



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2021 – 04:19 pm BST

PDB ID : 7A18
Title : 50S Deinococcus radiodurans ribosome bounded with mycinamicin IV
Authors : Breiner, E.; Eyal, Z.; Matzov, D.; Halfon, Y.; Camicata, G.; Rozenberg, H.;
Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2020-08-12
Resolution : 3.40 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 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 : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

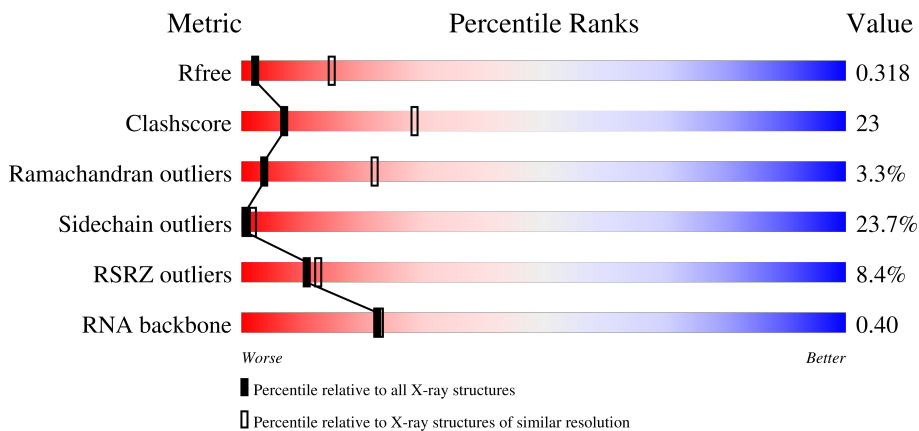
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



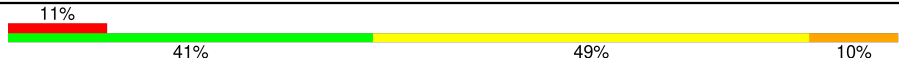


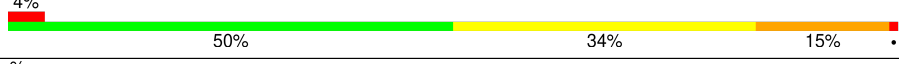
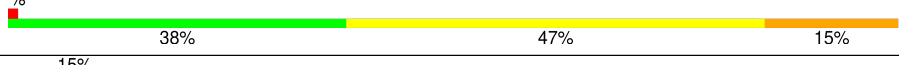
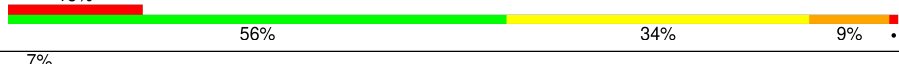
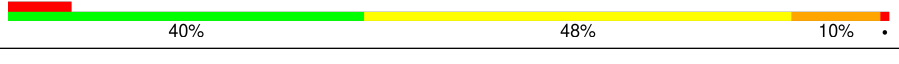
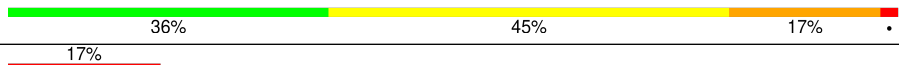

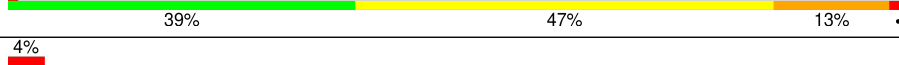

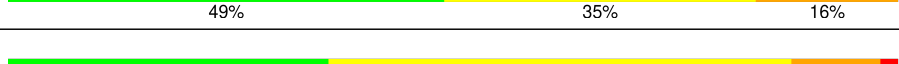
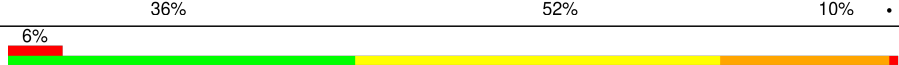
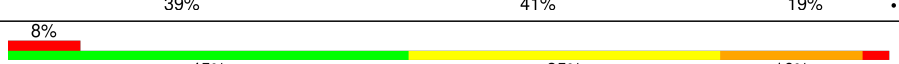

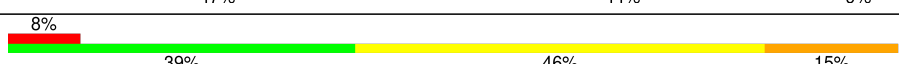
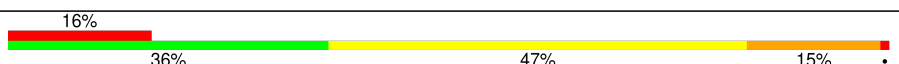
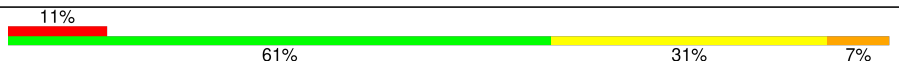
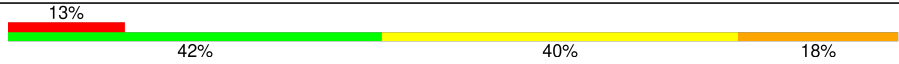
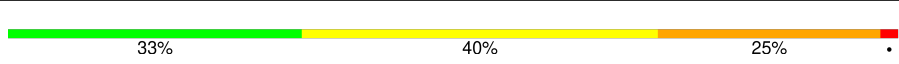


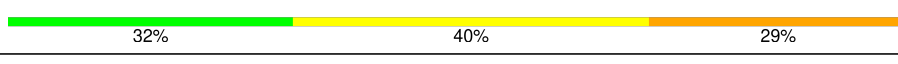

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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	2699	
2	Y	122	
3	A	271	
4	B	206	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	195	
6	D	176	
7	E	171	
8	G	142	
9	H	134	
10	I	137	
11	J	134	
12	K	115	
13	L	104	
14	M	118	
15	N	117	
16	O	98	
17	P	129	
18	Q	93	
19	R	110	
20	S	175	
21	T	72	
22	U	74	
23	V	54	
24	W	55	
25	Z	57	
26	1	49	
27	2	46	
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	2	101	-	-	-	X
30	MG	X	2925	-	-	-	X
30	MG	X	2950	-	-	-	X
30	MG	X	2969	-	-	-	X
30	MG	X	2976	-	-	-	X
30	MG	X	2979	-	-	-	X
30	MG	X	3002	-	-	-	X
30	MG	X	3045	-	-	-	X
30	MG	X	3050	-	-	-	X
30	MG	X	3052	-	-	-	X
30	MG	X	3057	-	-	-	X
30	MG	X	3060	-	-	-	X
30	MG	X	3071	-	-	-	X
30	MG	X	3074	-	-	-	X
30	MG	X	3086	-	-	-	X
30	MG	X	3090	-	-	-	X
30	MG	X	3096	-	-	-	X
30	MG	X	3097	-	-	-	X
30	MG	X	3102	-	-	-	X
30	MG	X	3104	-	-	-	X
30	MG	X	3105	-	-	-	X
30	MG	X	3109	-	-	-	X
30	MG	X	3115	-	-	-	X
30	MG	X	3122	-	-	-	X
30	MG	X	3131	-	-	-	X
30	MG	X	3141	-	-	-	X
30	MG	X	3144	-	-	-	X
30	MG	X	3146	-	-	-	X
30	MG	X	3149	-	-	-	X
30	MG	X	3151	-	-	-	X
30	MG	X	3154	-	-	-	X
30	MG	X	3159	-	-	-	X
30	MG	X	3163	-	-	-	X
30	MG	Y	202	-	-	-	X
31	SPD	X	3166	-	-	-	X
31	SPD	X	3167	-	-	X	-

2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 84387 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 (2699-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2699	57957	25853	10701	18704	2699	0	1	0

- Molecule 2 is a RNA chain called RNA (122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	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	271	2001	1246	390	362	3	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	206	1544	968	296	272	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	195	1467	912	280	273	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	176	1367	870	238	253	6	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 L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	G	142	1107	698	208	198	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	134	993	611	197	180	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	I	137	982	603	194	184	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	J	134	1042	668	188	179	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	115	897	552	183	159	3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	L	104	751	457	154	140	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	M	118	923	578	178	167	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	N	117	962	599	203	159	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	O	98	734	459	135	139	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	12	ALA	TYR	conflict	UNP Q9RY64

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	P	129	1020	643	199	176	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	Q	93	718	452	134	130	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	R	110	793	492	149	151	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	S	175	1290	811	224	251	4	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	T	72	542	343	104	94	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	U	74	539	336	107	96		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	V	54	438	270	89	78	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	Z	57	448	275	92	76	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	1	49	315	199	54	62		0	0	0

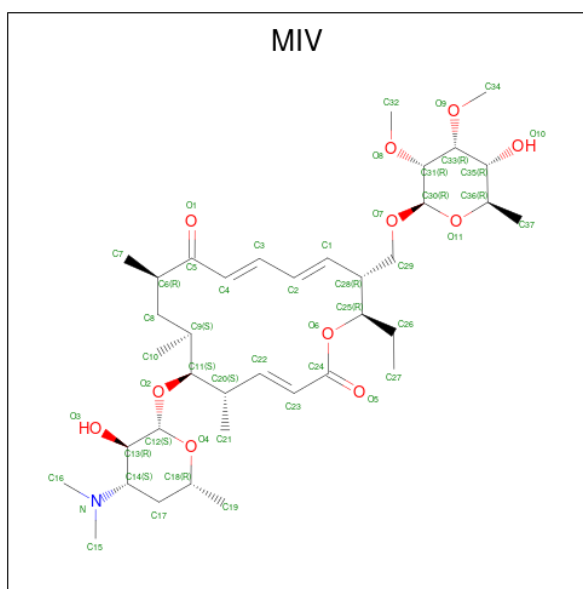
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	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
			470	295	97	75	3			

- Molecule 29 is MYCINAMICIN IV (three-letter code: MIV) (formula: C₃₇H₆₁NO₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	X	1	Total	C	N	O	0	0
			49	37	1	11		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

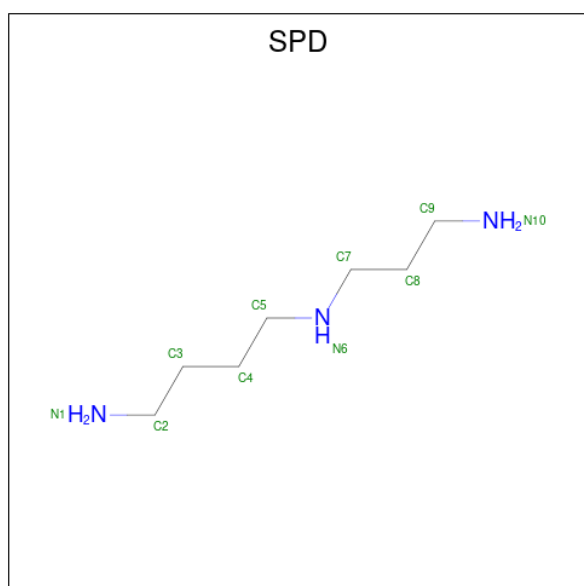
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	264	Total	Mg	0	0
			264	264		
30	Y	4	Total	Mg	0	0
			4	4		
30	A	1	Total	Mg	0	0
			1	1		
30	I	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	N	1	Total Mg 1 1	0	0
30	Q	2	Total Mg 2 2	0	0
30	W	1	Total Mg 1 1	0	0
30	2	2	Total Mg 2 2	0	0
30	3	1	Total Mg 1 1	0	0

- Molecule 31 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



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

Continued on next page...

