



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 07:00 AM UTC

PDB ID : 4IOC / pdb_00004ioc
Title : Crystal structure of compound 4f bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.60 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

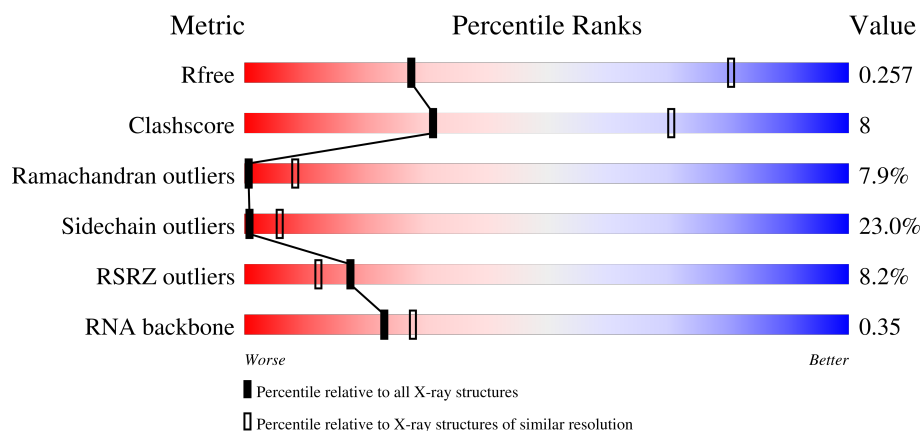
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2880	4% 43% 34% 14% 7%
2	Y	123	4% 48% 29% 18%
3	A	274	9% 45% 29% 11% 12%
4	B	211	% 59% 26% 9%

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	62% 68% 30%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	M	201	-	-	-	X
31	MG	X	2903	-	-	-	X
31	MG	X	2905	-	-	-	X
31	MG	X	2906	-	-	-	X
31	MG	X	2907	-	-	-	X
31	MG	X	2909	-	-	-	X
31	MG	X	2910	-	-	-	X
31	MG	X	2913	-	-	-	X
31	MG	X	2917	-	-	-	X
31	MG	X	2920	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2928	-	-	-	X
31	MG	Y	202	-	-	-	X
31	MG	Y	204	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83877 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	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
			1506	935	287	282	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
			1400	892	247	254	7			

- 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
			1286	812	237	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

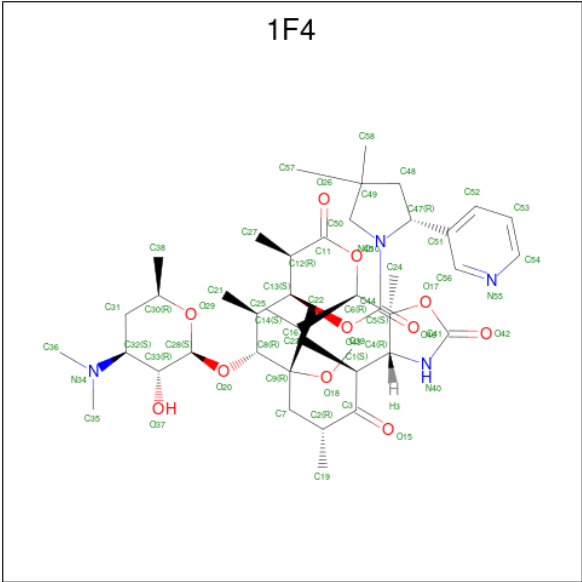
- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	Y	6	Total Mg 6 6	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15S,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-[[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy]tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-4,4-dimethyl-2-(pyridin-3-yl)pyrrolidine-1-carboxylate (CCD ID: 1F4) (formula: C₄₃H₆₈N₄O₁₁).

