



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:08 PM UTC

PDB ID : 5NRG / pdb_00005nrg
Title : The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with RB02
Authors : Yonath, A.; Matzov, D.; Eyal, Z.; Ben Hamou, R.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Fridman, M.
Deposited on : 2017-04-23
Resolution : 3.44 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

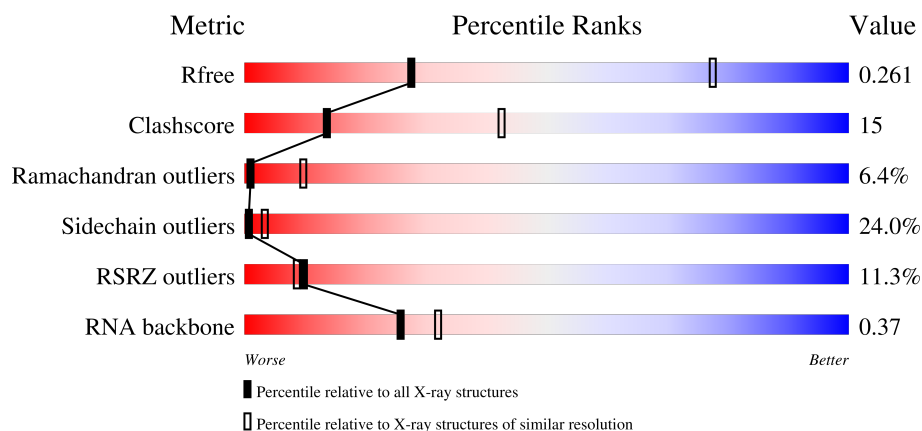
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)
RNA backbone	3983	1170 (3.88-3.00)

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

Mol	Chain	Length	Quality of chain
1	X	2923	
2	Y	114	
3	A	277	

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Mol	Chain	Length	Quality of chain
4	B	220	
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	140	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	V	69	
23	W	59	
24	Z	58	
25	2	45	
26	3	66	

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
30	MG	J	201	-	-	-	X
30	MG	X	3223	-	-	-	X
30	MG	X	3260	-	-	-	X
30	MG	X	3271	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 80800 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	2710	Total	C	N	O	P	0	1	0
			58141	25956	10658	18816	2711			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	260	Total	C	N	O	S	0	0	0
			1641	1008	314	315	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1534	961	287	281	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	198	Total	C	N	O	S	0	0	0
			1365	852	256	255	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	137	Total	C	N	O	S	0	0	0
			926	580	165	177	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	147	Total	C	N	O	0	0	0
			793	481	154	158			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1062	664	194	201	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			902	561	173	166	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	0	0	0
			780	467	162	151			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1011	651	184	172	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			883	539	176	167	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			672	410	126	136			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	111	Total	C	N	O	0	0	0
			779	492	147	140			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S	0	0	0
			937	590	186	157	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	101	Total	C	N	O	0	0	0
			700	445	128	127			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S	0	0	0
			852	532	161	156	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	90	Total	C	N	O	S	0	0	0
			656	411	111	132	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	102	Total	C	N	O	0	0	0
			596	365	111	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	174	Total	C	N	O	S	0	0	0
			1145	722	204	217	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	76	Total	C	N	O	0	0	0
			561	349	107	105			

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	0	0	0
			519	319	96	104			

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	W	57	Total	C	N	O	0	0	0
			437	272	83	82			

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Z	44	Total	C	N	O	S	0	0	0
			337	205	75	54	3			

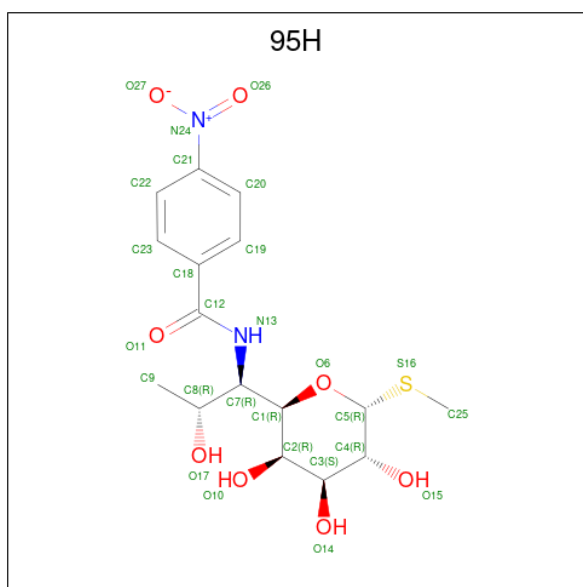
- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	44	Total	C	N	O	S	0	0	0
			360	219	87	53	1			

- Molecule 26 is a protein called 50S ribosomal protein L35.

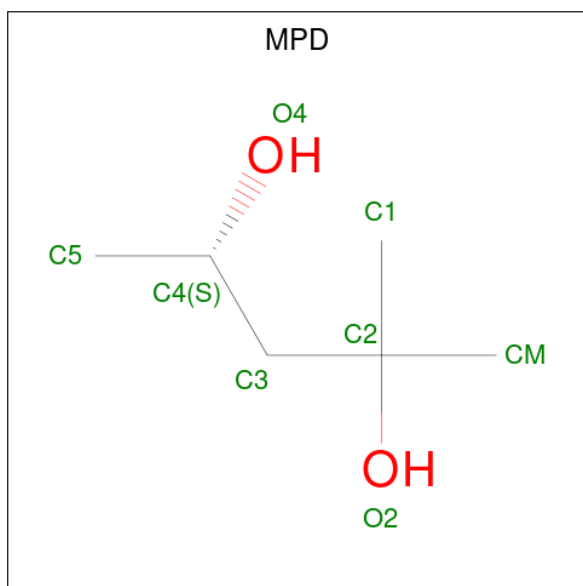
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	65	Total	C	N	O	S	0	0	0
			419	257	83	78	1			

- Molecule 27 is {N}-[(1 {R},2 {R})-1-[(2 {R},3 {R},4 {S},5 {R},6 {R})-6-methylsulfanyl-3,4,5-tris(oxidanyl)oxan-2-yl]-2-oxidanyl-propyl]-4-nitro-benzamide (CCD ID: 95H) (formula: C₁₆H₂₂N₂O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	X	1	Total	C	N	O	S	1	0
			27	16	2	8	1		

- Molecule 28 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		

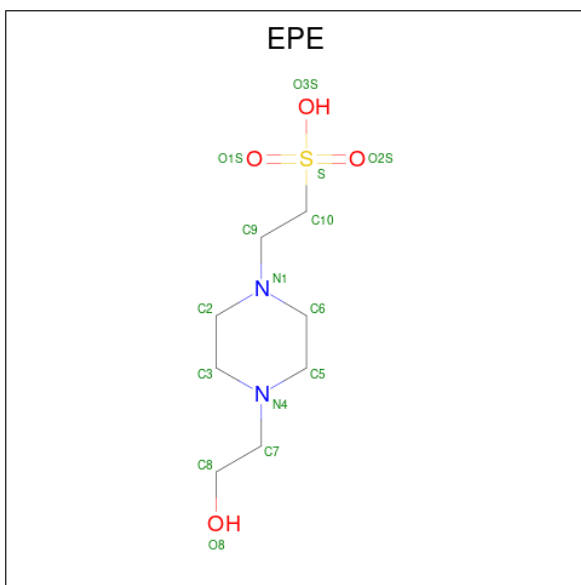
- Molecule 29 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	X	203	Total 203	Mn 203	0	0
29	Y	1	Total 1	Mn 1	0	0
29	E	1	Total 1	Mn 1	0	0
29	I	1	Total 1	Mn 1	0	0
29	Z	1	Total 1	Mn 1	0	0
29	3	3	Total 3	Mn 3	0	0

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

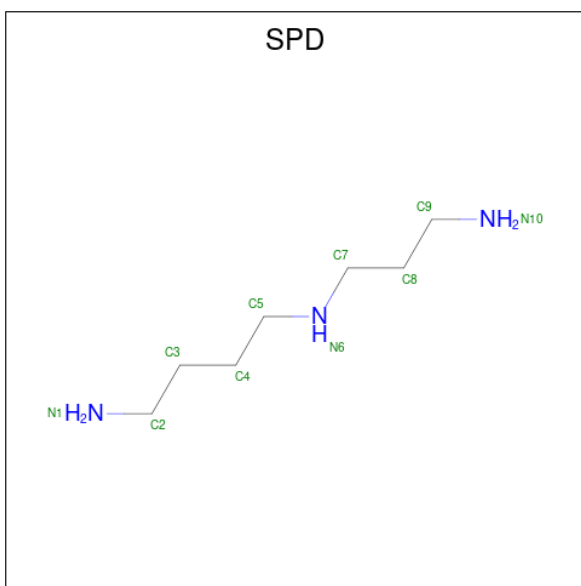
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	78	Total 78	Mg 78	0	0
30	Y	2	Total 2	Mg 2	0	0
30	C	1	Total 1	Mg 1	0	0
30	G	1	Total 1	Mg 1	0	0
30	J	1	Total 1	Mg 1	0	0
30	3	1	Total 1	Mg 1	0	0

- Molecule 31 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 32 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).

