



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:33 am GMT

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

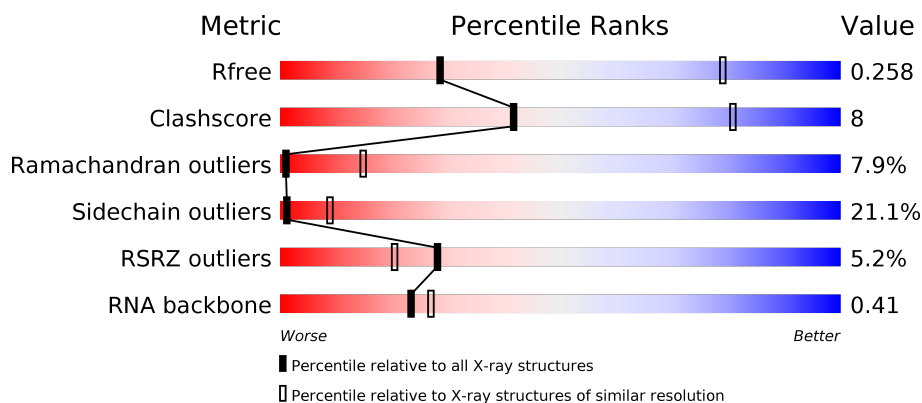
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)
RNA backbone	2435	1002 (4.30-2.90)

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. 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	<div> <div>2%</div> <div>31% 39% 20% 7%</div> </div>
2	Y	123	<div> <div>2%</div> <div>28% 40% 27% 5%</div> </div>
3	A	274	<div> <div>2%</div> <div>50% 26% 11% 12%</div> </div>
4	B	211	<div> <div></div> <div>62% 26% 9%</div> </div>

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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	

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	2901	-	-	-	X
31	MG	X	2907	-	-	-	X
31	MG	X	2914	-	-	-	X
31	MG	X	2915	-	-	-	X
31	MG	X	2917	-	-	-	X
31	MG	X	2922	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2926	-	-	-	X
31	MG	Y	202	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

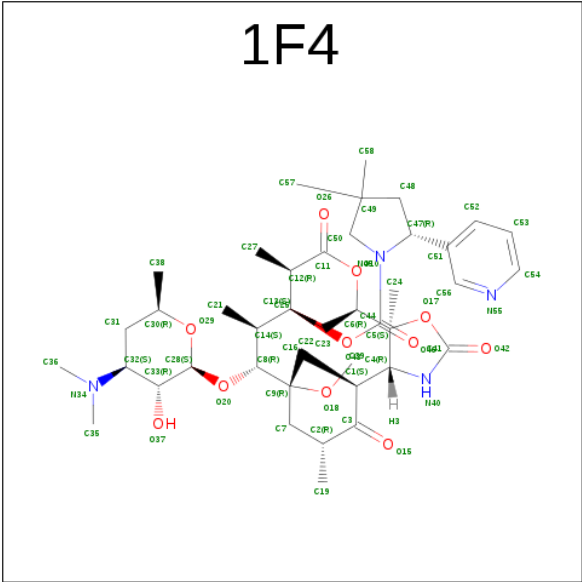
- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 32 is (3AS,4R,7R,8S,9S,10R,11R,13R,15S,15AR)-4-ETHYL-11-METHOXY-3A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-10-{{3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSYL}OXY}TETRADECAHYDRO-2H-OXACYCLO TETRADECINO[4,3-D][1,3]OXAZOL-8-YL (2R)-4,4-DIMETHYL-2-(PYRIDIN-3-YL)PYRROLIDINE-1-CARBOXYLATE (three-letter code: 1F4) (formula: C₄₃H₆₈N₄O₁₁).