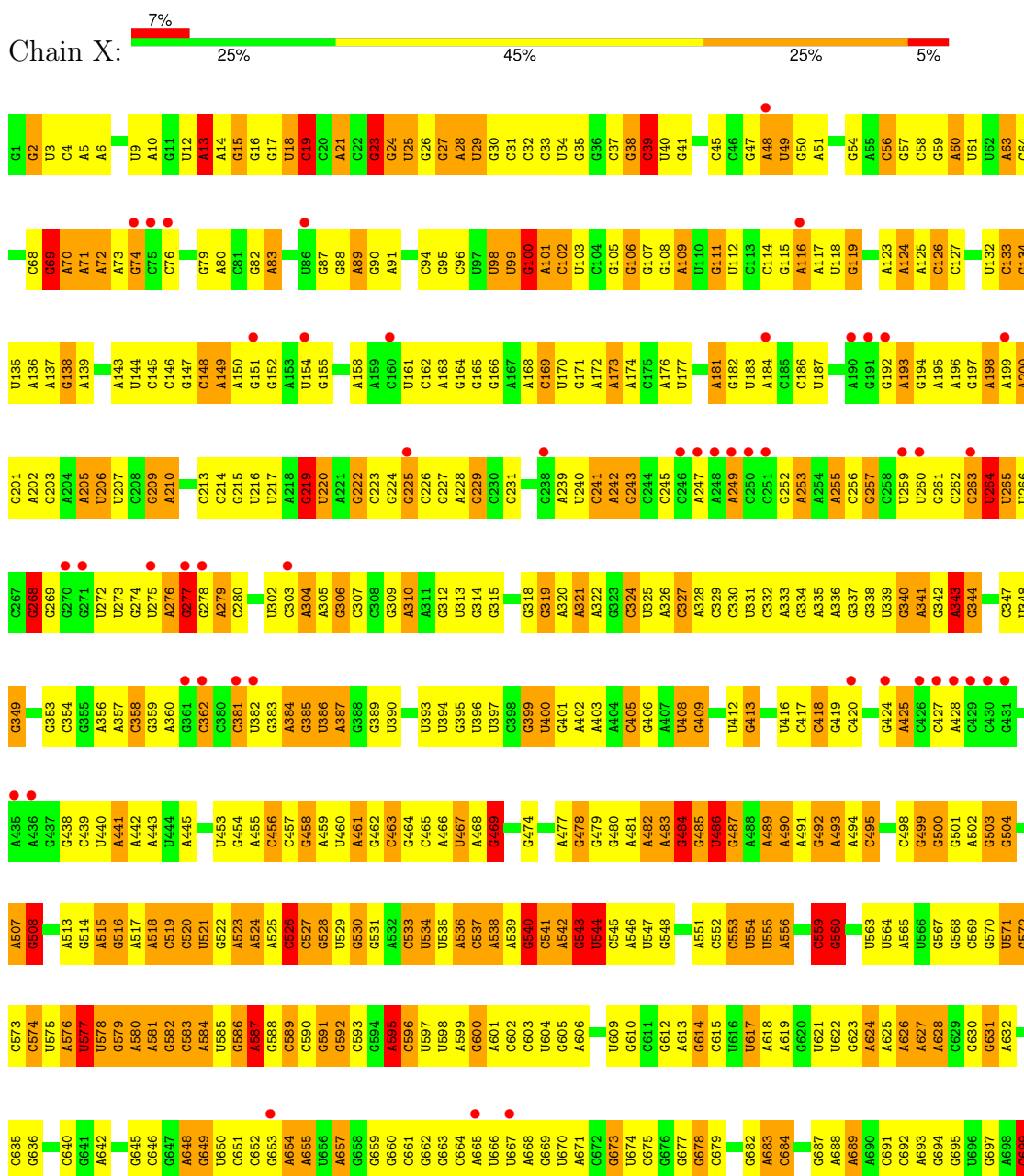
Continued from previous page...

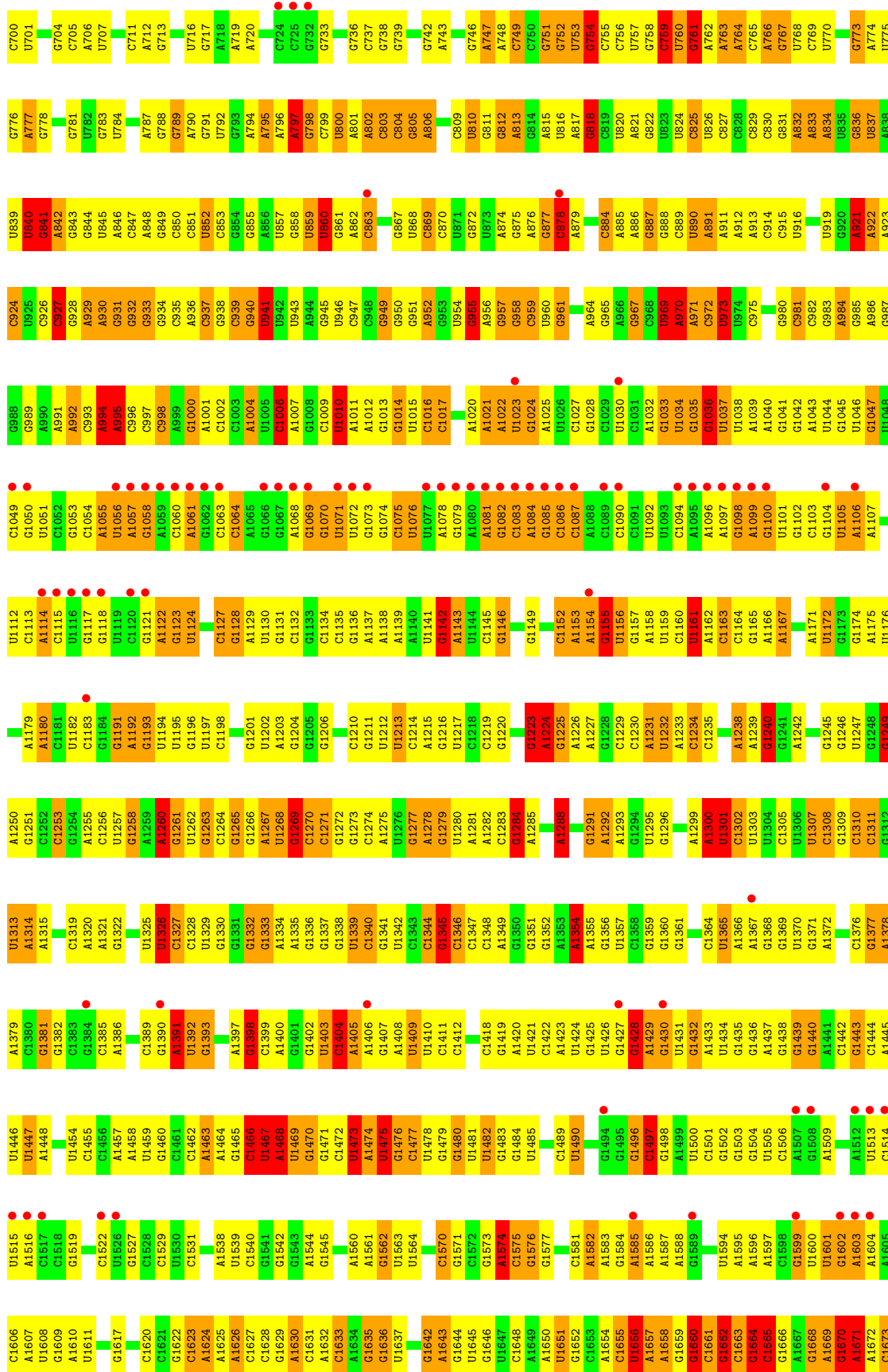
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
31	V	1	10	7	3	0	0

3 Residue-property plots [i](#)

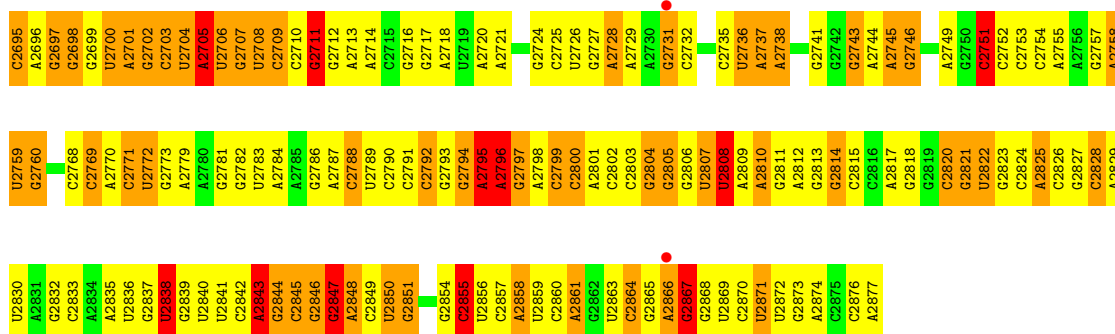
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RNA (2699-MER)

