



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 10:31 am BST

PDB ID : 4IO9
Title : Crystal structure of compound 4d bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.20 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	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

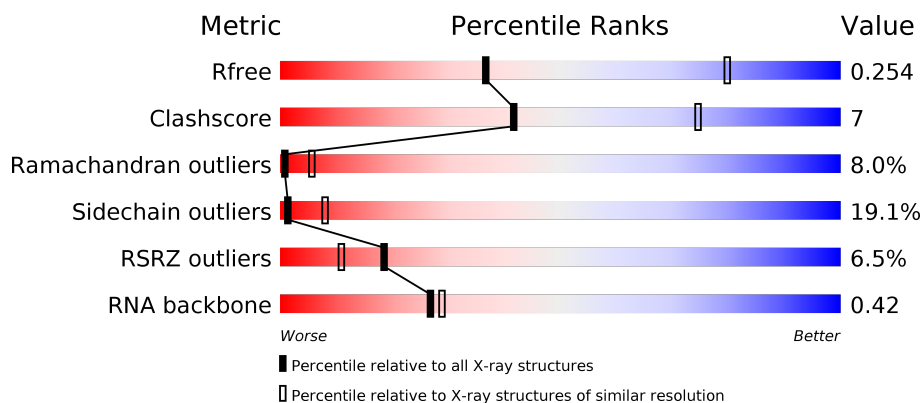
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 on 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	 3% 36% 35% 18% 7%
2	Y	123	 2% 37% 38% 20% 5%
3	A	274	 3% 51% 31% 5% 12%
4	B	211	 0% 70% 19% 8% 4%

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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	<div> <div>97%</div> <div> <div></div> <div>76%</div> <div>22%</div> </div> </div>

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	X	2902	-	-	-	X
31	MG	X	2903	-	-	-	X
31	MG	X	2912	-	-	-	X
31	MG	Y	201	-	-	-	X
31	MG	Y	203	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83875 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

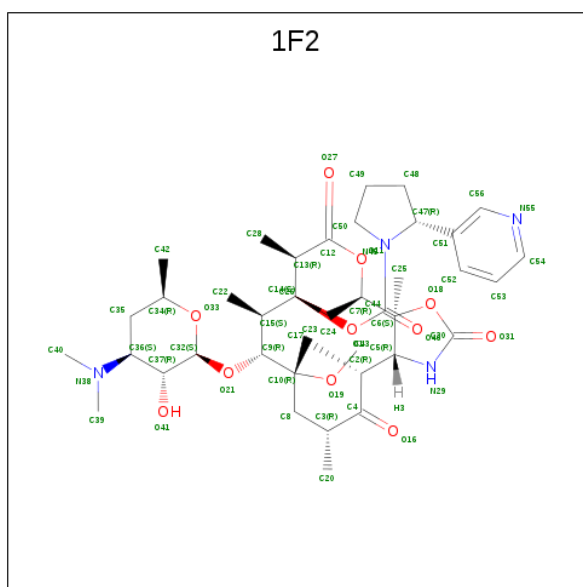
- Molecule 30 is a protein called 50S ribosomal protein L36.

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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	J	1	Total Mg 1 1	0	0
31	Y	5	Total Mg 5 5	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15R,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)-2-(pyridin-3-yl)pyrrolidine-1-carboxylate (three-letter code: 1F2) (formula: C₄₁H₆₄N₄O₁₁).