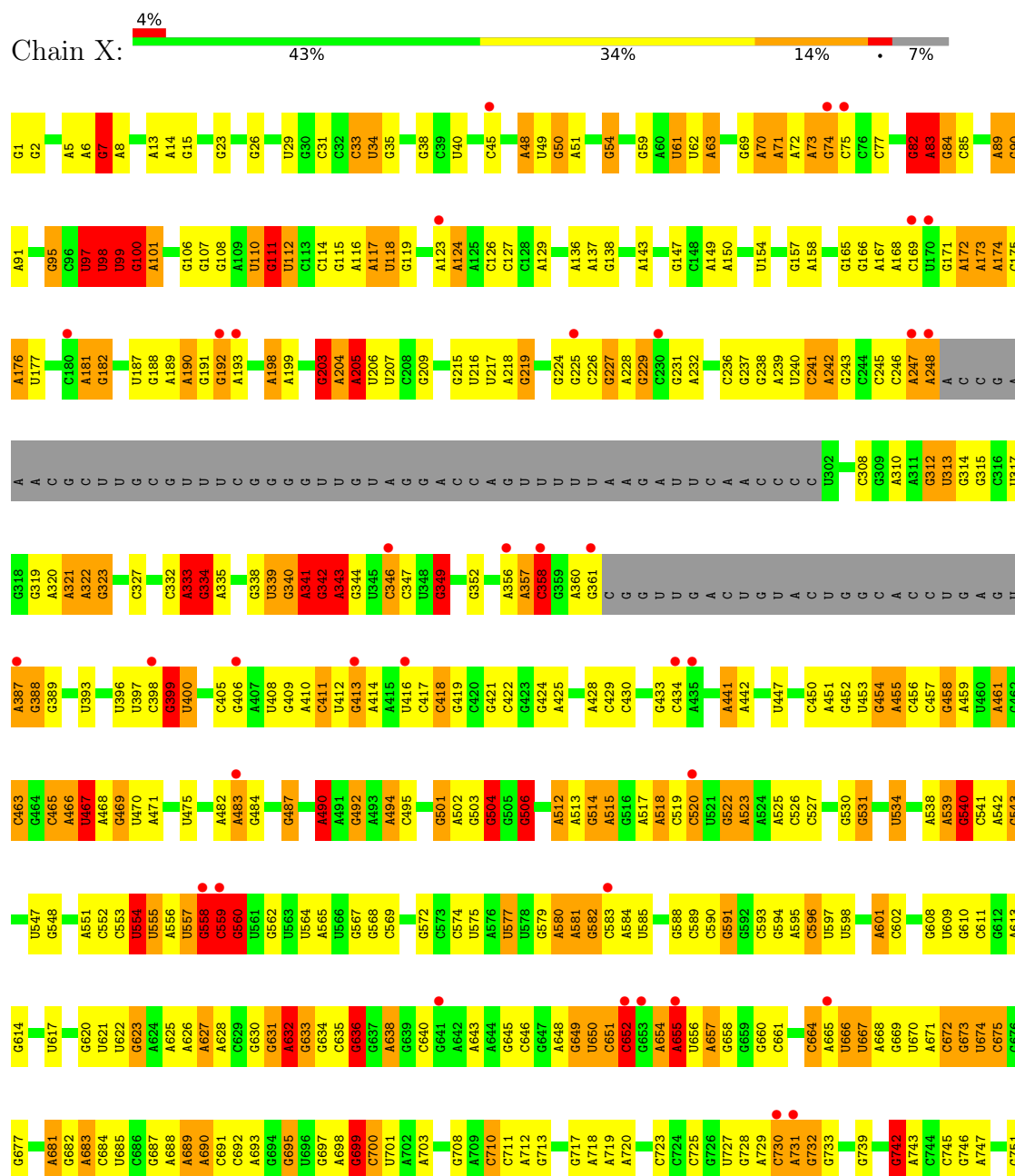


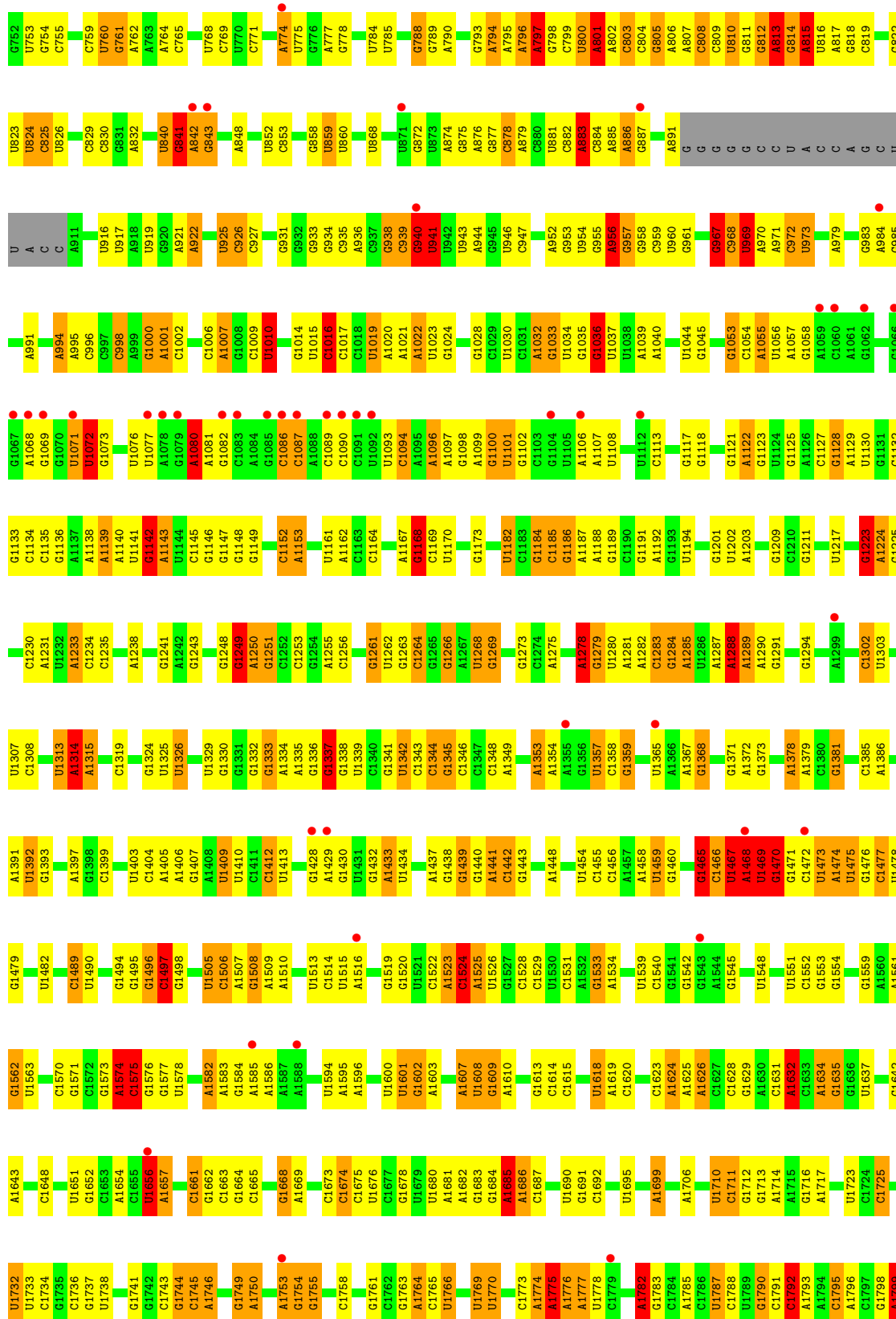
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			58	43	4	11		