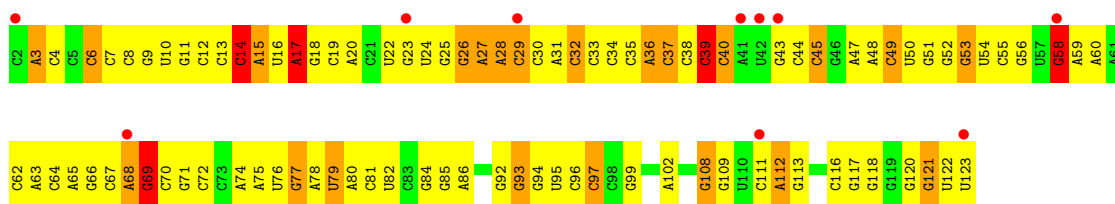




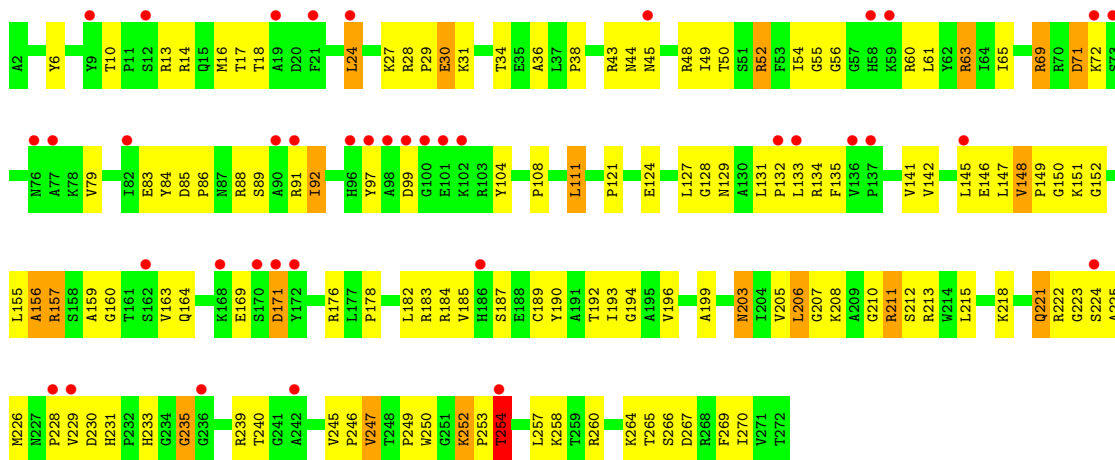
U6696	U6697	U6698	U6699	U6700	U6701	U6702	U6703	U6704	U6705	U6706	U6707	U6708	U6709	U6710	U6711	U6712	U6713	U6714	U6715	U6716	U6717	U6718	U6719	U6720	U6721	U6722	U6723	U6724	U6725
C2556	C2557	C2558	C2559	C2560	C2561	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585
C2489	C2490	C2491	C2492	C2493	C2494	C2495	C2496	C2497	C2498	C2499	C2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2508	C2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	C2518
A2429	A2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	A2438	A2439	A2440	A2441	A2442	A2443	A2444	A2445	A2446	A2447	A2448	A2449	A2450	A2451	A2452	A2453	A2454	A2455	A2456	A2457	A2458
G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389	G2390	G2391	
U2090	A2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	
C2028	G2029	U2030	G2031	G2032	G2033	G2034	G2035	G2036	G2037	G2038	G2039	G2040	G2041	G2042	G2043	G2044	G2045	G2046	G2047	G2048	G2049	G2050	G2051	G2052	G2053	G2054	G2055	G2056	
U1966	U1967	G1968	G1969	G1970	G1971	G1972	G1973	G1974	G1975	G1976	G1977	G1978	G1979	G1980	G1981	G1982	G1983	G1984	G1985	G1986	G1987	G1988	G1989	G1990	G1991	G1992	G1993	G1994	
G1886	G1887	G1888	G1889	G1890	G1891	G1892	G1893	G1894	G1895	G1896	G1897	G1898	G1899	G1900	G1901	G1902	G1903	G1904	G1905	G1906	G1907	G1908	G1909	G1910	G1911	G1912	G1913	G1914	
C1808	C1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	
G1742	G1743	G1744	G1745	G1746	G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1754	G1755	G1756	G1757	G1758	G1759	G1760	G1761	G1762	G1763	G1764	G1765	G1766	G1767	G1768	G1769	G1770	
C1674	C1675	U1676	U1677	G1678	G1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	



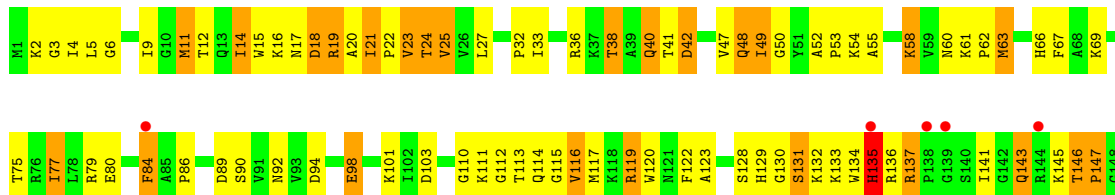
• Molecule 2: RNA (122-MER)



• Molecule 3: 50S ribosomal protein L2

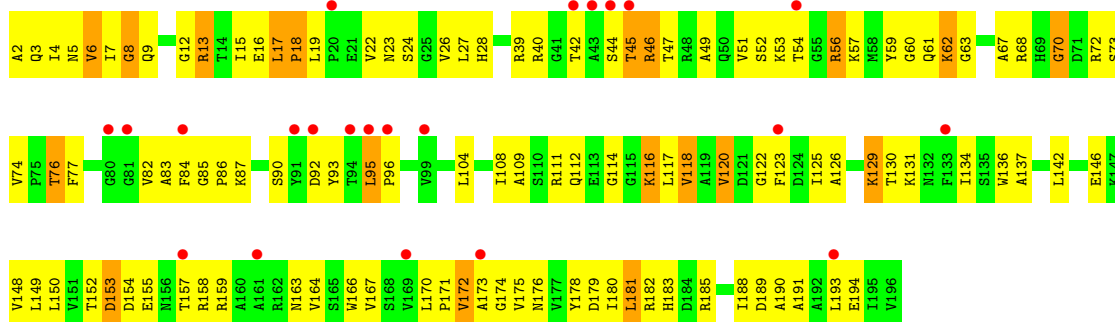


• Molecule 4: 50S ribosomal protein L3

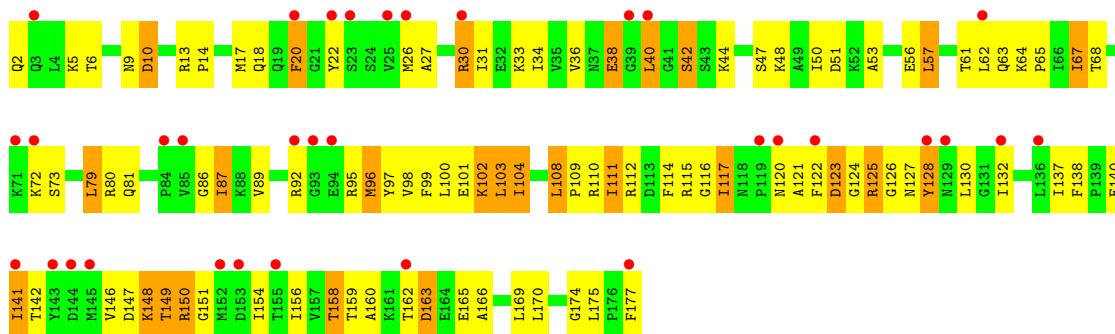
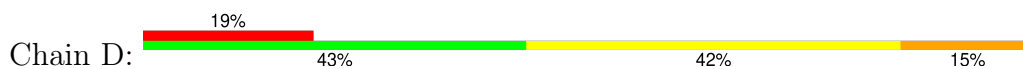




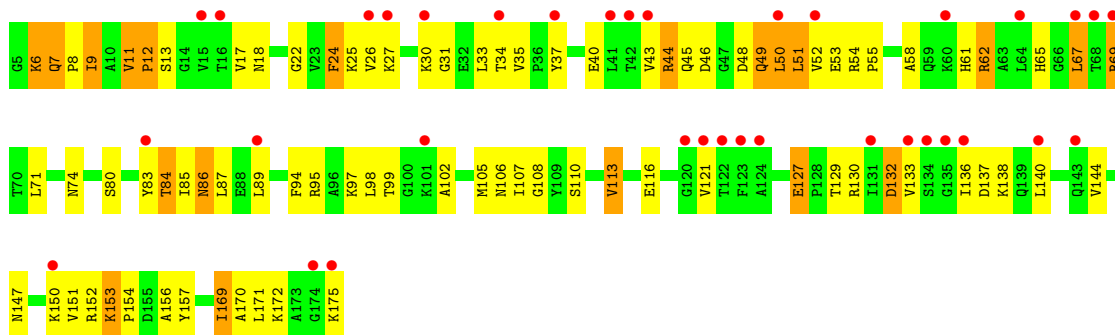
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

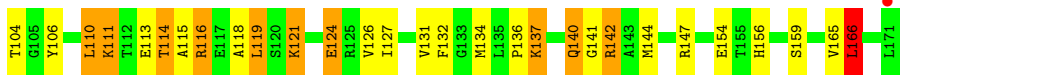
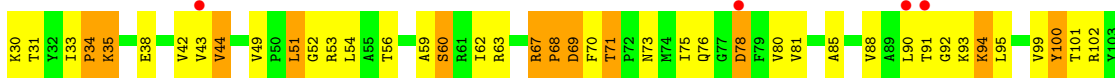


- Molecule 7: 50S ribosomal protein L6

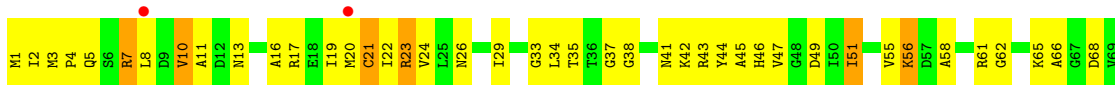


- Molecule 8: 50S ribosomal protein L13

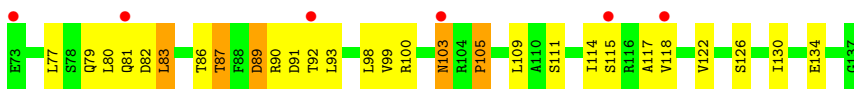
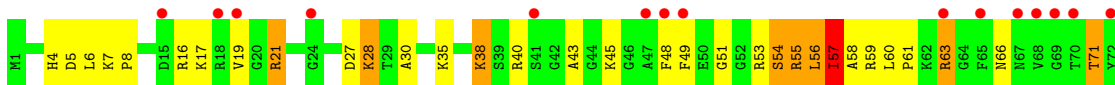




