



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 06:11 AM EDT

PDB ID : 4U67 / pdb_00004u67
Title : Crystal structure of the large ribosomal subunit (50S) of *Deinococcus radiodurans* containing a three residue insertion in L22
Authors : Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on : 2014-07-28
Resolution : 3.65 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

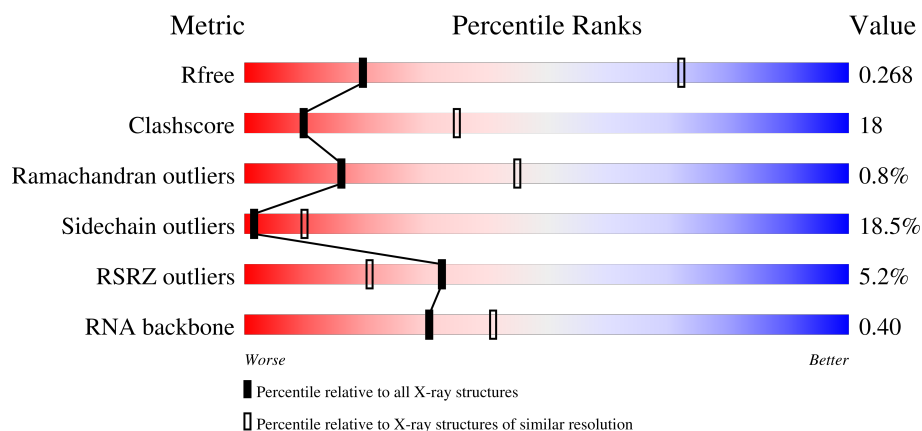
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)
RNA backbone	3983	1027 (4.26-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	275	
2	B	211	
3	C	205	
4	D	180	

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Mol	Chain	Length	Quality of chain
5	E	185	
6	G	174	
7	H	134	
8	I	156	
9	J	141	
10	K	116	
11	L	114	
12	M	166	
13	N	118	
14	O	100	
15	P	137	
16	Q	95	
17	R	114	
18	S	237	
19	T	91	
20	U	81	
21	V	67	
22	W	55	
23	Z	60	
24	1	55	
25	2	47	
26	3	66	
27	X	2880	
28	Y	123	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MG	X	2908	-	-	-	X
29	MG	X	2910	-	-	-	X
29	MG	X	2924	-	-	-	X
29	MG	X	2926	-	-	-	X
29	MG	X	2944	-	-	-	X
29	MG	X	2948	-	-	-	X

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 83768 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1987	1235	399	350	3			

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L13.

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

- Molecule 7 is a protein called 50S ribosomal protein L14.

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	134	Total	C	N	O		0	0	0
			1011	619	206	186				

- Molecule 9 is a protein called 50S ribosomal protein L16.

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

- Molecule 10 is a protein called 50S ribosomal protein L17.

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

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L19.

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

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

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

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	P	130	Total	C	N	O	S		
			1038	655	205	176	2	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	110	VAL	-	insertion	UNP Q9RXJ7
P	111	PRO	-	insertion	UNP Q9RXJ7
P	112	ARG	-	insertion	UNP Q9RXJ7

- Molecule 16 is a protein called 50S ribosomal protein L23.

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

- Molecule 17 is a protein called 50S ribosomal protein L24.

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

- Molecule 18 is a protein called 50S ribosomal protein L25.

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

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	T	74	Total	C	N	O	S		
			556	351	107	97	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L28.

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

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	65	Total	C	N	O	S			
			525	322	106	95	2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L30.

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

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	56	Total	C	N	O	S			
			443	272	91	75	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	53	Total	C	N	O	S			
			431	274	80	76	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	46	Total	C	N	O	S			
			383	230	91	60	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	S			
			462	290	95	73	4	0	0	0

- Molecule 27 is a RNA chain called 23s RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	2667	Total	C	N	O	P	0	0	0
			57254	25538	10574	18475	2667			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

- Molecule 28 is a RNA chain called 5s RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

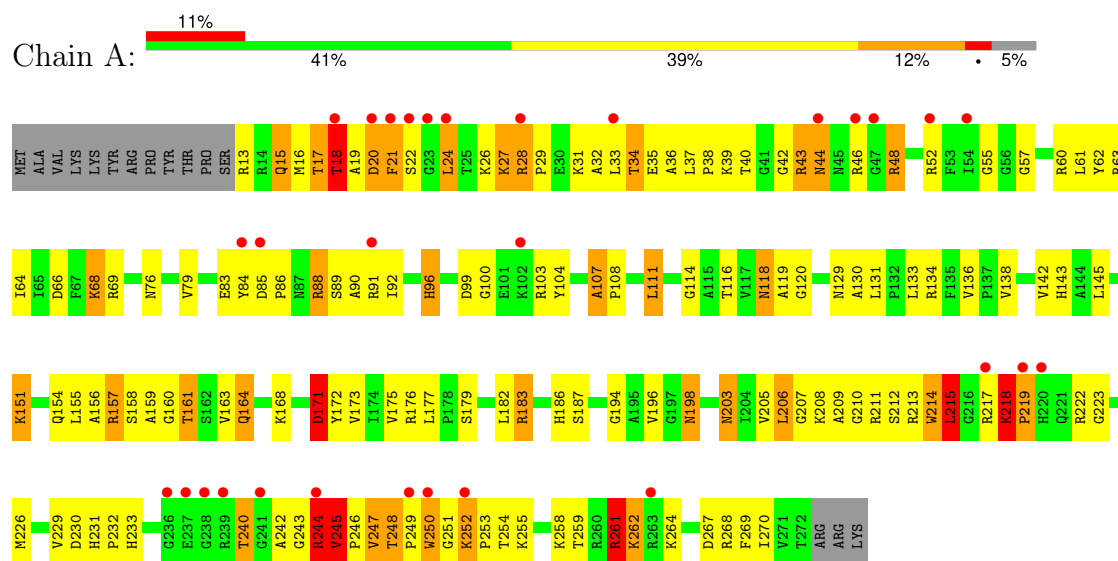
- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	K	1	Total	Mg	0	0
			1	1		
29	X	50	Total	Mg	0	0
			50	50		

