87	0.34	58,58,58,58	0
30	MG	Y	214	1/1	0.87	0.20	94,94,94,94	0
30	MG	X	3015	1/1	0.87	0.31	64,64,64,64	0
30	MG	X	2950	1/1	0.87	0.22	52,52,52,52	0
30	MG	X	2985	1/1	0.87	0.50	77,77,77,77	0
30	MG	A	303	1/1	0.87	0.46	88,88,88,88	0
30	MG	X	2963	1/1	0.87	0.20	48,48,48,48	0
30	MG	X	3047	1/1	0.87	0.50	84,84,84,84	0
30	MG	X	3079	1/1	0.88	0.13	69,69,69,69	0
30	MG	X	3205	1/1	0.88	0.39	61,61,61,61	0
30	MG	X	2914	1/1	0.88	0.44	54,54,54,54	0
30	MG	X	2954	1/1	0.88	0.24	86,86,86,86	0
30	MG	X	3106	1/1	0.88	0.25	100,100,100,100	0
30	MG	X	3144	1/1	0.88	0.23	83,83,83,83	0
30	MG	X	2912	1/1	0.88	0.48	55,55,55,55	0
30	MG	X	3219	1/1	0.88	0.22	51,51,51,51	0
30	MG	X	3077	1/1	0.88	0.35	59,59,59,59	0
30	MG	X	2994	1/1	0.88	0.48	79,79,79,79	0
30	MG	X	3152	1/1	0.88	0.21	82,82,82,82	0
30	MG	X	3200	1/1	0.88	0.24	69,69,69,69	0
30	MG	X	3024	1/1	0.89	0.17	83,83,83,83	0
30	MG	X	3214	1/1	0.89	0.37	88,88,88,88	0
30	MG	X	3215	1/1	0.89	0.18	91,91,91,91	0
30	MG	X	3201	1/1	0.89	0.17	81,81,81,81	0
30	MG	X	2960	1/1	0.89	0.47	73,73,73,73	0
30	MG	X	3062	1/1	0.89	0.27	61,61,61,61	0
30	MG	X	3160	1/1	0.89	0.16	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3093	1/1	0.89	0.23	64,64,64,64	0
30	MG	X	2934	1/1	0.89	0.20	51,51,51,51	0
30	MG	X	3074	1/1	0.89	0.22	73,73,73,73	0
30	MG	X	3185	1/1	0.90	0.29	100,100,100,100	0
30	MG	X	2905	1/1	0.90	0.31	57,57,57,57	0
30	MG	X	2988	1/1	0.90	0.18	67,67,67,67	0
30	MG	X	3188	1/1	0.90	0.31	79,79,79,79	0
30	MG	X	3053	1/1	0.90	0.34	68,68,68,68	0
30	MG	X	3014	1/1	0.90	0.30	95,95,95,95	0
30	MG	X	3035	1/1	0.90	0.29	68,68,68,68	0
30	MG	X	3128	1/1	0.90	0.07	67,67,67,67	0
30	MG	X	3196	1/1	0.90	0.24	56,56,56,56	0
30	MG	X	3166	1/1	0.90	0.15	49,49,49,49	0
30	MG	X	3135	1/1	0.90	0.61	85,85,85,85	0
30	MG	X	2952	1/1	0.90	0.18	88,88,88,88	0
30	MG	X	3059	1/1	0.90	0.15	57,57,57,57	0
30	MG	X	3143	1/1	0.90	0.19	63,63,63,63	0
30	MG	X	3204	1/1	0.90	0.50	76,76,76,76	0
30	MG	X	3040	1/1	0.90	0.04	60,60,60,60	0
30	MG	X	2980	1/1	0.90	0.23	78,78,78,78	0
30	MG	X	3178	1/1	0.90	0.14	63,63,63,63	0
30	MG	X	3108	1/1	0.90	0.50	104,104,104,104	0