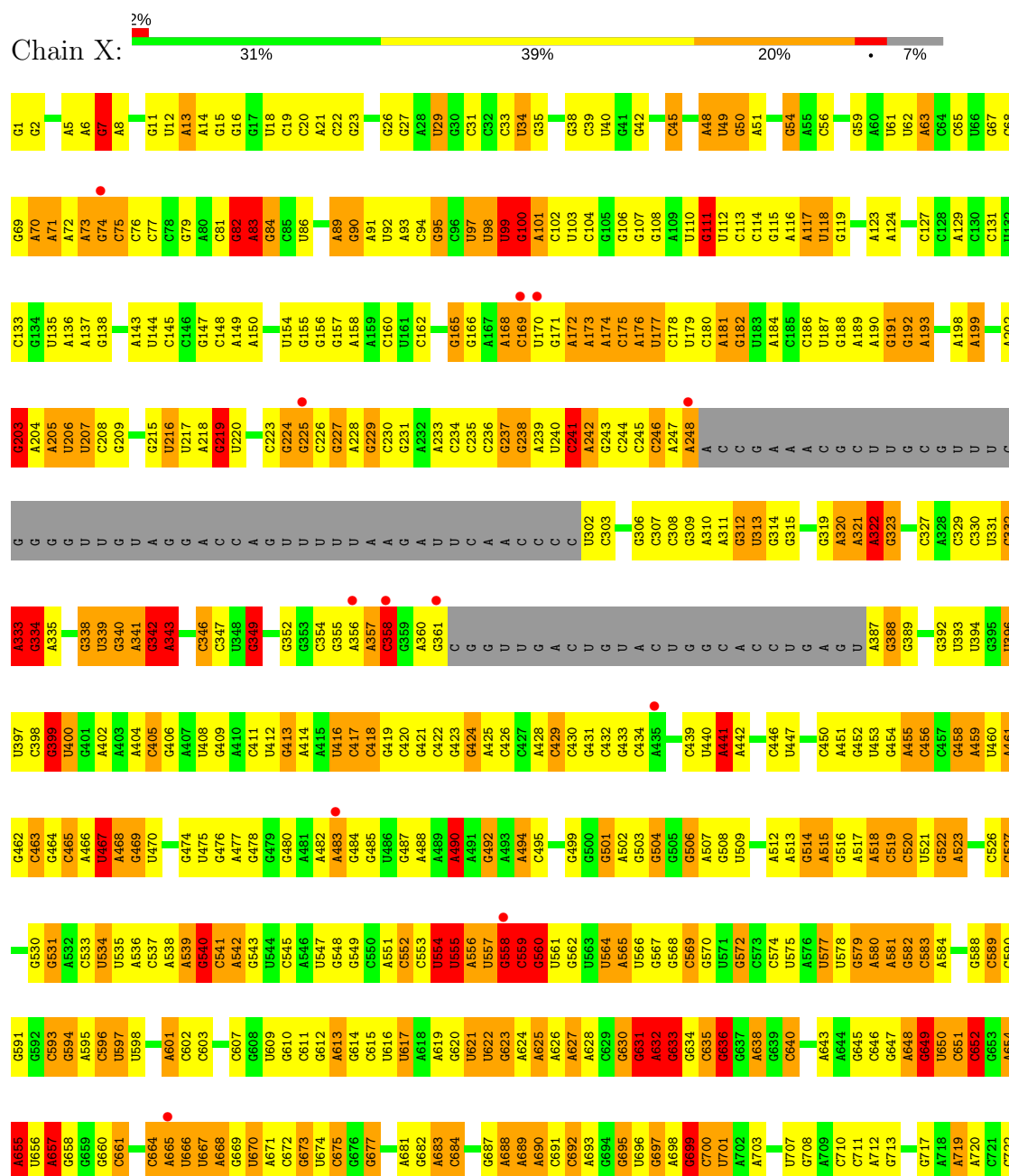


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			58	43	4	11		

3 Residue-property plots

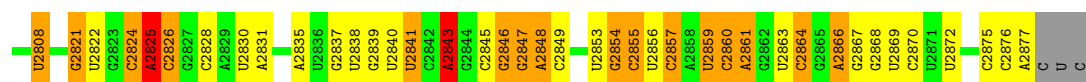
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