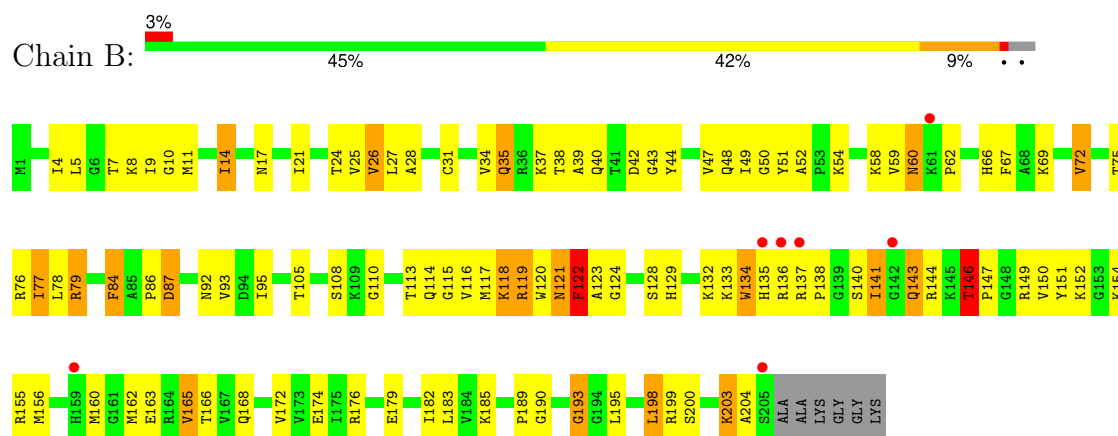
3 Residue-property plots [i](#)