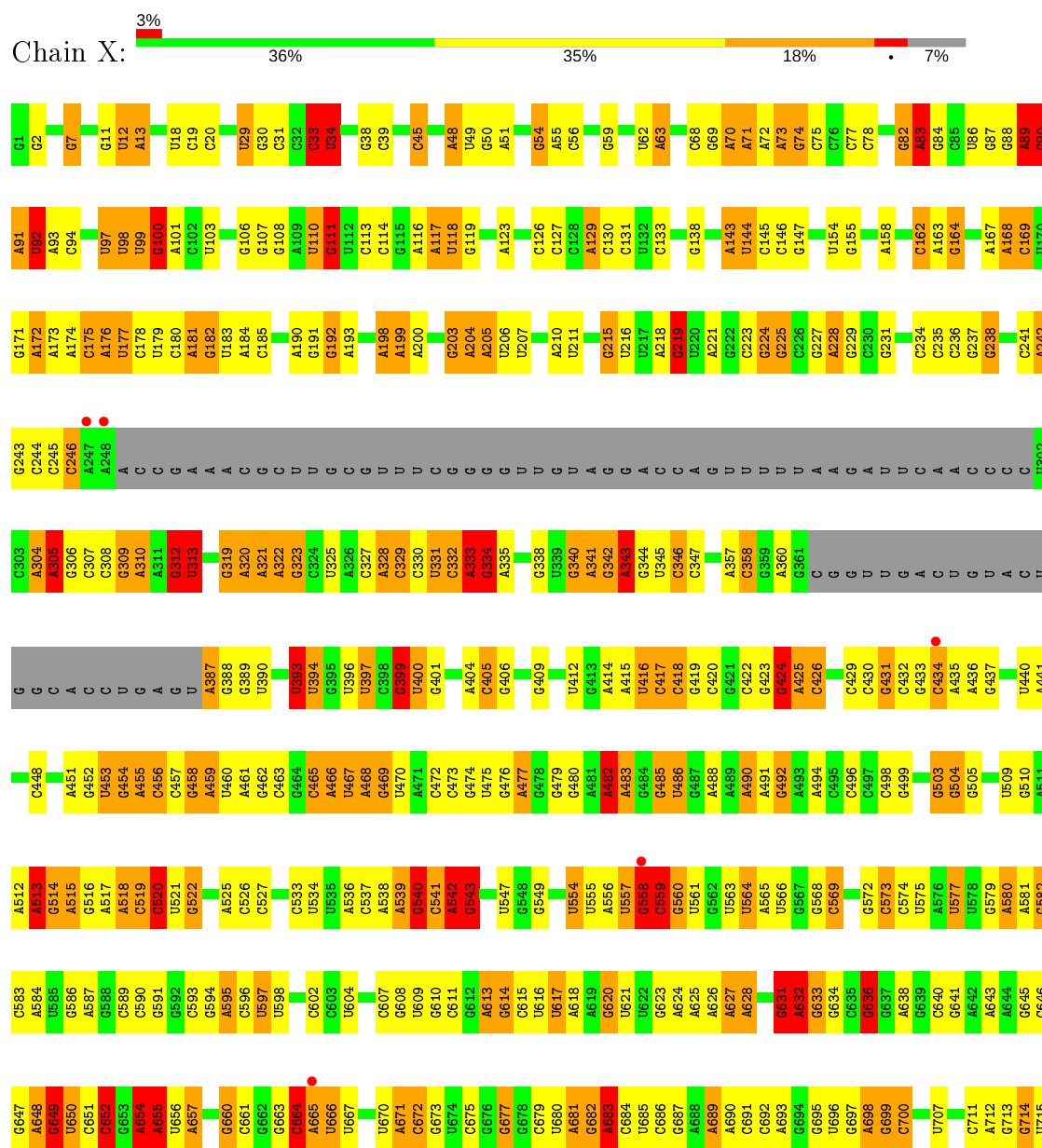


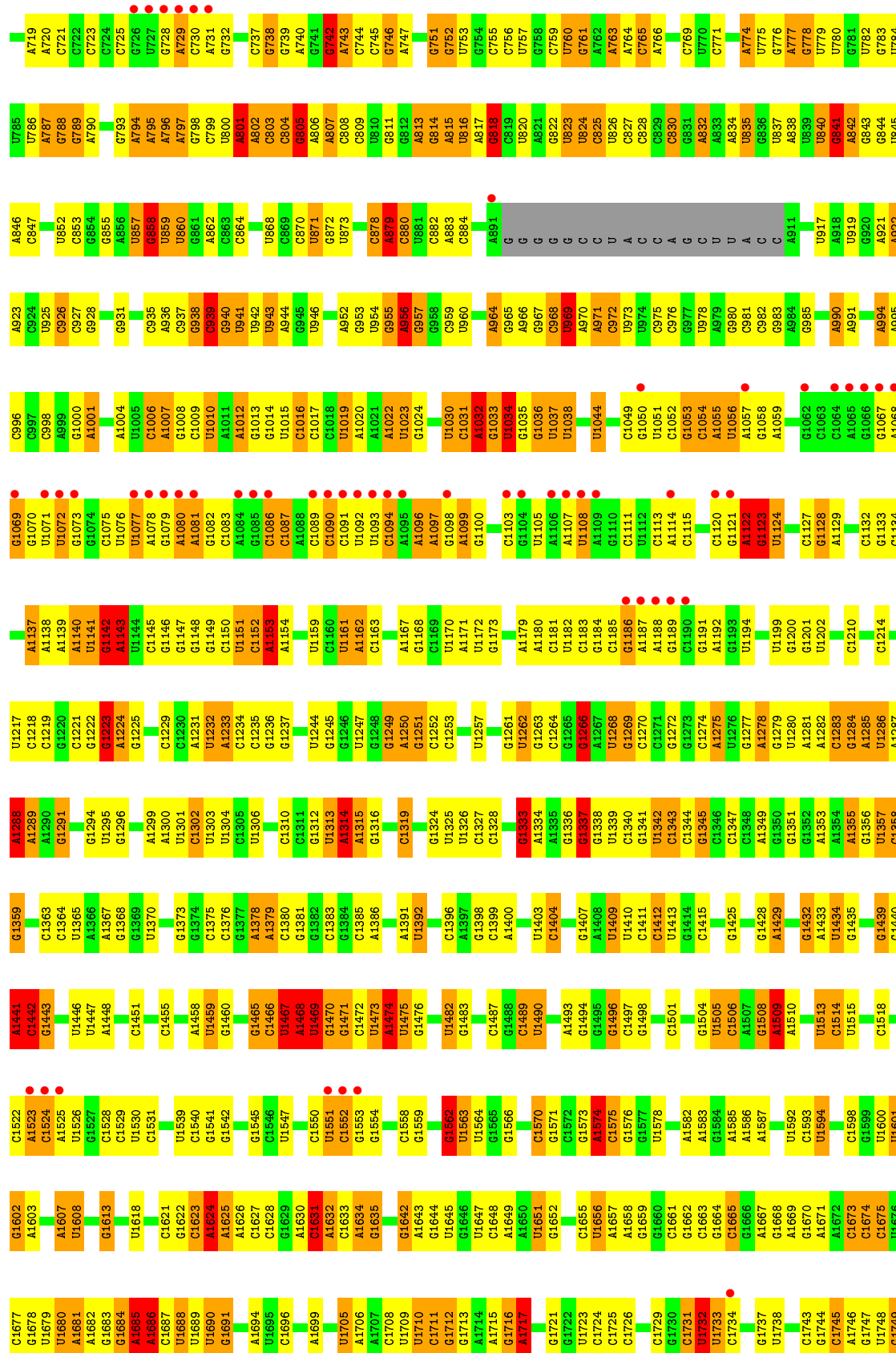
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			56	41	4	11		

3 Residue-property plots

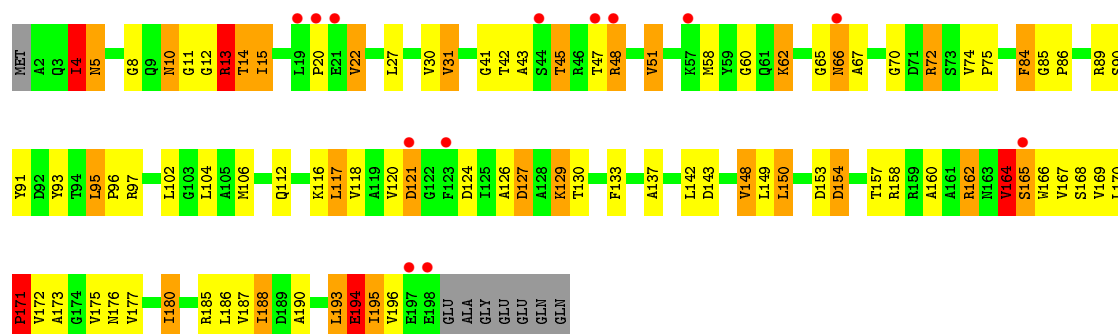
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