3 Residue-property plots

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

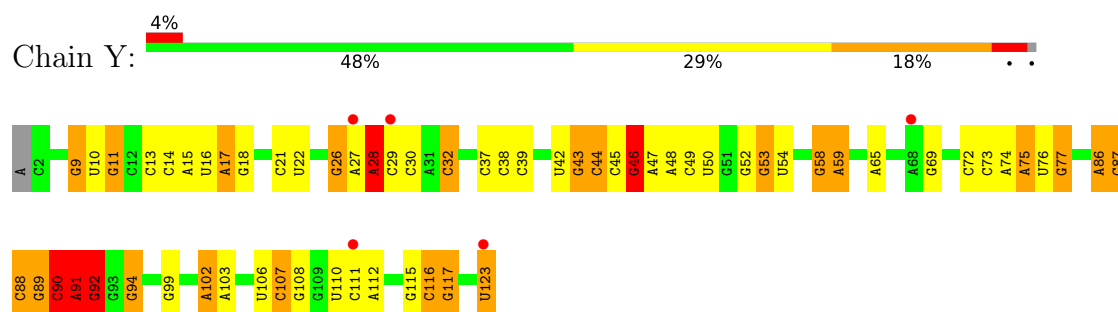
• Molecule 1: 23S ribosomal RNA



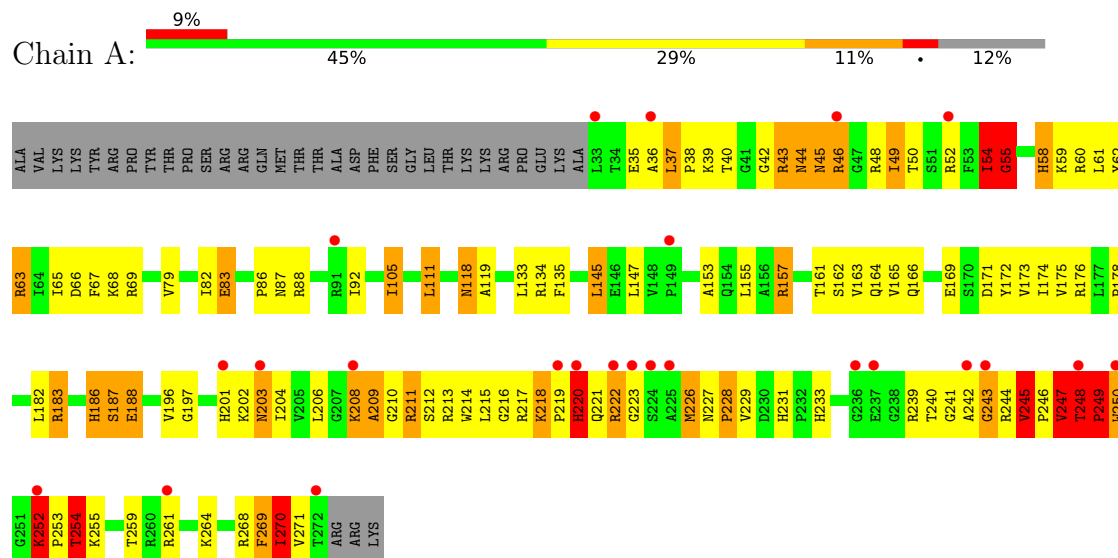


A1800	C1801	U1804	G1805	G1806	A1807	C1808	U1809	U1810	A1811	U1812	A1813	U1817	U1818	U1819	G1820	A1821	C1825	C1830	G1831	G1832	U1833	G1834	C1835	C1836	G1837	G1850	A1851	G1852	U1856	A1859	A1860	G1861	A1867	G1874	U1881	G1882	A1883	A1884	C1885	G1886	G1887	C1888	G													
G	C	C	C	G	U	A	U	A	U	A	A	C	G	G	U	C	U1909	G1903	A1911	G1912	G1913	G1918	A1919	A1920	A1921	U1922	U1923	C1924	C1925	U1926	U1927	U1928	U1929	C1930	A1935	A1936	G1937	U1938	U1939	C1940	A1943	U1946	G1947	C1948	A1949	C1950	G1951	A1952	A1953	A1954	G1955	G1958				
U1959	A1960	G1963	U1964	A1965	C1966	C1971	G1972	C1973	U1974	G1975	U1976	C1977	U1978	U1979	A1980	A1981	C1982	G1983	A1984	G1985	G1986	G1987	A1988	C1989	U1990	C1991	G1992	U1993	U1994	G1995	A1996	A1997	A1998	U1999	A2002	A2003	U2004	U2005	G2006	G2007	U2008	U2009	G2010	U2011	A2012	A2013	G2014	G2015	A2016	U2017	G2018	C2019	U2024	A2025	C2026	
C2027	C2028	G2029	A2030	G2031	C2032	C2033	A2034	C2035	C2038	G2039	A2040	A2041	A2042	G2043	G2044	A2045	C2046	C2047	C2048	U2051	G2052	G2053	A2054	C2055	C2056	U2057	A2063	U2064	A2065	G2066	G2070	C2071	C2072	U2075	G2076	G2077	G2078	A2079	U2080	U2081	C2082	G2083	U2088	C2089	U2090	C	U	A	G	C	U	G	U	A	C	C
G	A	U	A	G	U	U	G	G	G	C	C	C	U	U	G	G	A	A	C	C	G	C	C	U	U	U	U	U	G	G	G	U	U	U	U	U	G	G	C	G	G	U	C	U	C	A	A	C	C	C	C					
A	C	C	C	U	G	A2165	G2166	C2170	U2171	U2172	G2173	G2174	A2181	U2185	A2189	A2190	A2191	U2192	C2193	A2194	C2195	U2196	U2197	U2198	C2199	G2200	G2201	A2204	G2205	U2208	G2209	C2210	U2211	U2212	G2213	G2214	C2215	G2216	G2217	U2218	U2219	A2220	G2221	U2222	U2223	U2224	G2225	A2226	C2227	U2228	G2229	G2230	G			
G2235	U2236	C2237	U2241	A2245	A2246	A2247	A2252	A2253	C2254	G2255	G2256	A2257	G2258	G2261	C2262	A2265	A2266	A2267	G2268	U2269	U2270	C2271	A2277	A2278	G2283	U2284	U2285	G2286	G2287	A2288	A2289	A2290	U2291	C2295	U2298	A2299	G2300	A2301	C2305	A2306	A2312	G2313	G2314	A2315	G2320	C2321	U2322									
U2323	G2324	A2325	C2326	U2327	C2328	C2329	G2330	A2333	C2338	A2339	C2340	C2343	G2344	G2351	A2352	G2353	A2357	C2358	G2362	G2363	C2364	A2367	G2368	U2369	G2370	A2371	C2372	G2373	C2374	G2375	G2376	A2381	C2382	G2383	G2384	U2386	G2386	U2387	G2388	G2389	G2392	G2393	G2394	C2395	C2396	A2397	U2398	G2399	G2400	A2401						
U2402	C2403	A2404	A2405	C2406	G2407	G2408	A2409	U2410	A2413	A2414	G2415	A2418	C2420	A2421	G2422	G2423	G2426	A2427	U2428	A2438	U2439	C2446	A2448	U2452	C2453	C2454	A2455	U2456	A2457	U2458	C2459	G2460	G2461	C2462	G2463	G2466	U2470	U2471	U2472	C2477	C2480	G2481	A2482	U2483	G2484	U2485	C2486									
G2487	G2488	C2489	U2490	C2491	G2492	U2493	C2494	G2495	A2496	C2497	U2498	C2499	G2504	G2505	C2506	U2507	G2508	A2509	A2510	G2511	A2512	G2513	G2514	G2515	U2516	C2517	G2518	C2519	G2522	G2523	U2526	G2527	G2528	G2529	C2530	A2543	A2544	A2545	G2546	C2547	G2548	A2551	C2552	G2553	A2556	G2557	C2558	U2559	G2560	G2561	U2562	U2564				
C2565	A2566	C2567	A2568	U2572	C2573	G2574	A2577	C2578	U2579	A2581	G2582	C2585	G2586	U2587	U2588	C2589	U2590	C2591	U2592	A2593	U2594	C2595	C2596	C2597	G2598	U2599	G2604	C2605	U2608	G2609	G2610	A2611	G2612	A2613	U2614	U2615	U2616	G2617	A2618	U2619	G2620	C2621	G2627	C2628	A2633	G2634	G2640	A2641	U2642	C2643						
A2644	A2649	C2650	A2653	A2654	C2655	G2656	G2657	A2658	C2659	C2660	G2661	C2662	U2663	C2667	U2668	C2669	C2670	C2671	C2678	C2683	A2684	C2687	U2688	C2689	A2690	C2691	U2692	U2693	C2694	C2695	A2696	G2697	G2698	C2699	U2700	C2703	U2704	A2705	U2706	G2707	U2708	A2713	U2714	C2715	A2718	U2719	U2720	A2721	G2724							
U2728	A2729	A2730	G2731	C2732	C2735	U2736	A2737	A2745	C2748	U2758	U2759	G2760	C2767	C2768	C2769	A2770	C2771	U2774	U2775	U2776	A2777	U2778	C2779	A2780	C2781	U2782	U2783	A2784	A2785	C2788	C2791	G2792	G2793	C2794	A2795	U2796	G2797	A2798	C2799	C2800	C2803	G2804	G2805	U2806	U2807	U2808	A2809	U2810	G2811							
G2813	G2821	U2822	G2823	C2824	A2825	G2832	G2837	U2841	C2842	A2843	G2846	U2847	C2848	U2849	G2854	C2855	U2856	C2857	A2858	U2859	C2860	A2861	C2864	G2865	A2866	C2867	G2868	A2877	C	U	C																									