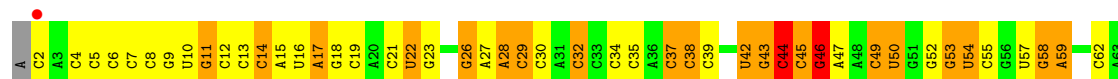




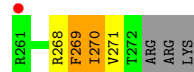
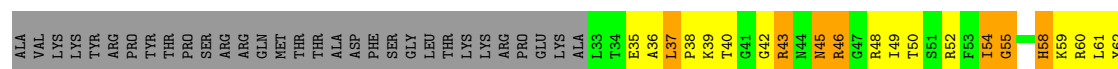
G2727	C2659	U2592	G2528	G2464	G2393	U2323	G2255	A2188	C2066	U1994	G1925	A1859	C1788
A2728	C2660	A2593	G2529	G2465	G2394	G2324	G2256	A2189	A2066	G1995	U1926	A1860	U1789
A2729	G2661	C2594	C2530	G2466	C2395	A2325	A2257	A2190	C2060	A1996	U1927	G1861	G1790
A2730	C2662	C2595	U2531	G2467	C2396	C2326	G2258	A2191	C2061	A1997	U1928	C1862	G1791
G2731	U2663	G2596	G2532	G2468	A2397			U2192	U2062	U1998	U1929	G1863	C1792
C2732	G2664	G2597	U2533	G2469				C2193	A2063	U1999	G1930	G1864	A1793
A2733	G2665	C2598	U2534	U2470	U2402	C2329	G2261	A2194	U2064	U2000	G1931	C1865	
U2734	U2666	U2472	U2471	U2473	C2403	G2330	C2262	C2195	A2065	G2001	G1932	G1866	A1796
C2735	G2667				A2404		C2263	C2196	A2066	A2002	G1933	G1867	
U2736	U2668				A2405	A2333	C2264	U2197	U2067	G2003	U1934		A1799
A2737	C2669	G2603	C2537		C2406	U2335	A2265	U2198	U2068	U2004	U1935	A1800	A1800
	C2670	G2604	C2539		G2407	G2336	A2267	C2199	U2069	U2005	A1936		C1801
C2740	G2671	A2540	U2541	C2476	A2408	A2337	G2268	G2200	G2070	G2006	G1937		
	U2672	C2606	U2542	U2479	A2409	C2338	G2269	G2201	G2071		U1938		U1804
A2745	U2677	A2608	A2543	C2480	U2410	A2339	U2270	A2204	C2072	U2009	U1939	C1876	G1805
C2748	G2678	C2609	A2544	G2481		C2340	C2271	C2205	U2075	G2010	C1940	C1877	G1806
C2754	U2680	G2610	A2545	U2482	G2415		C2274	C2206	G2076	U2011			A1807
		A2611	G2546	U2483	U2416	G2344	U2275	G2207	A2013	A1943		U1881	G1808
A2758	C2683	G2612	C2547	U2484	U2417	C2347	C2276	U2208	G2078		U1946	A1882	G1809
U2759	A2684	A2614	G2548	U2485	A2418	A2348	A2277	C2209	G2079	A2014	G1947	A1883	U1810
G2760		U2615	C2550	G2486	C2419	G2349	A2278	U2080	U2081	A2016	U1948	C1885	A1811
		U2616	G2551	G2487	C2420	G2350	U2211	C2081		U2017	A1949	G1886	A1812
U2764	G2687	G2617	A2551	G2488	C2421	G2351	G2281	U2212	C2082	G2018	G1950	G1887	A1813
	C2688	G2618	C2552	U2489	C2422	A2352	G2282	U2213	G2083	G2019	G1951	C1888	G1816
C2689	A2690	A2618	G2553	U2490	G2423	G2353	G2283	G2214			A1952	G	U1817
G2690	C2691	G2619	C2554	C2491	G2426		U2284	C2215	U2088	C2022	A1953	G	G1819
U2766	U2692	U2620	G2555	G2492	A2427	C2357	U2285	G2216	C2089	C2023	A1954	C	U1819
	G2693	G2621	A2556	U2493	U2428	C2358	G2286	G2217	U2090	U2024	G1955	C	G1820
C2771	U2694	G2622	G2557	G2494		U2359	G2287	G2218	C	A2025		G	A1821
	C2695		G2558	G2495			U2288	U2219	U	G2026	G1958	U	
C2772	C2695	U2625	U2559	C2496	C2431	G2362	A2289	A2220	U	G2027		A	G1824
G2773	A2696	U2626	C2560	C2497	A2432	G2363	A2290	C2028	C	C2028	G1963	A	C1825
U2774	G2697	G2627	U2561	U2498		U2364	G2291	U2222	U	U2030	A1964	C	C1828
	G2698	C2628		C2499	C2435	U2365	U2292	U2223	C	A2031	U1965	U	C1829
U2776	G2699		U2564	C2500		U2366	U2294	G2224	A	G2032	C1966	U	C1830
A2777	U2700	C2631	C2565		U2438	A2367	G2295	C2033	G	G2033		A	C1831
U2778	A2701	U2632	A2566	G2503	U2439	G2368	U2296	A2226	A	C2034	G1971	A	G1832
C2779	G2702	A2633	G2567	G2504	C2440	U2369	G2297	C2227	C	A2034	G1972	A	G1833
G2780	C2703	G2634	U2568	G2505	U2441	U2370	U2298	G2228	C	G2035	G1973	C	U1834
U2781	U2704	U2635	C2569	C2506	C2442	A2371	A2299	G2229	C	A2036	U1974	G	G1835
G2782	U2705	A2636	G2571	U2507	C2443	A2372	G2300	G2230	A	G2037	G1975	G	C1835
U2783	U2706	U2637	C2572	G2508	C2444	C2373	G2301		U	G2038	U1976	U	C1836
A2784	G2707	G2640	U2573	A2509		C2374	G2302	G2039	U	C2039	C1977	C	
	U2708	A2641	U2574	U2510	G2447	G2375	C2303	A2040	G	A2040	U1978	C	A1839
C2788	C2709	G2643	G2577	G2511	A2448	G2376	G2304	A2041	G	A2041	C1979		A1840
G2790	U2644	C2645	A2578		G2449	U2377	C2305	A2042	G	A2042	C1980		G1841
C2791	A2713	C2645	A2579	G2514		A2306	A2306	A2043	A	A2043	A1981		G1842
G2792	U2714	U2649	A2581	U2515	U2452	U2380	U2311	G2240	G	G2044	G1982		U1843
G2793	C2715	G2650	C2582	C2517	C2453	A2381	A2312	U2241	C	G2045	G1983		C1844
G2794	U2651	U2651	G2518	G2516	A2455	C2382	G2313	C2242	U	C2046	A1984		A1845
A2795	G2717	C2519	G2519	C2517	U2456	C2383	A2314	C2244	C	C2047	G1985		A1846
A2796	U2718	G2652	G2585		A2457	G2384	A2315	G2245	C	C2048	G1986		G1850
G2797	U2719	G2586	G2586	U2458	U2458	G2385	A2315	A2246	G	C2049	G1987		G1851
U2798	A2654	G2587	G2587	C2459	U2458	G2386	U2318	A2247	A	U2051	A1988		G1852
C2799	U2720	G2588	G2588	G2523	G2460	C2388	G2319	A2247	A	G2050	C1989		
	G2724	U2525	G2589	G2524	C2461	G2389	C2320	A2252	C	G2051	U1990		U1856
C2800	C2725	U2526	C2462	U2525	G2462		C2321	A2253	A	G2052	C1991		G1857
G2805	U2726	A2658	G2527	G2527	G2463	G2392	U2322	C2254	U	G2055	G1992		C1924