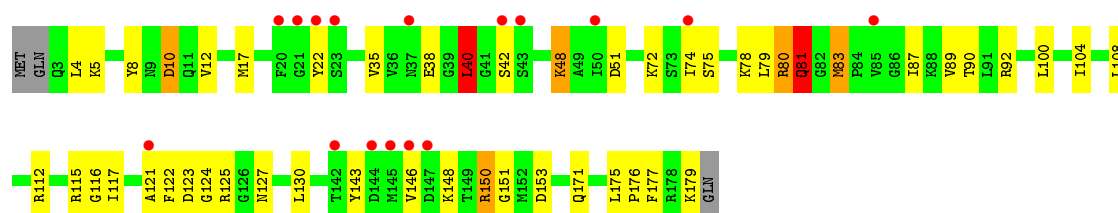




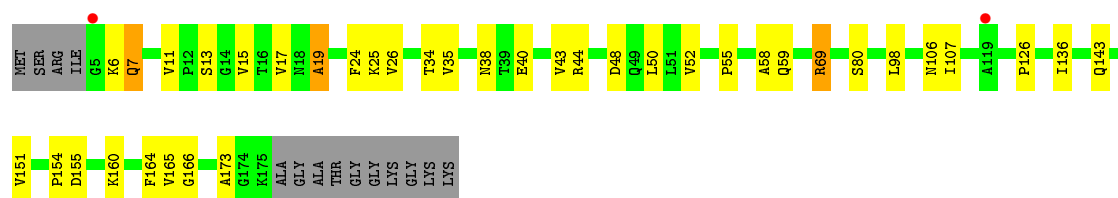
C2678	C2680	C2681	C2689	C2690	C2691	C2692	C2693	C2694	C2695	C2696	C2697	C2698	C2699	C2700	C2701	C2702	C2703	C2704	C2705	C2706	C2707	C2708	C2709	C2710	A2713	A2718	A2719	A2720	A2726	A2727	A2728	A2729	A2730	A2731	A2732	A2733	A2734	C2735	C2736	A2737	A2738	C2742	C2743	A2744	A2745	C2746	C2747	C2750	C2751	C2754	A2755	A2756																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C2601	C2605	A2608	A2611	G2612	A2613	A2614	A2615	A2616	A2617	G2620	G2621	G2622	G2625	G2626	G2627	G2632	A2633	G2634	G2635	A2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	A2649	A2650	A2653	A2654	C2659	C2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	C2669	C2670	C2671	G2672	G2673	C2674	C2675	C2676																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
U2533	U2534	C2535	C2538	C2539	A2540	U2541	U2542	A2543	A2544	A2545	G2546	C2550	A2551	C2552	C2553	C2554	C2555	A2556	C2557	C2558	C2559	A2560	G2561	C2562	C2563	C2564	C2565	A2566	C2567	A2568	C2569	C2570	C2571	C2572	C2573	C2576	C2580	A2581	C2582	U2583	U2584	C2585	G2586	G2587	U2588	C2589	U2590	C2591	U2592	A2593	A2594	C2595	C2596	A2600																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
A2467	U2472	G2473	G2474	C2475	A2476	C2477	C2478	U2479	C2480	G2481	A2482	U2483	C2484	U2485	C2486	G2487	G2488	C2489	U2490	C2491	G2492	U2493	C2494	G2495	C2496	A2497	U2498	A2499	C2500	G2504	G2505	U2507	C2508	A2509	G2511	G2514	G2515	U2516	C2517	C2518	C2519	G2522	G2523	G2524	U2525	U2526	G2527	C2528	G2529	U2530	U2531	G2532																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A2397	U2398	C2399	G2400	C2399	A2401	G2402	C2403	A2404	A2405	C2406	C2407	C2408	A2409	U2410	A2414	G2415	U2416	G2417	A2418	C2419	C2420	C2421	C2422	G2423	G2426	A2427	U2428	A2429	A2430	C2431	C2434	C2435	U2436	G2437	A2438	U2439	U2441	C2442	C2443	C2444	C2445	G2446	A2448	G2449	U2452	C2453	C2454	U2455	U2456	C2459	G2460	G2463																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A2325	C2326	U2327	C2328	C2329	G2330	A2331	G2332	C2336	A2337	C2338	U2342	C2343	C2347	G2351	A2352	G2354	A2355	A2356	A2357	C2358	U2359	G2360	A2361	C2362	C2363	C2364	U2365	A2366	G2367	G2368	U2369	C2370	A2371	A2372	U2377	G2378	G2379	A2381	C2382	C2383	U2385	G2386	C2387	C2388	U2389	G2392	G2393	C2394	C2395	C2396																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G2255	G2256	A2257	G2258	C2259	C2260	C2261	C2262	A2265	A2266	A2267	G2268	G2269	U2270	C2271	C2272	A2273	C2274	U2275	C2276	G2279	A2280	C2281	G2282	G2283	U2284	G2285	G2286	C2287	A2288	U2289	A2290	U2291	U2298	A2299	G2300	A2301	C2302	C2303	G2304	C2305	A2306	G2310	U2311	A2312	G2313	A2314	A2315	U2318	G2319	G2320	C2321	U2322	U2323	G2324																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
U2177	U2178	A2181	C2184	U2185	A2188	A2189	A2190	A2191	U2192	C2193	A2194	C2195	U2196	U2197	U2198	C2199	A2204	C2205	C2206	G2207	U2208	G2217	G2218	U2219	U2222	U2223	U2224	G2225	G2226	C2227	U2228	G2229	G2230	G2231	U2236	C2237	C2238	C2239	U2241	C2242	C2243	A2244	A2245	A2246	G2250	U2251	A2252	C2253	C2254																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A2045	C2046	C2047	C2048	G2049	G2050	U2051	G2052	U2062	A2063	U2064	A2065	G2066	U2069	G2070	G2071	C2072	U2075	G2076	G2077	U2080	U2081	C2082	G2083	G2084	U2087	U2088	C2089	U2090	C2091	U2098	A2099	C2103	C2104	G2105	U2106	U2107	C2108	C2109	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A2148	A2149	A2150	A2151	A2152	A2153	A2154	A2155	A2156	A2157	A2158	A2159	A2160	A2161	A2162	A2163	A2164	A2165	A2166	A2167	A2168	A2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252	A2253	A2254	A2255	A2256	A2257	A2258	A2259	A2260	A2261	A2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2321	A2322	A2323	A2324	A2325	A2326	A2327	A2328	A2329	A2330	A2331	A2332	A2333	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416	A2417	A2418	A2419	A2420	A2421	A2422	A2423	A2424	A2425	A2426	A2427	A2428	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	A2459	A2460	A2461	A2462	A2463	A2464	A2465	A2466	A2467	A2468	A2469	A2470	A2471	A2472	A2473	A2474	A2475	A2476	A2477	A2478	A2479	A2480	A2481	A2482	A2483	A2484	A2485	A2486	A2487	A2488	A2489	A2490	A2491	A2492	A2493	A2494	A2495	A2496	A2497	A2498	A2499	A2500	A2501	A2502	A2503	A2504	A2505	A2506	A2507	A2508	A2509	A2510	A2511	A2512	A2513	A2514	A2515	A2516	A2517	A2518	A2519	A2520	A2521	A2522	A2523	A2524	A2525	A2526	A2527	A2528	A2529	A2530	A2531	A2532	A2533	A2534	A2535	A2536	A2537	A2538	A2539	A2540	A2541	A2542	A2543	A2544	A2545	A2546	A2547	A2548	A2549	A2550	A2551	A2552	A2553	A2554	A2555	A2556	A2557	A2558	A2559	A2560	A2561	A2562	A2563	A2564	A2565	A2566	A2567	A2568	A2569	A2570	A2571	A2572	A2573	A2574	A2575	A2576	A2577	A2578	A2579	A2580	A2581	A2582	A2583	A2584	A2585	A2586	A2587	A2588	A2589	A2590	A2591	A2592	A2593	A2594	A2595	A2596	A2597	A2598	A2599	A2600	A2601	A2602	A2603	A2604	A2605	A2606	A2607	A2608	A2609	A2610	A2611	A2612	A2613	A2614	A2615	A2616	A2617	A2618	A2619	A2620	A2621	A2622	A2623	A2624	A2625	A2626	A2627	A2628	A2629	A2630	A2631	A2632	A2633	A2634	A2635	A2636	A2637	A2638	A2639	A2640	A2641	A2642	A2643	A2644	A2645	A2646	A2647	A2648	A2649	A2650	A2651	A2652	A2653	A2654	A2655	A2656	A2657	A2658	A2659	A2660	A2661	A2662	A2663	A2664	A2665	A2666	A2667	A2668	A2669	A2670	A2671	A2672	A2673	A2674	A2675	A2676	A2677	A2678	A2679	A2680	A2681	A2682	A2683	A2684	A2685	A2686	A2687	A2688	A2689	A2690	A2691	A2692	A2693	A2694	A2695	A2696	A2697	A2698	A2699	A2700	A2701	A2702	A2703	A2704	A2705	A2706	A2707	A2708	A2709	A2710	A2711	A2712	A2713	A2714	A2715	A2716	A2717	A2718	A2719	A2720	A2721	A2722	A2723	A2724	A2725	A2726	A2727	A2728	A2729	A2730	A2731	A2732	A2733	A2734	A2735	A2736	A2737	A2738	A2739	A2740	A2741	A2742	A2743	A2744	A2745	A2746	A2747	A2748	A2749	A2750	A2751	A2752	A2753	A2754	A2755	A2756	A2757	A2758	A2759	A2760	A2761	A2762	A2763	A2764	A2765	A2766	A2767	A2768	A2769	A2770	A2771	A2772	A2773	A2774	A2775	A2776	A2777	A2778	A2779	A2780	A2781	A2782	A2783	A2784	A2785	A2786	A2787	A2788	A2789	A2790	A2791	A2792	A2793	A2794	A2795	A2796	A2797	A2798	A2799	A2800	A2801	A2802	A2803	A2804	A2805	A2806	A2807	A2808	A2809	A2810	A2811	A2812	A2813	A2814	A2815	A2816	A2817	A2818	A2819	A2820	A2821	A2822	A2823	A2824	A2825	A2826	A2827	A2828	A2829	A2830	A2831	A2832	A2833	A2834	A2835	A2836	A2837	A2838	A2839	A2840	A2841	A2842	A2843	A2844	A2845	A2846	A2847	A2848	A2849	A2850	A2851	A2852	A2853	A2854	A2855	A2856	A2857	A2858	A2859	A2860	A2861	A2862	A2863	A2864	A2865	A2866	A2867	A2868	A2869	A2870	A2871	A2872	A2873	A2874	A2875	A2876	A2877	A2878	A2879	A2880	A2881	A2882	A2883	A2884	A2885	A2886	A2887	A2888	A2889	A2890	A2891	A2892	A2893	A2894	A2895	A2896	A2897	A2898	A2899	A2900	A2901	A2902	A2903	A2904	A2905	A2906	A2907	A2908	A2909	A2910	A2911	A2912	A2913	A2914	A2915	A2916	A2917	A2918	A2919	A2920	A2921	A2922	A2923	A2924	A2925	A2926	A2927	A2928	A2929	A2930	A2931	A2932	A2933	A2934	A2935	A2936	A2937	A2938	A2939	A2940	A2941	A2942	A2943	A2944	A2945	A2946	A2947	A2948	A2949	A2950	A2951	A2952	A2953	A2954	A2955	A2956	A2957	A2958	A2959	A2960	A2961	A2962	A2963	A2964	A2965	A2966	A2967	A2968	A2969	A2970	A2971	A2972	A2973	A2974	A2975	A2976	A2977	A2978	A2979	A2980	A2981	A2982	A2983	A2984	A2985	A2986	A2987	A2988	A2989	A2990	A2991	A2992	A2993	A2994	A2995	A2996	A2997</