30	MG	X	3183	1/1	0.90	0.09	75,75,75,75	0
30	MG	X	2907	1/1	0.91	0.26	50,50,50,50	0
30	MG	X	3000	1/1	0.91	0.22	83,83,83,83	0
30	MG	X	3055	1/1	0.91	0.18	119,119,119,119	0
30	MG	X	2929	1/1	0.91	0.32	60,60,60,60	0
30	MG	X	3109	1/1	0.91	0.29	60,60,60,60	0
30	MG	X	2977	1/1	0.91	0.34	66,66,66,66	0
30	MG	X	3216	1/1	0.91	0.12	75,75,75,75	0
30	MG	X	3158	1/1	0.91	0.23	109,109,109,109	0
30	MG	X	3220	1/1	0.91	0.56	56,56,56,56	0
30	MG	Y	201	1/1	0.91	0.17	101,101,101,101	0
30	MG	X	2925	1/1	0.91	0.21	76,76,76,76	0
30	MG	X	2965	1/1	0.91	0.34	69,69,69,69	0
30	MG	X	3164	1/1	0.91	0.61	85,85,85,85	0
30	MG	X	3043	1/1	0.91	0.30	102,102,102,102	0
30	MG	X	3194	1/1	0.91	0.08	75,75,75,75	0
30	MG	X	3195	1/1	0.91	0.27	80,80,80,80	0
30	MG	X	3087	1/1	0.91	0.11	65,65,65,65	0
30	MG	X	3168	1/1	0.91	0.07	60,60,60,60	0
30	MG	X	3088	1/1	0.91	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3132	1/1	0.91	0.07	62,62,62,62	0
30	MG	X	3044	1/1	0.91	0.21	68,68,68,68	0
30	MG	X	3069	1/1	0.91	0.26	78,78,78,78	0
30	MG	X	3174	1/1	0.91	0.16	88,88,88,88	0
30	MG	X	3010	1/1	0.91	0.27	70,70,70,70	0
30	MG	X	2958	1/1	0.91	0.23	50,50,50,50	0
30	MG	X	3207	1/1	0.91	0.16	84,84,84,84	0
30	MG	X	3120	1/1	0.92	0.12	83,83,83,83	0
30	MG	X	3156	1/1	0.92	0.16	112,112,112,112	0
30	MG	X	2961	1/1	0.92	0.33	60,60,60,60	0
30	MG	X	3159	1/1	0.92	0.16	102,102,102,102	0
30	MG	X	3125	1/1	0.92	0.47	51,51,51,51	0
30	MG	X	3190	1/1	0.92	0.42	129,129,129,129	0
30	MG	X	3161	1/1	0.92	0.30	74,74,74,74	0
30	MG	X	2969	1/1	0.92	0.32	63,63,63,63	0
30	MG	X	3163	1/1	0.92	0.18	68,68,68,68	0
30	MG	X	3101	1/1	0.92	0.21	68,68,68,68	0
30	MG	X	3130	1/1	0.92	0.09	55,55,55,55	0
30	MG	X	3102	1/1	0.92	0.32	78,78,78,78	0
30	MG	X	3103	1/1	0.92	0.08	62,62,62,62	0
30	MG	X	3084	1/1	0.92	0.20	99,99,99,99	0
30	MG	X	3199	1/1	0.92	0.22	76,76,76,76	0
30	MG	X	2975	1/1	0.92	0.07	61,61,61,61	0
30	MG	X	3008	1/1	0.92	0.21	73,73,73,73	0
30	MG	X	3061	1/1	0.92	0.27	82,82,82,82	0
30	MG	X	3146	1/1	0.92	0.17	73,73,73,73	0
30	MG	X	3110	1/1	0.92	0.49	81,81,81,81	0
30	MG	X	3021	1/1	0.92	0.43	63,63,63,63	0
30	MG	X	2995	1/1	0.92	0.09	74,74,74,74	0