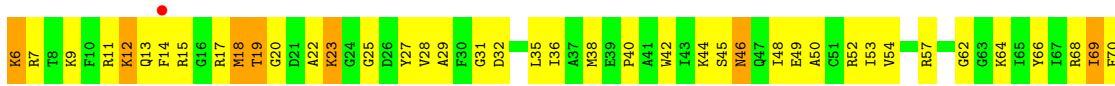
• Molecule 9: 50S ribosomal protein L14



• Molecule 10: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L16

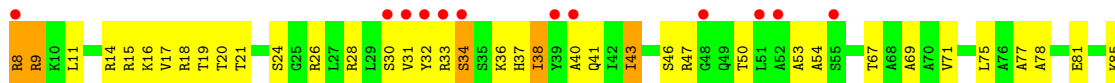


• Molecule 12: 50S ribosomal protein L17

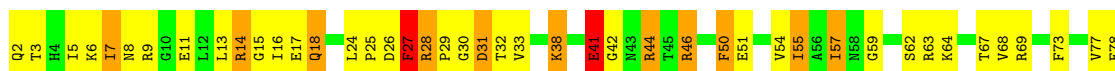




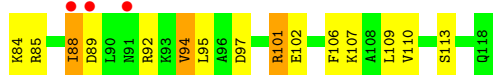
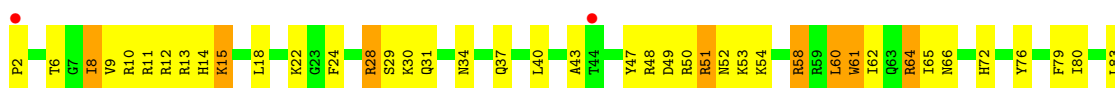
- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L21

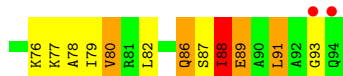


- Molecule 17: 50S ribosomal protein L22

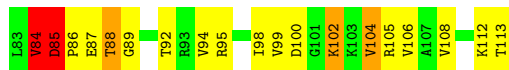
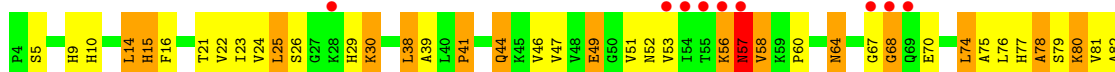
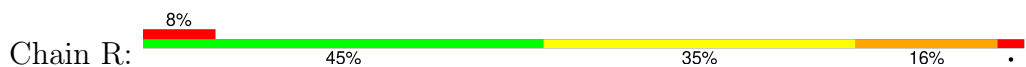




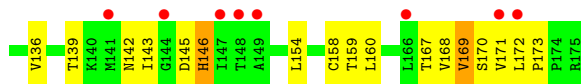
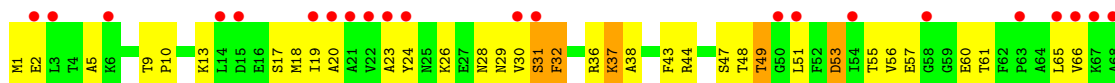
• Molecule 18: 50S ribosomal protein L23



• Molecule 19: 50S ribosomal protein L24



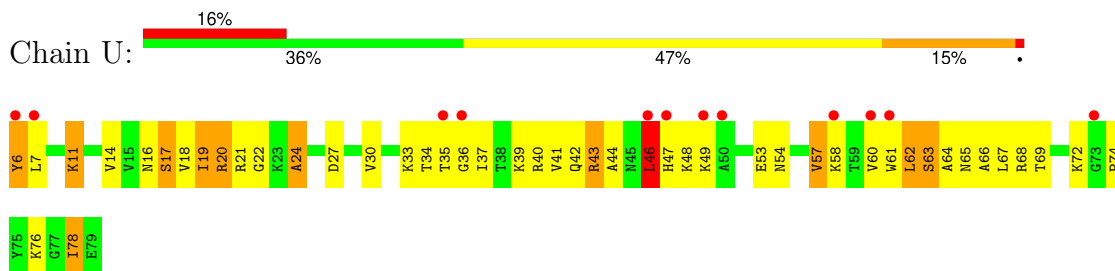
• Molecule 20: 50S ribosomal protein L25



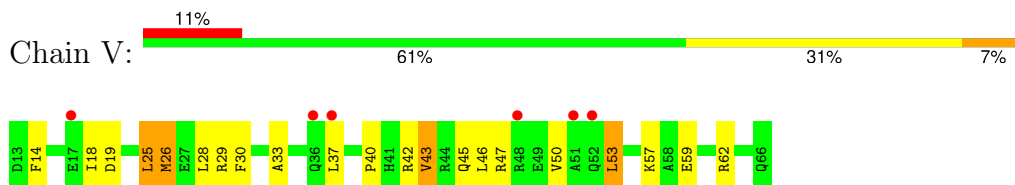
• Molecule 21: 50S ribosomal protein L27



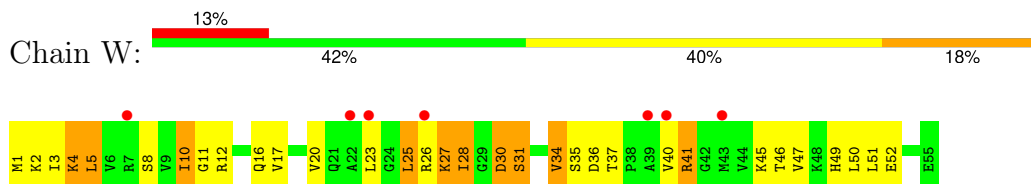
- Molecule 22: 50S ribosomal protein L28



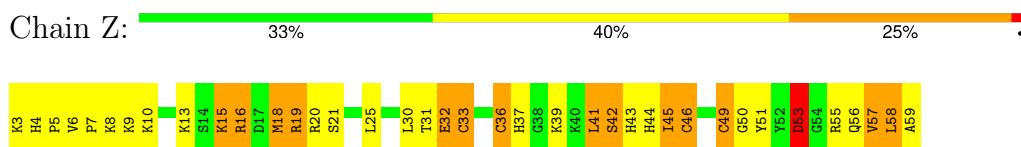
- Molecule 23: 50S ribosomal protein L29



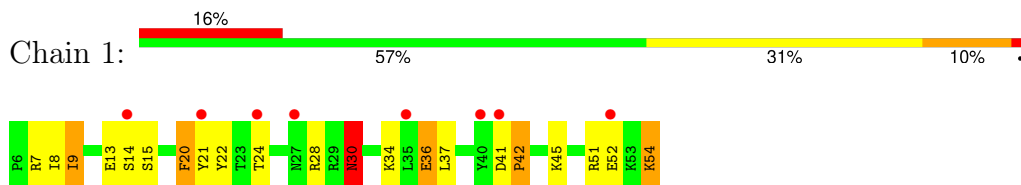
- Molecule 24: 50S ribosomal protein L30



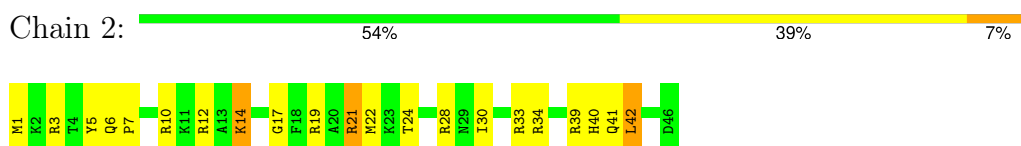
- Molecule 25: 50S ribosomal protein L32



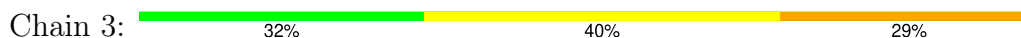
- Molecule 26: 50S ribosomal protein L33



- 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	169.59Å 410.13Å 690.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 50.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-3.40) 91.9 (50.07-3.30)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.284 , 0.318 0.284 , 0.318	Depositor DCC
R_{free} test set	16405 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	84387	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: MIV, SPD, 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	0.81	33/64897 (0.1%)	1.48	1063/101217 (1.1%)
2	Y	0.56	0/2904	1.27	26/4525 (0.6%)
3	A	0.37	0/2041	0.59	0/2765
4	B	0.59	0/1572	0.78	0/2112
5	C	0.44	0/1490	0.67	1/2021 (0.0%)
6	D	0.34	0/1385	0.58	0/1863
7	E	0.34	0/1308	0.59	0/1771
8	G	0.46	0/1131	0.68	1/1531 (0.1%)
9	H	0.71	1/1003 (0.1%)	0.85	0/1348
10	I	0.46	0/994	0.74	0/1338
11	J	0.50	0/1064	0.70	0/1425
12	K	0.71	0/905	0.92	1/1212 (0.1%)
13	L	0.31	0/755	0.65	0/1011
14	M	0.68	0/936	0.86	0/1257
15	N	0.53	0/978	0.75	1/1305 (0.1%)
16	O	0.43	0/741	0.66	0/992
17	P	0.62	0/1033	0.79	1/1383 (0.1%)
18	Q	0.38	0/729	0.60	0/980
19	R	0.44	0/803	0.66	0/1087
20	S	0.36	0/1312	0.59	0/1791
21	T	0.43	0/549	0.65	0/728
22	U	0.32	0/544	0.61	0/732
23	V	0.38	0/441	0.48	0/586
24	W	0.43	0/426	0.68	0/568
25	Z	0.69	0/460	0.87	2/618 (0.3%)
26	1	0.41	0/319	0.66	0/438
27	2	0.41	0/387	0.64	0/509
28	3	0.44	0/475	0.70	1/623 (0.2%)
All	All	0.73	34/91582 (0.0%)	1.33	1097/137736 (0.8%)

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
4	B	0	5
5	C	0	1
8	G	0	1
10	I	0	2
11	J	0	2
12	K	0	1
14	M	0	2
16	O	0	1
19	R	0	2
20	S	0	1
25	Z	0	2
All	All	0	20

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1278	A	N3-C4	-8.26	1.29	1.34
1	X	1981	A	N3-C4	-7.72	1.30	1.34
9	H	21	CYS	CB-SG	-7.46	1.69	1.82
1	X	1278	A	N9-C4	-7.20	1.33	1.37
1	X	2823	G	N7-C5	-6.66	1.35	1.39