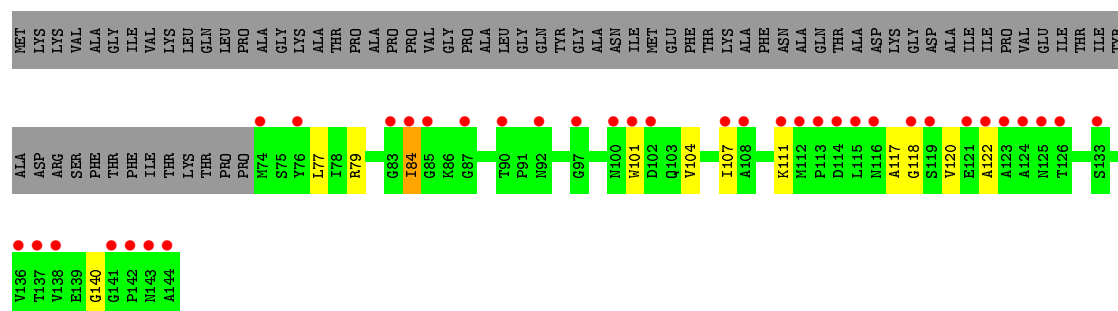
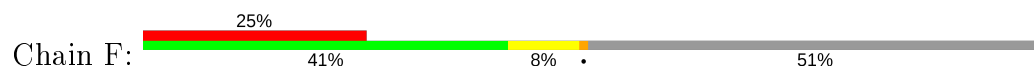
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

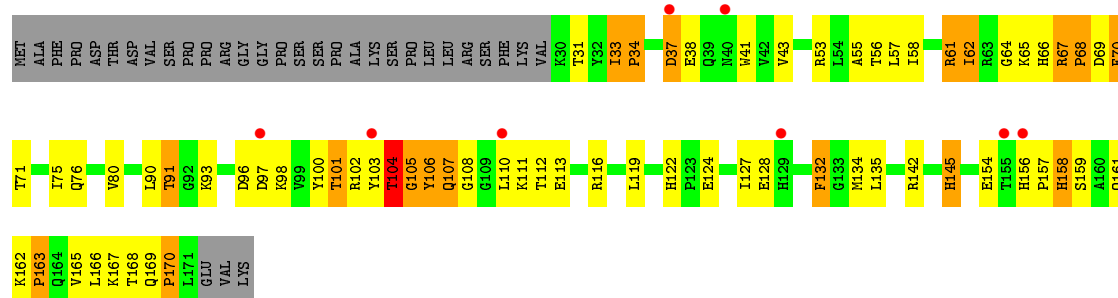


• Molecule 8: 50S ribosomal protein L11



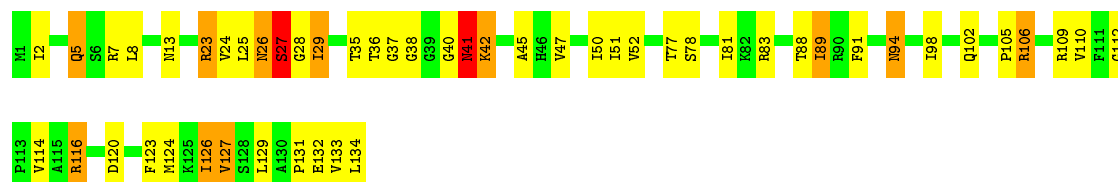
• Molecule 9: 50S ribosomal protein L13





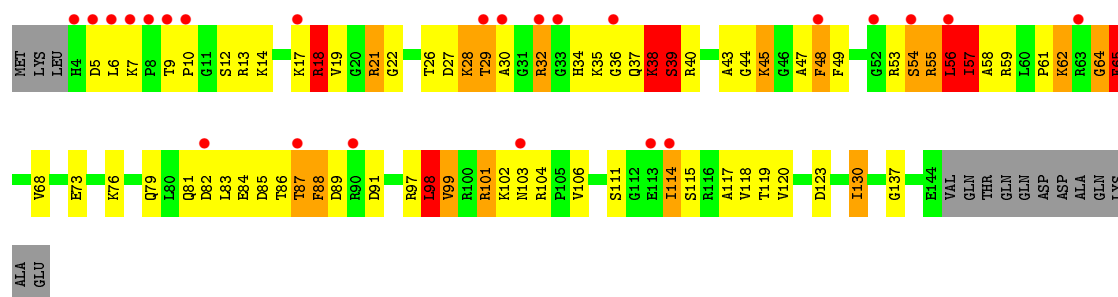
- Molecule 10: 50S ribosomal protein L14

Chain H: 62% 28% 8%



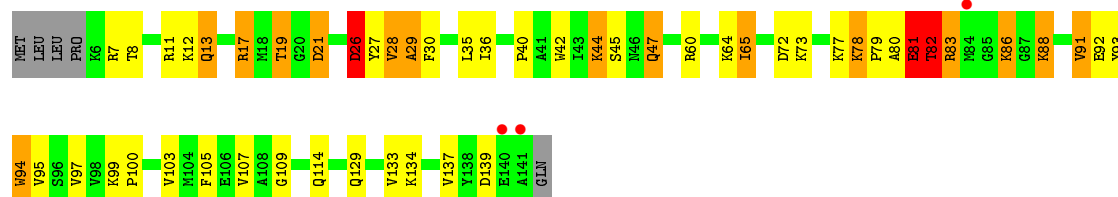
- Molecule 11: 50S ribosomal protein L15

Chain I: 15% 42% 33% 10% 10%



- Molecule 12: 50S ribosomal protein L16

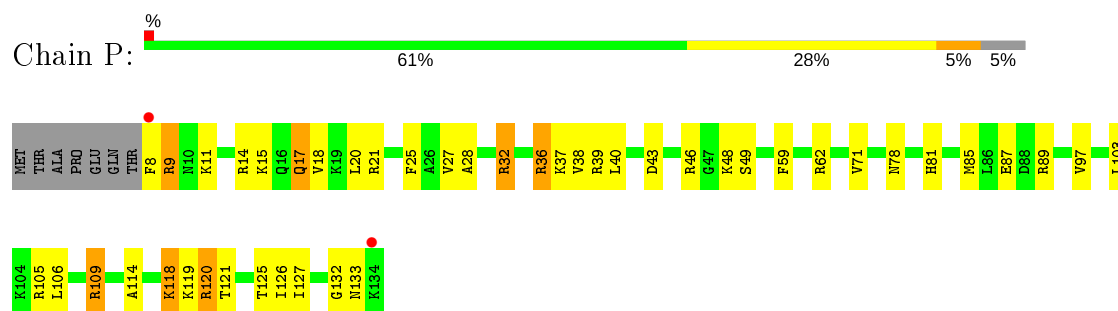
Chain J: 2% 60% 24% 11%



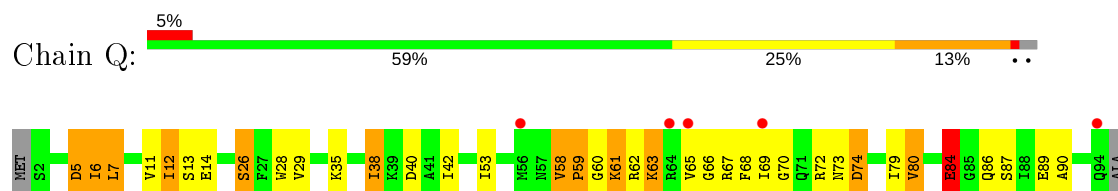
- Molecule 13: 50S ribosomal protein L17

Chain K: 59% 23% 13%

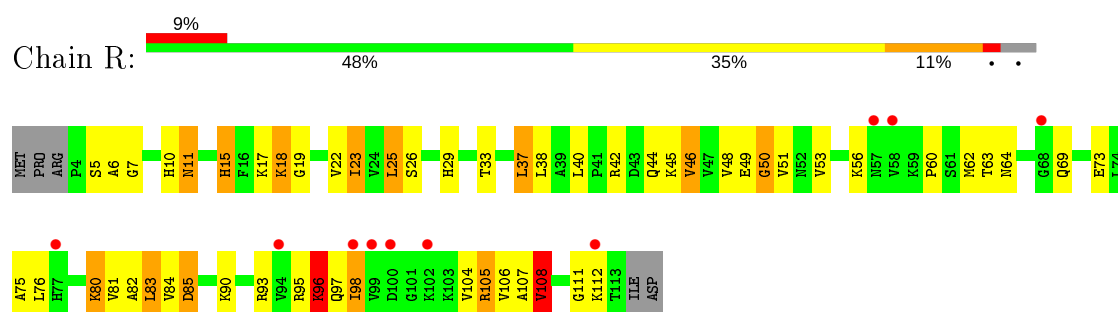
- Molecule 18: 50S ribosomal protein L22