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

• Molecule 1: 50S ribosomal protein L2

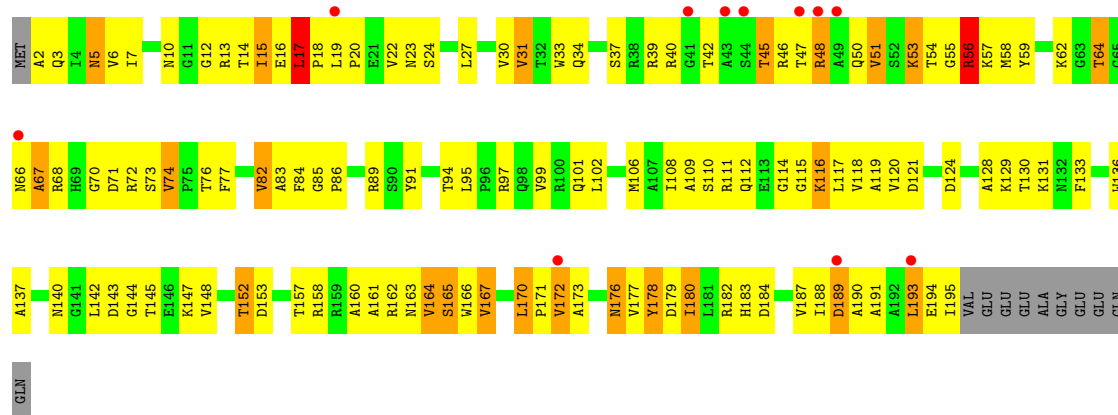


• Molecule 2: 50S ribosomal protein L3

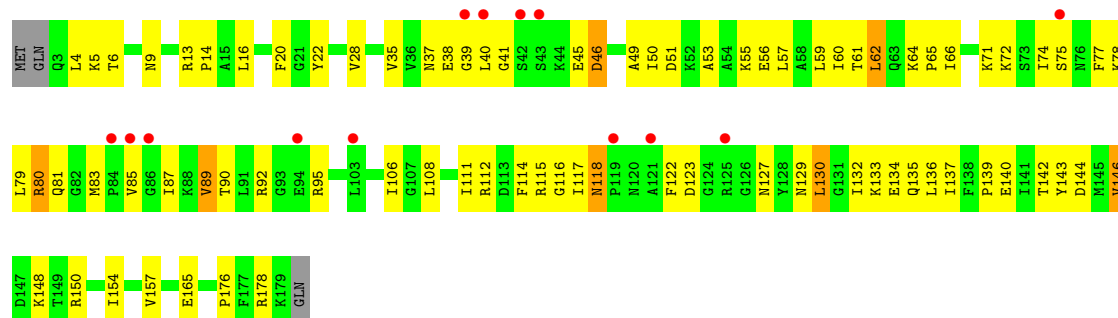


• Molecule 3: 50S ribosomal protein L4

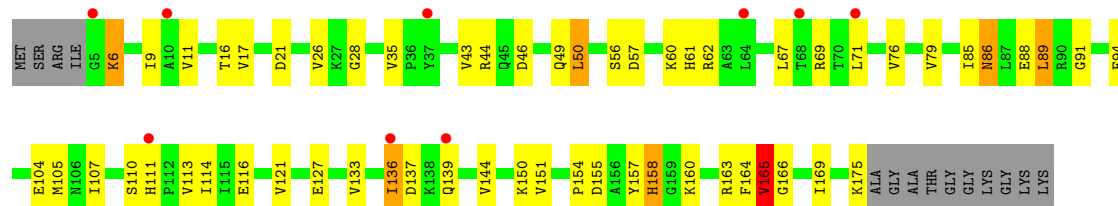




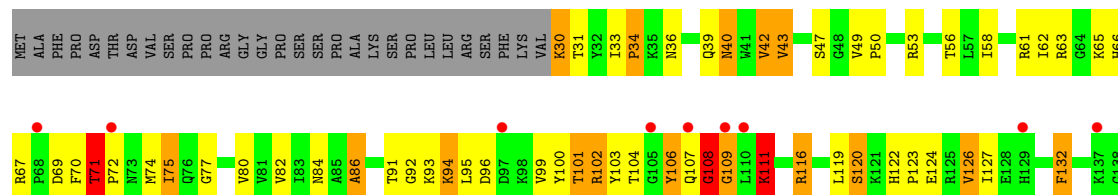
• Molecule 4: 50S ribosomal protein L5



• Molecule 5: 50S ribosomal protein L6



• Molecule 6: 50S ribosomal protein L13

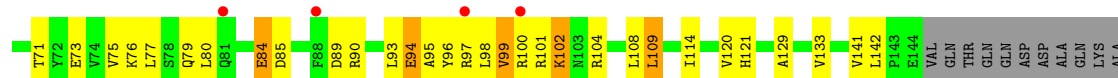
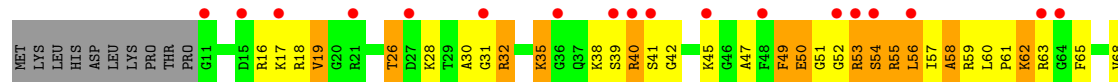
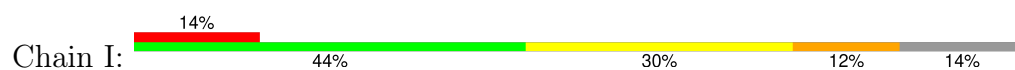




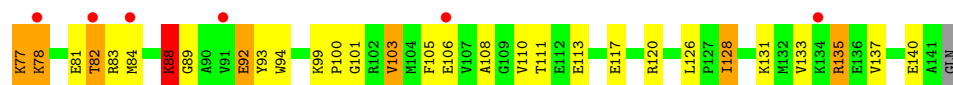
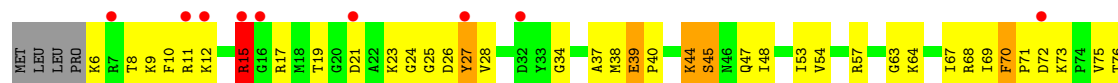
• Molecule 7: 50S ribosomal protein L14