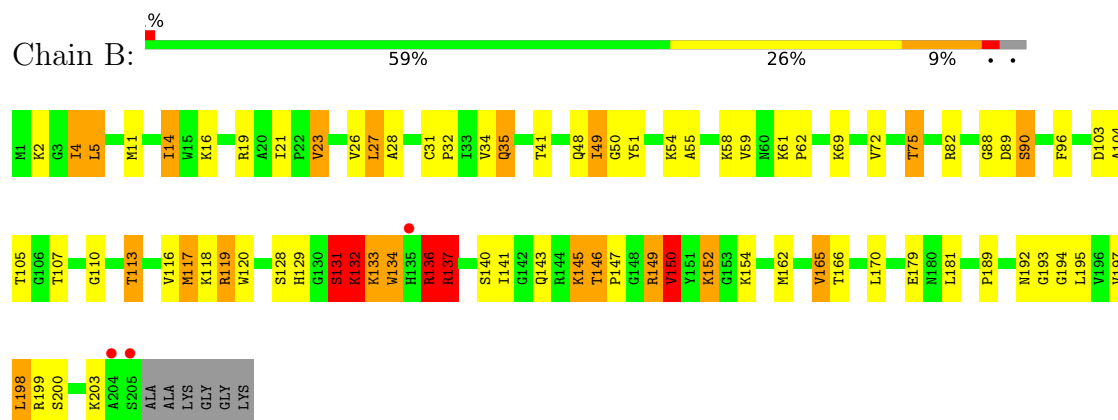
• Molecule 2: 5S ribosomal RNA



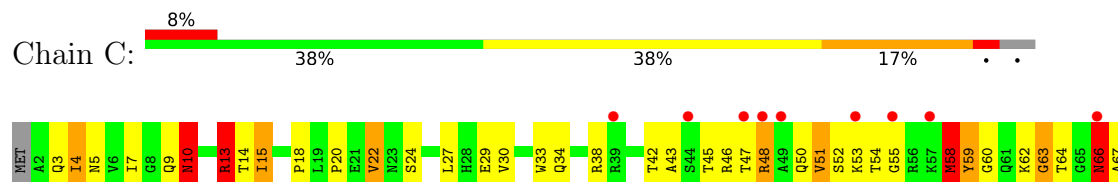
• Molecule 3: 50S ribosomal protein L2

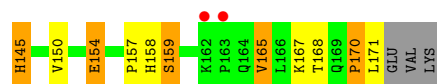


• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

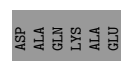
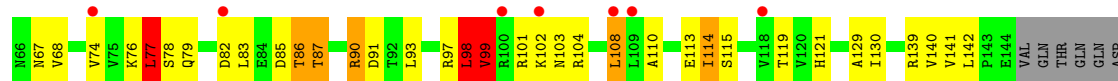
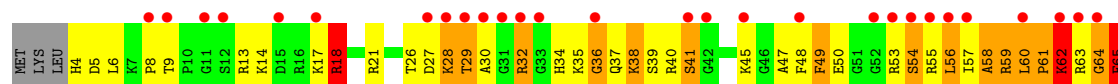
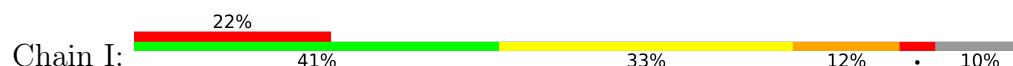




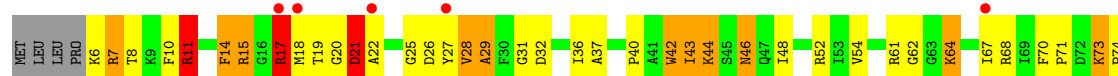
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



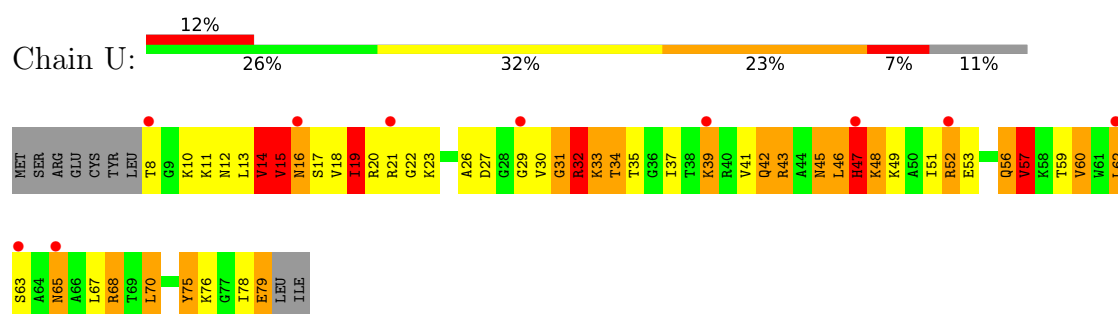
- Molecule 12: 50S ribosomal protein L16