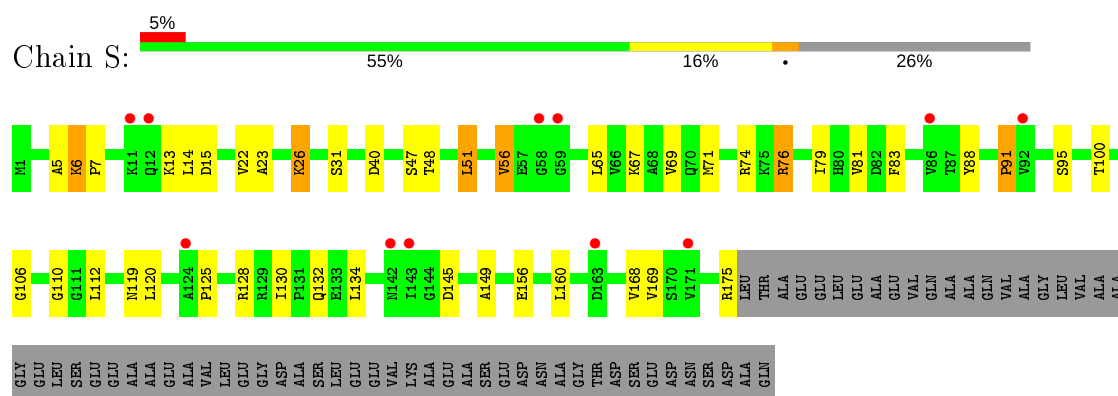
- Molecule 19: 50S ribosomal protein L23



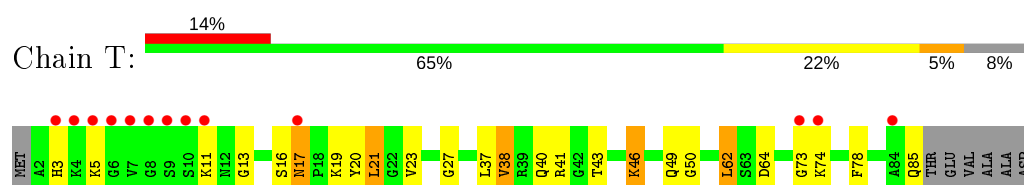
- Molecule 20: 50S ribosomal protein L24



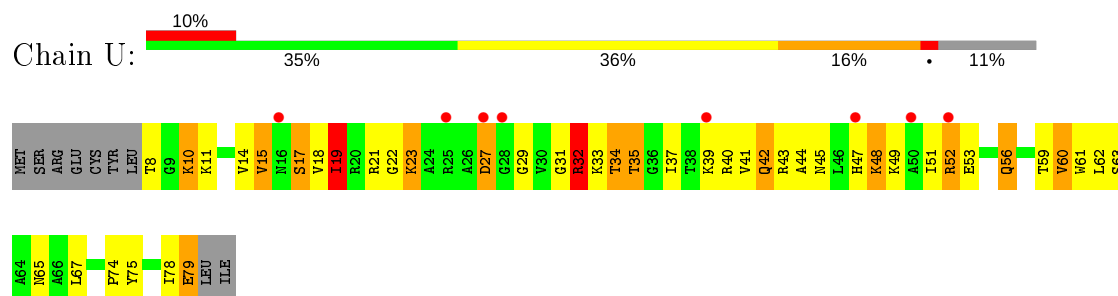
- Molecule 21: 50S ribosomal protein L25



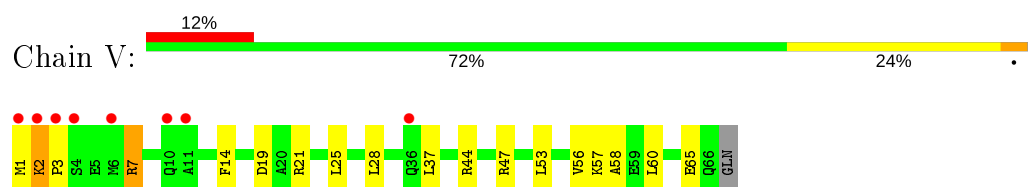
- Molecule 22: 50S ribosomal protein L27



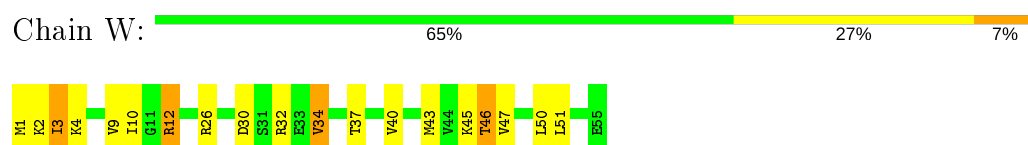
- Molecule 23: 50S ribosomal protein L28



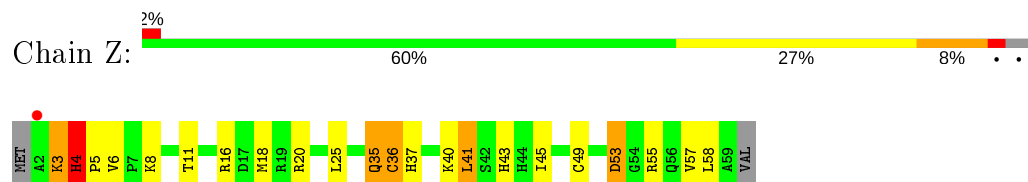
- Molecule 24: 50S ribosomal protein L29



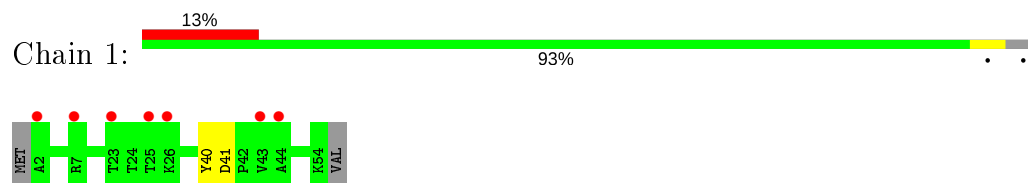
- Molecule 25: 50S ribosomal protein L30



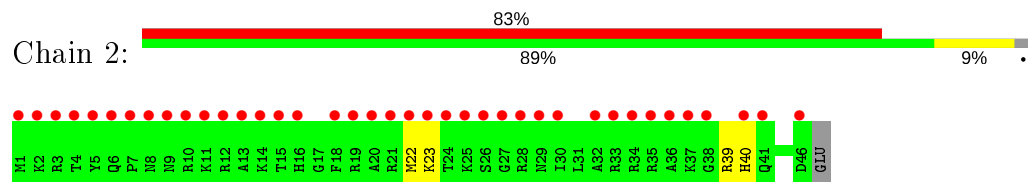
- Molecule 26: 50S ribosomal protein L32



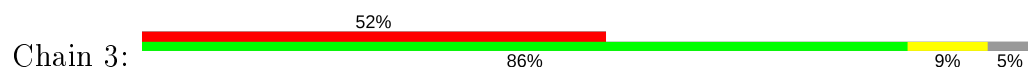
- Molecule 27: 50S ribosomal protein L33