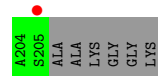
• Molecule 2: 5S ribosomal RNA



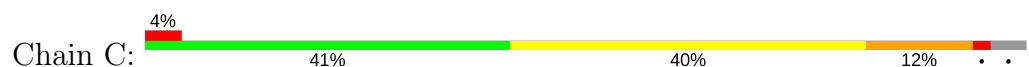
• Molecule 3: 50S ribosomal protein L2

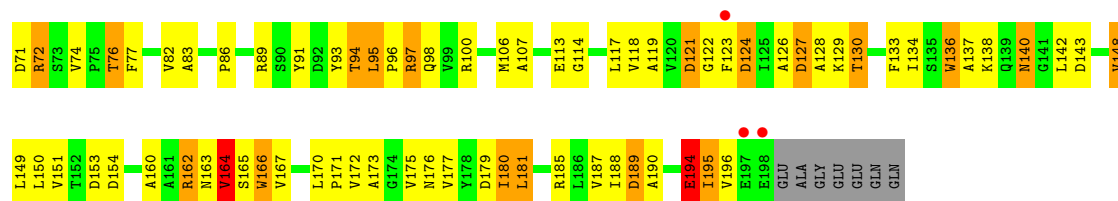


• Molecule 4: 50S ribosomal protein L3

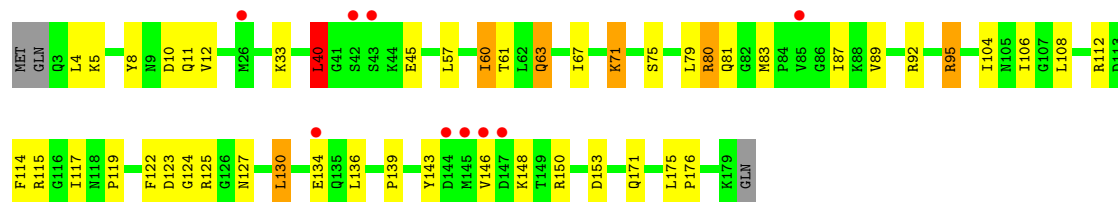


• Molecule 5: 50S ribosomal protein L4

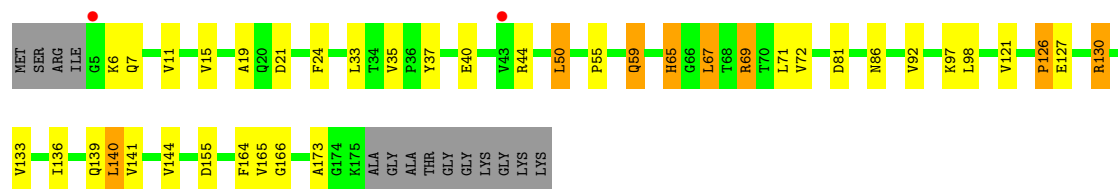




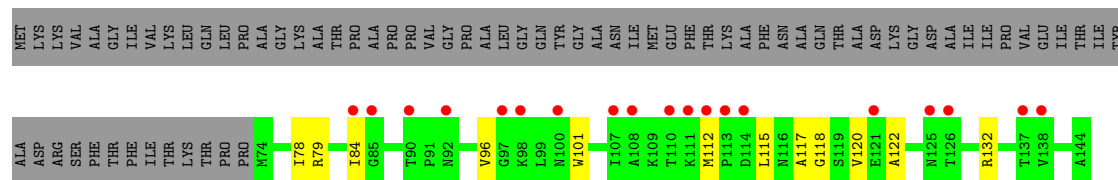
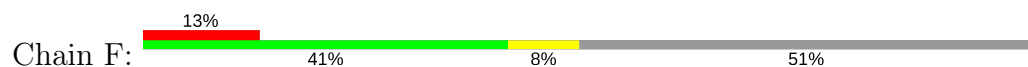
• Molecule 6: 50S ribosomal protein L5



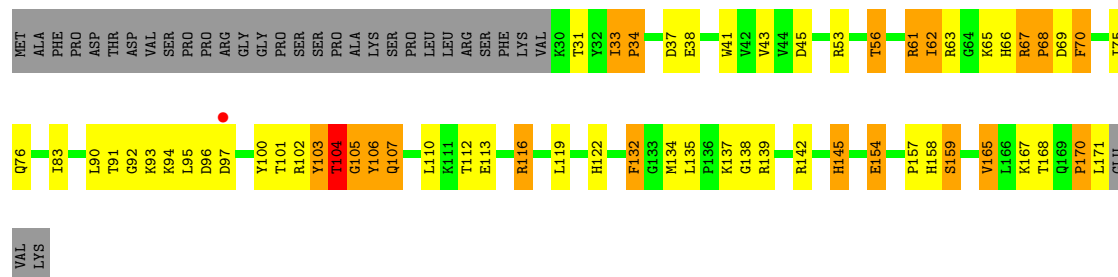
• Molecule 7: 50S ribosomal protein L6



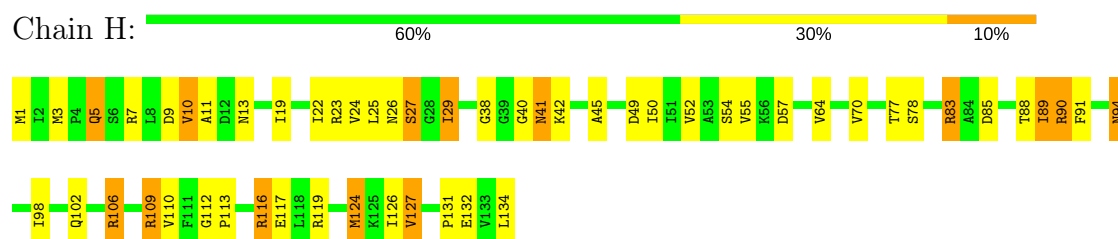
• Molecule 8: 50S ribosomal protein L11



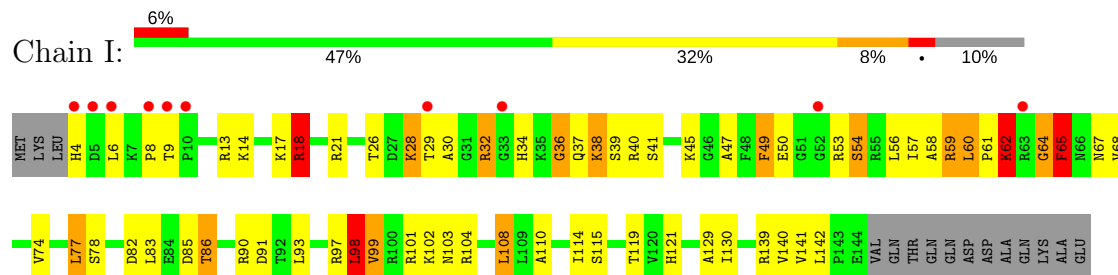
• Molecule 9: 50S ribosomal protein L13



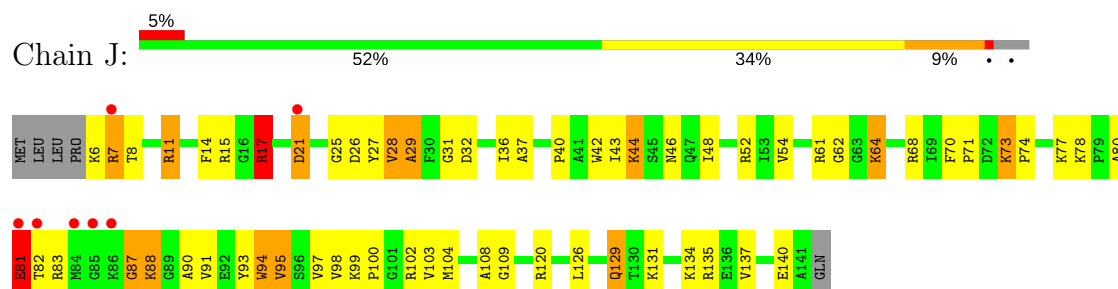
- Molecule 10: 50S ribosomal protein L14