The worst 5 of 1097 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2489	C	C6-N1-C2	-19.63	112.45	120.30
1	X	1675	C	O5'-P-OP1	-17.57	89.61	110.70
1	X	2532	G	O5'-P-OP2	-13.57	93.48	105.70
1	X	2489	C	N3-C4-C5	-13.52	116.49	121.90
1	X	1973	C	C6-N1-C2	-12.59	115.27	120.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	130	GLY	Peptide
4	B	131	SER	Peptide
4	B	135	HIS	Peptide
4	B	146	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	B	149	ARG	Peptide

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	57957	0	29205	1932	0
2	Y	2598	0	1328	88	0
3	A	2001	0	1994	121	0
4	B	1544	0	1605	107	0
5	C	1467	0	1472	100	0
6	D	1367	0	1423	81	0
7	E	1286	0	1336	61	0
8	G	1107	0	1124	66	0
9	H	993	0	1035	84	0
10	I	982	0	973	49	0
11	J	1042	0	1059	64	0
12	K	897	0	955	68	0
13	L	751	0	770	40	0
14	M	923	0	942	76	0
15	N	962	0	987	65	0
16	O	734	0	736	35	0
17	P	1020	0	1096	72	0
18	Q	718	0	731	48	0
19	R	793	0	804	68	0
20	S	1290	0	1268	56	0
21	T	542	0	566	39	0
22	U	539	0	556	37	0
23	V	438	0	456	18	0
24	W	424	0	470	18	0
25	Z	448	0	446	41	0
26	1	315	0	252	16	0
27	2	383	0	414	19	0
28	3	470	0	512	48	0
29	X	49	0	61	8	0
30	2	2	0	0	0	0
30	3	1	0	0	0	0
30	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	1	0	0	0	0
30	N	1	0	0	0	0
30	Q	2	0	0	0	0
30	W	1	0	0	0	0
30	X	264	0	0	0	0
30	Y	4	0	0	0	0
31	V	10	0	19	0	0
31	X	60	0	104	15	0
All	All	84387	0	54699	3132	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 23.

The worst 5 of 3132 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)
13:L:30:SER:O	13:L:40:ALA:HA	1.55	1.03
15:N:66:ASN:HB3	15:N:76:TYR:HB2	1.40	1.03
1:X:1673:C:H5'	4:B:136:ARG:HB3	1.39	1.02
8:G:119:LEU:HD12	8:G:126:VAL:HG23	1.41	1.01
1:X:2796:A:H2'	1:X:2797:G:H8	1.24	1.01

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%)	234 (87%)	26 (10%)	9 (3%)	4	22
4	B	204/206 (99%)	176 (86%)	22 (11%)	6 (3%)	4	24
5	C	193/195 (99%)	168 (87%)	14 (7%)	11 (6%)	1	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	174/176 (99%)	147 (84%)	21 (12%)	6 (3%)	3	21
7	E	169/171 (99%)	156 (92%)	11 (6%)	2 (1%)	13	41
8	G	140/142 (99%)	121 (86%)	14 (10%)	5 (4%)	3	21
9	H	132/134 (98%)	122 (92%)	8 (6%)	2 (2%)	10	36
10	I	135/137 (98%)	103 (76%)	22 (16%)	10 (7%)	1	7
11	J	132/134 (98%)	105 (80%)	22 (17%)	5 (4%)	3	19
12	K	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	5	26
13	L	102/104 (98%)	83 (81%)	17 (17%)	2 (2%)	7	30
14	M	116/118 (98%)	102 (88%)	10 (9%)	4 (3%)	3	21
15	N	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
16	O	96/98 (98%)	79 (82%)	13 (14%)	4 (4%)	3	18
17	P	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	34
18	Q	91/93 (98%)	79 (87%)	9 (10%)	3 (3%)	4	22
19	R	108/110 (98%)	92 (85%)	11 (10%)	5 (5%)	2	15
20	S	172/175 (98%)	147 (86%)	19 (11%)	6 (4%)	3	21
21	T	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11	37
22	U	72/74 (97%)	55 (76%)	13 (18%)	4 (6%)	2	12
23	V	52/54 (96%)	49 (94%)	2 (4%)	1 (2%)	8	31
24	W	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
25	Z	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	8	32
26	1	47/49 (96%)	35 (74%)	7 (15%)	5 (11%)	0	3
27	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
28	3	61/63 (97%)	46 (75%)	13 (21%)	2 (3%)	4	22
All	All	3042/3095 (98%)	2636 (87%)	307 (10%)	99 (3%)	4	22

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	30	GLU
3	A	247	VAL
3	A	254	THR
4	B	131	SER
4	B	147	PRO

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	196/212 (92%)	168 (86%)	28 (14%)	3	13
4	B	155/155 (100%)	120 (77%)	35 (23%)	1	2
5	C	150/155 (97%)	127 (85%)	23 (15%)	2	11
6	D	147/152 (97%)	111 (76%)	36 (24%)	0	2
7	E	136/136 (100%)	109 (80%)	27 (20%)	1	4
8	G	116/118 (98%)	89 (77%)	27 (23%)	1	2
9	H	102/103 (99%)	79 (78%)	23 (22%)	1	2
10	I	93/105 (89%)	72 (77%)	21 (23%)	1	2
11	J	103/109 (94%)	76 (74%)	27 (26%)	0	1
12	K	92/92 (100%)	63 (68%)	29 (32%)	0	1
13	L	68/74 (92%)	55 (81%)	13 (19%)	1	4
14	M	97/101 (96%)	72 (74%)	25 (26%)	0	2
15	N	93/96 (97%)	75 (81%)	18 (19%)	1	4
16	O	71/77 (92%)	51 (72%)	20 (28%)	0	1
17	P	109/111 (98%)	82 (75%)	27 (25%)	0	2
18	Q	73/75 (97%)	49 (67%)	24 (33%)	0	1
19	R	84/91 (92%)	57 (68%)	27 (32%)	0	1
20	S	137/149 (92%)	111 (81%)	26 (19%)	1	4
21	T	54/54 (100%)	41 (76%)	13 (24%)	0	2
22	U	52/59 (88%)	35 (67%)	17 (33%)	0	1
23	V	43/43 (100%)	36 (84%)	7 (16%)	2	9
24	W	48/48 (100%)	30 (62%)	18 (38%)	0	0
25	Z	50/51 (98%)	33 (66%)	17 (34%)	0	1
26	1	23/44 (52%)	15 (65%)	8 (35%)	0	1
27	2	39/39 (100%)	33 (85%)	6 (15%)	2	11
28	3	45/50 (90%)	24 (53%)	21 (47%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2376/2499 (95%)	1813 (76%)	563 (24%)	1 2

5 of 563 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	T	59	LEU
22	U	43	ARG
21	T	57	HIS
25	Z	41	LEU
9	H	121	ARG

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

Mol	Chain	Res	Type
9	H	102	GLN
14	M	2	GLN
28	3	32	GLN
21	T	71	ASN
22	U	47	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2685/2699 (99%)	770 (28%)	65 (2%)
2	Y	121/122 (99%)	28 (23%)	4 (3%)
All	All	2806/2821 (99%)	798 (28%)	69 (2%)

5 of 798 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	13	A
1	X	19	C
1	X	23	G
1	X	25	U

5 of 69 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	2414	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2460	G
2	Y	14	C
1	X	843	G
1	X	813	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 285 ligands modelled in this entry, 277 are monoatomic - leaving 8 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	MIV	X	2901	-	51,51,51	0.72	2 (3%)	62,71,71	1.42	7 (11%)
31	SPD	X	3166	-	9,9,9	0.38	0	8,8,8	0.64	0
31	SPD	X	3167	1	9,9,9	0.32	0	8,8,8	1.00	0
31	SPD	X	3168	1	9,9,9	0.42	0	8,8,8	0.96	0
31	SPD	X	3170	1	9,9,9	0.47	0	8,8,8	1.19	1 (12%)
31	SPD	X	3171	-	9,9,9	0.28	0	8,8,8	0.66	0
31	SPD	V	101	-	9,9,9	0.29	0	8,8,8	0.85	0
31	SPD	X	3169	1	9,9,9	0.37	0	8,8,8	1.08	1 (12%)

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	MIV	X	2901	-	-	25/55/91/91	0/2/3/3
31	SPD	X	3166	-	-	3/7/7/7	-
31	SPD	X	3167	1	-	2/7/7/7	-
31	SPD	X	3168	1	-	3/7/7/7	-
31	SPD	X	3170	1	-	4/7/7/7	-
31	SPD	X	3171	-	-	3/7/7/7	-
31	SPD	V	101	-	-	5/7/7/7	-
31	SPD	X	3169	1	-	3/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	MIV	O6-C24	2.84	1.40	1.34
29	X	2901	MIV	C31-C33	2.81	1.58	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	MIV	O6-C25-C26	-5.97	97.39	106.92
29	X	2901	MIV	O6-C25-C28	4.22	116.68	107.42
29	X	2901	MIV	C32-O8-C31	3.85	124.64	114.52
29	X	2901	MIV	O11-C30-C31	3.55	116.55	109.51
31	X	3170	SPD	C8-C7-N6	2.87	119.88	112.14

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	2901	MIV	C17-C14-N-C15
29	X	2901	MIV	C13-C14-N-C15
29	X	2901	MIV	C5-C6-C8-C9
29	X	2901	MIV	O1-C5-C6-C7
29	X	2901	MIV	C4-C5-C6-C7

There are no ring outliers.