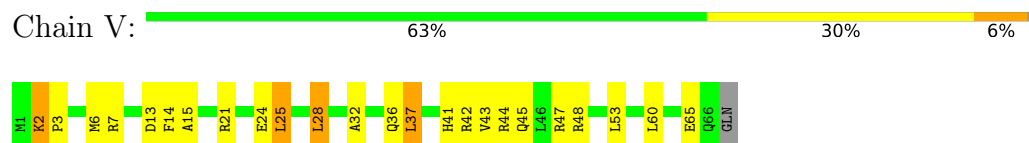
- Molecule 13: 50S ribosomal protein L17



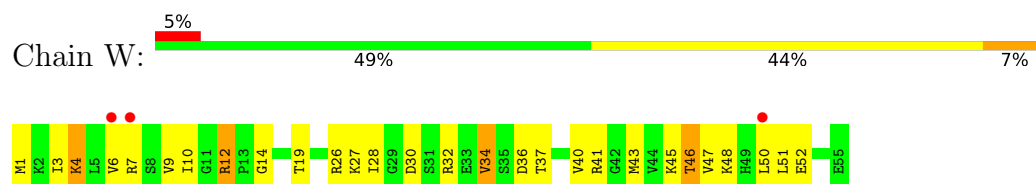
- Molecule 14: 50S ribosomal protein L18



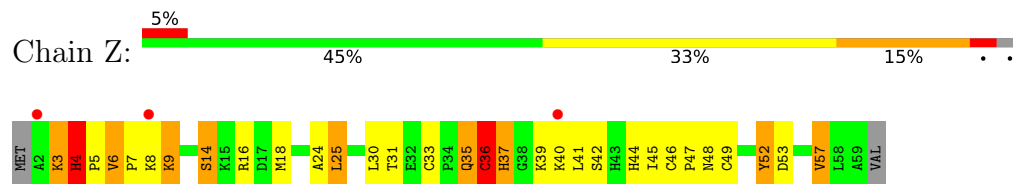
- Molecule 24: 50S ribosomal protein L29



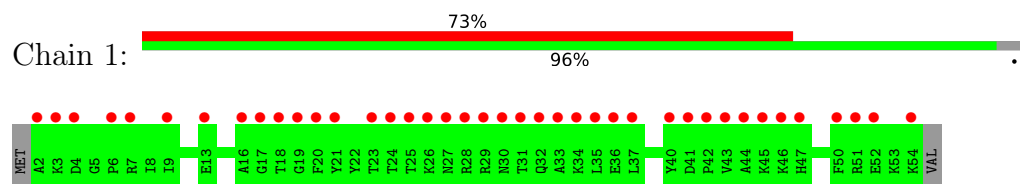
- Molecule 25: 50S ribosomal protein L30



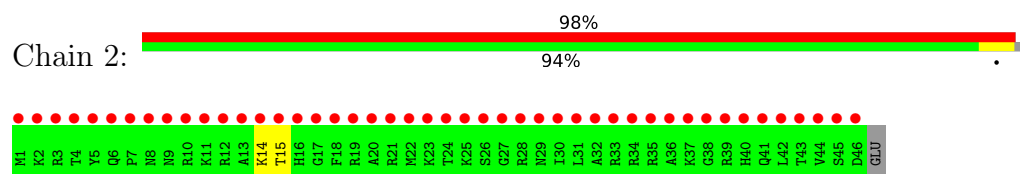
- Molecule 26: 50S ribosomal protein L32



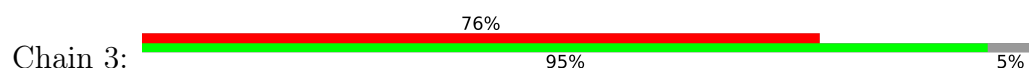
- Molecule 27: 50S ribosomal protein L33

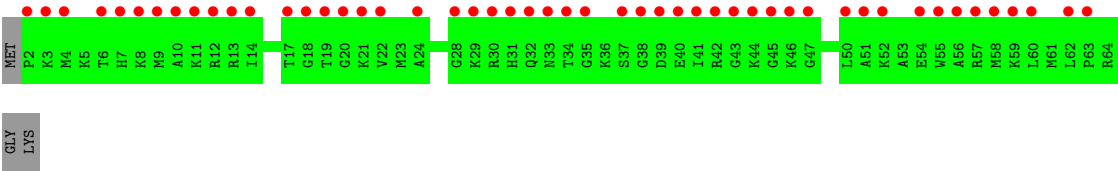


- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35





● Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.00 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.3 (30.00-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.65Å)	Xtriage
Refinement program	autoBUSTER	Depositor
R, R_{free}	0.198 , 0.239 0.215 , 0.257	Depositor DCC
R_{free} test set	12232 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	129.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 91.4	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	83877	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: 1F4, 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	0.71	27/64561 (0.0%)	1.39	857/100708 (0.9%)
2	Y	0.82	2/2904 (0.1%)	1.35	31/4525 (0.7%)
3	A	0.97	6/1862 (0.3%)	1.58	38/2510 (1.5%)
4	B	0.94	1/1567 (0.1%)	1.51	16/2105 (0.8%)
5	C	1.03	3/1529 (0.2%)	1.70	28/2070 (1.4%)
6	D	0.87	0/1419	1.35	5/1903 (0.3%)
7	E	0.86	0/1308	1.39	5/1771 (0.3%)
8	F	0.93	0/508	1.36	1/683 (0.1%)
9	G	0.94	1/1138 (0.1%)	1.62	18/1539 (1.2%)
10	H	0.90	2/1007 (0.2%)	1.44	11/1352 (0.8%)
11	I	1.14	4/1081 (0.4%)	1.80	32/1448 (2.2%)
12	J	1.46	7/1113 (0.6%)	1.75	36/1486 (2.4%)
13	K	1.08	5/886 (0.6%)	1.64	20/1188 (1.7%)
14	L	0.90	0/785	1.71	17/1048 (1.6%)
15	M	0.97	1/884 (0.1%)	1.66	18/1186 (1.5%)
16	N	0.87	0/994	1.57	14/1323 (1.1%)
17	O	0.89	0/750	1.62	14/1000 (1.4%)
18	P	0.95	1/1027 (0.1%)	1.57	11/1373 (0.8%)
19	Q	0.93	0/737	1.67	14/988 (1.4%)
20	R	1.09	1/835 (0.1%)	1.78	25/1121 (2.2%)
21	S	1.11	0/1370	1.50	12/1862 (0.6%)
22	T	0.93	0/633	1.54	11/838 (1.3%)
23	U	1.28	4/556 (0.7%)	1.94	27/741 (3.6%)
24	V	0.91	0/537	1.62	6/714 (0.8%)
25	W	0.88	0/426	1.53	3/568 (0.5%)
26	Z	1.02	0/469	1.68	8/629 (1.3%)
30	4	0.98	0/298	1.33	0/390
All	All	0.80	65/91184 (0.1%)	1.44	1278/137069 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	3