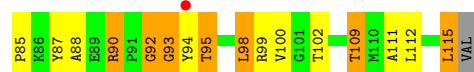
• Molecule 8: 50S ribosomal protein L15



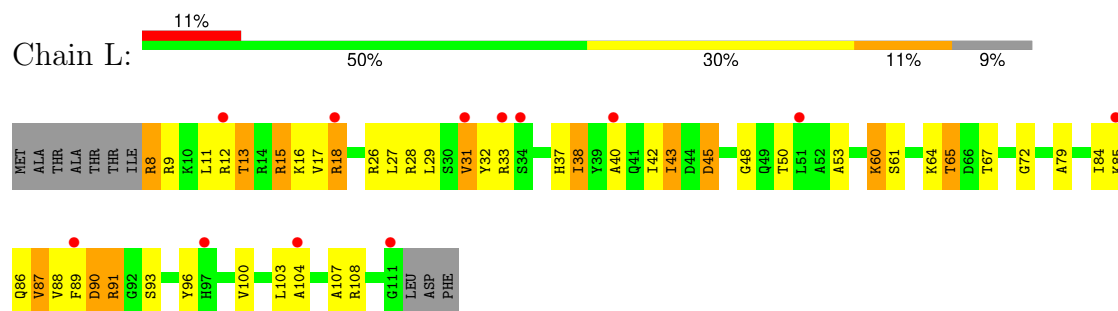
• Molecule 9: 50S ribosomal protein L16



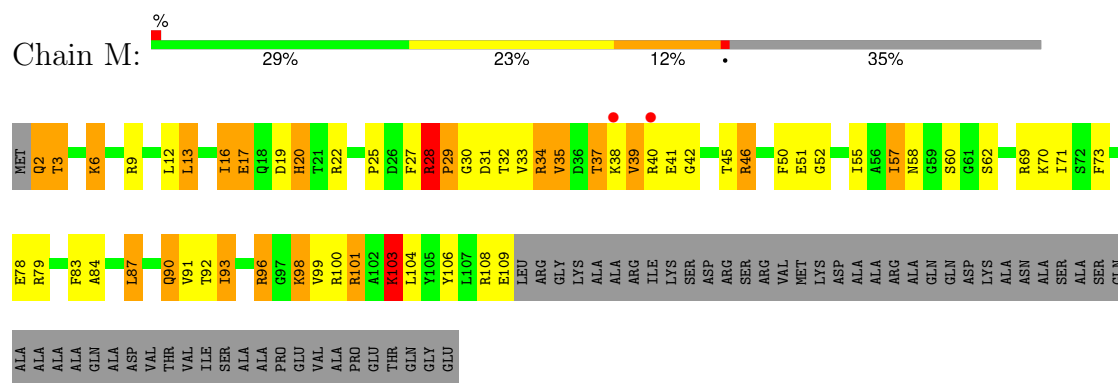
• Molecule 10: 50S ribosomal protein L17



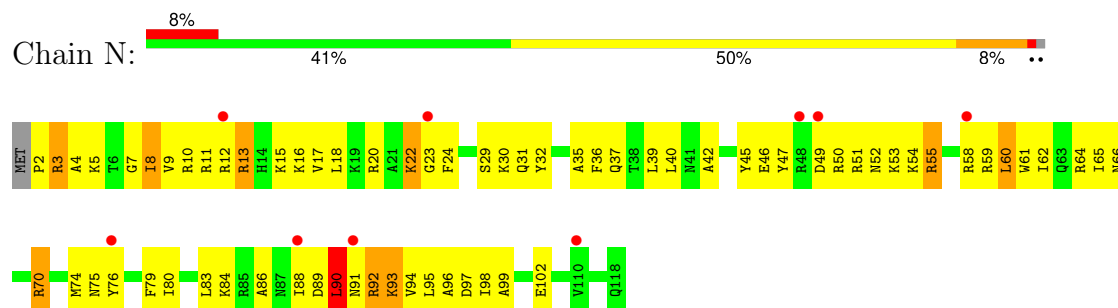
- Molecule 11: 50S ribosomal protein L18



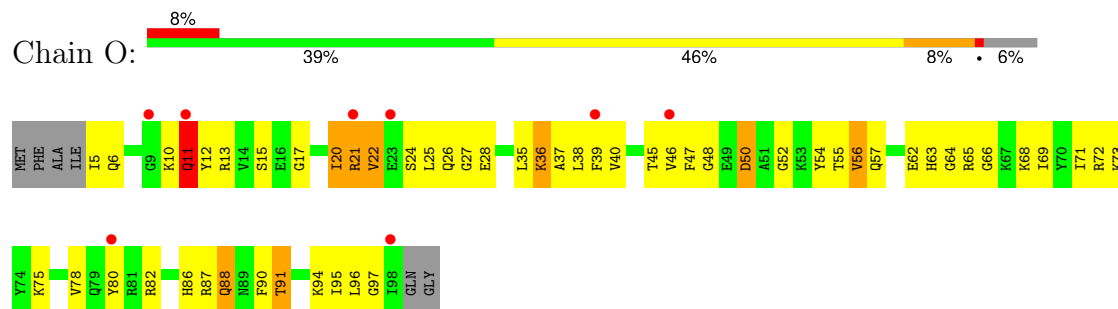
- Molecule 12: 50S ribosomal protein L19