6 monomers are involved in 23 short contacts:

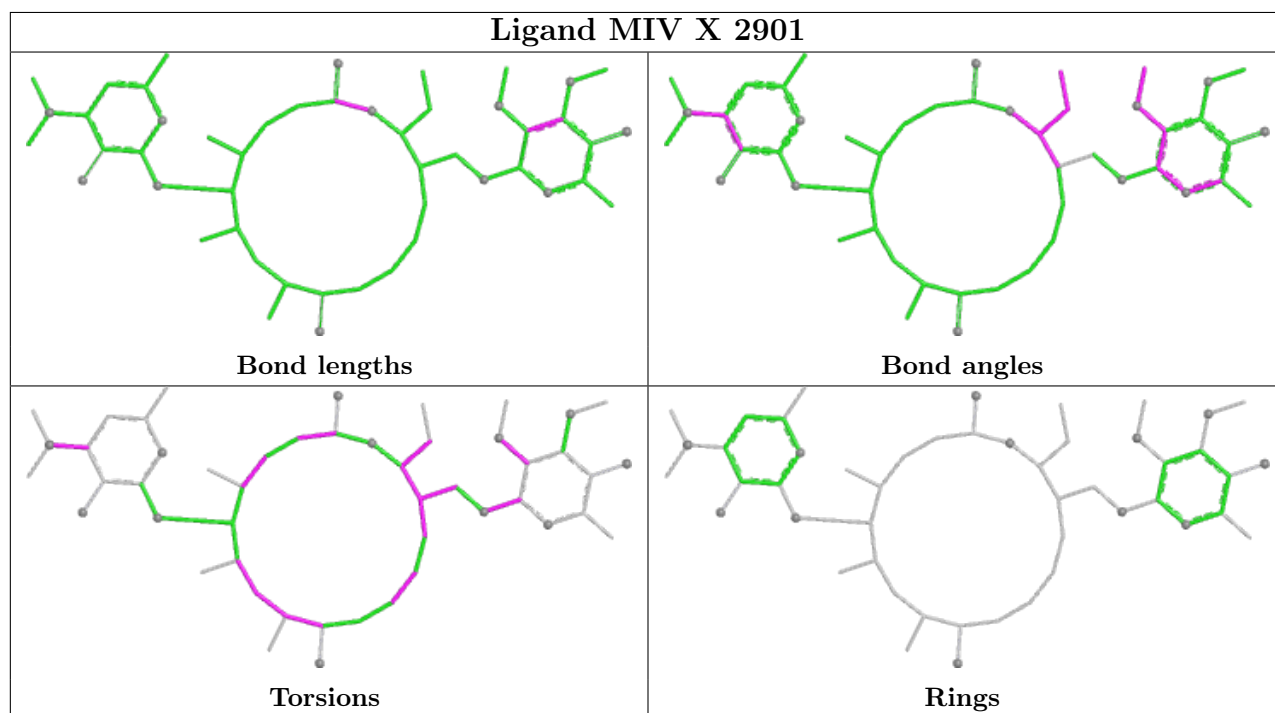
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	2901	MIV	8	0
31	X	3167	SPD	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	3168	SPD	3	0
31	X	3170	SPD	3	0
31	X	3171	SPD	2	0
31	X	3169	SPD	1	0

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	12

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	282:A	O3'	302:U	P	65.10
1	X	362:C	O3'	380:C	P	54.16
1	X	2090:U	O3'	2165:A	P	19.14
1	X	1184:G	O3'	1191:G	P	18.52
1	X	2773:G	O3'	2779:A	P	17.92

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	2699/2699 (100%)	0.43	183 (6%) 17 19	37, 96, 191, 312	0
2	Y	122/122 (100%)	0.51	10 (8%) 11 13	95, 183, 226, 251	0
3	A	271/271 (100%)	0.76	39 (14%) 2 3	79, 131, 162, 170	0
4	B	206/206 (100%)	0.16	8 (3%) 39 38	40, 64, 80, 85	0
5	C	195/195 (100%)	0.47	22 (11%) 5 6	60, 122, 150, 159	0
6	D	176/176 (100%)	0.80	33 (18%) 1 1	168, 207, 227, 235	0
7	E	171/171 (100%)	0.76	35 (20%) 1 1	98, 144, 186, 190	0
8	G	142/142 (100%)	0.22	5 (3%) 44 43	60, 95, 107, 115	0
9	H	134/134 (100%)	0.04	2 (1%) 73 72	46, 57, 64, 69	0
10	I	137/137 (100%)	0.78	21 (15%) 2 2	67, 141, 180, 192	0
11	J	134/134 (100%)	0.43	9 (6%) 17 19	71, 103, 126, 132	0
12	K	115/115 (100%)	-0.01	0 100 100	40, 47, 54, 58	0
13	L	104/104 (100%)	0.72	18 (17%) 1 1	159, 198, 226, 237	0
14	M	118/118 (100%)	-0.14	1 (0%) 86 85	46, 56, 69, 74	0
15	N	117/117 (100%)	0.42	5 (4%) 35 35	59, 94, 121, 127	0
16	O	98/98 (100%)	0.32	6 (6%) 21 22	66, 114, 134, 138	0
17	P	129/129 (100%)	-0.13	0 100 100	49, 59, 82, 97	0
18	Q	93/93 (100%)	0.34	6 (6%) 18 20	85, 109, 125, 126	0
19	R	110/110 (100%)	0.35	9 (8%) 11 13	86, 103, 146, 156	0
20	S	175/175 (100%)	1.15	48 (27%) 0 0	113, 157, 176, 182	0
21	T	72/72 (100%)	0.54	6 (8%) 11 13	87, 133, 147, 153	0
22	U	74/74 (100%)	0.88	12 (16%) 1 2	106, 144, 175, 178	0
23	V	54/54 (100%)	0.48	6 (11%) 5 6	116, 127, 154, 162	0
24	W	55/55 (100%)	0.83	7 (12%) 3 4	88, 108, 128, 133	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/57 (100%)	0.02	0 100 100	47, 56, 70, 74	0
26	1	49/49 (100%)	0.69	8 (16%) 1 2	132, 148, 166, 168	0
27	2	46/46 (100%)	0.11	0 100 100	63, 86, 94, 96	0
28	3	63/63 (100%)	0.44	0 100 100	105, 115, 128, 134	0
All	All	5916/5916 (100%)	0.45	499 (8%) 11 13	37, 105, 203, 312	0

The worst 5 of 499 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	S	82	ASP	9.5
1	X	248	A	8.9
7	E	123	PHE	8.6
6	D	153	ASP	8.6
1	X	1095	A	8.1