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	R	77	HIS	CA-C	9.55	1.56	1.52
4	B	117	MET	SD-CE	9.25	2.02	1.79
11	I	29	THR	CA-C	7.92	1.63	1.52
1	X	559	C	C3'-O3'	7.65	1.53	1.42
1	X	655	A	C3'-O3'	7.32	1.53	1.42

The worst 5 of 1278 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-24.41	85.29	109.70
1	X	1288	A	C5'-C4'-O4'	15.03	131.64	109.10
1	X	1019	U	P-O3'-C3'	14.88	142.51	120.20
1	X	559	C	C4'-C3'-C2'	-14.06	88.54	102.60
3	A	203	ASN	CA-CB-CG	12.60	125.20	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1251	G	Sidechain
1	X	699	G	Sidechain
1	X	967	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	540	0
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1539	0	1600	60	0
5	C	1506	0	1525	58	0
6	D	1400	0	1481	20	0
7	E	1286	0	1336	10	0
8	F	503	0	520	6	0
9	G	1114	0	1144	49	0
10	H	997	0	1046	30	0
11	I	1067	0	1103	40	0
12	J	1090	0	1125	35	0
13	K	878	0	930	24	0
14	L	779	0	820	20	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	26	0
19	Q	726	0	753	11	0
20	R	825	0	881	27	0
21	S	1345	0	1372	32	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	17	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1108	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 8.

The worst 5 of 1108 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)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.38	1.03
1:X:558:G:H4'	1:X:559:C:H5'	1.40	1.02
1:X:1448:A:H61	1:X:1574:A:H61	1.09	1.00

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	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	1	9
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	4	28
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0	3
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	2	20
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	1	14
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	2	18
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	0	5
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	5	30
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0	3
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	0	6
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	1	14
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	0	4
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	1	13
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	1	13
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	3
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	3	24
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0	2
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	1	12
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	1	13
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0	1
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	3	25
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	6	33
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	0	7
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	3	26
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1	8

5 of 235 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	209	ALA
3	A	217	ARG
3	A	248	THR
3	A	249	PRO

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	185/215 (86%)	146 (79%)	39 (21%)	1	7
4	B	155/157 (99%)	118 (76%)	37 (24%)	1	5
5	C	157/163 (96%)	108 (69%)	49 (31%)	0	2
6	D	153/156 (98%)	127 (83%)	26 (17%)	2	13
7	E	136/144 (94%)	115 (85%)	21 (15%)	2	16
8	F	51/107 (48%)	45 (88%)	6 (12%)	5	24
9	G	118/146 (81%)	86 (73%)	32 (27%)	0	3
10	H	103/103 (100%)	83 (81%)	20 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	I	108/121 (89%)	74 (68%)	34 (32%)	0	2
12	J	110/115 (96%)	90 (82%)	20 (18%)	2	11
13	K	90/93 (97%)	72 (80%)	18 (20%)	1	8
14	L	74/82 (90%)	53 (72%)	21 (28%)	0	3
15	M	94/134 (70%)	69 (73%)	25 (27%)	0	3
16	N	96/97 (99%)	74 (77%)	22 (23%)	1	6
17	O	75/79 (95%)	53 (71%)	22 (29%)	0	2
18	P	109/115 (95%)	89 (82%)	20 (18%)	2	11
19	Q	75/76 (99%)	59 (79%)	16 (21%)	1	7
20	R	91/96 (95%)	70 (77%)	21 (23%)	1	6
21	S	149/192 (78%)	113 (76%)	36 (24%)	1	5
22	T	62/67 (92%)	54 (87%)	8 (13%)	4	22
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	0
24	V	54/55 (98%)	43 (80%)	11 (20%)	1	8
25	W	48/48 (100%)	35 (73%)	13 (27%)	0	3
26	Z	51/53 (96%)	39 (76%)	12 (24%)	1	5
30	4	35/35 (100%)	28 (80%)	7 (20%)	1	8
All	All	2436/2715 (90%)	1876 (77%)	560 (23%)	1	6

5 of 560 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	S	66	VAL
21	S	130	ILE
21	S	65	LEU
24	V	14	PHE
9	G	104	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
20	R	29	HIS
23	U	16	ASN
20	R	44	GLN
22	T	3	HIS

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Mol	Chain	Res	Type
26	Z	43	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	739 (27%)	250 (9%)
2	Y	121/123 (98%)	43 (35%)	12 (9%)
All	All	2804/3003 (93%)	782 (27%)	262 (9%)

5 of 782 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	13	A
1	X	14	A
1	X	15	G

5 of 262 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	2660	C
1	X	2759	U
2	Y	116	C
1	X	1000	G
1	X	970	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	1F4	X	2929	-	61,62,62	1.27	6 (9%)	81,95,95	2.75	37 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	1F4	X	2929	-	-	33/74/119/119	1/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	C41-N40	4.52	1.39	1.33
32	X	2929	1F4	C52-C51	3.41	1.44	1.39
32	X	2929	1F4	C22-C9	2.87	1.58	1.52
32	X	2929	1F4	O46-C44	2.19	1.24	1.21
32	X	2929	1F4	C4-N40	2.09	1.49	1.45

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C51-C47-N45	-8.29	98.37	113.03
32	X	2929	1F4	C6-O10-C11	6.74	129.97	118.20
32	X	2929	1F4	C22-C9-C7	-5.34	103.00	111.17
32	X	2929	1F4	C21-C14-C13	5.10	120.37	111.40
32	X	2929	1F4	O43-C13-C14	5.05	119.16	107.52

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C4-C5-C6-O10

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Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C4-C5-C6-C23
32	X	2929	1F4	O17-C5-C6-O10
32	X	2929	1F4	O17-C5-C6-C23
32	X	2929	1F4	C24-C5-C6-O10