- Molecule 13: 50S ribosomal protein L20

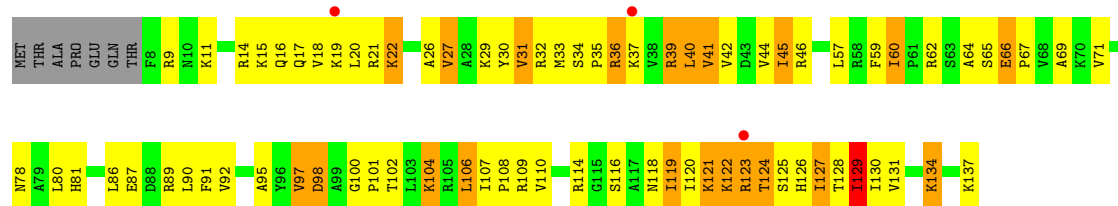


- Molecule 14: 50S ribosomal protein L21

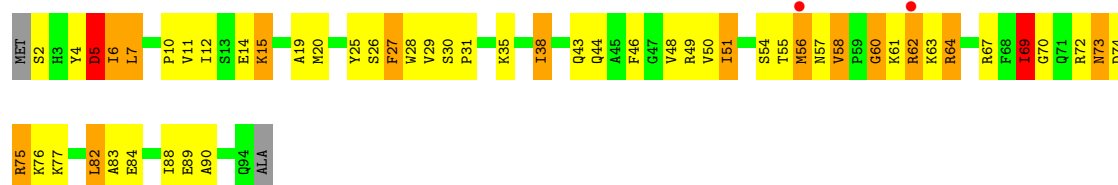


- Molecule 15: 50S ribosomal protein L22

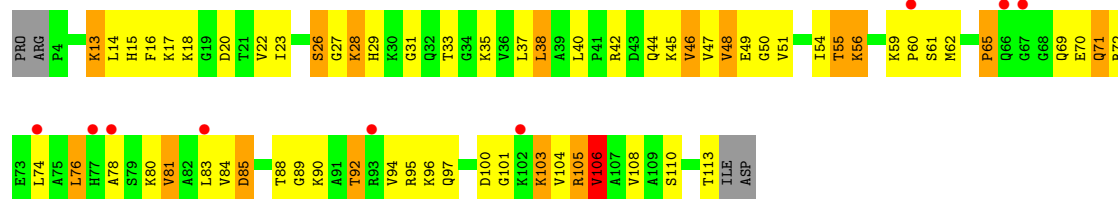




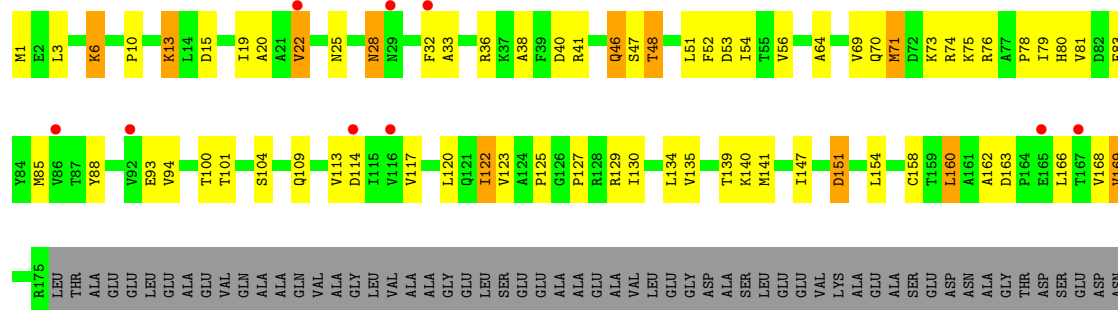
• Molecule 16: 50S ribosomal protein L23



• Molecule 17: 50S ribosomal protein L24

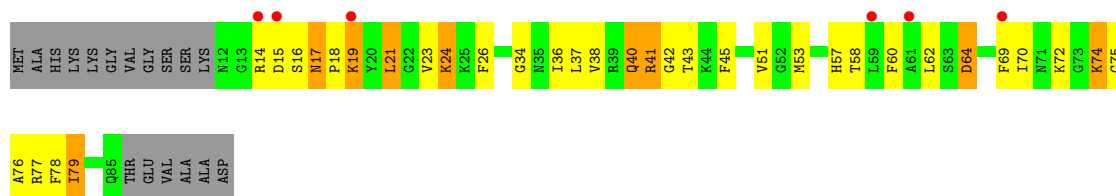


• Molecule 18: 50S ribosomal protein L25

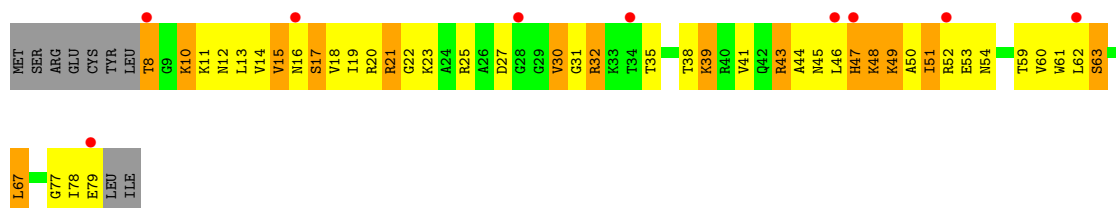


• Molecule 19: 50S ribosomal protein L27

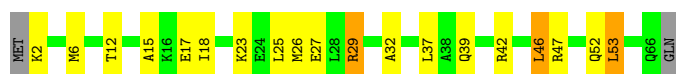




- Molecule 20: 50S ribosomal protein L28



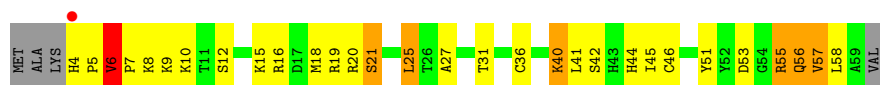
- Molecule 21: 50S ribosomal protein L29



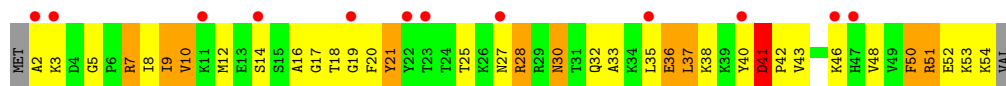
- Molecule 22: 50S ribosomal protein L30