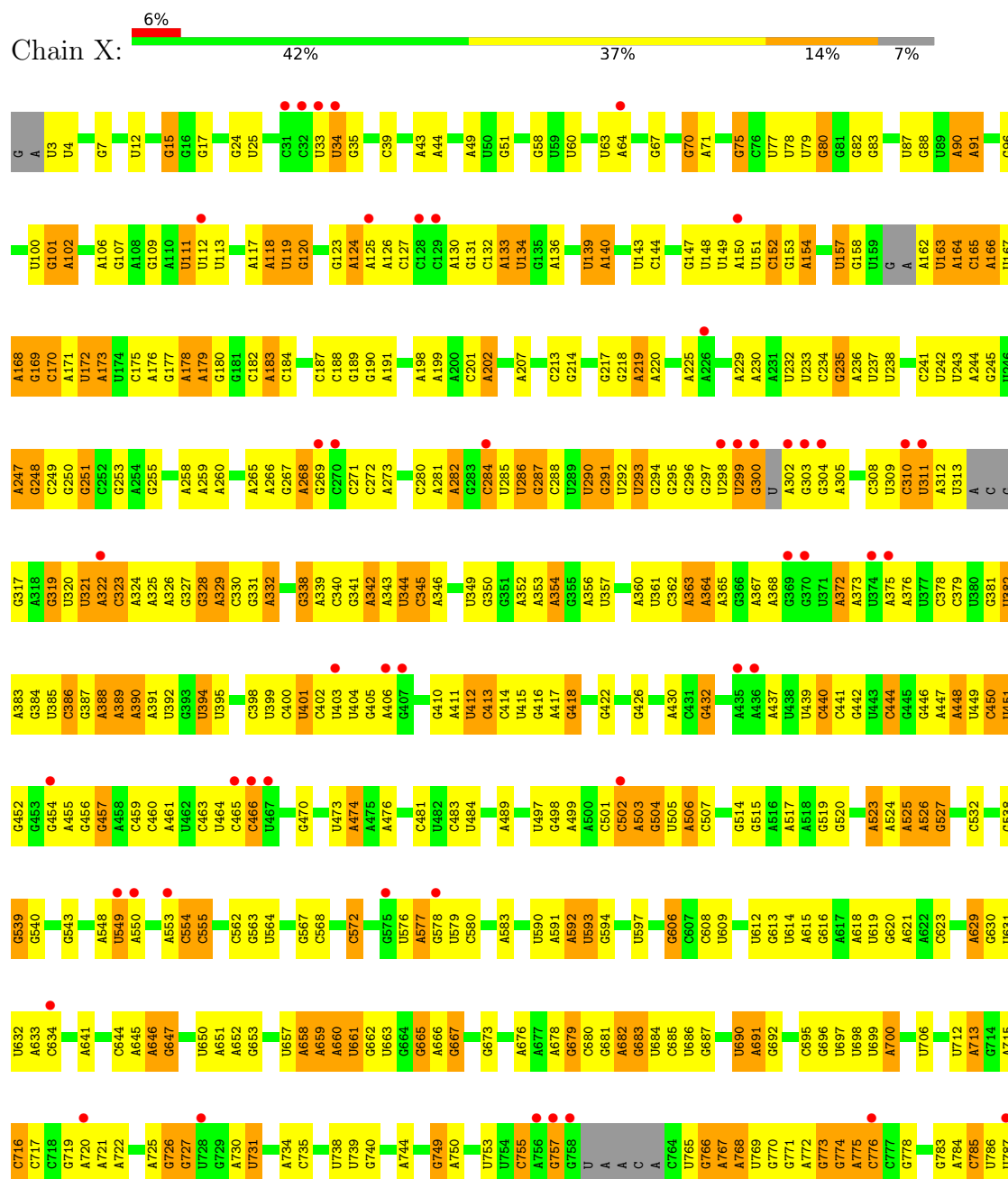


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	N	0	0
			10	7	3		

3 Residue-property plots

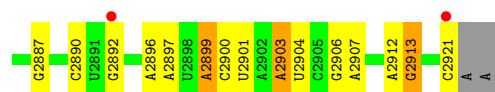
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

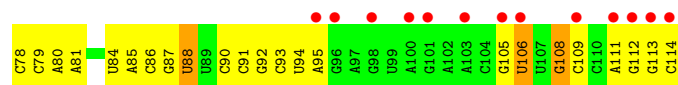
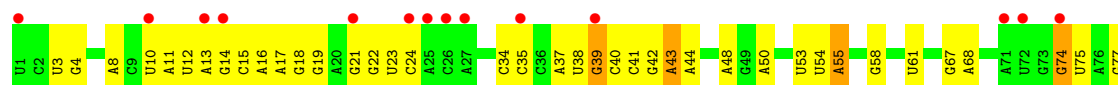




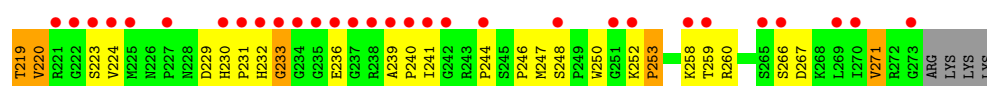
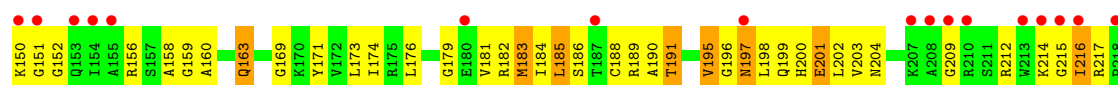
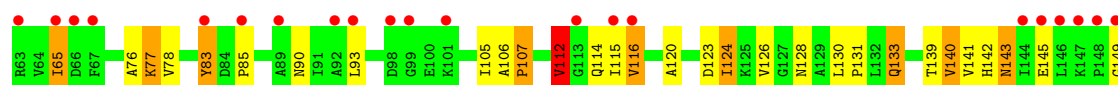
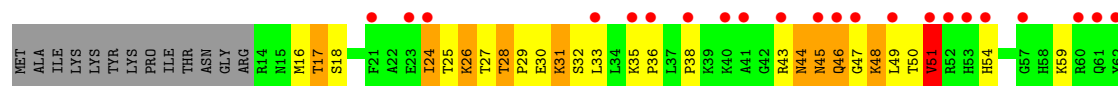
U2783	U2784	C2787	A2792	C2793	C2801	A2802	A2805	U2806	C2807	C2816	A2817	A2818	C2819	U2820	C	G2823	G2824	A2827	U2828	A2832	A2843	U2844	G2845	U2846	U2847	A2848	A2849	G2850	U2851	U2751	A2752	A2854	A2855	U2856	A2857	U2860	G2863	C2873	A2874	U2875	G2876	G2877	U2878	A2882	U2883	G2884																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
U2607	G2608	G2609	G2610	U2611	U2612	C2618	U2619	U2620	C2621	U2622	U2623	G2624	A2625	A2628	U2629	C2632	G2633	G2634	G2635	U2636	G2637	C2638	G2639	U2640	A2641	U2642	U2646	U2649	G2650	A2656	G2657	G2658	A2659	U2663	U2664	A2668	G2669	G2670	A2671	G2672	G2673	U2674	U2677	U2682	U2683	A2687	G2688	C2693	G2694																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G2695	G2696	G2697	A2698	U2701	A2704	U2705	A2706	C2707	U2708	U2709	U2710	G2711	G2712	U2715	U2716	A2717	G2718	C2719	A2720	U2725	C2726	G2729	C2730	U2731	A2732	U2733	C2734	G2735	C2736	C2737	A2740	G2741	U2751	A2752	A2854	U2855	A2856	A2857	A2760	U2766	U2771	G2774	A2775	U2776	G2777	U2778	C2779	A2780	U2781	C2782																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G2513	G2514	C2528	G2529	U2530	U2531	G2532	U2533	G2534	A2540	A2545	U2546	G2547	C2548	U2549	G2550	G2551	G2552	G2553	G2554	U2555	G2556	U2557	C2561	G2562	G2563	U2564	G2565	G2570	G2571	U2574	G2575	G2576	U2579	G2580	U2581	U2582	C2587	A2588	U2589	U2590	A2591	A2592	A2593	G2594	C2600	G2603	A2604	G2605	G2606																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G2442	A2445	U2446	C2447	G2448	C2449	U2450	C2451	A2452	A2453	C2454	G2455	G2456	A2457	U2458	A2459	A2462	U2465	A2466	C2467	C2468	G2469	G2470	G2471	G2472	G2473	G2474	A2475	U2476	C2479	A2480	U2485	A2486	C2492	G2493	C2494	A2495	A2496	G2497	A2498	U2499	U2500	U2501	C2502	A2503	G2504	A2505	U2506	C2507	G2508	G2511	G2512																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C2359	A2360	A2361	A2362	G2363	G2364	G2365	G2366	A2367	G2368	G2369	U2370	U2371	G2372	A2373	C2374	U2375	G2376	C2377	G2378	C2382	C2383	A2384	A2385	C2386	A2387	A2388	C2391	G2392	A2393	G2398	G2399	U2400	G2401	G2402	A2407	C2408	G2409	G2410	A2411	C2412	G2416	U2417	G2418	A2419	C2422	G2423	U2429	C2430	C2431	G2432	A2434																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
A2293	A2294	A2295	G2298	U2299	A2300	A2301	C2302	G2303	G2304	A2305	G2306	G2307	G2308	G2309	C2310	U2311	A2314	A2315	U2319	U2320	C2321	C2322	U2323	C2324	A2325	G2326	U2329	G2330	G2331	U2332	U2333	G2334	G2335	A2336	A2337	A2338	G2339	C2340	A2341	U2342	U2343	A2347	G2348	A2349	G2350	U2351	G2352	U2353	A2354	A2355	A2356	G2358																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G	U	G	U	U2216	G2217	G2218	U2219	U2220	U2221	U2222	C2223	U2224	A2225	C2229	G2230	G2231	A2232	C2233	C2234	A2235	G2236	U2237	U2238	A2239	U2240	C2241	G2242	U2243	G2244	G2245	U2246	G2247	G2248	G2249	A2250	G2251	A2252	C2253	G2254	G2255	U2256	A2260	A2261	G2262	G2265	G2266	C2267	A2268	G2269	U2270	C2271	G2272	G2273	G2274	G2275	G2276	G2277	G2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	G2286	G2287	G2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2298	G2299	G2300	G2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	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	G2392	G2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	G2401	G2402	G2403	G2404	G2405	G2406	G2407	G2408	G2409	G2410	G2411	G2412	G2413	G2414	G2415	G2416	G2417	G2418	G2419	G2420	G2421	G2422	G2423	G2424	G2425	G2426	G2427	G2428	G2429	G2430	G2431	G2432	G2433	G2434	G2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	G2448	G2449	G2450	G2451	G2452	G2453	G2454	G2455	G2456	G2457	G2458	G2459	G2460	G2461	G2462	G2463	G2464	G2465	G2466	G2467	G2468	G2469	G2470	G2471	G2472	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	G2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2552	G2553	G2554	G2555	G2556	G2557	G2558	G2559	G2560	G2561	G2562	G2563	G2564	G2565	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	G2579	G2580	G2581	G2582	G2583	G2584	G2585	G2586	G2587	G2588	G2589	G2590	G2591	G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601	G2602	G2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	G2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	G2764	G2765	G2766	G2767	G2768	G2769	G2770	G2771	G2772	G2773	G2774	G2775	G2776	G2777	G2778	G2779	G2780	G2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	G2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	G2799	G2800	G2801	G2802	G2803	G2804	G2805	G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2919	G2920	G2921	G2922	G2923	G2924	G2925	G2926	G2927	G2928	G2929	G2930	G2931	G2932	G2933	G2934	G2935	G2936	G2937	G2938	G2939	G2940	G2941	G2942	G2943	G2944	G2945	G2946	G2947	G2948	G2949	G2950	G2951	G2952	G2953	G2954	G2955	G2956	G2957	G2958	G2959	G2960	G2961	G2962	G2963	G2964	G2965	G2966	G2967	G2968	G2969	G2970	G2971	G2972	G2973	G2974	G2975	G2976	G2977	G2978	G2979	G2980	G2981	G2982	G2983	G2984	G2985	G2986	G2987	G2988	G2989	G2990	G2991	G2992	G2993	G2994	G2995	G2996	G2997	G2998	G2999	G3000	G3001	G3002	G3003	G3004	G3005	G3006	G3007	G3008	G3009	G3010	G3011	G3012	G3013	G3014	G3015	G3016	G3017	G3018	G3019	G3020	G3021	G3022	G3023	G3024	G3025	G3026	G3027	G3028	G3029	G3030	G3031	G3032	G3033	G3034	G3035	G3036	G3037	G3038	G3039	G3040	G3041	G3042	G3043	G3044	G3045	G3046	G3047	G3048	G3049	G3050	G3051	G3052	G3053	G3054	G3055	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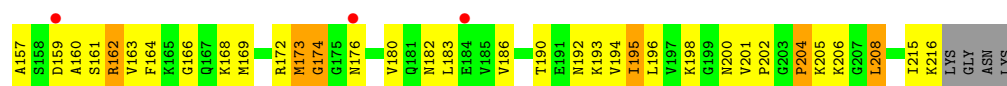
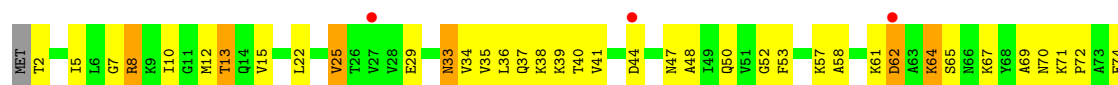
• Molecule 2: 5S ribosomal RNA