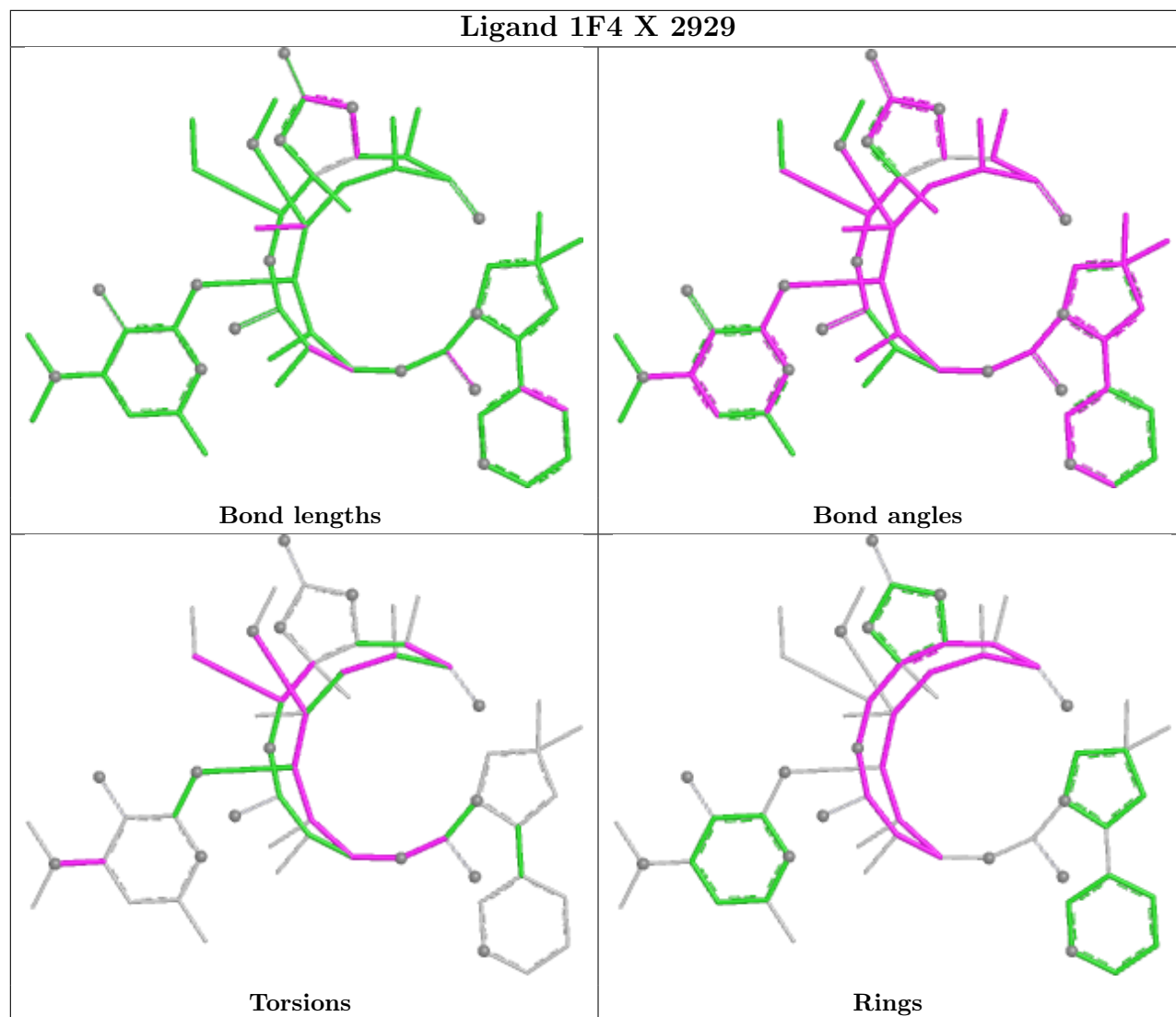
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C1-C11-C12-C13-C14-C2-C3-C4-C5-C6-C7-C8-C9-O10

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2929	1F4	19	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2686/2880 (93%)	0.11	116 (4%) 40 22	43, 92, 197, 276	0
2	Y	122/123 (99%)	0.32	5 (4%) 41 23	83, 135, 170, 191	0
3	A	240/274 (87%)	0.49	24 (10%) 12 10	68, 115, 146, 172	0
4	B	205/211 (97%)	0.08	3 (1%) 72 44	45, 73, 105, 154	0
5	C	197/205 (96%)	0.57	17 (8%) 16 12	57, 114, 154, 187	0
6	D	177/180 (98%)	0.33	7 (3%) 42 24	146, 183, 216, 227	0
7	E	171/185 (92%)	0.10	7 (4%) 41 23	92, 143, 192, 206	0
8	F	71/144 (49%)	0.76	6 (8%) 16 12	211, 236, 252, 257	0
9	G	142/174 (81%)	0.38	9 (6%) 26 16	72, 97, 144, 161	0
10	H	134/134 (100%)	0.02	1 (0%) 84 61	50, 70, 97, 121	0
11	I	141/156 (90%)	1.26	35 (24%) 2 2	67, 129, 174, 204	0
12	J	136/141 (96%)	0.43	11 (8%) 18 12	74, 103, 149, 184	0
13	K	113/116 (97%)	0.22	6 (5%) 32 19	35, 60, 79, 91	0
14	L	104/114 (91%)	0.63	15 (14%) 6 6	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.04	1 (0%) 81 56	50, 73, 111, 145	0
16	N	117/118 (99%)	0.36	9 (7%) 19 13	59, 90, 128, 159	0
17	O	94/100 (94%)	0.38	8 (8%) 16 12	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.15	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	0.27	5 (5%) 31 18	73, 106, 162, 195	0
20	R	110/115 (95%)	0.67	13 (11%) 9 8	88, 117, 170, 178	0
21	S	175/237 (73%)	0.42	11 (6%) 26 16	121, 155, 175, 190	0
22	T	84/91 (92%)	0.43	7 (8%) 17 12	79, 107, 186, 200	0
23	U	72/81 (88%)	0.97	10 (13%) 6 6	92, 128, 153, 161	0
24	V	66/67 (98%)	-0.24	0 100 100	100, 132, 211, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	0.08	3 (5%) 30 18	80, 98, 126, 152	0
26	Z	58/60 (96%)	0.39	3 (5%) 33 19	49, 70, 105, 114	0
27	1	53/55 (96%)	6.95	40 (75%) 0 0	8, 32, 62, 93	0
28	2	46/47 (97%)	10.41	46 (100%) 0 0	3, 15, 38, 59	0
29	3	63/66 (95%)	8.83	50 (79%) 0 0	3, 25, 40, 61	0
30	4	37/37 (100%)	2.84	23 (62%) 0 0	228, 254, 266, 269	0
All	All	5997/6561 (91%)	0.49	491 (8%) 17 12	3, 100, 196, 276	0

The worst 5 of 491 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	58.7
28	2	31	LEU	54.2
29	3	28	GLY	43.9
29	3	41	ILE	37.1
27	1	34	LYS	31.9

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.