- Molecule 23: 50S ribosomal protein L32

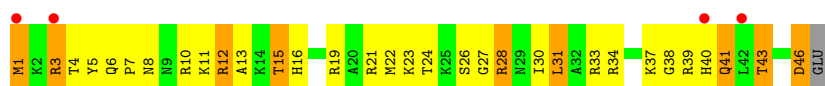


- Molecule 24: 50S ribosomal protein L33

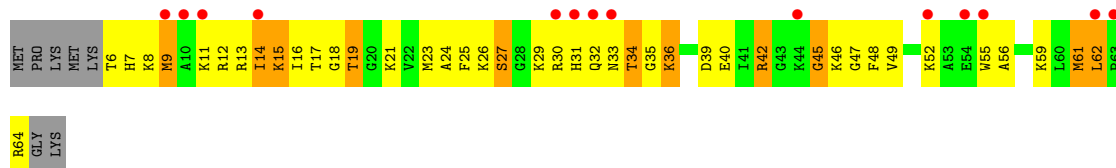


- Molecule 25: 50S ribosomal protein L34

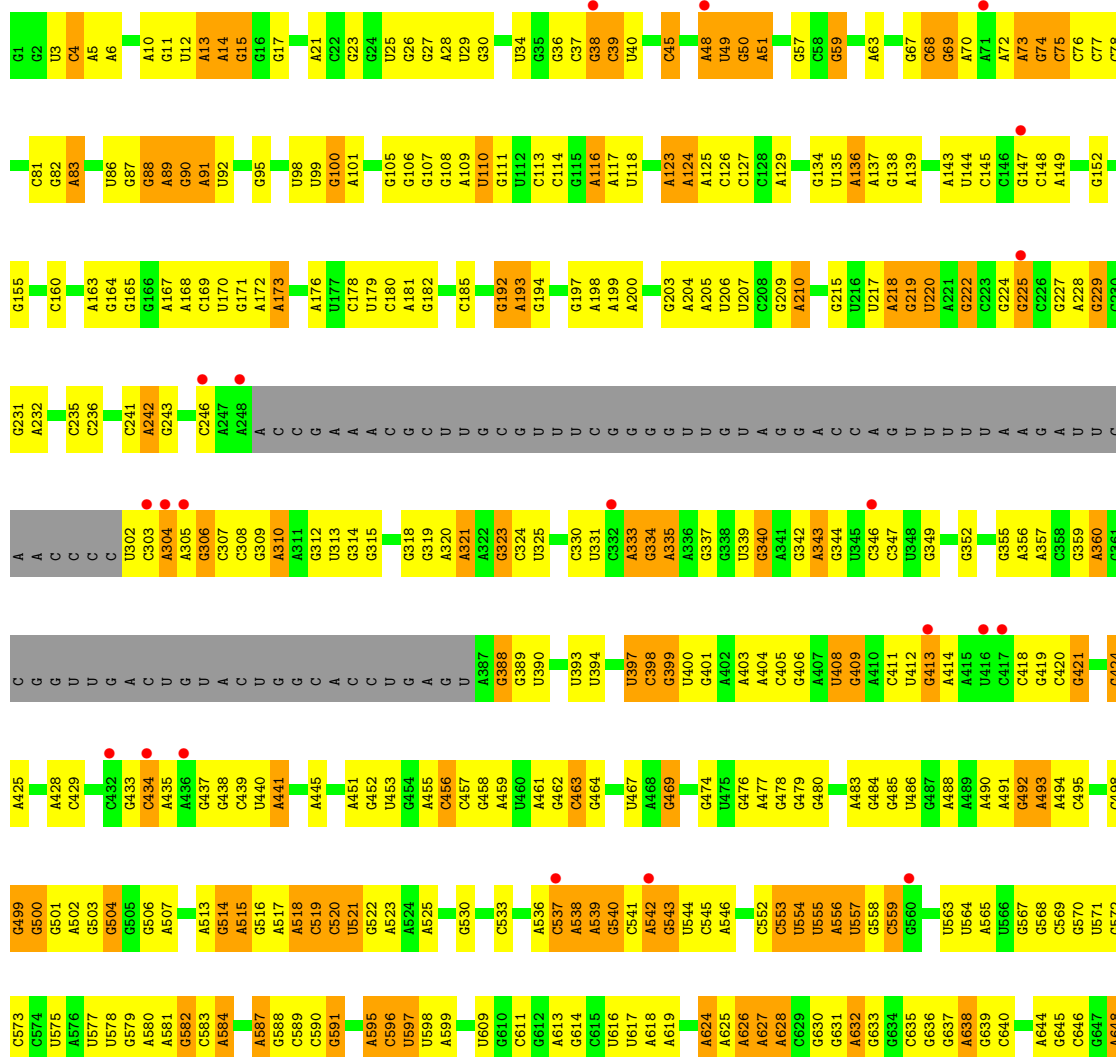


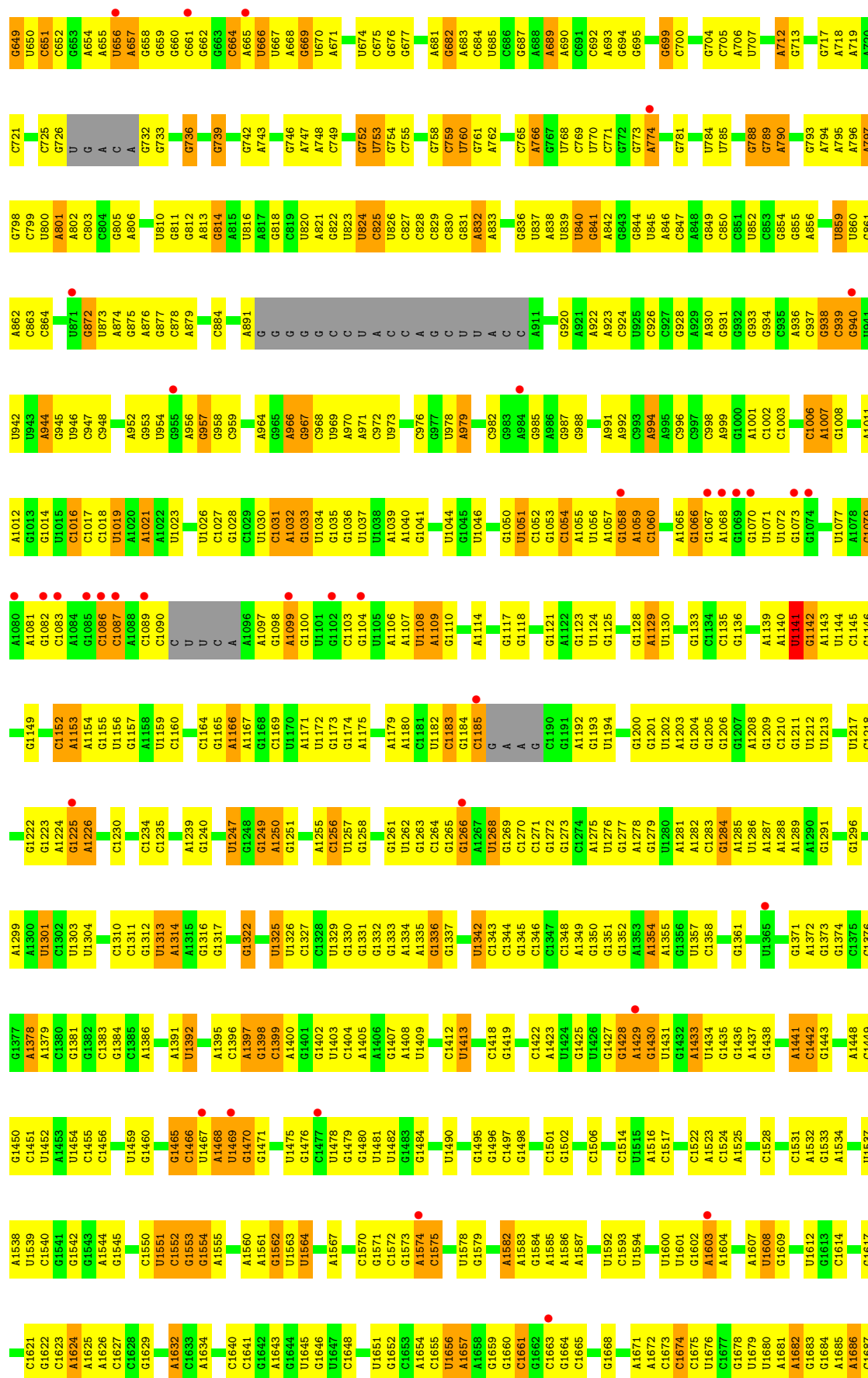


• Molecule 26: 50S ribosomal protein L35

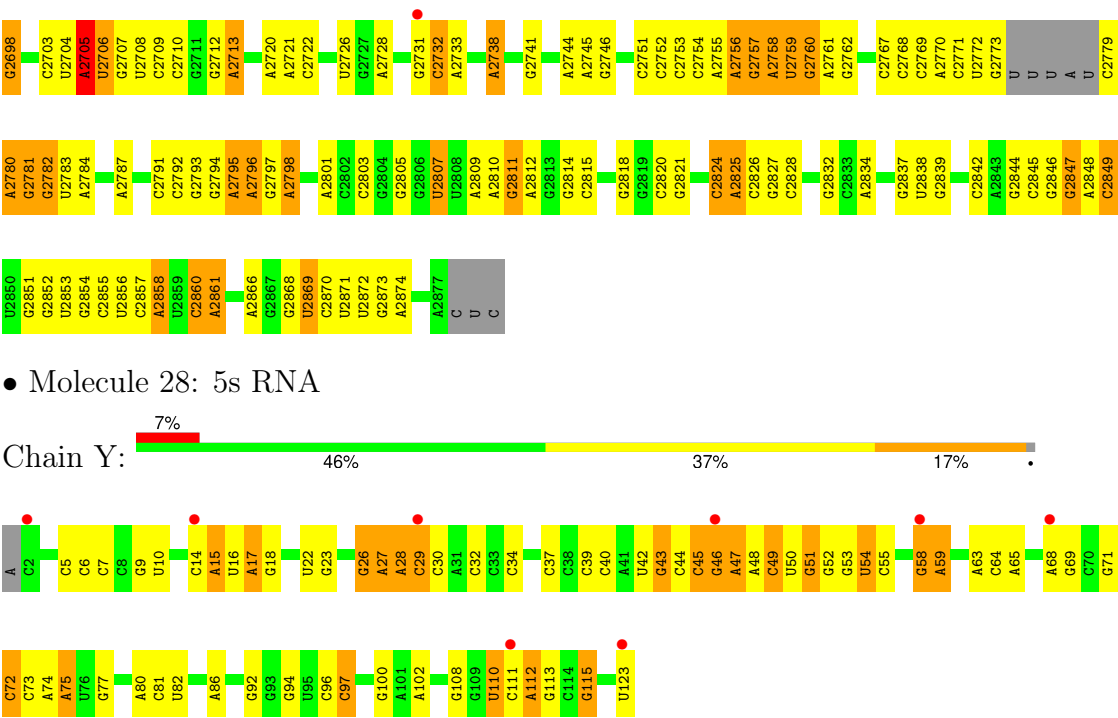


• Molecule 27: 23s RNA





G2620	G2621	G2624	G2625	G2626	G2627	G2628	G2629	A2633	G2634	G2635	A2636	G2637	G2640	A2641	G2642	G2645	G2646	G2650	G2651	G2652	G2653	G2654	A2655	G2656	G2657	A2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	A2690	A2691	A2692	U2693	G2694	G2695	A2696	G2697													
C2547	C2548	G2549	C2550	A2551	C2552	G2553	G2554	G2555	A2556	G2557	G2558	G2559	G2560	G2561	G2562	U2563	U2564	G2565	A2566	G2571	U2572	C2573	G2576	A2577	G2578	A2579	C2580	A2581	G2582	U2583	G2587	U2588	C2591	G2592	A2593	U2594	C2595	G2596	U2597	G2598	G2599	A2600	G2604	C2605	G2606	G2607	A2608										