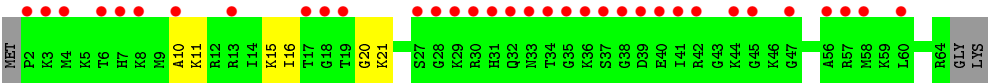


- Molecule 28: 50S ribosomal protein L34

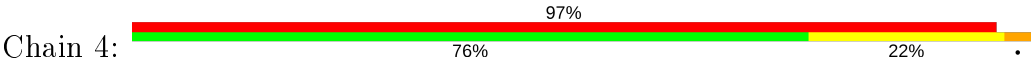


- Molecule 29: 50S ribosomal protein L35





● 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	169.94Å 409.69Å 694.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.20 – 3.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 94.1 (30.20-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 3.24Å)	Xtriage
Refinement program	autobuster	Depositor
R, R_{free}	0.199 , 0.235 0.214 , 0.254	Depositor DCC
R_{free} test set	18481 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 93.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83875	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 1.92% 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: MG, 1F2

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	1.00	46/64561 (0.1%)	1.87	1961/100708 (1.9%)
2	Y	1.05	0/2904	1.78	84/4525 (1.9%)
3	A	0.61	0/1862	0.92	1/2510 (0.0%)
4	B	0.57	0/1567	0.94	1/2105 (0.0%)
5	C	0.62	0/1529	0.98	2/2070 (0.1%)
6	D	0.45	0/1419	0.66	0/1903
7	E	0.45	0/1308	0.67	0/1771
8	F	0.46	0/508	0.64	0/683
9	G	0.58	0/1138	0.94	1/1539 (0.1%)
10	H	0.55	0/1007	0.88	1/1352 (0.1%)
11	I	0.73	1/1081 (0.1%)	1.12	6/1448 (0.4%)
12	J	0.68	1/1113 (0.1%)	0.95	1/1486 (0.1%)
13	K	0.77	2/886 (0.2%)	1.02	3/1188 (0.3%)
14	L	0.53	0/785	0.88	1/1048 (0.1%)
15	M	0.64	0/884	0.98	1/1186 (0.1%)
16	N	0.51	0/994	0.77	0/1323
17	O	0.52	0/750	0.95	1/1000 (0.1%)
18	P	0.56	0/1027	0.85	0/1373
19	Q	0.60	0/737	1.03	5/988 (0.5%)
20	R	0.61	0/835	0.99	0/1121
21	S	0.48	0/1370	0.73	0/1862
22	T	0.55	0/633	0.82	0/838
23	U	0.75	0/556	1.10	1/741 (0.1%)
24	V	0.47	0/537	0.71	0/714
25	W	0.48	0/426	0.81	0/568
26	Z	0.62	0/469	0.97	0/629
30	4	0.44	0/298	0.62	0/390
All	All	0.91	50/91184 (0.1%)	1.69	2070/137069 (1.5%)

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	6

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1688	U	C4-O4	9.12	1.30	1.23
1	X	774	A	C5-C4	8.90	1.45	1.38
1	X	1685	A	C3'-O3'	7.74	1.52	1.42
1	X	1468	A	N9-C4	7.70	1.42	1.37
1	X	1333	G	N9-C4	-7.09	1.32	1.38

The worst 5 of 2070 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1631	C	C1'-O4'-C4'	-33.72	82.92	109.90
1	X	1288	A	C1'-O4'-C4'	-32.93	83.55	109.90
1	X	1288	A	C5'-C4'-O4'	20.68	133.91	109.10
1	X	1288	A	O4'-C1'-N9	20.52	124.61	108.20
1	X	1019	U	P-O3'-C3'	19.59	143.21	119.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1143	A	Sidechain
1	X	474	G	Sidechain
1	X	671	A	Sidechain
1	X	683	A	Sidechain
1	X	805	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	404	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	2598	0	1328	17	0
3	A	1826	0	1885	61	0
4	B	1539	0	1600	61	0
5	C	1506	0	1525	49	0
6	D	1400	0	1481	22	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	68	0
10	H	997	0	1046	31	0
11	I	1067	0	1103	37	0
12	J	1090	0	1125	36	0
13	K	878	0	930	36	0
14	L	779	0	820	25	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	34	0
18	P	1014	0	1096	20	0
19	Q	726	0	753	15	0
20	R	825	0	881	27	0
21	S	1345	0	1372	18	0
22	T	625	0	655	11	0
23	U	552	0	604	26	0
24	V	533	0	558	5	0
25	W	424	0	470	8	0
26	Z	457	0	462	12	0
27	1	53	0	0	1	0
28	2	46	0	0	2	0
29	3	63	0	0	3	0
30	4	297	0	330	5	0
31	J	1	0	0	0	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	5	0	0	0	0
32	X	56	0	64	3	0
All	All	83875	0	54807	954	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 7.

The worst 5 of 954 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)
15:M:57:ILE:CD1	15:M:57:ILE:CG1	1.79	1.58
11:I:57:ILE:CD1	11:I:57:ILE:CG1	1.92	1.45
13:K:52:ILE:CD1	13:K:52:ILE:CG1	1.95	1.45
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.66	1.08
11:I:62:LYS:HE2	11:I:64:GLY:HA2	1.34	1.03

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%)	178 (75%)	39 (16%)	21 (9%)	1	4
4	B	203/211 (96%)	171 (84%)	24 (12%)	8 (4%)	3	22
5	C	195/205 (95%)	129 (66%)	45 (23%)	21 (11%)	0	2
6	D	175/180 (97%)	141 (81%)	27 (15%)	7 (4%)	3	21
7	E	169/185 (91%)	139 (82%)	20 (12%)	10 (6%)	1	12
8	F	69/144 (48%)	57 (83%)	10 (14%)	2 (3%)	4	28
9	G	140/174 (80%)	105 (75%)	21 (15%)	14 (10%)	0	3
10	H	132/134 (98%)	115 (87%)	11 (8%)	6 (4%)	2	18
11	I	139/156 (89%)	85 (61%)	28 (20%)	26 (19%)	0	0
12	J	134/141 (95%)	101 (75%)	19 (14%)	14 (10%)	0	3
13	K	111/116 (96%)	92 (83%)	11 (10%)	8 (7%)	1	7
14	L	102/114 (90%)	75 (74%)	19 (19%)	8 (8%)	1	6
15	M	106/166 (64%)	89 (84%)	13 (12%)	4 (4%)	3	22
16	N	115/118 (98%)	92 (80%)	17 (15%)	6 (5%)	2	15
17	O	92/100 (92%)	67 (73%)	13 (14%)	12 (13%)	0	1
18	P	125/134 (93%)	108 (86%)	12 (10%)	5 (4%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	91/95 (96%)	64 (70%)	14 (15%)	13 (14%)	0	1
20	R	108/115 (94%)	66 (61%)	24 (22%)	18 (17%)	0	0
21	S	173/237 (73%)	135 (78%)	28 (16%)	10 (6%)	1	13
22	T	82/91 (90%)	64 (78%)	11 (13%)	7 (8%)	1	4
23	U	70/81 (86%)	43 (61%)	16 (23%)	11 (16%)	0	1
24	V	64/67 (96%)	58 (91%)	4 (6%)	2 (3%)	4	26
25	W	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
26	Z	56/60 (93%)	48 (86%)	5 (9%)	3 (5%)	2	14
30	4	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	4	28
All	All	2977/3390 (88%)	2303 (77%)	437 (15%)	237 (8%)	1	6

5 of 237 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	56	GLY
3	A	89	SER
3	A	198	ASN
3	A	199	ALA
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%)	151 (82%)	34 (18%)	1	8
4	B	155/157 (99%)	128 (83%)	27 (17%)	2	10
5	C	157/163 (96%)	120 (76%)	37 (24%)	1	3
6	D	153/156 (98%)	133 (87%)	20 (13%)	4	19
7	E	136/144 (94%)	125 (92%)	11 (8%)	11	42
8	F	51/107 (48%)	49 (96%)	2 (4%)	32	67
9	G	118/146 (81%)	93 (79%)	25 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	103/103 (100%)	87 (84%)	16 (16%)	2	12
11	I	108/121 (89%)	76 (70%)	32 (30%)	0	1
12	J	110/115 (96%)	88 (80%)	22 (20%)	1	6
13	K	90/93 (97%)	68 (76%)	22 (24%)	0	2
14	L	74/82 (90%)	56 (76%)	18 (24%)	0	2
15	M	94/134 (70%)	66 (70%)	28 (30%)	0	1
16	N	96/97 (99%)	81 (84%)	15 (16%)	2	12
17	O	75/79 (95%)	57 (76%)	18 (24%)	0	3
18	P	109/115 (95%)	89 (82%)	20 (18%)	1	8
19	Q	75/76 (99%)	62 (83%)	13 (17%)	2	10
20	R	91/96 (95%)	70 (77%)	21 (23%)	1	3
21	S	149/192 (78%)	130 (87%)	19 (13%)	4	20
22	T	62/67 (92%)	53 (86%)	9 (14%)	3	15
23	U	57/66 (86%)	37 (65%)	20 (35%)	0	0
24	V	54/55 (98%)	46 (85%)	8 (15%)	3	14
25	W	48/48 (100%)	35 (73%)	13 (27%)	0	1
26	Z	51/53 (96%)	39 (76%)	12 (24%)	1	3
30	4	35/35 (100%)	31 (89%)	4 (11%)	5	24
All	All	2436/2715 (90%)	1970 (81%)	466 (19%)	1	8