30	MG	X	3151	1/1	0.92	0.32	80,80,80,80	0
30	MG	X	3003	1/1	0.92	0.17	90,90,90,90	0
30	MG	X	3039	1/1	0.93	0.20	64,64,64,64	0
30	MG	X	3148	1/1	0.93	0.30	75,75,75,75	0
30	MG	X	2944	1/1	0.93	0.14	50,50,50,50	0
30	MG	X	3086	1/1	0.93	0.18	59,59,59,59	0
30	MG	X	2920	1/1	0.93	0.14	66,66,66,66	0
30	MG	X	3115	1/1	0.93	0.28	78,78,78,78	0
30	MG	X	3117	1/1	0.93	0.44	66,66,66,66	0
30	MG	X	3155	1/1	0.93	0.15	119,119,119,119	0
30	MG	X	2978	1/1	0.93	0.15	68,68,68,68	0
30	MG	X	3012	1/1	0.93	0.09	72,72,72,72	0
30	MG	X	3066	1/1	0.93	0.22	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	Y	205	1/1	0.93	0.36	92,92,92,92	0
30	MG	X	3046	1/1	0.93	0.41	83,83,83,83	0
30	MG	X	3013	1/1	0.93	0.25	45,45,45,45	0
30	MG	X	3048	1/1	0.93	0.12	66,66,66,66	0
30	MG	X	3050	1/1	0.93	0.06	70,70,70,70	0
30	MG	X	3134	1/1	0.93	0.49	71,71,71,71	0
30	MG	X	2915	1/1	0.93	0.28	58,58,58,58	0
30	MG	X	3136	1/1	0.93	0.33	85,85,85,85	0
30	MG	X	3137	1/1	0.93	0.15	72,72,72,72	0
30	MG	X	3138	1/1	0.93	0.13	69,69,69,69	0
30	MG	X	3028	1/1	0.93	0.57	58,58,58,58	0
30	MG	X	2991	1/1	0.93	0.17	62,62,62,62	0
30	MG	A	301	1/1	0.93	0.45	84,84,84,84	0
29	QTZ	X	2901	51/51	0.93	0.16	55,57,60,60	20
30	MG	X	2930	1/1	0.93	0.23	67,67,67,67	0
30	MG	J	202	1/1	0.93	0.12	111,111,111,111	0
30	MG	K	201	1/1	0.93	0.07	71,71,71,71	0
30	MG	X	3019	1/1	0.93	0.33	64,64,64,64	0
30	MG	X	3176	1/1	0.93	0.07	129,129,129,129	0
30	MG	X	3036	1/1	0.94	0.25	58,58,58,58	0
30	MG	X	3218	1/1	0.94	0.29	44,44,44,44	0
30	MG	X	3011	1/1	0.94	0.21	46,46,46,46	0
30	MG	X	2931	1/1	0.94	0.11	69,69,69,69	0
30	MG	X	2964	1/1	0.94	0.47	73,73,73,73	0
30	MG	Y	202	1/1	0.94	0.32	95,95,95,95	0
30	MG	X	2993	1/1	0.94	0.19	46,46,46,46	0
30	MG	X	2972	1/1	0.94	0.16	83,83,83,83	0
30	MG	X	3114	1/1	0.94	0.27	75,75,75,75	0
30	MG	X	2936	1/1	0.94	0.23	53,53,53,53	0
30	MG	X	3076	1/1	0.94	0.15	90,90,90,90	0
30	MG	X	3118	1/1	0.94	0.13	70,70,70,70	0
30	MG	X	3096	1/1	0.94	0.39	75,75,75,75	0
30	MG	X	3058	1/1	0.94	0.21	115,115,115,115	0
30	MG	X	3100	1/1	0.94	0.12	124,124,124,124	0
30	MG	X	2937	1/1	0.94	0.18	68,68,68,68	0
30	MG	X	3180	1/1	0.94	0.21	58,58,58,58	0