C2477	U2478	U2479	C2480	G2481	A2482	U2483	G2484	U2485	G2486	G2487	G2488	G2489	U2490	C2491	G2492	U2493	C2494	G2495	A2496	A2497	U2498	C2499	C2500	G2504	G2508	A2509	A2510	A2513	G2514	G2515	U2516	C2517	G2518	U2519	C2520	A2521	G2522	G2523	U2526	G2527	G2528	U2529	G2530	U2531	G2532	U2533	U2534	A2540	U2541	U2542	A2543	A2544	G2545	G2546			
A2401	U2402	C2403	A2404	A2405	C2406	G2407	G2408	A2409	U2410	A2413	U2417	A2418	G2419	A2420	C2421	C2422	G2423	G2424	G2425	G2426	A2427	U2428	A2429	A2430	C2431	A2432	G2433	G2434	G2435	U2436	G2437	A2438	U2441	C2442	C2443	C2444	G2447	A2448	G2449	A2450	G2451	U2452	C2453	C2454	A2455	U2456	A2457	U2458	G2463	U2471	U2475	A2476					
C2329	G2330	A2331	G2332	C2333	C2334	U2335	G2336	A2337	C2338	A2339	C2340	C2343	G2344	A2345	G2346	G2351	A2352	G2353	G2354	A2355	A2356	A2357	G2358	U2359	C2360	G2361	G2362	G2363	G2364	G2368	U2369	G2370	A2371	A2372	G2375	U2376	U2377	G2378	U2379	U2380	A2381	C2382	G2386	U2387	G2388	G2389	G2394	C2395	G2396	A2397	U2398	G2399	C2400				
C2260	G2261	C2262	C2263	C2264	A2265	A2266	G2267	G2268	G2269	U2270	C2271	A2272	A2277	A2278	G2281	G2282	G2283	U2284	U2285	G2286	G2287	A2288	A2289	A2290	U2291	G2292	G2293	U2294	G2297	U2298	A2299	G2300	A2301	G2302	C2303	G2304	C2305	A2306	A2307	A2308	G2309	G2310	U2311	A2312	G2313	A2314	A2315	U2318	U2324	U2325	A2326	U2327	G2328				