5 of 466 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	45	SER
14	L	89	PHE
24	V	7	ARG
12	J	82	THR
13	K	51	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
16	N	31	GLN
17	O	88	GLN
26	Z	29	ASN

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Mol	Chain	Res	Type
16	N	91	ASN
18	P	78	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	672 (25%)	252 (9%)
2	Y	121/123 (98%)	26 (21%)	7 (5%)
All	All	2804/3003 (93%)	698 (24%)	259 (9%)

5 of 698 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	34	U
1	X	45	C
1	X	48	A

5 of 259 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1142	G
1	X	1442	C
1	X	2738	A
1	X	1186	G
1	X	1333	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1F2	X	2929	-	58,60,60	1.98	13 (22%)	81,90,90	2.09	26 (32%)

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	1F2	X	2929	-	-	1/74/115/115	0/5/5/5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F2	C30-N29	9.08	1.46	1.33
32	X	2929	1F2	C8-C10	4.43	1.59	1.52
32	X	2929	1F2	C5-N29	3.51	1.52	1.45
32	X	2929	1F2	O11-C12	-3.49	1.26	1.34
32	X	2929	1F2	C17-C2	3.22	1.60	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F2	C24-C7-C6	-5.42	107.76	115.23
32	X	2929	1F2	C25-C6-C5	-4.99	109.41	116.42
32	X	2929	1F2	C48-C47-N45	4.90	107.56	101.94
32	X	2929	1F2	O16-C4-C2	-4.29	114.51	120.60
32	X	2929	1F2	O31-C30-N29	-4.26	124.25	129.22

There are no chirality outliers.

All (1) torsion outliers are listed below:

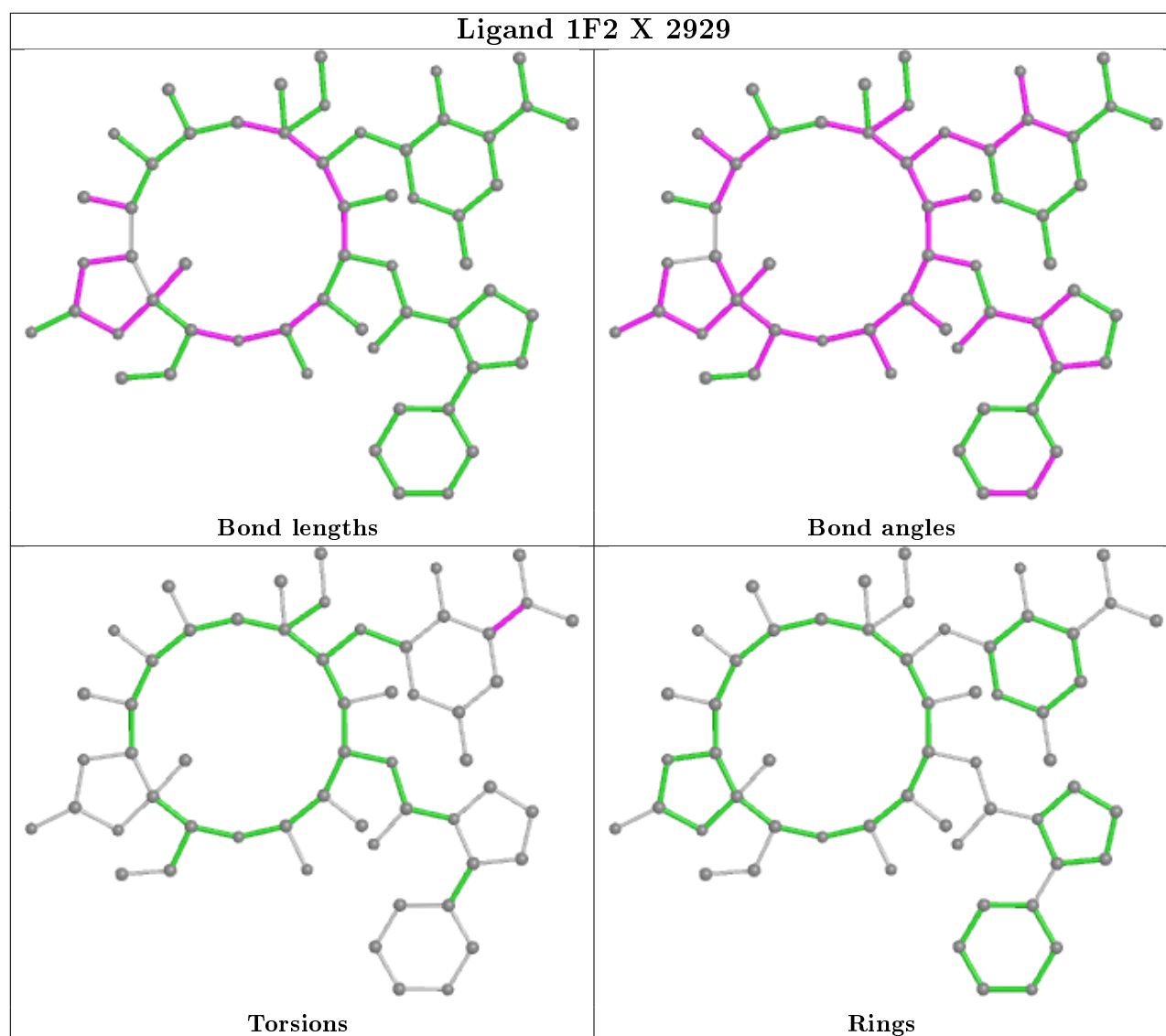
Mol	Chain	Res	Type	Atoms
32	X	2929	1F2	C35-C36-N38-C40

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2929	1F2	3	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%)	-0.18	85 (3%) 47 31	43, 92, 197, 276	0
2	Y	122/123 (99%)	-0.05	2 (1%) 72 59	83, 136, 170, 192	0
3	A	240/274 (87%)	0.06	9 (3%) 40 26	69, 116, 146, 173	0
4	B	205/211 (97%)	-0.29	3 (1%) 73 61	45, 73, 106, 154	0
5	C	197/205 (96%)	0.17	13 (6%) 18 11	57, 114, 155, 187	0
6	D	177/180 (98%)	0.53	16 (9%) 9 5	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.20	2 (1%) 79 67	92, 143, 192, 206	0
8	F	71/144 (49%)	2.27	36 (50%) 0 0	211, 236, 252, 257	0
9	G	142/174 (81%)	0.08	8 (5%) 24 13	73, 97, 145, 161	0
10	H	134/134 (100%)	-0.42	0 100 100	50, 70, 96, 120	0
11	I	141/156 (90%)	0.81	24 (17%) 1 1	67, 129, 174, 204	0
12	J	136/141 (96%)	0.11	3 (2%) 62 48	74, 103, 149, 184	0
13	K	113/116 (97%)	-0.42	0 100 100	35, 60, 79, 91	0
14	L	104/114 (91%)	0.39	9 (8%) 10 5	98, 134, 156, 169	0
15	M	108/166 (65%)	-0.41	0 100 100	50, 73, 111, 144	0
16	N	117/118 (99%)	-0.29	0 100 100	60, 90, 127, 160	0
17	O	94/100 (94%)	-0.22	3 (3%) 47 31	67, 115, 156, 173	0
18	P	127/134 (94%)	-0.39	2 (1%) 72 59	50, 67, 108, 158	0
19	Q	93/95 (97%)	-0.04	5 (5%) 25 14	73, 106, 162, 195	0
20	R	110/115 (95%)	0.22	10 (9%) 9 5	88, 117, 170, 178	0
21	S	175/237 (73%)	0.14	11 (6%) 20 11	121, 155, 175, 190	0
22	T	84/91 (92%)	0.58	13 (15%) 2 1	80, 108, 186, 199	0
23	U	72/81 (88%)	0.47	8 (11%) 5 3	92, 128, 153, 162	0
24	V	66/67 (98%)	0.55	8 (12%) 4 2	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%)	-0.39	0 100 100	81, 98, 126, 152	0
26	Z	58/60 (96%)	-0.14	1 (1%) 70 57	49, 71, 105, 113	0
27	1	53/55 (96%)	0.84	7 (13%) 3 2	8, 32, 61, 96	0
28	2	46/47 (97%)	3.75	39 (84%) 0 0	3, 16, 37, 59	0
29	3	63/66 (95%)	2.54	34 (53%) 0 0	3, 25, 40, 60	0
30	4	37/37 (100%)	6.83	36 (97%) 0 0	227, 254, 265, 269	0
All	All	5997/6561 (91%)	0.07	387 (6%) 18 11	3, 100, 196, 276	0