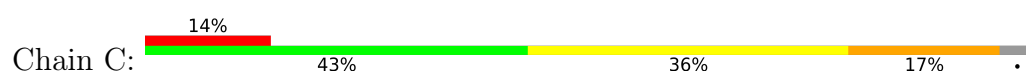
• Molecule 3: 50S ribosomal protein L2

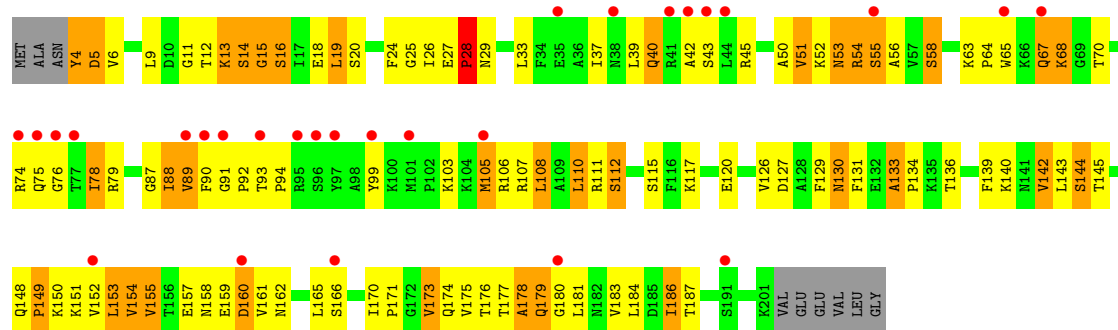


• Molecule 4: 50S ribosomal protein L3

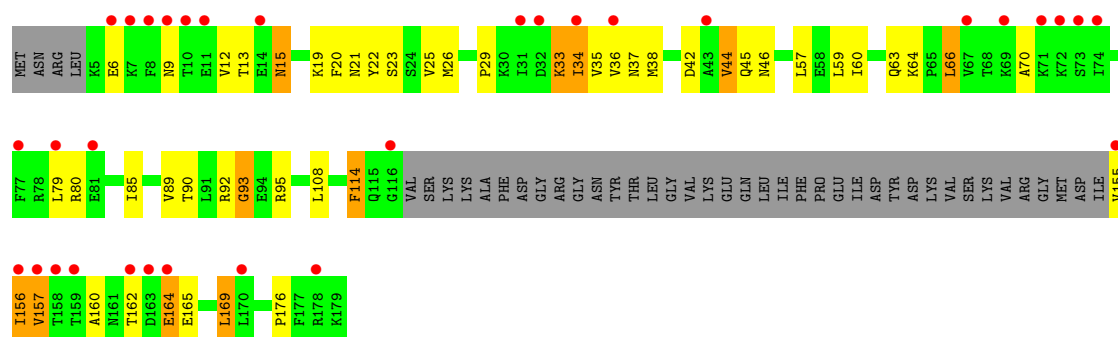


• Molecule 5: 50S ribosomal protein L4

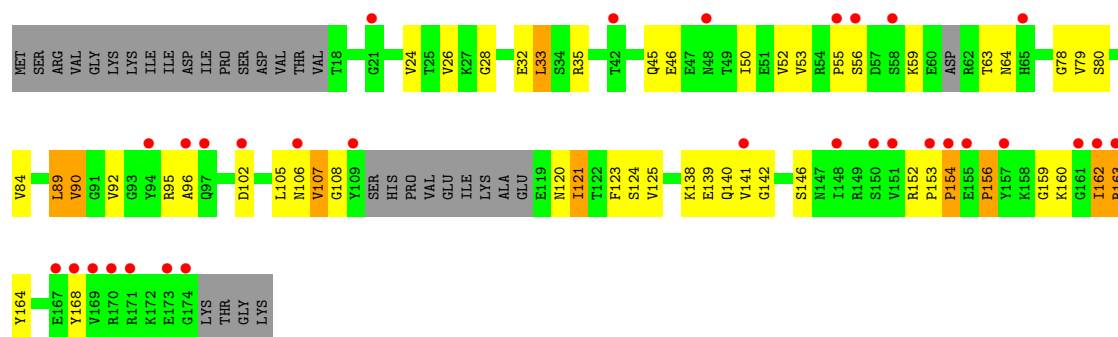




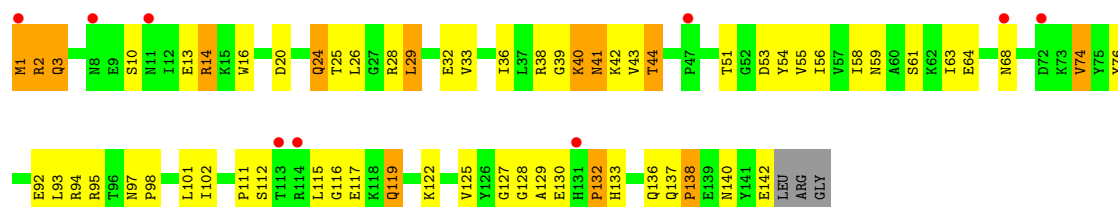
• Molecule 6: 50S ribosomal protein L5



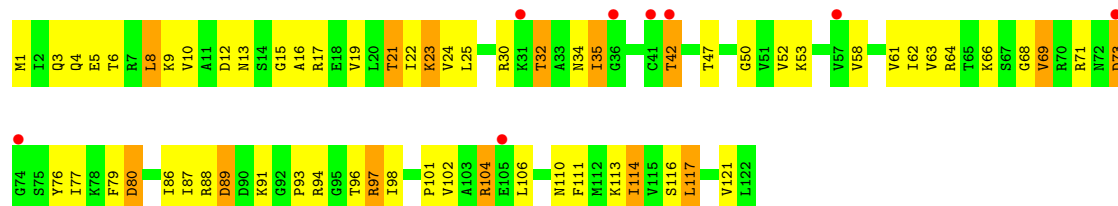
• Molecule 7: 50S ribosomal protein L6



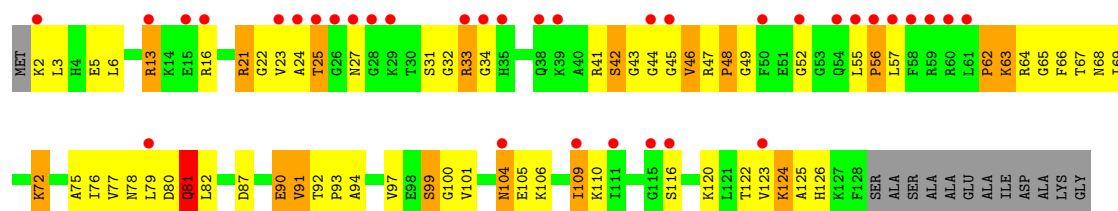
• Molecule 8: 50S ribosomal protein L13



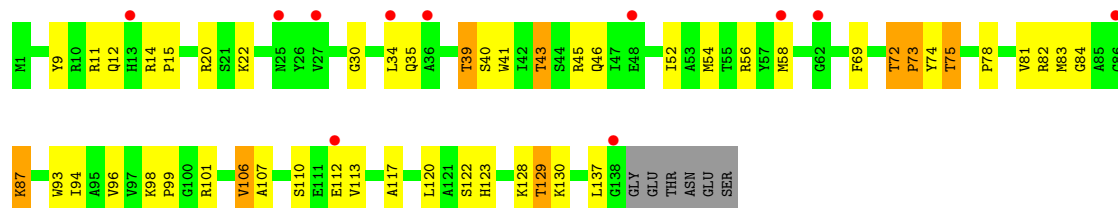
- Molecule 9: 50S ribosomal protein L14



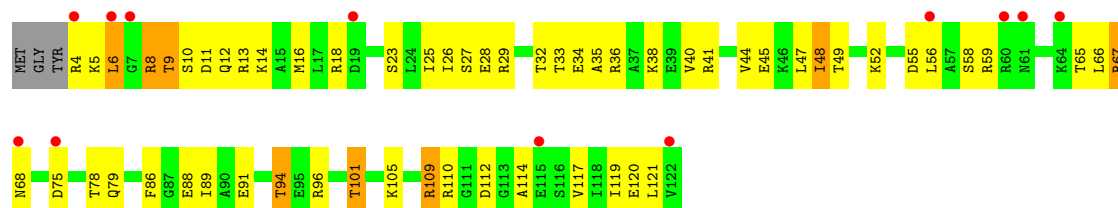
- Molecule 10: 50S ribosomal protein L15



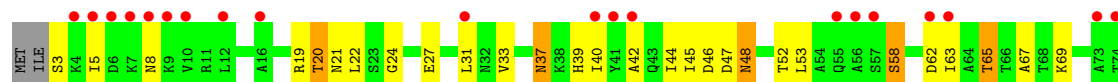
- Molecule 11: 50S ribosomal protein L16

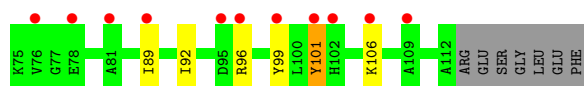


- Molecule 12: 50S ribosomal protein L17

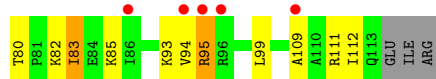
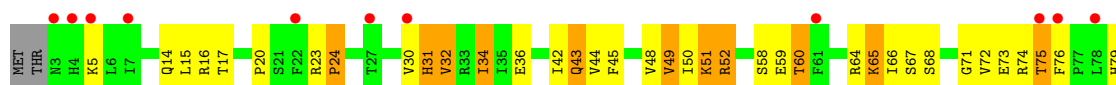