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
30	MG	X	2976	1/1	0.39	0.78	125,125,125,125	0
30	MG	X	3060	1/1	0.40	0.85	54,54,54,54	0
30	MG	X	3097	1/1	0.44	0.64	102,102,102,102	0
30	MG	X	3154	1/1	0.46	1.29	74,74,74,74	0
30	MG	X	3050	1/1	0.54	0.63	108,108,108,108	0
31	SPD	X	3166	10/10	0.56	0.69	92,95,99,99	0
30	MG	X	3104	1/1	0.58	1.46	119,119,119,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MG	X	3002	1/1	0.59	0.48	138,138,138,138	0
30	MG	X	3096	1/1	0.61	0.44	71,71,71,71	0
30	MG	X	3146	1/1	0.61	0.82	178,178,178,178	0
30	MG	Y	202	1/1	0.62	0.58	98,98,98,98	0
30	MG	X	3074	1/1	0.63	0.46	59,59,59,59	0
30	MG	X	3121	1/1	0.63	0.38	79,79,79,79	0
30	MG	X	3090	1/1	0.64	0.55	81,81,81,81	0
31	SPD	V	101	10/10	0.67	0.28	126,128,135,136	0
30	MG	X	3109	1/1	0.68	0.54	63,63,63,63	0
30	MG	X	3122	1/1	0.68	0.52	65,65,65,65	0
30	MG	X	3141	1/1	0.68	0.44	145,145,145,145	0
30	MG	X	3115	1/1	0.68	0.73	54,54,54,54	0
30	MG	X	3144	1/1	0.69	1.39	105,105,105,105	0
30	MG	X	3151	1/1	0.69	0.89	53,53,53,53	0
30	MG	X	3163	1/1	0.70	0.52	60,60,60,60	0
30	MG	X	3113	1/1	0.70	0.39	55,55,55,55	0
30	MG	X	2969	1/1	0.73	0.81	55,55,55,55	0
30	MG	X	3102	1/1	0.73	0.76	112,112,112,112	0
30	MG	X	3130	1/1	0.73	0.39	60,60,60,60	0
30	MG	X	2950	1/1	0.73	0.45	88,88,88,88	0
30	MG	X	3052	1/1	0.74	0.74	105,105,105,105	0
30	MG	X	3057	1/1	0.74	0.51	80,80,80,80	0
30	MG	X	2984	1/1	0.74	0.36	62,62,62,62	0
30	MG	X	3071	1/1	0.75	0.54	95,95,95,95	0
30	MG	X	3131	1/1	0.76	0.59	98,98,98,98	0
30	MG	X	3149	1/1	0.76	0.56	83,83,83,83	0
30	MG	X	3086	1/1	0.76	0.72	78,78,78,78	0
30	MG	X	3045	1/1	0.76	0.55	92,92,92,92	0
30	MG	X	2979	1/1	0.77	0.71	83,83,83,83	0
30	MG	X	3116	1/1	0.77	0.26	60,60,60,60	0
30	MG	X	3105	1/1	0.78	0.54	69,69,69,69	0
30	MG	X	3017	1/1	0.79	0.34	114,114,114,114	0
30	MG	X	3159	1/1	0.79	0.49	93,93,93,93	0
30	MG	X	3018	1/1	0.79	0.30	76,76,76,76	0
30	MG	X	2988	1/1	0.79	0.35	87,87,87,87	0
30	MG	2	101	1/1	0.79	1.45	80,80,80,80	0
30	MG	X	3048	1/1	0.79	0.30	124,124,124,124	0
30	MG	X	2925	1/1	0.79	0.71	50,50,50,50	0
30	MG	X	3046	1/1	0.80	0.47	78,78,78,78	0
30	MG	X	3145	1/1	0.80	0.37	77,77,77,77	0
30	MG	X	3123	1/1	0.81	0.34	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MG	X	3110	1/1	0.81	0.71	41,41,41,41	0
30	MG	X	3032	1/1	0.81	0.74	112,112,112,112	0
30	MG	X	3051	1/1	0.81	0.37	118,118,118,118	0
30	MG	X	2958	1/1	0.81	0.46	77,77,77,77	0
30	MG	X	3120	1/1	0.81	0.37	78,78,78,78	0
30	MG	X	3026	1/1	0.81	0.43	81,81,81,81	0
30	MG	X	3030	1/1	0.81	0.40	48,48,48,48	0
30	MG	X	2944	1/1	0.82	1.21	102,102,102,102	0
30	MG	X	3091	1/1	0.82	0.90	53,53,53,53	0
30	MG	X	3139	1/1	0.82	0.41	182,182,182,182	0
30	MG	X	3095	1/1	0.82	0.40	65,65,65,65	0
30	MG	X	3164	1/1	0.82	0.42	39,39,39,39	0
30	MG	X	3082	1/1	0.82	0.86	112,112,112,112	0
30	MG	X	3003	1/1	0.82	0.25	77,77,77,77	0
30	MG	X	3098	1/1	0.82	0.36	120,120,120,120	0
30	MG	X	3124	1/1	0.82	0.81	67,67,67,67	0
30	MG	X	3021	1/1	0.83	0.63	73,73,73,73	0
30	MG	3	101	1/1	0.83	1.69	126,126,126,126	0
30	MG	X	2989	1/1	0.83	0.39	103,103,103,103	0
31	SPD	X	3170	10/10	0.83	0.29	62,63,64,64	0
30	MG	X	3044	1/1	0.83	0.55	73,73,73,73	0
30	MG	X	2923	1/1	0.84	0.34	75,75,75,75	0
30	MG	Y	203	1/1	0.84	0.45	132,132,132,132	0
30	MG	N	201	1/1	0.84	1.01	75,75,75,75	0
30	MG	Q	101	1/1	0.84	0.56	104,104,104,104	0
30	MG	X	3153	1/1	0.84	0.57	47,47,47,47	0
30	MG	X	2914	1/1	0.84	0.31	65,65,65,65	0
30	MG	X	2920	1/1	0.84	0.55	74,74,74,74	0
30	MG	X	3077	1/1	0.84	1.50	56,56,56,56	0
30	MG	X	3093	1/1	0.84	0.23	117,117,117,117	0
30	MG	X	3117	1/1	0.85	0.26	48,48,48,48	0
30	MG	X	3152	1/1	0.85	0.65	49,49,49,49	0
30	MG	X	2903	1/1	0.85	0.54	60,60,60,60	0
30	MG	X	3055	1/1	0.85	0.39	66,66,66,66	0
30	MG	X	2939	1/1	0.85	0.26	50,50,50,50	0
30	MG	X	2990	1/1	0.85	0.15	62,62,62,62	0
30	MG	X	3040	1/1	0.85	0.60	103,103,103,103	0
30	MG	X	2971	1/1	0.85	0.49	59,59,59,59	0
30	MG	X	3010	1/1	0.86	0.52	111,111,111,111	0
30	MG	X	3034	1/1	0.86	0.16	66,66,66,66	0
30	MG	X	3036	1/1	0.86	0.28	75,75,75,75	0
30	MG	X	2924	1/1	0.86	0.26	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MG	X	2959	1/1	0.86	0.49	78,78,78,78	0
30	MG	W	101	1/1	0.86	0.32	111,111,111,111	0
30	MG	X	2999	1/1	0.86	0.61	81,81,81,81	0
30	MG	X	3111	1/1	0.86	0.30	53,53,53,53	0
30	MG	X	3065	1/1	0.86	0.46	99,99,99,99	0
30	MG	X	2986	1/1	0.86	0.47	57,57,57,57	0
30	MG	X	2961	1/1	0.86	0.39	78,78,78,78	0
30	MG	X	3004	1/1	0.87	0.52	61,61,61,61	0
30	MG	X	3158	1/1	0.87	0.25	64,64,64,64	0
30	MG	X	3009	1/1	0.87	0.31	54,54,54,54	0
30	MG	X	2981	1/1	0.87	0.30	79,79,79,79	0
30	MG	X	3140	1/1	0.87	0.20	159,159,159,159	0
30	MG	Y	201	1/1	0.87	0.33	114,114,114,114	0
30	MG	X	2934	1/1	0.87	0.18	58,58,58,58	0
30	MG	X	2964	1/1	0.87	0.34	67,67,67,67	0
30	MG	X	2982	1/1	0.88	0.15	101,101,101,101	0
30	MG	X	3023	1/1	0.88	0.75	70,70,70,70	0
30	MG	X	3056	1/1	0.88	0.32	47,47,47,47	0
30	MG	X	2937	1/1	0.88	0.42	83,83,83,83	0
30	MG	X	3035	1/1	0.88	0.39	104,104,104,104	0
30	MG	Q	102	1/1	0.88	0.44	75,75,75,75	0
30	MG	X	2917	1/1	0.89	0.40	71,71,71,71	0
30	MG	X	2985	1/1	0.89	0.23	63,63,63,63	0
30	MG	X	3062	1/1	0.89	0.30	109,109,109,109	0
30	MG	X	3022	1/1	0.89	0.12	64,64,64,64	0
30	MG	X	3119	1/1	0.89	0.30	69,69,69,69	0
30	MG	X	2977	1/1	0.89	0.23	66,66,66,66	0
30	MG	X	2957	1/1	0.89	0.70	73,73,73,73	0
30	MG	X	3008	1/1	0.89	0.32	49,49,49,49	0
29	MIV	X	2901	49/49	0.89	0.26	52,53,57,58	0
30	MG	X	2936	1/1	0.89	0.25	69,69,69,69	0
30	MG	X	3127	1/1	0.89	0.16	49,49,49,49	0
30	MG	X	3016	1/1	0.89	0.73	72,72,72,72	0
30	MG	X	2993	1/1	0.89	0.26	128,128,128,128	0
30	MG	X	3160	1/1	0.89	0.50	40,40,40,40	0
30	MG	X	3069	1/1	0.90	0.27	90,90,90,90	0
30	MG	Y	204	1/1	0.90	0.28	151,151,151,151	0
30	MG	A	301	1/1	0.90	0.69	94,94,94,94	0
30	MG	X	3112	1/1	0.90	0.60	54,54,54,54	0
30	MG	X	2962	1/1	0.90	0.70	97,97,97,97	0
30	MG	X	2911	1/1	0.90	0.36	39,39,39,39	0
30	MG	X	3143	1/1	0.90	0.72	133,133,133,133	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MG	X	3007	1/1	0.90	0.19	71,71,71,71	0
30	MG	X	3125	1/1	0.90	0.62	71,71,71,71	0
30	MG	X	3126	1/1	0.90	0.51	76,76,76,76	0
31	SPD	X	3167	10/10	0.90	0.32	56,56,57,57	0
30	MG	X	2912	1/1	0.90	0.80	64,64,64,64	0
30	MG	X	3068	1/1	0.90	0.27	97,97,97,97	0
30	MG	X	3033	1/1	0.91	0.24	45,45,45,45	0
30	MG	X	3132	1/1	0.91	0.28	88,88,88,88	0
30	MG	X	2908	1/1	0.91	0.47	39,39,39,39	0
30	MG	X	2910	1/1	0.91	0.37	41,41,41,41	0
30	MG	X	2978	1/1	0.91	0.85	85,85,85,85	0
30	MG	X	3094	1/1	0.91	1.22	69,69,69,69	0
30	MG	X	2913	1/1	0.91	0.36	59,59,59,59	0
30	MG	X	2927	1/1	0.91	0.60	69,69,69,69	0
30	MG	X	3067	1/1	0.91	0.21	94,94,94,94	0
30	MG	X	3000	1/1	0.91	0.26	67,67,67,67	0
30	MG	X	2928	1/1	0.91	0.20	68,68,68,68	0
30	MG	X	2983	1/1	0.91	0.56	89,89,89,89	0
30	MG	2	102	1/1	0.91	0.57	62,62,62,62	0
30	MG	X	2956	1/1	0.91	0.35	69,69,69,69	0
30	MG	X	2970	1/1	0.91	0.34	61,61,61,61	0
30	MG	X	2921	1/1	0.91	0.46	66,66,66,66	0
30	MG	X	3129	1/1	0.91	0.15	86,86,86,86	0
31	SPD	X	3171	10/10	0.91	0.26	45,47,50,50	0
30	MG	X	3084	1/1	0.91	0.79	82,82,82,82	0
30	MG	X	3059	1/1	0.92	0.36	55,55,55,55	0
30	MG	X	3006	1/1	0.92	0.32	44,44,44,44	0
30	MG	X	3061	1/1	0.92	0.18	95,95,95,95	0
30	MG	X	2922	1/1	0.92	0.76	51,51,51,51	0
30	MG	X	3092	1/1	0.92	0.20	77,77,77,77	0
30	MG	X	2902	1/1	0.92	0.64	82,82,82,82	0
30	MG	X	2951	1/1	0.92	0.39	54,54,54,54	0
30	MG	X	2942	1/1	0.92	0.28	49,49,49,49	0
30	MG	X	3012	1/1	0.92	0.31	47,47,47,47	0
30	MG	X	3118	1/1	0.92	0.54	45,45,45,45	0
30	MG	X	3053	1/1	0.92	0.22	53,53,53,53	0
30	MG	X	3039	1/1	0.92	0.29	67,67,67,67	0
31	SPD	X	3169	10/10	0.92	0.21	77,79,80,81	0
30	MG	X	3165	1/1	0.92	0.29	39,39,39,39	0
30	MG	X	3015	1/1	0.92	0.66	105,105,105,105	0
30	MG	X	3028	1/1	0.92	0.76	69,69,69,69	0
30	MG	X	2987	1/1	0.93	0.26	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MG	X	3064	1/1	0.93	0.30	113,113,113,113	0
30	MG	X	3088	1/1	0.93	0.17	78,78,78,78	0
30	MG	X	3108	1/1	0.93	0.31	61,61,61,61	0
30	MG	X	2906	1/1	0.93	0.33	75,75,75,75	0
30	MG	X	2941	1/1	0.93	0.23	73,73,73,73	0
30	MG	X	2918	1/1	0.93	0.91	71,71,71,71	0
30	MG	X	3147	1/1	0.93	1.02	95,95,95,95	0
30	MG	X	2963	1/1	0.93	0.48	96,96,96,96	0
30	MG	X	3058	1/1	0.93	0.36	63,63,63,63	0
30	MG	X	3128	1/1	0.93	0.45	95,95,95,95	0
30	MG	X	3073	1/1	0.93	0.20	118,118,118,118	0
30	MG	X	2995	1/1	0.93	0.23	54,54,54,54	0
30	MG	X	3156	1/1	0.93	0.44	71,71,71,71	0
30	MG	X	2930	1/1	0.93	0.52	50,50,50,50	0
30	MG	X	2948	1/1	0.93	0.40	83,83,83,83	0
31	SPD	X	3168	10/10	0.93	0.43	44,45,46,46	0
30	MG	X	3134	1/1	0.93	0.40	39,39,39,39	0
30	MG	X	3161	1/1	0.93	0.47	38,38,38,38	0
30	MG	X	3162	1/1	0.93	0.43	69,69,69,69	0
30	MG	X	3136	1/1	0.93	0.27	79,79,79,79	0
30	MG	X	3080	1/1	0.94	0.28	51,51,51,51	0
30	MG	X	3107	1/1	0.94	0.17	83,83,83,83	0
30	MG	X	2947	1/1	0.94	0.15	87,87,87,87	0
30	MG	X	3150	1/1	0.94	0.18	70,70,70,70	0
30	MG	I	201	1/1	0.94	0.27	81,81,81,81	0
30	MG	X	3014	1/1	0.94	0.49	75,75,75,75	0
30	MG	X	2974	1/1	0.94	0.20	61,61,61,61	0
30	MG	X	3031	1/1	0.94	0.55	38,38,38,38	0
30	MG	X	3049	1/1	0.94	0.56	124,124,124,124	0
30	MG	X	2953	1/1	0.94	0.28	57,57,57,57	0
30	MG	X	2968	1/1	0.94	0.47	75,75,75,75	0
30	MG	X	2915	1/1	0.94	0.47	57,57,57,57	0
30	MG	X	2996	1/1	0.94	0.27	76,76,76,76	0
30	MG	X	2935	1/1	0.94	0.33	90,90,90,90	0
30	MG	X	3072	1/1	0.94	0.15	115,115,115,115	0
30	MG	X	2980	1/1	0.94	0.50	88,88,88,88	0
30	MG	X	3024	1/1	0.94	0.31	41,41,41,41	0
30	MG	X	3076	1/1	0.94	0.43	65,65,65,65	0
30	MG	X	3042	1/1	0.94	0.20	58,58,58,58	0
30	MG	X	2972	1/1	0.95	0.40	81,81,81,81	0
30	MG	X	2946	1/1	0.95	0.21	51,51,51,51	0
30	MG	X	3078	1/1	0.95	0.22	59,59,59,59	0