The worst 5 of 387 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	24	LEU	18.2
30	4	17	VAL	15.6
27	1	7	ARG	15.5
30	4	25	VAL	14.0
8	F	125	ASN	12.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

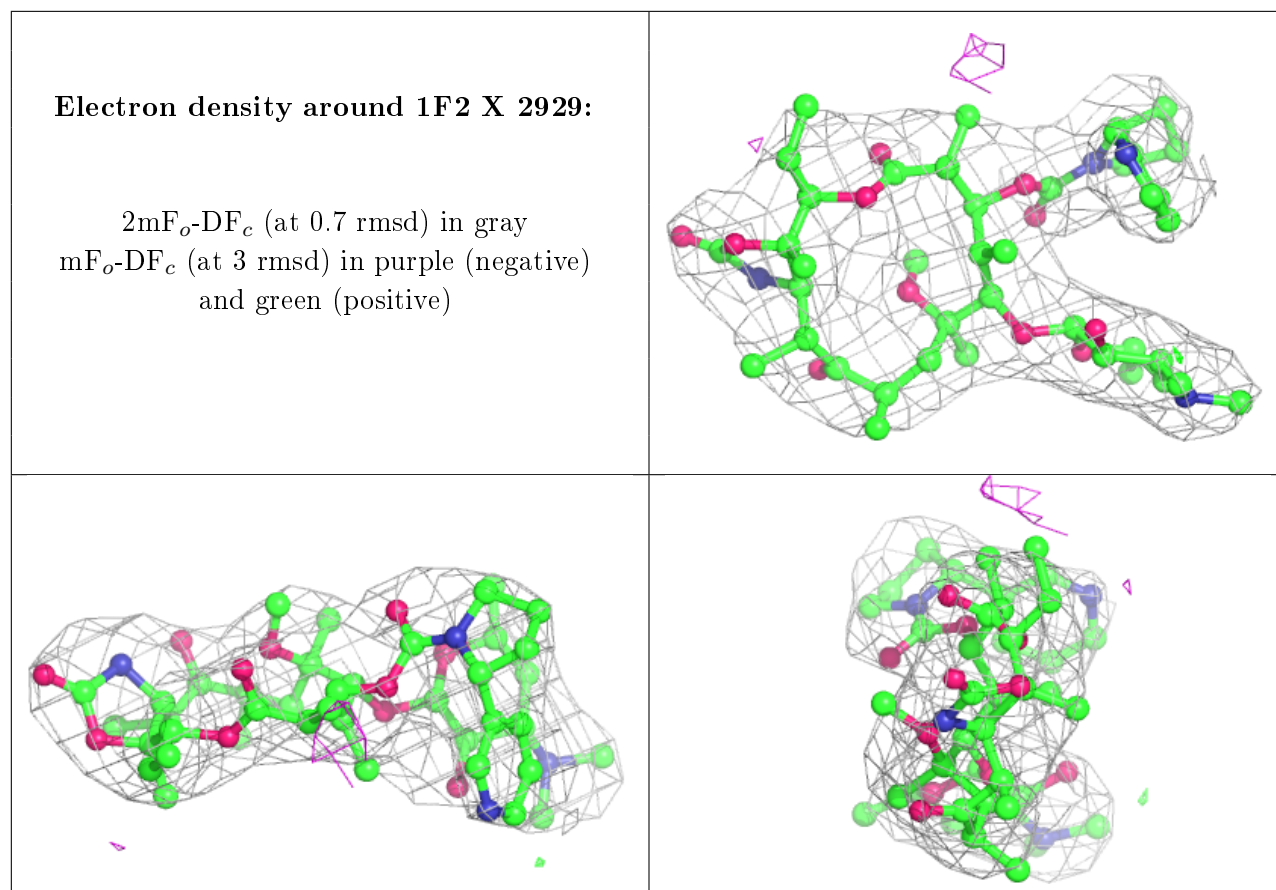
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	Y	203	1/1	0.45	0.72	87,87,87,87	0
31	MG	X	2902	1/1	0.60	0.63	94,94,94,94	0
31	MG	X	2903	1/1	0.64	0.67	89,89,89,89	0
31	MG	Y	201	1/1	0.66	0.82	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	2905	1/1	0.78	0.27	65,65,65,65	0
31	MG	X	2912	1/1	0.78	0.50	71,71,71,71	0
31	MG	J	201	1/1	0.79	0.30	100,100,100,100	0
31	MG	X	2928	1/1	0.84	0.53	62,62,62,62	0
31	MG	Y	205	1/1	0.85	0.30	79,79,79,79	0
31	MG	X	2909	1/1	0.90	0.51	96,96,96,96	0
31	MG	X	2924	1/1	0.91	1.20	69,69,69,69	0
31	MG	X	2907	1/1	0.91	0.65	51,51,51,51	0
31	MG	X	2917	1/1	0.92	0.54	55,55,55,55	0
31	MG	X	2904	1/1	0.92	0.29	107,107,107,107	0
31	MG	X	2925	1/1	0.94	0.53	122,122,122,122	0
31	MG	X	2906	1/1	0.94	0.41	58,58,58,58	0
31	MG	X	2915	1/1	0.95	0.68	57,57,57,57	0
31	MG	X	2920	1/1	0.95	0.20	115,115,115,115	0
31	MG	X	2911	1/1	0.95	0.31	68,68,68,68	0
31	MG	X	2919	1/1	0.95	0.47	30,30,30,30	0
31	MG	X	2918	1/1	0.95	0.67	42,42,42,42	0
31	MG	X	2913	1/1	0.96	0.63	61,61,61,61	0
31	MG	Y	202	1/1	0.96	0.51	58,58,58,58	0
31	MG	X	2922	1/1	0.96	0.65	44,44,44,44	0
31	MG	Y	204	1/1	0.96	0.31	82,82,82,82	0
31	MG	X	2921	1/1	0.97	0.42	81,81,81,81	0
32	1F2	X	2929	56/56	0.97	0.19	42,68,77,83	0
31	MG	X	2927	1/1	0.97	0.50	62,62,62,62	0
31	MG	X	2914	1/1	0.97	0.40	27,27,27,27	0
31	MG	X	2901	1/1	0.98	0.36	50,50,50,50	0
31	MG	X	2908	1/1	0.98	0.92	37,37,37,37	0
31	MG	M	201	1/1	0.98	0.55	23,23,23,23	0
31	MG	X	2910	1/1	0.98	0.44	42,42,42,42	0
31	MG	X	2923	1/1	0.98	0.38	34,34,34,34	0
31	MG	X	2916	1/1	0.98	0.62	37,37,37,37	0
31	MG	X	2926	1/1	0.99	0.97	45,45,45,45	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.