- Molecule 13: 50S ribosomal protein L18

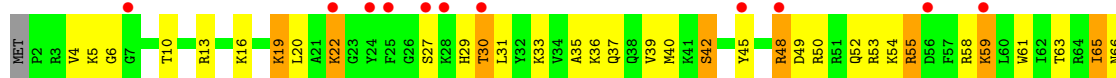




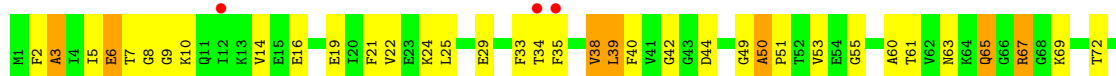
• Molecule 14: 50S ribosomal protein L19



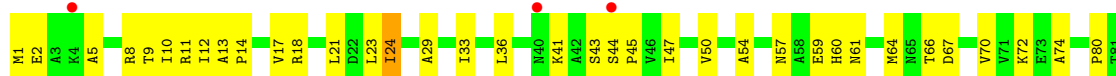
• Molecule 15: 50S ribosomal protein L20



• Molecule 16: 50S ribosomal protein L21

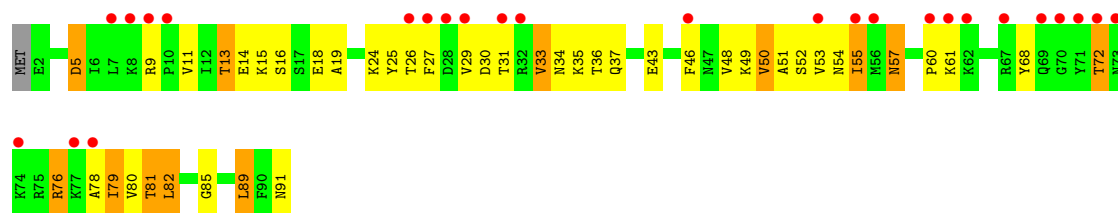


• Molecule 17: 50S ribosomal protein L22

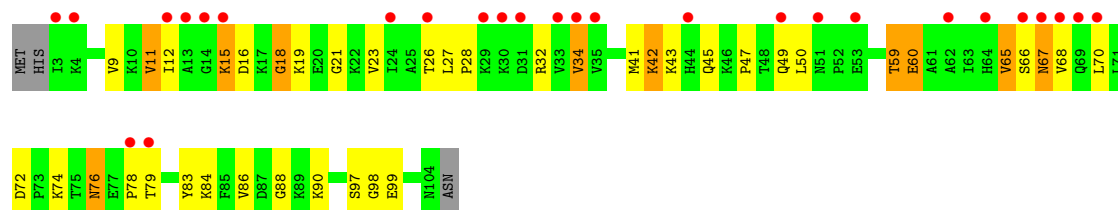


• Molecule 18: 50S ribosomal protein L23

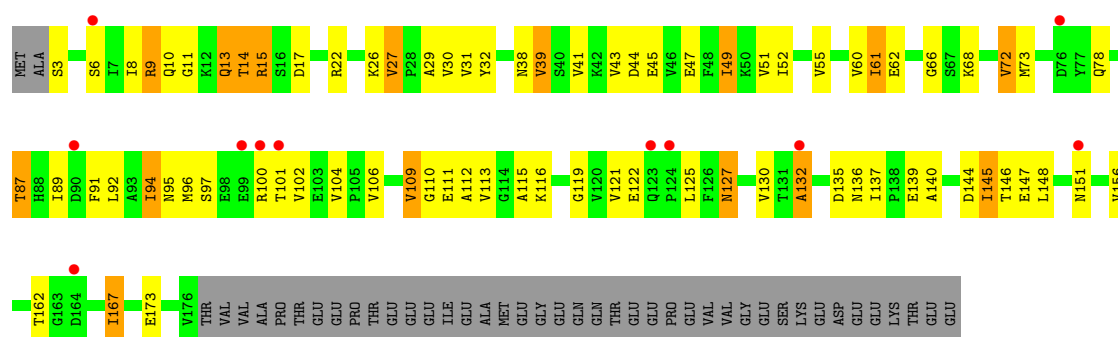
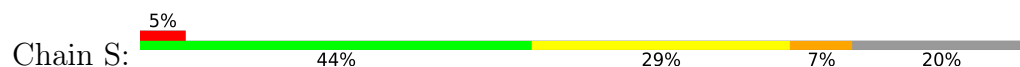




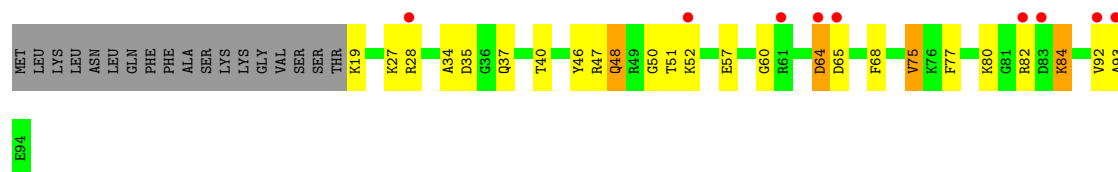
• Molecule 19: 50S ribosomal protein L24



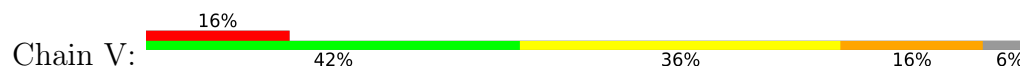
• Molecule 20: 50S ribosomal protein L25



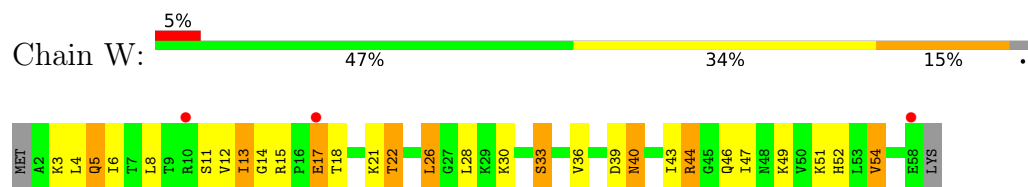
• Molecule 21: 50S ribosomal protein L27



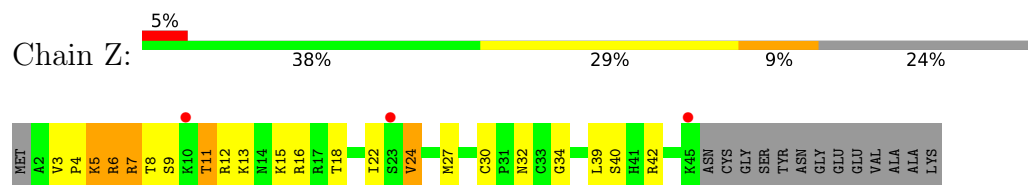
• Molecule 22: 50S ribosomal protein L29



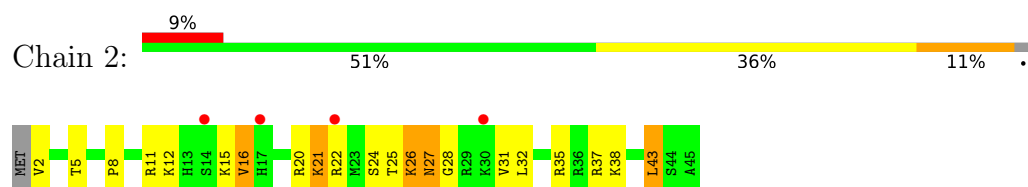
• Molecule 23: 50S ribosomal protein L30



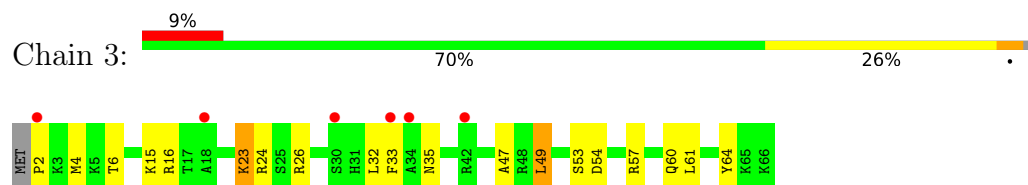
• Molecule 24: 50S ribosomal protein L32



• Molecule 25: 50S ribosomal protein L34



• Molecule 26: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.80Å 279.80Å 873.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.37 – 3.44 49.37 – 3.44	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.37-3.44) 96.1 (49.37-3.44)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.219 , 0.261 0.219 , 0.261	Depositor DCC
R_{free} test set	12721 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	99.6	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	80800	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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: 95H, MG, MPD, SPD, MN, EPE

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	0.46	0/65104	0.65	4/101503 (0.0%)
2	Y	0.41	0/2717	0.58	0/4232
3	A	0.53	0/1665	0.85	0/2275
4	B	0.54	0/1557	0.80	1/2102 (0.0%)
5	C	0.62	0/1386	0.96	2/1890 (0.1%)
6	D	0.40	1/934 (0.1%)	0.57	1/1273 (0.1%)
7	E	0.30	0/798	0.72	0/1102
8	G	0.44	0/1083	0.72	0/1466
9	H	0.44	0/908	0.72	0/1221
10	I	0.53	0/789	0.90	2/1073 (0.2%)
11	J	0.53	1/1034 (0.1%)	0.72	1/1401 (0.1%)
12	K	0.38	0/885	0.64	0/1185
13	L	0.36	0/678	0.64	0/934
14	M	0.54	0/790	0.90	1/1071 (0.1%)
15	N	0.60	0/949	0.84	2/1258 (0.2%)
16	O	0.59	0/710	0.86	0/962
17	P	0.61	0/860	0.81	0/1159
18	Q	0.43	0/662	0.67	0/898
19	R	0.48	0/601	0.75	0/830
20	S	0.42	0/1158	0.64	0/1588
21	T	0.45	0/567	0.68	0/756
22	V	0.36	0/520	0.61	0/694
23	W	0.54	0/439	0.71	0/592
24	Z	0.57	0/342	0.77	0/456
25	2	0.61	0/363	0.79	0/475
26	3	0.47	0/424	0.86	0/578
All	All	0.46	2/87923 (0.0%)	0.67	14/132974 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	3
4	B	0	5
5	C	0	5
7	E	0	1
8	G	0	5
9	H	0	1
10	I	0	4
11	J	0	1
14	M	0	1
16	O	0	2
18	Q	0	1
19	R	0	2
All	All	0	31