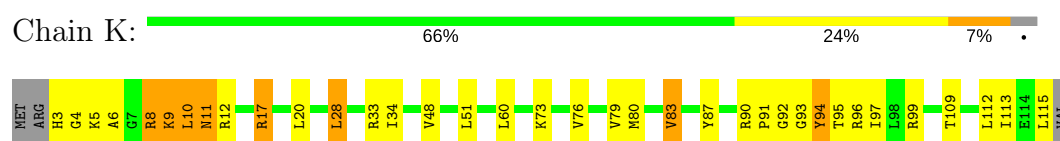
- Molecule 11: 50S ribosomal protein L15



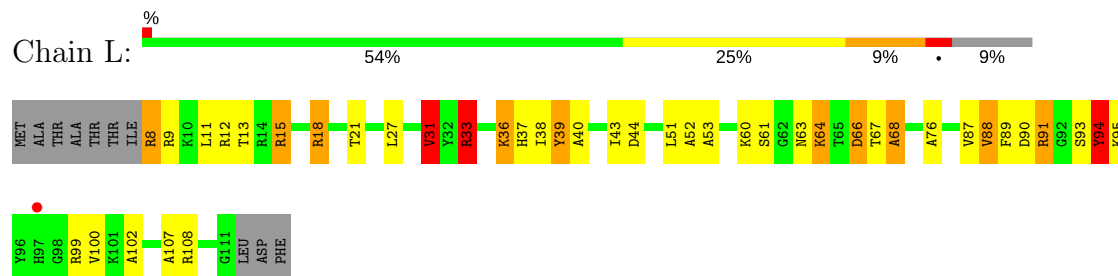
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

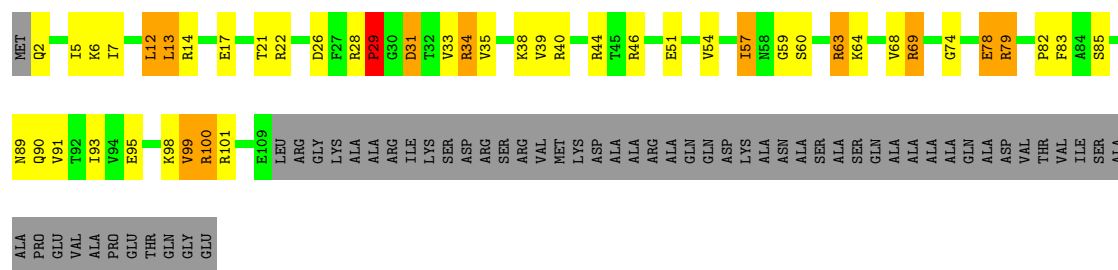


- Molecule 14: 50S ribosomal protein L18



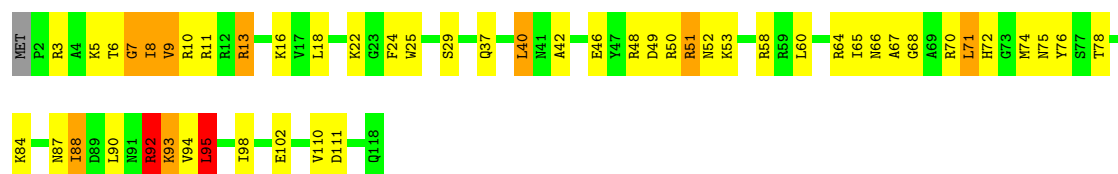
- Molecule 15: 50S ribosomal protein L19





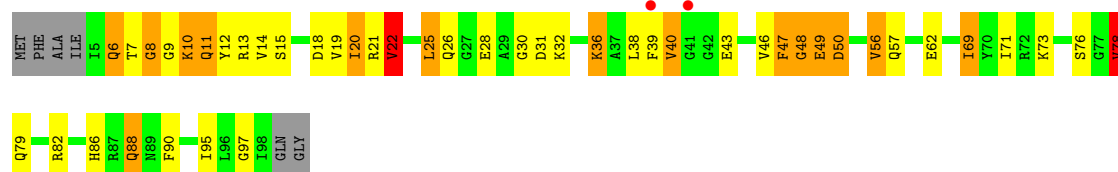
- Molecule 16: 50S ribosomal protein L20

Chain N: 56% 34% 8% ..



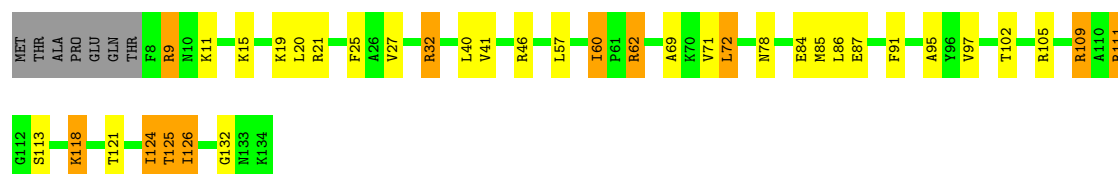
- Molecule 17: 50S ribosomal protein L21

Chain O: 2% 48% 29% 15% 6%



- Molecule 18: 50S ribosomal protein L22

Chain P: 67% 19% 8% 5%



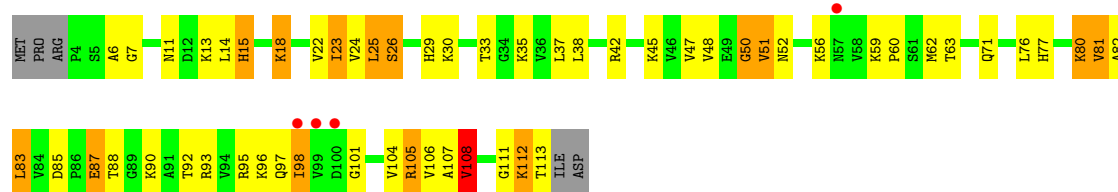
- Molecule 19: 50S ribosomal protein L23

Chain Q: 2% 61% 27% 7% ..