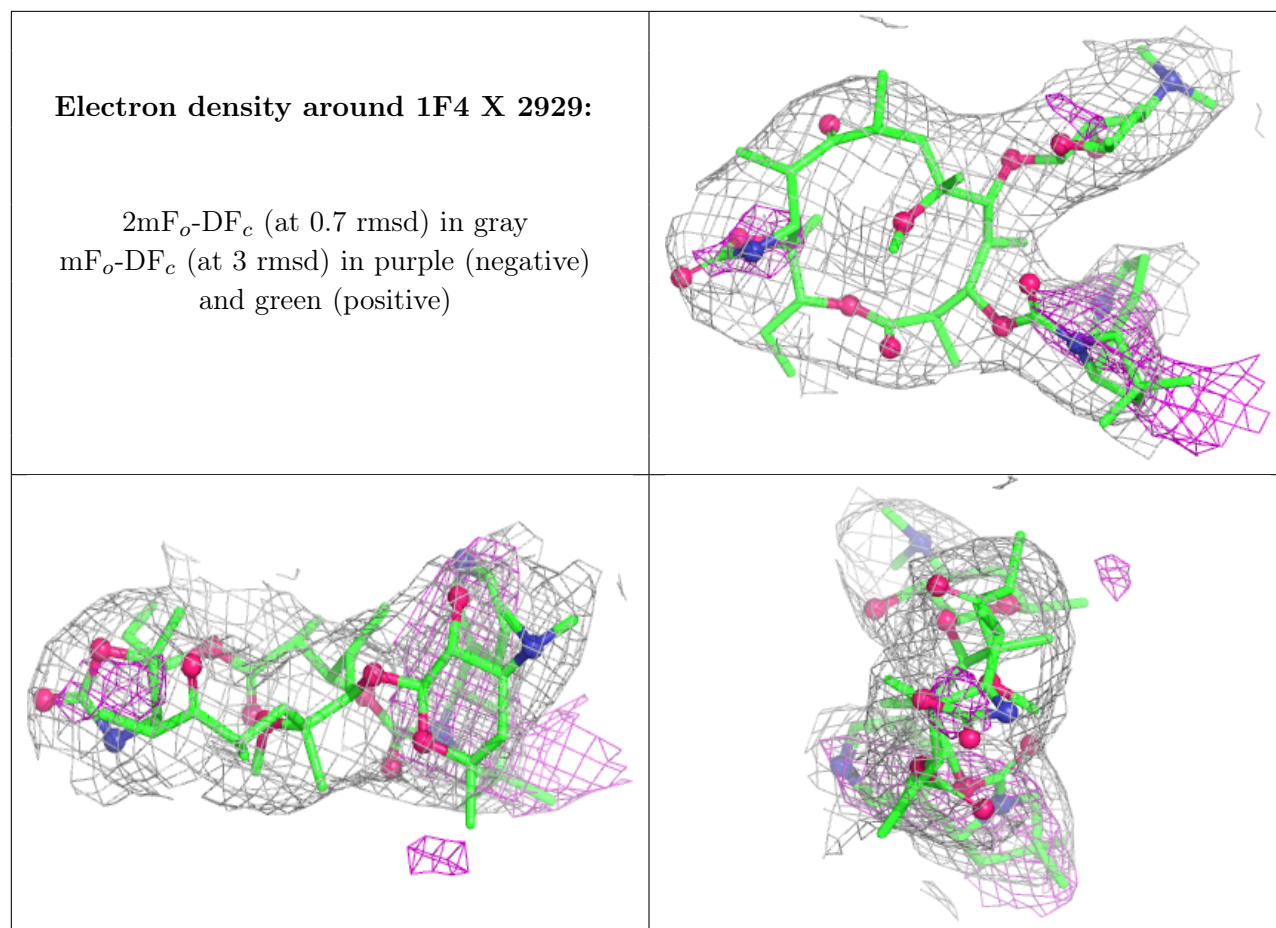
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	Y	204	1/1	0.20	0.51	86,86,86,86	0
31	MG	X	2909	1/1	0.25	0.45	97,97,97,97	0
31	MG	Y	202	1/1	0.49	0.92	88,88,88,88	0
31	MG	X	2924	1/1	0.53	0.79	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	2903	1/1	0.65	1.03	89,89,89,89	0
31	MG	Y	206	1/1	0.67	0.11	78,78,78,78	0
31	MG	X	2913	1/1	0.68	2.56	60,60,60,60	0
31	MG	X	2920	1/1	0.68	0.81	113,113,113,113	0
31	MG	X	2917	1/1	0.70	0.62	55,55,55,55	0
31	MG	X	2928	1/1	0.73	1.28	61,61,61,61	0
31	MG	X	2906	1/1	0.75	0.75	58,58,58,58	0
31	MG	M	201	1/1	0.75	0.47	23,23,23,23	0
31	MG	X	2910	1/1	0.77	0.41	41,41,41,41	0
31	MG	X	2905	1/1	0.78	0.46	65,65,65,65	0
31	MG	X	2907	1/1	0.79	0.77	51,51,51,51	0
31	MG	X	2902	1/1	0.80	0.17	94,94,94,94	0
31	MG	Y	201	1/1	0.80	0.17	98,98,98,98	0
31	MG	X	2914	1/1	0.83	0.40	27,27,27,27	0
31	MG	X	2922	1/1	0.85	0.89	44,44,44,44	0
31	MG	X	2912	1/1	0.86	0.54	71,71,71,71	0
31	MG	X	2925	1/1	0.86	0.20	122,122,122,122	0
31	MG	X	2919	1/1	0.87	0.60	30,30,30,30	0
31	MG	X	2918	1/1	0.88	0.84	42,42,42,42	0
31	MG	X	2915	1/1	0.88	1.64	57,57,57,57	0
31	MG	X	2927	1/1	0.88	0.64	64,64,64,64	0
31	MG	X	2911	1/1	0.89	0.35	68,68,68,68	0
31	MG	X	2921	1/1	0.89	0.82	80,80,80,80	0
31	MG	X	2923	1/1	0.90	0.47	34,34,34,34	0
31	MG	X	2926	1/1	0.90	0.88	45,45,45,45	0
31	MG	X	2908	1/1	0.90	0.73	37,37,37,37	0
31	MG	X	2916	1/1	0.93	0.96	37,37,37,37	0
31	MG	Y	203	1/1	0.94	0.41	59,59,59,59	0
32	1F4	X	2929	58/58	0.94	0.09	20,20,20,20	0
31	MG	Y	205	1/1	0.96	0.19	82,82,82,82	0
31	MG	X	2901	1/1	0.97	1.85	50,50,50,50	0
31	MG	X	2904	1/1	0.97	0.11	110,110,110,110	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.