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	69	PHE	C-N	-7.64	1.16	1.33
6	D	108	LEU	C-N	7.17	1.50	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	6	GLU	CB-CA-C	-7.06	107.63	117.23
11	J	84	GLY	N-CA-C	6.29	128.08	113.18
10	I	25	THR	N-CA-C	6.21	124.03	110.80
4	B	98	ALA	CB-CA-C	-6.02	107.91	116.34
1	X	1702	C	OP1-P-OP2	5.61	136.42	119.60

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	156	ARG	Peptide
3	A	195	VAL	Peptide
3	A	50	THR	Peptide
4	B	58	ALA	Peptide
4	B	97	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58141	0	29232	1122	0
2	Y	2430	0	1229	57	0
3	A	1641	0	1415	76	0
4	B	1534	0	1495	56	0
5	C	1365	0	1258	90	0
6	D	926	0	824	34	0
7	E	793	0	475	17	0
8	G	1062	0	1000	35	0
9	H	902	0	956	41	0
10	I	780	0	621	38	0
11	J	1011	0	988	32	0
12	K	883	0	890	44	0
13	L	672	0	515	14	0
14	M	779	0	726	28	0
15	N	937	0	1003	51	0
16	O	700	0	629	32	0
17	P	852	0	905	33	0
18	Q	656	0	615	34	0
19	R	596	0	450	23	0
20	S	1145	0	991	40	0
21	T	561	0	555	17	0
22	V	519	0	530	25	0
23	W	437	0	474	18	0
24	Z	337	0	343	20	0
25	2	360	0	402	16	0
26	3	419	0	323	11	0
27	X	27	0	0	2	0
28	X	16	0	28	2	0
29	3	3	0	0	0	0
29	E	1	0	0	0	0
29	I	1	0	0	0	0
29	X	203	0	0	0	0
29	Y	1	0	0	0	0
29	Z	1	0	0	0	0
30	3	1	0	0	0	0
30	C	1	0	0	0	0
30	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	J	1	0	0	0	0
30	X	78	0	0	0	0
30	Y	2	0	0	0	0
31	X	15	0	17	0	0
32	X	10	0	19	3	0
All	All	80800	0	48908	1825	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 15.

The worst 5 of 1825 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)
5:C:40:GLN:HE22	5:C:178:ALA:HB2	1.24	1.00
1:X:1835:U:H2'	1:X:1836:A:H5''	1.45	0.98
1:X:1515:G:H1	1:X:1564:G:H1	1.11	0.96
1:X:2850:G:OP2	4:B:86:ARG:NH2	2.00	0.93
1:X:630:G:OP2	10:I:21:ARG:NH2	2.03	0.92

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	258/277 (93%)	189 (73%)	47 (18%)	22 (8%)	0	6
4	B	213/220 (97%)	180 (84%)	22 (10%)	11 (5%)	1	13
5	C	196/207 (95%)	147 (75%)	30 (15%)	19 (10%)	0	5
6	D	133/179 (74%)	115 (86%)	14 (10%)	4 (3%)	3	23
7	E	141/178 (79%)	79 (56%)	35 (25%)	27 (19%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	G	140/145 (97%)	127 (91%)	9 (6%)	4 (3%)	3	23
9	H	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7	32
10	I	125/140 (89%)	65 (52%)	34 (27%)	26 (21%)	0	1
11	J	136/144 (94%)	121 (89%)	11 (8%)	4 (3%)	3	23
12	K	117/122 (96%)	105 (90%)	7 (6%)	5 (4%)	2	16
13	L	108/119 (91%)	83 (77%)	15 (14%)	10 (9%)	0	5
14	M	109/116 (94%)	88 (81%)	14 (13%)	7 (6%)	1	10
15	N	114/118 (97%)	111 (97%)	2 (2%)	1 (1%)	14	45
16	O	99/102 (97%)	81 (82%)	14 (14%)	4 (4%)	2	17
17	P	110/117 (94%)	103 (94%)	6 (6%)	1 (1%)	14	45
18	Q	88/91 (97%)	75 (85%)	12 (14%)	1 (1%)	11	40
19	R	100/105 (95%)	71 (71%)	19 (19%)	10 (10%)	0	5
20	S	172/217 (79%)	133 (77%)	25 (14%)	14 (8%)	1	6
21	T	74/94 (79%)	61 (82%)	11 (15%)	2 (3%)	4	24
22	V	63/69 (91%)	59 (94%)	3 (5%)	1 (2%)	7	33
23	W	55/59 (93%)	52 (94%)	3 (6%)	0	100	100
24	Z	42/58 (72%)	37 (88%)	4 (10%)	1 (2%)	4	26
25	2	42/45 (93%)	39 (93%)	2 (5%)	1 (2%)	4	26
26	3	63/66 (96%)	49 (78%)	11 (18%)	3 (5%)	2	14
All	All	2818/3110 (91%)	2280 (81%)	358 (13%)	180 (6%)	1	10

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	35	LYS
3	A	36	PRO
3	A	38	PRO
3	A	51	VAL
3	A	77	LYS

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	125/224 (56%)	85 (68%)	40 (32%)	0	1
4	B	146/177 (82%)	110 (75%)	36 (25%)	1	3
5	C	118/169 (70%)	88 (75%)	30 (25%)	0	3
6	D	78/158 (49%)	60 (77%)	18 (23%)	1	4
7	E	26/155 (17%)	20 (77%)	6 (23%)	1	4
8	G	103/123 (84%)	83 (81%)	20 (19%)	1	7
9	H	95/100 (95%)	72 (76%)	23 (24%)	1	3
10	I	51/108 (47%)	34 (67%)	17 (33%)	0	1
11	J	92/119 (77%)	78 (85%)	14 (15%)	3	14
12	K	84/102 (82%)	67 (80%)	17 (20%)	1	6
13	L	40/95 (42%)	28 (70%)	12 (30%)	0	2
14	M	68/102 (67%)	48 (71%)	20 (29%)	0	2
15	N	95/98 (97%)	81 (85%)	14 (15%)	3	15
16	O	56/86 (65%)	40 (71%)	16 (29%)	0	2
17	P	89/94 (95%)	75 (84%)	14 (16%)	2	13
18	Q	64/82 (78%)	47 (73%)	17 (27%)	0	2
19	R	36/90 (40%)	27 (75%)	9 (25%)	0	3
20	S	91/190 (48%)	66 (72%)	25 (28%)	0	2
21	T	53/75 (71%)	45 (85%)	8 (15%)	3	14
22	V	55/62 (89%)	39 (71%)	16 (29%)	0	2
23	W	50/53 (94%)	34 (68%)	16 (32%)	0	1
24	Z	35/51 (69%)	26 (74%)	9 (26%)	0	3
25	2	37/40 (92%)	28 (76%)	9 (24%)	1	3
26	3	26/57 (46%)	21 (81%)	5 (19%)	1	7
All	All	1713/2610 (66%)	1302 (76%)	411 (24%)	1	3

5 of 411 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	L	96	ARG
17	P	66	THR
25	2	15	LYS

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Mol	Chain	Res	Type
14	M	43	GLN
15	N	59	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
22	V	17	GLN
25	2	13	HIS
14	M	79	HIS
15	N	108	GLN
17	P	97	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2690/2923 (92%)	711 (26%)	31 (1%)
2	Y	113/114 (99%)	17 (15%)	0
All	All	2803/3037 (92%)	728 (25%)	31 (1%)

5 of 728 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	12	U
1	X	15	G
1	X	34	U
1	X	35	G
1	X	39	C

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1323	A
1	X	2433	C
1	X	1520	A
1	X	2783	U
1	X	2062	G

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 299 ligands modelled in this entry, 294 are monoatomic - leaving 5 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	SPD	X	3286	-	9,9,9	0.33	0	8,8,8	0.32	0
27	95H	X	3001	-	26,28,28	1.80	5 (19%)	33,40,40	2.58	11 (33%)
28	MPD	X	3002	-	7,7,7	0.30	0	9,10,10	0.19	0
31	EPE	X	3285	-	15,15,15	0.54	0	19,20,20	0.95	1 (5%)
28	MPD	X	3003	-	7,7,7	1.52	1 (14%)	9,10,10	0.72	0

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	SPD	X	3286	-	-	0/7/7/7	-
27	95H	X	3001	-	-	6/20/42/42	0/2/2/2
28	MPD	X	3002	-	-	3/5/5/5	-
31	EPE	X	3285	-	-	5/9/19/19	0/1/1/1
28	MPD	X	3003	-	-	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)
27	X	3001	95H	C12-N13	6.06	1.48	1.34
28	X	3003	MPD	C3-C2	3.36	1.64	1.54
27	X	3001	95H	C18-C12	-3.11	1.43	1.50
27	X	3001	95H	C21-N24	2.91	1.52	1.45
27	X	3001	95H	C20-C21	2.64	1.43	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	3001	95H	C22-C21-N24	-7.84	112.49	119.34
27	X	3001	95H	C20-C21-N24	6.17	124.73	119.34
27	X	3001	95H	C20-C19-C18	-4.65	115.83	120.80
27	X	3001	95H	C23-C18-C19	4.52	124.32	118.57
27	X	3001	95H	O6-C1-C7	3.32	113.67	105.79

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	X	3001	95H	O6-C5-S16-C25
31	X	3285	EPE	C10-C9-N1-C6
31	X	3285	EPE	C9-C10-S-O2S
27	X	3001	95H	C18-C12-N13-C7
27	X	3001	95H	O11-C12-N13-C7