30	MG	X	3060	1/1	0.94	0.19	58,58,58,58	0
30	MG	X	2998	1/1	0.94	0.38	77,77,77,77	0
30	MG	X	3184	1/1	0.94	0.18	84,84,84,84	0
30	MG	X	3131	1/1	0.94	0.08	75,75,75,75	0
30	MG	X	2939	1/1	0.94	0.27	59,59,59,59	0
30	MG	J	201	1/1	0.94	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3105	1/1	0.94	0.43	61,61,61,61	0
30	MG	X	3213	1/1	0.94	0.20	85,85,85,85	0
30	MG	X	3049	1/1	0.94	0.14	48,48,48,48	0
30	MG	X	3107	1/1	0.94	0.47	82,82,82,82	0
30	MG	X	2973	1/1	0.95	0.49	61,61,61,61	0
30	MG	X	3027	1/1	0.95	0.14	60,60,60,60	0
30	MG	X	3181	1/1	0.95	0.27	68,68,68,68	0
30	MG	X	3073	1/1	0.95	0.30	75,75,75,75	0
30	MG	X	3045	1/1	0.95	0.52	77,77,77,77	0
30	MG	X	2974	1/1	0.95	0.31	55,55,55,55	0
30	MG	X	2904	1/1	0.95	0.17	38,38,38,38	0
30	MG	X	2926	1/1	0.95	0.27	48,48,48,48	0
30	MG	X	2956	1/1	0.95	0.24	51,51,51,51	0
30	MG	X	3203	1/1	0.95	0.07	63,63,63,63	0
30	MG	X	2957	1/1	0.95	0.36	53,53,53,53	0
30	MG	X	2943	1/1	0.95	0.19	71,71,71,71	0
30	MG	X	2910	1/1	0.95	0.22	46,46,46,46	0
30	MG	X	3067	1/1	0.95	0.35	59,59,59,59	0
30	MG	X	2945	1/1	0.95	0.31	61,61,61,61	0
30	MG	X	2928	1/1	0.95	0.14	54,54,54,54	0
30	MG	X	3157	1/1	0.96	0.14	97,97,97,97	0
30	MG	X	2990	1/1	0.96	0.05	63,63,63,63	0
30	MG	X	3037	1/1	0.96	0.22	51,51,51,51	0
30	MG	X	3082	1/1	0.96	0.25	82,82,82,82	0
30	MG	X	3065	1/1	0.96	0.08	65,65,65,65	0
30	MG	X	3133	1/1	0.96	0.13	68,68,68,68	0
30	MG	X	2983	1/1	0.96	0.20	60,60,60,60	0
30	MG	X	3052	1/1	0.96	0.14	87,87,87,87	0
30	MG	X	3068	1/1	0.96	0.18	101,101,101,101	0
30	MG	X	3001	1/1	0.96	0.08	55,55,55,55	0
30	MG	X	3167	1/1	0.96	0.12	49,49,49,49	0
30	MG	X	2992	1/1	0.96	0.18	51,51,51,51	0
30	MG	X	3140	1/1	0.96	0.20	77,77,77,77	0
30	MG	X	3025	1/1	0.96	0.16	83,83,83,83	0
30	MG	X	3042	1/1	0.96	0.33	59,59,59,59	0
30	MG	X	2911	1/1	0.96	0.36	33,33,33,33	0
30	MG	X	2935	1/1	0.96	0.09	61,61,61,61	0
30	MG	X	3097	1/1	0.96	0.15	63,63,63,63	0
30	MG	X	3005	1/1	0.96	0.15	77,77,77,77	0
30	MG	X	3099	1/1	0.96	0.34	72,72,72,72	0
30	MG	X	3121	1/1	0.96	0.36	56,56,56,56	0
30	MG	X	3179	1/1	0.96	0.30	41,41,41,41	0