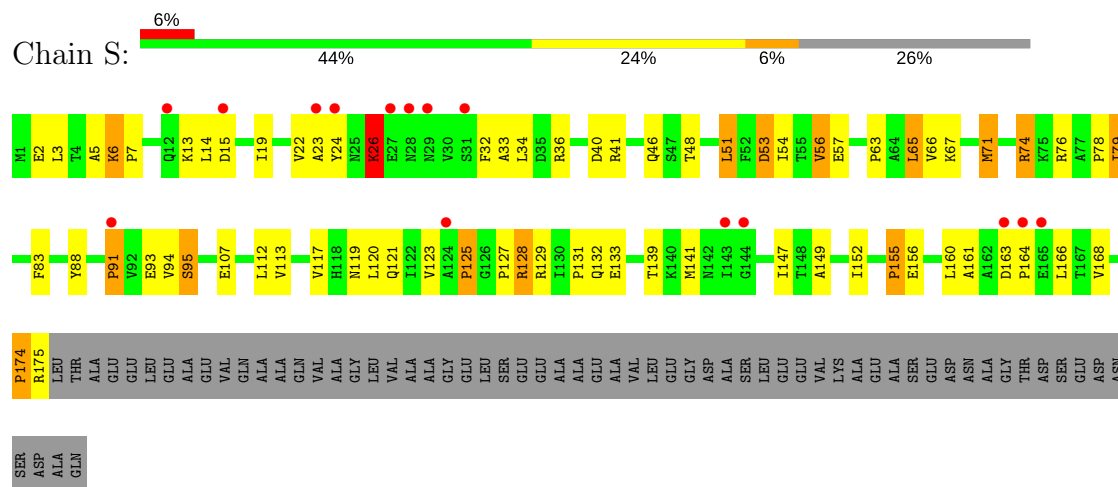


- Molecule 20: 50S ribosomal protein L24

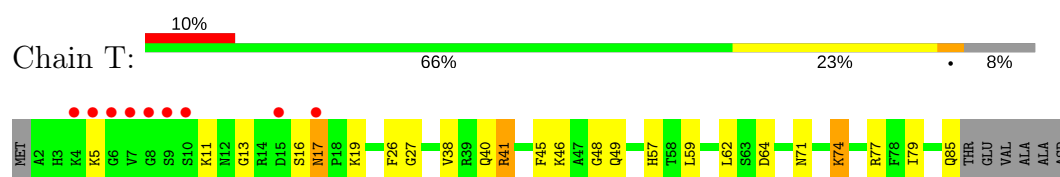
Chain R: 3% 47% 36% 12% ..



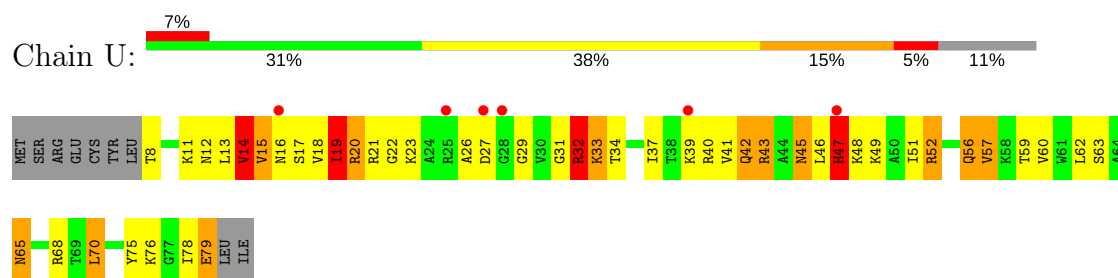
• Molecule 21: 50S ribosomal protein L25



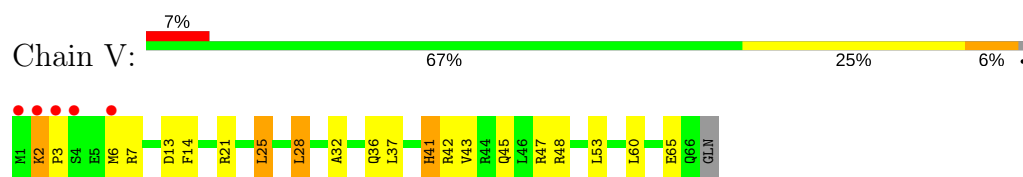
• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29



• Molecule 25: 50S ribosomal protein L30

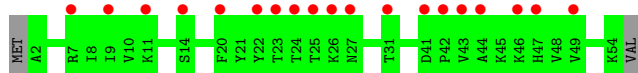




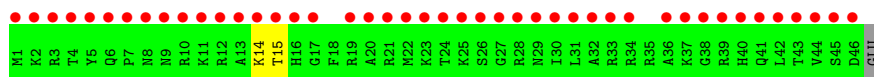
- Molecule 26: 50S ribosomal protein L32



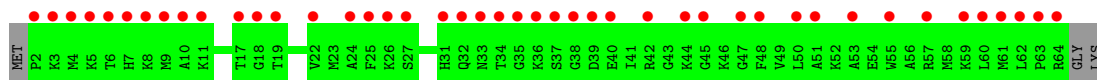
- Molecule 27: 50S ribosomal protein L33