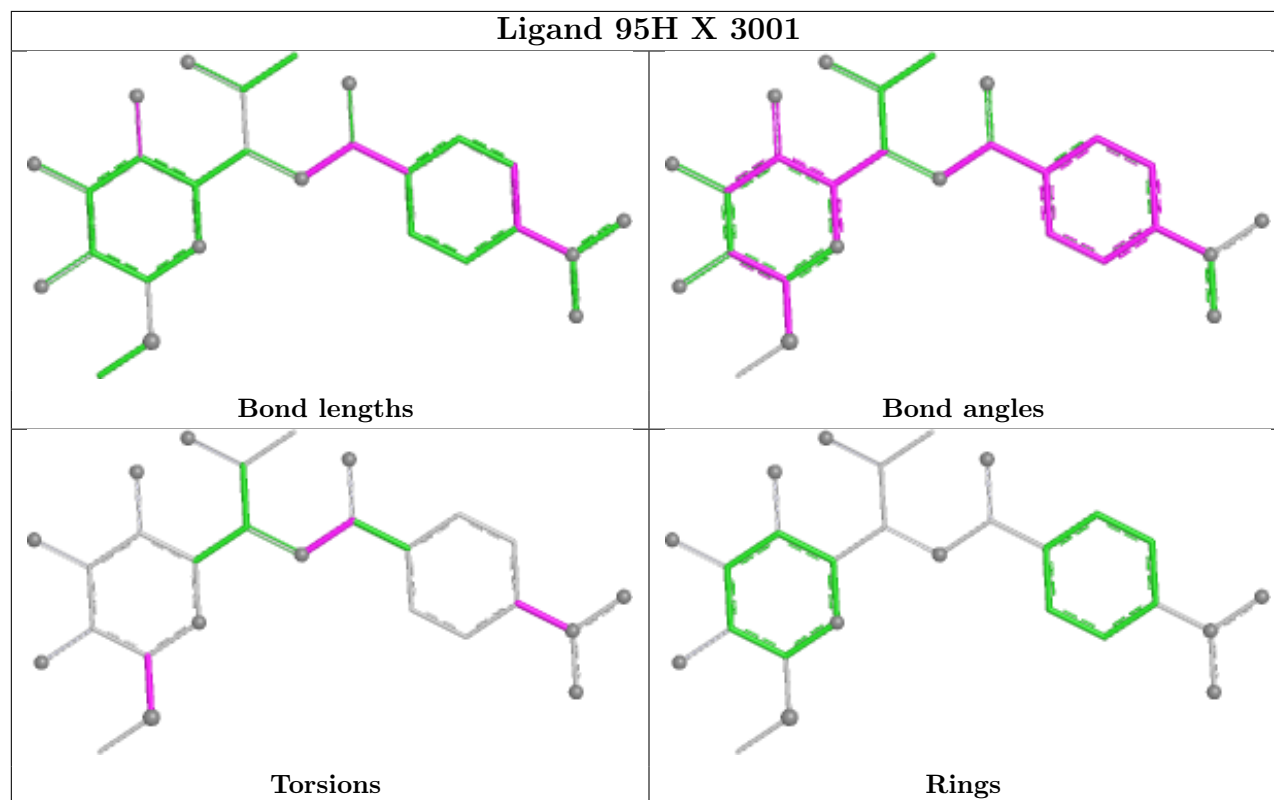
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	3286	SPD	3	0
27	X	3001	95H	2	0
28	X	3002	MPD	1	0
28	X	3003	MPD	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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	69:PHE	C	70:PRO	N	1.16

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	2710/2923 (92%)	0.34	175 (6%) 25 18	36, 97, 197, 300	1 (0%)
2	Y	114/114 (100%)	1.22	27 (23%) 2 3	68, 128, 188, 250	0
3	A	260/277 (93%)	1.72	90 (34%) 1 1	87, 134, 168, 183	0
4	B	215/220 (97%)	0.53	18 (8%) 17 13	50, 74, 96, 119	0
5	C	198/207 (95%)	1.05	28 (14%) 6 6	63, 92, 113, 140	0
6	D	137/179 (76%)	1.33	32 (23%) 2 3	162, 186, 212, 219	0
7	E	147/178 (82%)	1.13	31 (21%) 2 3	122, 156, 181, 185	0
8	G	142/145 (97%)	0.54	9 (6%) 26 18	58, 70, 87, 95	0
9	H	122/122 (100%)	0.48	8 (6%) 24 17	75, 93, 118, 125	0
10	I	127/140 (90%)	1.32	35 (27%) 1 2	49, 108, 135, 139	0
11	J	138/144 (95%)	0.78	11 (7%) 18 14	69, 89, 116, 141	0
12	K	119/122 (97%)	0.74	12 (10%) 12 10	63, 81, 115, 135	0
13	L	110/119 (92%)	1.45	31 (28%) 1 2	106, 120, 143, 152	0
14	M	111/116 (95%)	0.77	16 (14%) 6 6	77, 91, 127, 151	0
15	N	116/118 (98%)	0.68	12 (10%) 12 10	49, 65, 90, 102	0
16	O	101/102 (99%)	0.32	5 (4%) 34 22	47, 79, 98, 115	0
17	P	112/117 (95%)	0.41	4 (3%) 46 30	59, 70, 103, 129	0
18	Q	90/91 (98%)	1.51	26 (28%) 1 2	100, 123, 152, 170	0
19	R	102/105 (97%)	1.41	27 (26%) 1 2	95, 115, 171, 180	0
20	S	174/217 (80%)	0.52	11 (6%) 26 18	75, 102, 184, 192	0
21	T	76/94 (80%)	0.69	9 (11%) 9 8	76, 88, 113, 155	0
22	V	65/69 (94%)	1.08	11 (16%) 4 4	119, 136, 160, 164	0
23	W	57/59 (96%)	0.16	3 (5%) 32 21	59, 71, 95, 103	0
24	Z	44/58 (75%)	0.75	3 (6%) 23 17	55, 86, 144, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	44/45 (97%)	1.06	4 (9%) 15 12	80, 89, 96, 104	0
26	3	65/66 (98%)	0.81	6 (9%) 14 12	70, 81, 95, 100	0
All	All	5696/6147 (92%)	0.65	644 (11%) 10 9	36, 96, 186, 300	1 (0%)