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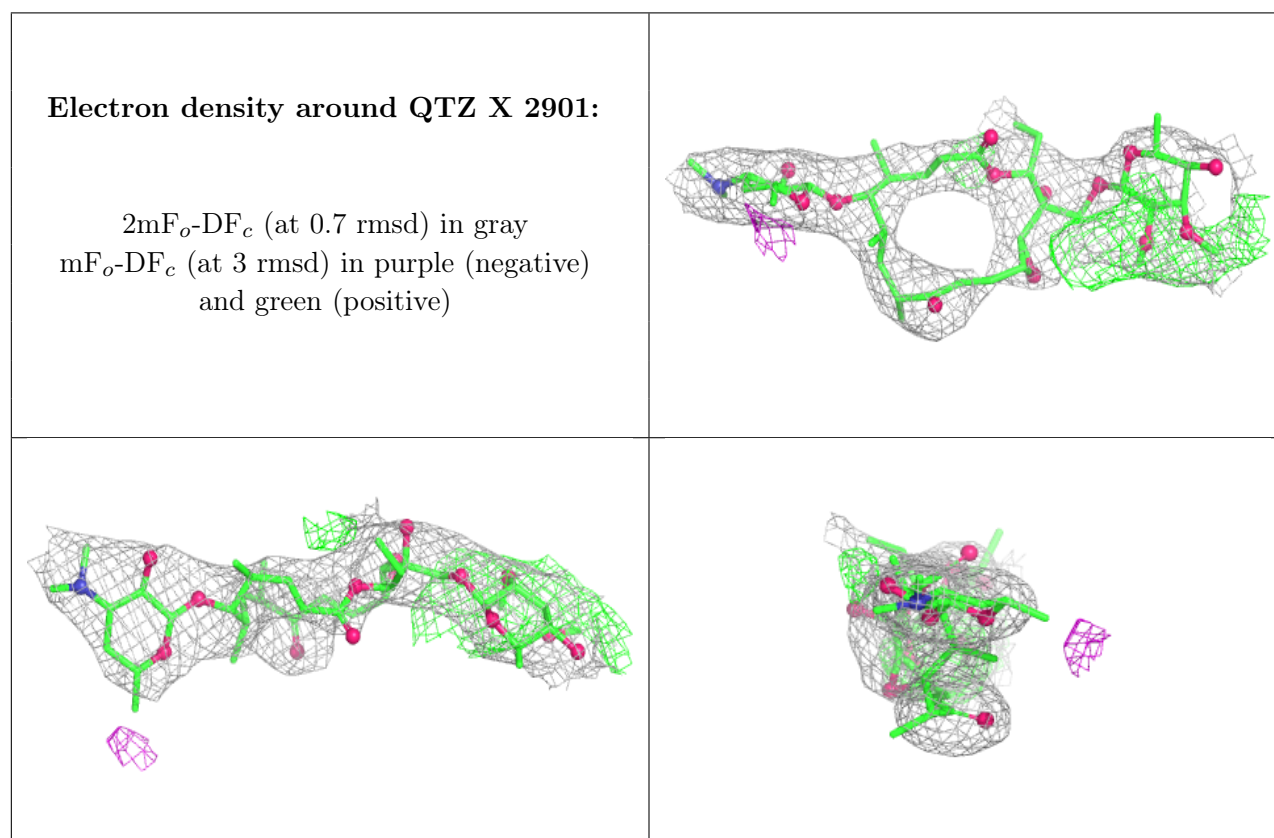
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3122	1/1	0.96	0.15	68,68,68,68	0
30	MG	I	201	1/1	0.96	0.08	60,60,60,60	0
30	MG	X	3123	1/1	0.96	0.20	50,50,50,50	0
30	MG	X	2916	1/1	0.96	0.15	55,55,55,55	0
30	MG	X	2909	1/1	0.96	0.12	41,41,41,41	0
30	MG	X	3126	1/1	0.96	0.40	45,45,45,45	0
30	MG	X	2924	1/1	0.96	0.15	75,75,75,75	0
30	MG	X	3221	1/1	0.97	0.32	61,61,61,61	0
30	MG	X	3091	1/1	0.97	0.27	62,62,62,62	0
30	MG	X	3153	1/1	0.97	0.27	86,86,86,86	0
30	MG	Y	203	1/1	0.97	0.31	73,73,73,73	0
30	MG	X	2966	1/1	0.97	0.14	73,73,73,73	0
30	MG	X	3075	1/1	0.97	0.16	81,81,81,81	0
30	MG	X	3033	1/1	0.97	0.09	56,56,56,56	0
30	MG	X	3009	1/1	0.97	0.43	62,62,62,62	0
30	MG	X	2976	1/1	0.97	0.12	58,58,58,58	0
30	MG	X	2940	1/1	0.97	0.13	48,48,48,48	0
30	MG	X	2938	1/1	0.97	0.55	62,62,62,62	0
30	MG	X	3139	1/1	0.97	0.14	61,61,61,61	0
30	MG	X	2979	1/1	0.97	0.26	65,65,65,65	0
30	MG	X	2987	1/1	0.97	0.41	61,61,61,61	0
30	MG	X	3083	1/1	0.97	0.10	105,105,105,105	0
30	MG	X	2917	1/1	0.97	0.10	69,69,69,69	0
30	MG	X	3211	1/1	0.97	0.25	52,52,52,52	0
30	MG	X	2997	1/1	0.97	0.07	81,81,81,81	0
30	MG	X	3145	1/1	0.97	0.06	81,81,81,81	0
30	MG	X	2981	1/1	0.97	0.29	57,57,57,57	0
30	MG	X	3029	1/1	0.97	0.30	42,42,42,42	0
30	MG	X	3030	1/1	0.97	0.30	32,32,32,32	0
30	MG	X	3217	1/1	0.97	0.41	60,60,60,60	0
30	MG	X	3031	1/1	0.97	0.16	95,95,95,95	0
30	MG	X	3129	1/1	0.97	0.21	55,55,55,55	0
30	MG	X	3090	1/1	0.97	0.10	69,69,69,69	0
30	MG	X	2908	1/1	0.98	0.34	21,21,21,21	0
30	MG	X	3095	1/1	0.98	0.32	44,44,44,44	0
30	MG	X	3018	1/1	0.98	0.06	60,60,60,60	0
30	MG	X	2959	1/1	0.98	0.23	43,43,43,43	0
30	MG	X	2955	1/1	0.98	0.21	47,47,47,47	0
30	MG	X	2923	1/1	0.98	0.41	57,57,57,57	0
30	MG	X	3116	1/1	0.98	0.05	74,74,74,74	0
30	MG	X	2932	1/1	0.98	0.13	57,57,57,57	0
30	MG	X	2968	1/1	0.98	0.10	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	MG	X	2919	1/1	0.99	0.21	42,42,42,42	0
30	MG	X	3119	1/1	0.99	0.04	72,72,72,72	0
30	MG	X	3171	1/1	1.00	0.02	53,53,53,53	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.