- 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	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.11 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.4 (30.11-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.65Å)	Xtriage
Refinement program	autobuster	Depositor
R, R_{free}	0.198 , 0.239 0.215 , 0.258	Depositor DCC
R_{free} test set	12232 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	129.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 93.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	83877	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1F4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	1.02	36/64561 (0.1%)	1.86	1991/100708 (2.0%)
2	Y	1.22	2/2904 (0.1%)	1.83	99/4525 (2.2%)
3	A	0.58	0/1862	0.93	4/2510 (0.2%)
4	B	0.55	0/1567	0.88	1/2105 (0.0%)
5	C	0.62	0/1529	0.96	0/2070
6	D	0.46	0/1419	0.68	0/1903
7	E	0.47	0/1308	0.71	0/1771
8	F	0.50	0/508	0.67	0/683
9	G	0.58	0/1138	0.92	2/1539 (0.1%)
10	H	0.53	0/1007	0.84	0/1352
11	I	0.67	0/1081	1.06	2/1448 (0.1%)
12	J	0.86	0/1113	0.96	1/1486 (0.1%)
13	K	0.66	0/886	0.92	0/1188
14	L	0.52	0/785	0.93	0/1048
15	M	0.59	0/884	1.00	2/1186 (0.2%)
16	N	0.53	0/994	0.79	0/1323
17	O	0.52	0/750	0.96	1/1000 (0.1%)
18	P	0.57	0/1027	0.88	0/1373
19	Q	0.56	0/737	0.99	2/988 (0.2%)
20	R	0.59	0/835	1.02	0/1121
21	S	0.61	0/1370	0.76	0/1862
22	T	0.54	0/633	0.88	0/838
23	U	0.71	0/556	1.08	2/741 (0.3%)
24	V	0.52	0/537	0.73	0/714
25	W	0.51	0/426	0.81	0/568
26	Z	0.62	0/469	0.98	0/629
30	4	0.49	0/298	0.73	0/390
All	All	0.94	38/91184 (0.0%)	1.68	2107/137069 (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	3

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	559	C	C3'-O3'	8.19	1.53	1.42
1	X	655	A	C3'-O3'	7.84	1.53	1.42
1	X	774	A	C5-C4	7.25	1.43	1.38
1	X	699	G	N9-C4	-6.97	1.32	1.38
1	X	1688	U	C2-N3	6.58	1.42	1.37

The worst 5 of 2107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-30.77	85.29	109.90
1	X	1019	U	P-O3'-C3'	19.01	142.51	119.70
1	X	1288	A	C5'-C4'-O4'	18.79	131.64	109.10
1	X	774	A	N1-C6-N6	17.73	129.24	118.60
1	X	559	C	O4'-C1'-N1	17.43	122.14	108.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts [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	535	0
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1539	0	1600	57	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	17	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	46	0
10	H	997	0	1046	30	0
11	I	1067	0	1103	39	0
12	J	1090	0	1125	31	0
13	K	878	0	930	24	0
14	L	779	0	820	19	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	23	0
19	Q	726	0	753	11	0
20	R	825	0	881	26	0
21	S	1345	0	1372	30	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	15	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1080 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	1	15
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	6	44
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0	5
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	3	32
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	2	25
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	3	30
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	0	9
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	7	46
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0	5
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	1	12
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	2	24
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	0	7
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	2	23
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	2	22
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	5
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	5	38
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0	4
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	1	21
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	2	22
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0	2
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	5	40
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	9	50
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	1	12
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	5	41
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1	15

5 of 235 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	185/215 (86%)	145 (78%)	40 (22%)	1	8
4	B	155/157 (99%)	119 (77%)	36 (23%)	1	6
5	C	157/163 (96%)	112 (71%)	45 (29%)	0	3
6	D	153/156 (98%)	130 (85%)	23 (15%)	3	23
7	E	136/144 (94%)	115 (85%)	21 (15%)	3	22
8	F	51/107 (48%)	49 (96%)	2 (4%)	37	73
9	G	118/146 (81%)	94 (80%)	24 (20%)	1	10
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	I	108/121 (89%)	79 (73%)	29 (27%)	0	4
12	J	110/115 (96%)	89 (81%)	21 (19%)	2	11
13	K	90/93 (97%)	76 (84%)	14 (16%)	3	21
14	L	74/82 (90%)	51 (69%)	23 (31%)	0	3
15	M	94/134 (70%)	71 (76%)	23 (24%)	1	6
16	N	96/97 (99%)	76 (79%)	20 (21%)	1	9
17	O	75/79 (95%)	56 (75%)	19 (25%)	0	5
18	P	109/115 (95%)	91 (84%)	18 (16%)	2	18
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	10
20	R	91/96 (95%)	75 (82%)	16 (18%)	2	14
21	S	149/192 (78%)	117 (78%)	32 (22%)	1	8
22	T	62/67 (92%)	53 (86%)	9 (14%)	4	25
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	1
24	V	54/55 (98%)	43 (80%)	11 (20%)	1	10
25	W	48/48 (100%)	37 (77%)	11 (23%)	1	7
26	Z	51/53 (96%)	41 (80%)	10 (20%)	1	11
30	4	35/35 (100%)	29 (83%)	6 (17%)	2	16
All	All	2436/2715 (90%)	1921 (79%)	515 (21%)	1	9

5 of 515 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	77	LEU
14	L	43	ILE
23	U	78	ILE
11	I	99	VAL
12	J	131	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	58	ASN
17	O	79	GLN
25	W	54	GLN
15	M	90	GLN

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Mol	Chain	Res	Type
16	N	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	701 (26%)	0
2	Y	121/123 (98%)	41 (33%)	0
All	All	2801/3003 (93%)	742 (26%)	0

5 of 742 RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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	1F4	X	2929	-	60,62,62	1.25	4 (6%)	84,95,95	2.83	40 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	1F4	X	2929	-	-	0/74/119/119	1/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	O46-C44	2.15	1.24	1.21
32	X	2929	1F4	C22-C9	2.57	1.58	1.52
32	X	2929	1F4	C52-C51	3.37	1.44	1.39
32	X	2929	1F4	C41-N40	4.23	1.39	1.33

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C51-C47-N45	-10.01	98.37	112.82
32	X	2929	1F4	C58-C49-C50	-5.64	104.57	110.66
32	X	2929	1F4	C22-C9-C7	-4.99	103.00	111.12
32	X	2929	1F4	C49-C48-C47	-4.81	101.42	106.10
32	X	2929	1F4	C9-C7-C2	-4.40	108.70	116.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

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

1 monomer is involved in 19 short contacts:

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

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%)	-0.14	67 (2%) 58 43	43, 92, 197, 276	0
2	Y	122/123 (99%)	-0.13	3 (2%) 58 43	83, 135, 170, 191	0
3	A	240/274 (87%)	-0.20	5 (2%) 64 50	68, 115, 146, 172	0
4	B	205/211 (97%)	-0.34	1 (0%) 90 84	45, 73, 105, 154	0
5	C	197/205 (96%)	-0.15	8 (4%) 38 27	57, 114, 154, 187	0
6	D	177/180 (98%)	-0.18	9 (5%) 29 20	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.52	2 (1%) 79 66	92, 143, 192, 206	0
8	F	71/144 (49%)	1.55	19 (26%) 1 1	211, 236, 252, 257	0
9	G	142/174 (81%)	-0.32	1 (0%) 87 78	72, 97, 144, 161	0
10	H	134/134 (100%)	-0.40	0 100 100	50, 70, 97, 121	0
11	I	141/156 (90%)	0.31	10 (7%) 17 12	67, 129, 174, 204	0
12	J	136/141 (96%)	0.25	7 (5%) 29 20	74, 103, 149, 184	0
13	K	113/116 (97%)	-0.37	0 100 100	35, 60, 79, 91	0
14	L	104/114 (91%)	-0.15	1 (0%) 82 70	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.62	0 100 100	50, 73, 111, 145	0
16	N	117/118 (99%)	-0.43	0 100 100	59, 90, 128, 159	0
17	O	94/100 (94%)	-0.30	2 (2%) 64 50	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.50	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	-0.25	2 (2%) 62 48	73, 106, 162, 195	0
20	R	110/115 (95%)	-0.17	4 (3%) 43 32	88, 117, 170, 178	0
21	S	175/237 (73%)	0.35	15 (8%) 11 9	121, 155, 175, 190	0
22	T	84/91 (92%)	0.46	9 (10%) 7 6	79, 107, 186, 200	0
23	U	72/81 (88%)	0.06	6 (8%) 12 10	92, 128, 153, 161	0
24	V	66/67 (98%)	0.03	5 (7%) 15 11	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%)	-0.48	1 (1%) 69 55	80, 98, 126, 152	0
26	Z	58/60 (96%)	-0.17	3 (5%) 28 20	49, 70, 105, 114	0
27	1	53/55 (96%)	2.49	19 (35%) 0 0	8, 32, 62, 93	0
28	2	46/47 (97%)	5.93	44 (95%) 0 0	3, 15, 38, 59	0
29	3	63/66 (95%)	3.45	44 (69%) 0 0	3, 25, 40, 61	0
30	4	37/37 (100%)	4.01	24 (64%) 0 0	228, 254, 266, 269	0
All	All	5997/6561 (91%)	-0.01	311 (5%) 28 20	3, 100, 196, 276	0

The worst 5 of 311 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	19.2
28	2	27	GLY	13.8
30	4	25	VAL	12.9
22	T	9	SER	12.8
28	2	8	ASN	12.4

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
31	MG	X	2926	1/1	0.79	1.78	49.54	45,45,45,45	0
31	MG	X	2917	1/1	0.94	1.09	36.48	55,55,55,55	0
31	MG	X	2924	1/1	0.79	1.09	25.37	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	2907	1/1	0.96	0.81	22.55	51,51,51,51	0
31	MG	Y	202	1/1	0.88	1.43	21.91	88,88,88,88	0
31	MG	X	2901	1/1	0.53	0.69	19.77	50,50,50,50	0
31	MG	X	2915	1/1	0.85	0.73	16.42	57,57,57,57	0
31	MG	X	2922	1/1	0.95	0.86	12.19	44,44,44,44	0
31	MG	X	2914	1/1	0.96	0.64	4.43	27,27,27,27	0
32	1F4	X	2929	58/58	0.96	0.21	-0.27	20,20,20,20	0
31	MG	X	2925	1/1	0.97	0.27	-	122,122,122,122	0
31	MG	X	2927	1/1	0.68	0.52	-	64,64,64,64	0
31	MG	M	201	1/1	0.98	1.39	-	23,23,23,23	0
31	MG	X	2902	1/1	0.93	0.31	-	94,94,94,94	0
31	MG	X	2910	1/1	0.99	0.69	-	41,41,41,41	0
31	MG	Y	201	1/1	0.93	0.46	-	98,98,98,98	0
31	MG	X	2921	1/1	0.91	0.70	-	80,80,80,80	0
31	MG	X	2913	1/1	0.36	1.00	-	60,60,60,60	0
31	MG	Y	204	1/1	0.34	0.97	-	86,86,86,86	0
31	MG	X	2920	1/1	0.54	0.46	-	113,113,113,113	0
31	MG	X	2928	1/1	0.56	0.81	-	61,61,61,61	0
31	MG	X	2916	1/1	0.86	1.18	-	37,37,37,37	0
31	MG	Y	203	1/1	0.81	0.89	-	59,59,59,59	0
31	MG	X	2903	1/1	0.45	0.63	-	89,89,89,89	0
31	MG	X	2906	1/1	0.94	0.95	-	58,58,58,58	0
31	MG	X	2919	1/1	0.92	0.92	-	30,30,30,30	0
31	MG	X	2905	1/1	0.89	0.49	-	65,65,65,65	0
31	MG	Y	205	1/1	0.92	0.40	-	82,82,82,82	0
31	MG	X	2923	1/1	0.96	0.34	-	34,34,34,34	0
31	MG	X	2909	1/1	0.33	0.62	-	97,97,97,97	0
31	MG	X	2908	1/1	0.82	2.34	-	37,37,37,37	0
31	MG	Y	206	1/1	0.84	0.29	-	78,78,78,78	0
31	MG	X	2911	1/1	0.77	0.39	-	68,68,68,68	0
31	MG	X	2904	1/1	0.92	0.30	-	110,110,110,110	0
31	MG	X	2918	1/1	0.84	1.24	-	42,42,42,42	0
31	MG	X	2912	1/1	0.70	0.58	-	71,71,71,71	0

6.5 Other polymers ⓘ

There are no such residues in this entry.