The worst 5 of 644 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	233	GLY	10.4
3	A	234	GLY	8.6
3	A	235	GLY	7.7
15	N	56	ASP	7.3
1	X	1993	A	7.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MG	X	3255	1/1	0.08	0.22	112,112,112,112	0
30	MG	X	3268	1/1	0.15	0.17	134,134,134,134	0
29	MN	X	3145	1/1	0.32	0.20	144,144,144,144	0
30	MG	X	3227	1/1	0.34	0.22	93,93,93,93	0
30	MG	J	201	1/1	0.36	0.61	107,107,107,107	0
30	MG	X	3224	1/1	0.45	0.16	97,97,97,97	0
30	MG	X	3267	1/1	0.47	0.13	91,91,91,91	0
30	MG	X	3240	1/1	0.48	0.23	87,87,87,87	0
30	MG	C	301	1/1	0.53	0.19	74,74,74,74	0
30	MG	X	3246	1/1	0.61	0.23	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3266	1/1	0.61	0.26	119,119,119,119	0
30	MG	X	3264	1/1	0.62	0.27	102,102,102,102	0
30	MG	X	3168	1/1	0.65	0.15	73,73,73,73	0
29	MN	X	3222	1/1	0.68	0.11	142,142,142,142	0
29	MN	X	3203	1/1	0.71	0.15	141,141,141,141	0
30	MG	X	3271	1/1	0.71	0.53	90,90,90,90	0
30	MG	X	3256	1/1	0.73	0.33	91,91,91,91	0
29	MN	X	3062	1/1	0.73	0.10	135,135,135,135	0
30	MG	X	3181	1/1	0.74	0.16	89,89,89,89	0
30	MG	X	3242	1/1	0.74	0.24	60,60,60,60	0
29	MN	X	3156	1/1	0.74	0.16	104,104,104,104	0
29	MN	X	3214	1/1	0.74	0.13	125,125,125,125	0
30	MG	X	3259	1/1	0.75	0.28	61,61,61,61	0
30	MG	X	3260	1/1	0.75	0.50	73,73,73,73	0
30	MG	X	3196	1/1	0.75	0.21	78,78,78,78	0
29	MN	X	3235	1/1	0.76	0.12	118,118,118,118	0
30	MG	X	3223	1/1	0.76	0.49	71,71,71,71	0
30	MG	X	3265	1/1	0.76	0.11	73,73,73,73	0
28	MPD	X	3003	8/8	0.77	0.26	80,80,80,80	0
30	MG	Y	203	1/1	0.78	0.09	122,122,122,122	0
30	MG	X	3269	1/1	0.78	0.39	104,104,104,104	0
30	MG	X	3250	1/1	0.78	0.24	66,66,66,66	0
29	MN	3	102	1/1	0.79	0.22	101,101,101,101	0
30	MG	X	3241	1/1	0.79	0.16	91,91,91,91	0
30	MG	X	3276	1/1	0.79	0.24	67,67,67,67	0
29	MN	X	3075	1/1	0.80	0.15	102,102,102,102	0
30	MG	X	3247	1/1	0.80	0.27	69,69,69,69	0
29	MN	X	3229	1/1	0.81	0.08	144,144,144,144	0
29	MN	X	3141	1/1	0.81	0.15	104,104,104,104	0
29	MN	X	3194	1/1	0.82	0.10	140,140,140,140	0
30	MG	X	3160	1/1	0.82	0.12	69,69,69,69	0
29	MN	X	3169	1/1	0.82	0.23	98,98,98,98	0
29	MN	X	3179	1/1	0.82	0.14	110,110,110,110	0
30	MG	X	3262	1/1	0.82	0.12	82,82,82,82	0
30	MG	X	3249	1/1	0.82	0.24	89,89,89,89	0
30	MG	X	3183	1/1	0.82	0.26	72,72,72,72	0
30	MG	X	3254	1/1	0.82	0.31	67,67,67,67	0
30	MG	X	3182	1/1	0.83	0.16	53,53,53,53	0
29	MN	X	3234	1/1	0.83	0.14	137,137,137,137	0
30	MG	X	3239	1/1	0.83	0.17	46,46,46,46	0
30	MG	X	3261	1/1	0.83	0.17	163,163,163,163	0
29	MN	X	3074	1/1	0.84	0.12	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3154	1/1	0.84	0.12	114,114,114,114	0
32	SPD	X	3286	10/10	0.84	0.23	65,65,65,65	0
30	MG	X	3251	1/1	0.85	0.14	65,65,65,65	0
29	MN	X	3008	1/1	0.85	0.11	50,50,50,50	0
29	MN	X	3172	1/1	0.85	0.07	126,126,126,126	0
29	MN	X	3198	1/1	0.85	0.11	100,100,100,100	0
29	MN	X	3171	1/1	0.86	0.13	117,117,117,117	0
30	MG	X	3226	1/1	0.86	0.31	74,74,74,74	0
30	MG	X	3270	1/1	0.86	0.17	68,68,68,68	0
30	MG	X	3193	1/1	0.86	0.42	78,78,78,78	0
30	MG	X	3274	1/1	0.86	0.28	69,69,69,69	0
30	MG	X	3228	1/1	0.86	0.26	65,65,65,65	0
30	MG	X	3283	1/1	0.86	0.24	59,59,59,59	0
29	MN	X	3189	1/1	0.86	0.08	123,123,123,123	0
30	MG	X	3197	1/1	0.86	0.07	54,54,54,54	0
30	MG	X	3202	1/1	0.86	0.16	64,64,64,64	0
29	MN	X	3162	1/1	0.86	0.09	110,110,110,110	0
29	MN	X	3205	1/1	0.87	0.14	143,143,143,143	0
30	MG	X	3195	1/1	0.87	0.15	57,57,57,57	0
30	MG	X	3257	1/1	0.87	0.08	156,156,156,156	0
30	MG	X	3072	1/1	0.87	0.24	41,41,41,41	0
30	MG	X	3112	1/1	0.87	0.14	84,84,84,84	0
30	MG	X	3152	1/1	0.87	0.14	57,57,57,57	0
29	MN	X	3006	1/1	0.87	0.14	49,49,49,49	0
29	MN	X	3191	1/1	0.87	0.09	126,126,126,126	0
29	MN	X	3150	1/1	0.87	0.08	98,98,98,98	0
28	MPD	X	3002	8/8	0.87	0.19	96,96,96,96	0
30	MG	3	104	1/1	0.87	0.18	56,56,56,56	0
29	MN	X	3184	1/1	0.87	0.09	126,126,126,126	0
30	MG	X	3280	1/1	0.88	0.22	66,66,66,66	0
29	MN	X	3231	1/1	0.88	0.11	125,125,125,125	0
30	MG	X	3263	1/1	0.88	0.27	81,81,81,81	0
30	MG	X	3258	1/1	0.88	0.09	64,64,64,64	0
29	MN	X	3178	1/1	0.88	0.08	108,108,108,108	0
30	MG	X	3069	1/1	0.88	0.20	52,52,52,52	0
30	MG	X	3238	1/1	0.88	0.30	58,58,58,58	0
29	MN	X	3219	1/1	0.89	0.06	118,118,118,118	0
29	MN	3	103	1/1	0.89	0.09	129,129,129,129	0
30	MG	X	3032	1/1	0.89	0.21	31,31,31,31	0
30	MG	X	3058	1/1	0.89	0.24	63,63,63,63	0
29	MN	X	3018	1/1	0.89	0.10	86,86,86,86	0
30	MG	X	3253	1/1	0.89	0.13	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3123	1/1	0.89	0.09	109,109,109,109	0
29	MN	X	3170	1/1	0.89	0.11	103,103,103,103	0
29	MN	X	3131	1/1	0.89	0.16	114,114,114,114	0
30	MG	X	3201	1/1	0.89	0.17	66,66,66,66	0
29	MN	X	3026	1/1	0.89	0.17	94,94,94,94	0
29	MN	E	201	1/1	0.90	0.14	125,125,125,125	0
29	MN	Z	101	1/1	0.90	0.13	109,109,109,109	0
29	MN	X	3221	1/1	0.90	0.06	141,141,141,141	0
30	MG	X	3279	1/1	0.90	0.28	66,66,66,66	0
29	MN	X	3199	1/1	0.90	0.08	131,131,131,131	0
29	MN	X	3165	1/1	0.90	0.07	109,109,109,109	0
30	MG	X	3204	1/1	0.90	0.07	67,67,67,67	0
30	MG	X	3218	1/1	0.90	0.19	74,74,74,74	0
29	MN	X	3192	1/1	0.90	0.11	106,106,106,106	0
29	MN	X	3063	1/1	0.90	0.07	140,140,140,140	0
29	MN	X	3067	1/1	0.90	0.08	103,103,103,103	0
29	MN	X	3174	1/1	0.91	0.15	115,115,115,115	0
29	MN	X	3096	1/1	0.91	0.23	98,98,98,98	0
29	MN	X	3064	1/1	0.91	0.18	124,124,124,124	0
29	MN	X	3130	1/1	0.91	0.11	94,94,94,94	0
29	MN	X	3185	1/1	0.91	0.07	100,100,100,100	0
30	MG	X	3277	1/1	0.91	0.13	59,59,59,59	0
29	MN	X	3164	1/1	0.91	0.09	110,110,110,110	0
29	MN	X	3061	1/1	0.91	0.07	119,119,119,119	0
29	MN	X	3138	1/1	0.91	0.07	102,102,102,102	0
29	MN	X	3073	1/1	0.91	0.09	120,120,120,120	0
29	MN	X	3044	1/1	0.91	0.14	93,93,93,93	0
29	MN	X	3053	1/1	0.91	0.07	96,96,96,96	0
29	MN	X	3200	1/1	0.91	0.11	136,136,136,136	0
31	EPE	X	3285	15/15	0.91	0.20	72,72,72,72	0
29	MN	3	101	1/1	0.91	0.11	96,96,96,96	0
29	MN	X	3035	1/1	0.92	0.12	104,104,104,104	0
30	MG	X	3252	1/1	0.92	0.26	60,60,60,60	0
29	MN	X	3167	1/1	0.92	0.06	110,110,110,110	0
29	MN	X	3147	1/1	0.92	0.09	113,113,113,113	0
29	MN	X	3206	1/1	0.92	0.14	127,127,127,127	0
29	MN	X	3136	1/1	0.92	0.08	106,106,106,106	0
29	MN	X	3037	1/1	0.92	0.14	78,78,78,78	0
29	MN	X	3139	1/1	0.92	0.08	102,102,102,102	0
29	MN	X	3016	1/1	0.92	0.07	87,87,87,87	0
29	MN	X	3176	1/1	0.92	0.06	128,128,128,128	0
29	MN	X	3142	1/1	0.92	0.07	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3155	1/1	0.93	0.11	105,105,105,105	0
30	MG	X	3237	1/1	0.93	0.14	93,93,93,93	0
30	MG	X	3126	1/1	0.93	0.12	58,58,58,58	0
29	MN	X	3134	1/1	0.93	0.08	84,84,84,84	0
29	MN	X	3135	1/1	0.93	0.10	108,108,108,108	0
29	MN	X	3187	1/1	0.93	0.05	112,112,112,112	0
29	MN	X	3188	1/1	0.93	0.11	117,117,117,117	0
29	MN	X	3051	1/1	0.93	0.10	100,100,100,100	0
29	MN	X	3190	1/1	0.93	0.07	117,117,117,117	0
29	MN	X	3104	1/1	0.93	0.14	86,86,86,86	0
29	MN	X	3106	1/1	0.93	0.05	99,99,99,99	0
29	MN	I	201	1/1	0.93	0.05	95,95,95,95	0
29	MN	X	3034	1/1	0.93	0.07	94,94,94,94	0
29	MN	X	3127	1/1	0.93	0.07	79,79,79,79	0
29	MN	X	3076	1/1	0.93	0.09	93,93,93,93	0
29	MN	X	3146	1/1	0.93	0.07	101,101,101,101	0
30	MG	X	3213	1/1	0.93	0.08	47,47,47,47	0
29	MN	X	3081	1/1	0.93	0.06	57,57,57,57	0
30	MG	X	3036	1/1	0.93	0.10	55,55,55,55	0
29	MN	X	3132	1/1	0.93	0.10	101,101,101,101	0
29	MN	X	3133	1/1	0.93	0.07	85,85,85,85	0
29	MN	X	3207	1/1	0.93	0.11	92,92,92,92	0
30	MG	X	3248	1/1	0.94	0.12	66,66,66,66	0
30	MG	X	3275	1/1	0.94	0.21	57,57,57,57	0
29	MN	X	3017	1/1	0.94	0.07	90,90,90,90	0
29	MN	X	3048	1/1	0.94	0.06	117,117,117,117	0
30	MG	X	3158	1/1	0.94	0.27	48,48,48,48	0
29	MN	X	3230	1/1	0.94	0.12	126,126,126,126	0
29	MN	X	3084	1/1	0.94	0.06	71,71,71,71	0
30	MG	X	3284	1/1	0.94	0.12	56,56,56,56	0
29	MN	X	3157	1/1	0.94	0.09	87,87,87,87	0
29	MN	X	3210	1/1	0.94	0.08	107,107,107,107	0
30	MG	G	201	1/1	0.94	0.26	25,25,25,25	0
29	MN	X	3090	1/1	0.94	0.08	69,69,69,69	0
30	MG	X	3245	1/1	0.94	0.17	63,63,63,63	0
29	MN	X	3055	1/1	0.94	0.07	129,129,129,129	0
29	MN	X	3057	1/1	0.94	0.07	93,93,93,93	0
29	MN	X	3114	1/1	0.95	0.09	65,65,65,65	0
29	MN	X	3116	1/1	0.95	0.08	78,78,78,78	0
29	MN	X	3027	1/1	0.95	0.10	89,89,89,89	0
29	MN	X	3166	1/1	0.95	0.06	95,95,95,95	0
29	MN	X	3212	1/1	0.95	0.12	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3125	1/1	0.95	0.07	86,86,86,86	0
29	MN	X	3215	1/1	0.95	0.09	119,119,119,119	0
29	MN	X	3092	1/1	0.95	0.05	87,87,87,87	0
30	MG	X	3281	1/1	0.95	0.18	69,69,69,69	0
30	MG	X	3243	1/1	0.95	0.14	54,54,54,54	0
29	MN	X	3220	1/1	0.95	0.04	112,112,112,112	0
30	MG	Y	202	1/1	0.95	0.14	54,54,54,54	0
29	MN	X	3068	1/1	0.95	0.11	84,84,84,84	0
29	MN	X	3100	1/1	0.95	0.05	59,59,59,59	0
29	MN	X	3101	1/1	0.95	0.07	60,60,60,60	0
29	MN	X	3102	1/1	0.95	0.14	77,77,77,77	0
29	MN	X	3103	1/1	0.95	0.14	81,81,81,81	0
29	MN	X	3029	1/1	0.95	0.13	82,82,82,82	0
29	MN	X	3011	1/1	0.95	0.11	40,40,40,40	0
29	MN	X	3163	1/1	0.96	0.05	99,99,99,99	0
29	MN	X	3088	1/1	0.96	0.05	68,68,68,68	0
29	MN	X	3208	1/1	0.96	0.12	77,77,77,77	0
29	MN	X	3209	1/1	0.96	0.05	105,105,105,105	0
29	MN	X	3007	1/1	0.96	0.18	61,61,61,61	0
27	95H	X	3001	27/27	0.96	0.15	52,52,52,52	19
29	MN	X	3094	1/1	0.96	0.07	83,83,83,83	0
29	MN	X	3045	1/1	0.96	0.06	88,88,88,88	0
29	MN	X	3066	1/1	0.96	0.07	91,91,91,91	0
29	MN	X	3047	1/1	0.96	0.11	87,87,87,87	0
29	MN	X	3028	1/1	0.96	0.10	90,90,90,90	0
29	MN	X	3071	1/1	0.96	0.07	83,83,83,83	0
29	MN	X	3225	1/1	0.96	0.08	101,101,101,101	0
29	MN	X	3175	1/1	0.96	0.08	103,103,103,103	0
29	MN	X	3140	1/1	0.96	0.07	100,100,100,100	0
29	MN	X	3177	1/1	0.96	0.21	110,110,110,110	0
29	MN	X	3021	1/1	0.96	0.05	68,68,68,68	0
29	MN	X	3052	1/1	0.96	0.09	121,121,121,121	0
29	MN	X	3236	1/1	0.96	0.04	104,104,104,104	0
30	MG	X	3273	1/1	0.96	0.11	57,57,57,57	0
30	MG	X	3232	1/1	0.96	0.09	67,67,67,67	0
29	MN	X	3144	1/1	0.96	0.08	80,80,80,80	0
29	MN	X	3109	1/1	0.96	0.07	87,87,87,87	0
29	MN	X	3186	1/1	0.96	0.08	104,104,104,104	0
29	MN	X	3111	1/1	0.96	0.04	80,80,80,80	0
29	MN	X	3113	1/1	0.96	0.07	75,75,75,75	0
29	MN	X	3148	1/1	0.96	0.08	91,91,91,91	0
30	MG	X	3282	1/1	0.96	0.06	63,63,63,63	0