Continued on next page...

Continued from previous page...

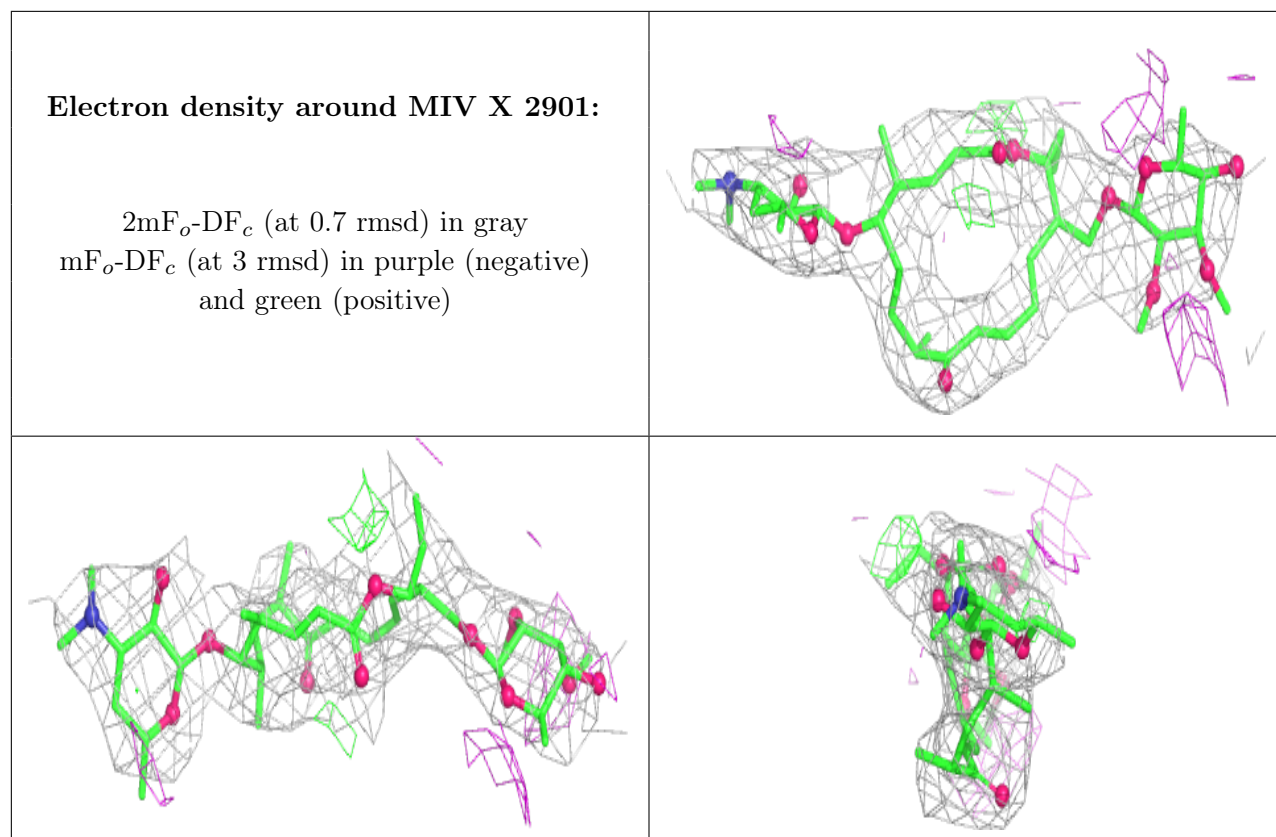
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MG	X	3037	1/1	0.95	0.36	104,104,104,104	0
30	MG	X	3038	1/1	0.95	0.30	67,67,67,67	0
30	MG	X	2975	1/1	0.95	0.32	84,84,84,84	0
30	MG	X	3029	1/1	0.95	0.39	66,66,66,66	0
30	MG	X	3001	1/1	0.95	0.08	91,91,91,91	0
30	MG	X	3089	1/1	0.95	0.29	61,61,61,61	0
30	MG	X	3019	1/1	0.95	0.45	91,91,91,91	0
30	MG	X	2992	1/1	0.95	0.55	73,73,73,73	0
30	MG	X	2904	1/1	0.95	0.32	49,49,49,49	0
30	MG	X	2931	1/1	0.95	0.42	68,68,68,68	0
30	MG	X	3135	1/1	0.96	0.18	148,148,148,148	0
30	MG	X	2938	1/1	0.96	0.17	52,52,52,52	0
30	MG	X	3137	1/1	0.96	0.12	83,83,83,83	0
30	MG	X	3066	1/1	0.96	0.37	81,81,81,81	0
30	MG	X	2998	1/1	0.96	0.47	78,78,78,78	0
30	MG	X	2960	1/1	0.96	0.37	62,62,62,62	0
30	MG	X	3011	1/1	0.96	0.48	53,53,53,53	0
30	MG	X	3070	1/1	0.96	0.14	136,136,136,136	0
30	MG	X	3025	1/1	0.96	0.64	38,38,38,38	0
30	MG	X	3054	1/1	0.96	0.26	101,101,101,101	0
30	MG	X	2926	1/1	0.96	0.28	55,55,55,55	0
30	MG	X	2954	1/1	0.96	0.42	56,56,56,56	0
30	MG	X	3101	1/1	0.96	0.26	95,95,95,95	0
30	MG	X	3041	1/1	0.96	0.17	114,114,114,114	0
30	MG	X	2940	1/1	0.96	0.38	60,60,60,60	0
30	MG	X	2905	1/1	0.96	0.48	62,62,62,62	0
30	MG	X	2966	1/1	0.96	0.49	101,101,101,101	0
30	MG	X	2994	1/1	0.96	0.29	88,88,88,88	0
30	MG	X	3047	1/1	0.96	0.38	92,92,92,92	0
30	MG	X	3063	1/1	0.96	0.16	112,112,112,112	0
30	MG	X	3087	1/1	0.96	0.68	116,116,116,116	0
30	MG	X	3133	1/1	0.96	0.13	50,50,50,50	0
30	MG	X	2919	1/1	0.96	0.54	44,44,44,44	0
30	MG	X	3100	1/1	0.97	0.11	77,77,77,77	0
30	MG	X	2929	1/1	0.97	0.20	71,71,71,71	0
30	MG	X	2952	1/1	0.97	0.51	52,52,52,52	0
30	MG	X	2945	1/1	0.97	1.19	104,104,104,104	0
30	MG	X	2916	1/1	0.97	0.96	62,62,62,62	0
30	MG	X	2965	1/1	0.97	0.51	117,117,117,117	0
30	MG	X	2973	1/1	0.97	0.41	69,69,69,69	0
30	MG	X	3083	1/1	0.97	0.63	79,79,79,79	0
30	MG	X	2955	1/1	0.97	0.23	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MG	X	3085	1/1	0.97	0.53	75,75,75,75	0
30	MG	X	3005	1/1	0.97	0.17	101,101,101,101	0
30	MG	X	2997	1/1	0.97	0.18	99,99,99,99	0
30	MG	X	3099	1/1	0.97	0.21	69,69,69,69	0
30	MG	X	3027	1/1	0.98	0.10	50,50,50,50	0
30	MG	X	3020	1/1	0.98	0.20	88,88,88,88	0
30	MG	X	3114	1/1	0.98	0.38	48,48,48,48	0
30	MG	X	3103	1/1	0.98	0.12	61,61,61,61	0
30	MG	X	3138	1/1	0.98	0.10	39,39,39,39	0
30	MG	X	2907	1/1	0.98	0.45	46,46,46,46	0
30	MG	X	2949	1/1	0.98	0.65	56,56,56,56	0
30	MG	X	2991	1/1	0.98	0.09	80,80,80,80	0
30	MG	X	2943	1/1	0.98	0.35	67,67,67,67	0
30	MG	X	2967	1/1	0.98	0.24	86,86,86,86	0
30	MG	X	2909	1/1	0.98	0.18	44,44,44,44	0
30	MG	X	3043	1/1	0.98	0.09	47,47,47,47	0
30	MG	X	3013	1/1	0.99	0.24	62,62,62,62	0
30	MG	X	2933	1/1	0.99	0.25	61,61,61,61	0
30	MG	X	3155	1/1	0.99	0.15	54,54,54,54	0
30	MG	X	3079	1/1	0.99	0.07	55,55,55,55	0
30	MG	X	3157	1/1	0.99	0.10	45,45,45,45	0
30	MG	X	3075	1/1	0.99	0.21	72,72,72,72	0
30	MG	X	3148	1/1	0.99	0.13	72,72,72,72	0
30	MG	X	3081	1/1	0.99	0.14	76,76,76,76	0
30	MG	X	3106	1/1	0.99	0.21	64,64,64,64	0
30	MG	X	3142	1/1	0.99	0.10	83,83,83,83	0
30	MG	X	2932	1/1	0.99	0.31	49,49,49,49	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.