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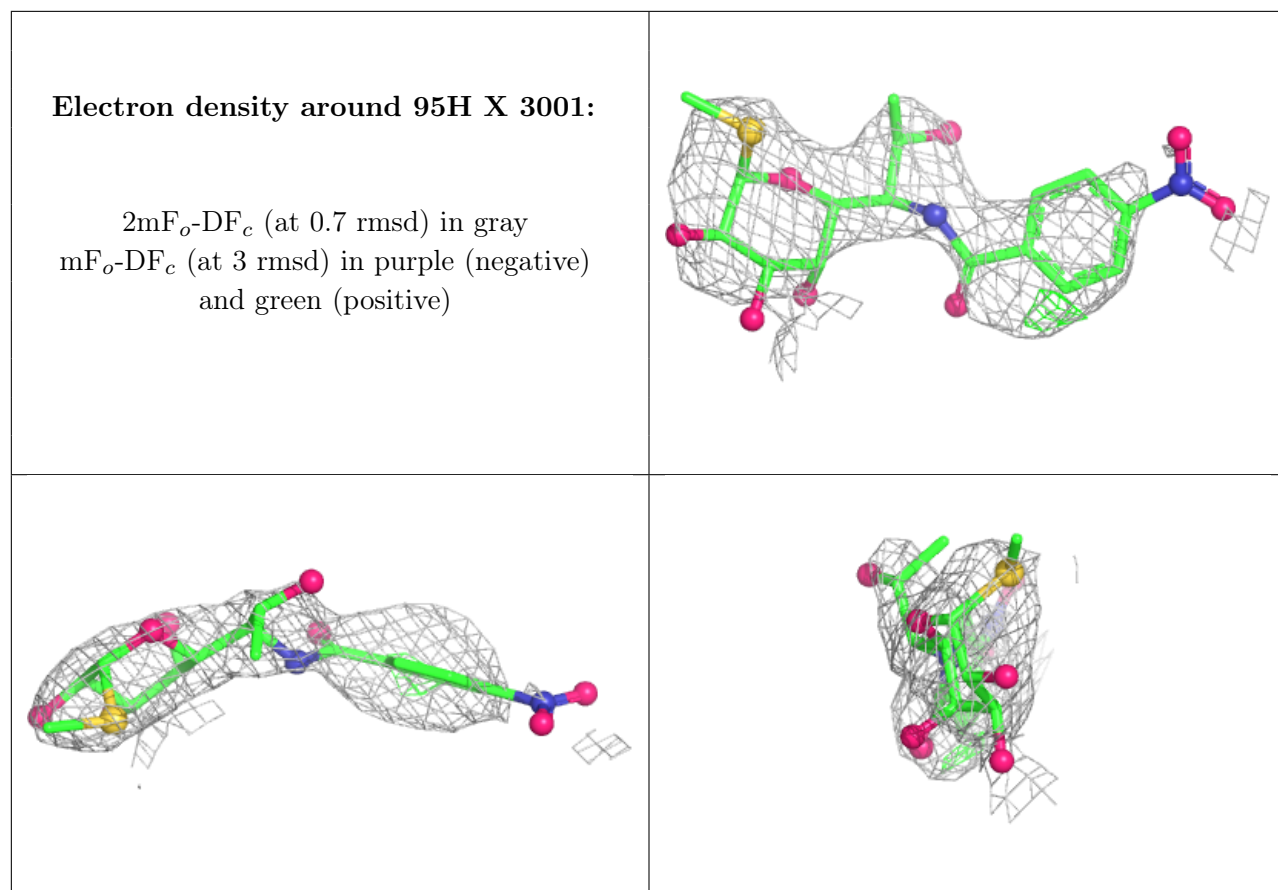
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3031	1/1	0.96	0.07	80,80,80,80	0
30	MG	X	3244	1/1	0.96	0.08	57,57,57,57	0
29	MN	X	3151	1/1	0.96	0.07	97,97,97,97	0
29	MN	X	3115	1/1	0.96	0.05	63,63,63,63	0
29	MN	X	3033	1/1	0.96	0.20	90,90,90,90	0
29	MN	X	3079	1/1	0.96	0.06	70,70,70,70	0
29	MN	X	3023	1/1	0.96	0.08	70,70,70,70	0
29	MN	X	3159	1/1	0.96	0.16	104,104,104,104	0
29	MN	X	3161	1/1	0.96	0.05	130,130,130,130	0
29	MN	X	3025	1/1	0.96	0.05	79,79,79,79	0
29	MN	X	3014	1/1	0.97	0.06	56,56,56,56	0
29	MN	X	3085	1/1	0.97	0.10	61,61,61,61	0
29	MN	X	3211	1/1	0.97	0.05	100,100,100,100	0
29	MN	X	3065	1/1	0.97	0.04	85,85,85,85	0
29	MN	X	3149	1/1	0.97	0.05	102,102,102,102	0
29	MN	X	3089	1/1	0.97	0.04	69,69,69,69	0
29	MN	X	3015	1/1	0.97	0.05	63,63,63,63	0
29	MN	X	3038	1/1	0.97	0.09	73,73,73,73	0
29	MN	X	3054	1/1	0.97	0.05	82,82,82,82	0
29	MN	X	3129	1/1	0.97	0.09	74,74,74,74	0
29	MN	X	3070	1/1	0.97	0.11	97,97,97,97	0
29	MN	X	3098	1/1	0.97	0.10	70,70,70,70	0
29	MN	X	3099	1/1	0.97	0.06	73,73,73,73	0
29	MN	X	3030	1/1	0.97	0.06	89,89,89,89	0
29	MN	X	3233	1/1	0.97	0.04	59,59,59,59	0
29	MN	X	3056	1/1	0.97	0.06	94,94,94,94	0
29	MN	X	3009	1/1	0.97	0.11	59,59,59,59	0
29	MN	X	3059	1/1	0.97	0.09	92,92,92,92	0
29	MN	Y	201	1/1	0.97	0.09	95,95,95,95	0
29	MN	X	3046	1/1	0.97	0.05	94,94,94,94	0
29	MN	X	3012	1/1	0.97	0.08	72,72,72,72	0
30	MG	X	3216	1/1	0.97	0.13	43,43,43,43	0
30	MG	X	3217	1/1	0.97	0.32	64,64,64,64	0
29	MN	X	3107	1/1	0.97	0.10	68,68,68,68	0
29	MN	X	3108	1/1	0.97	0.10	70,70,70,70	0
29	MN	X	3013	1/1	0.97	0.14	67,67,67,67	0
29	MN	X	3110	1/1	0.97	0.07	65,65,65,65	0
29	MN	X	3082	1/1	0.97	0.06	59,59,59,59	0
29	MN	X	3095	1/1	0.98	0.04	69,69,69,69	0
29	MN	X	3077	1/1	0.98	0.03	88,88,88,88	0
29	MN	X	3097	1/1	0.98	0.06	79,79,79,79	0
29	MN	X	3173	1/1	0.98	0.12	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3143	1/1	0.98	0.06	44,44,44,44	0
29	MN	X	3040	1/1	0.98	0.03	79,79,79,79	0
29	MN	X	3117	1/1	0.98	0.04	66,66,66,66	0
29	MN	X	3118	1/1	0.98	0.03	69,69,69,69	0
29	MN	X	3119	1/1	0.98	0.11	77,77,77,77	0
30	MG	X	3272	1/1	0.98	0.07	60,60,60,60	0
29	MN	X	3120	1/1	0.98	0.04	72,72,72,72	0
29	MN	X	3121	1/1	0.98	0.05	67,67,67,67	0
29	MN	X	3122	1/1	0.98	0.07	82,82,82,82	0
29	MN	X	3080	1/1	0.98	0.07	59,59,59,59	0
29	MN	X	3153	1/1	0.98	0.06	99,99,99,99	0
29	MN	X	3005	1/1	0.98	0.17	53,53,53,53	0
29	MN	X	3020	1/1	0.98	0.06	78,78,78,78	0
29	MN	X	3010	1/1	0.98	0.15	59,59,59,59	0
29	MN	X	3022	1/1	0.98	0.04	74,74,74,74	0
29	MN	X	3086	1/1	0.98	0.03	62,62,62,62	0
29	MN	X	3278	1/1	0.98	0.04	99,99,99,99	0
29	MN	X	3105	1/1	0.98	0.05	71,71,71,71	0
29	MN	X	3004	1/1	0.98	0.08	60,60,60,60	0
29	MN	X	3049	1/1	0.98	0.08	81,81,81,81	0
29	MN	X	3050	1/1	0.98	0.05	98,98,98,98	0
29	MN	X	3091	1/1	0.98	0.04	61,61,61,61	0
29	MN	X	3137	1/1	0.98	0.07	72,72,72,72	0
29	MN	X	3024	1/1	0.98	0.08	74,74,74,74	0
29	MN	X	3039	1/1	0.98	0.05	94,94,94,94	0
29	MN	X	3043	1/1	0.99	0.03	79,79,79,79	0
29	MN	X	3180	1/1	0.99	0.07	70,70,70,70	0
29	MN	X	3087	1/1	0.99	0.04	63,63,63,63	0
29	MN	X	3019	1/1	0.99	0.03	73,73,73,73	0
29	MN	X	3128	1/1	0.99	0.03	62,62,62,62	0
29	MN	X	3041	1/1	0.99	0.06	75,75,75,75	0
29	MN	X	3042	1/1	0.99	0.02	80,80,80,80	0
29	MN	X	3083	1/1	0.99	0.05	56,56,56,56	0
29	MN	X	3060	1/1	0.99	0.05	84,84,84,84	0
29	MN	X	3093	1/1	0.99	0.04	61,61,61,61	0
29	MN	X	3078	1/1	0.99	0.04	55,55,55,55	0
29	MN	X	3124	1/1	1.00	0.03	76,76,76,76	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.