U2180	A2181	U2185	G2186	A2187	A2188	A2189	A2190	A2191	U2192	G2193	A2194	C2195	U2196	U2197	U2198	C2199	G2200	G2201	G2202	G2203	A2204	C2205	U2212	G2213	G2217	G2218	U2222	U2223	U2224	G2225	A2226	C2227	U2228	G2229	G2230	G2234	G2235	U2236	C2237	U2241	C2242	C2243	C2244	A2245	A2246	A2247	G2250	U2251	A2252	A2253	C2254						
A	C	U	G	G	C	U	U	U	U	G	G	G	G	G	C	C	U	U	G	G	G	G	C	A	A	C	C	U	U	A	G	C	A	C	C	C	C	C	G	A2165	A2166	A2167	A2168	A2169	C2170	U2171	G2174	A2175	U2176	U2177	U2178	C2179					
G1983	A1984	G1985	G1986	G1987	A1988	C1989	U1990	C1991	G1992	G1993	U1994	G1995	A1996	A1997	U1998	U1999	U2000	G2001	A2002	A2003	U2004	U2005	G2006	G2007	C2008	U2009	G2010	U2011	A2012	A2013	A2014	G2015	A2016	U2017	G2018	C2019	G2020	G2021	C2022	G2023	A2024	A2025	C2026	C2027	A2031	G2032	C2033	A2034	G2035	C2038	G2039	A2040	A2041	A2042	A2043	A2044	A2045
U1833	G1834	G1835	C1836	A1840	G1841	G1842	G1843	A1844	C1845	A1846	G1850	A1851	G1852	C1853	G1854	G1855	U1856	G1857	C1858	A1859	A1860	G1861	C1865	G1866	G1867	A1868	G1871	A1872	G1873	U1874	A1875	G1876	G1877	G1879	G1882	C1885	G1886	G1887	C1888	G1815	G1816	U1817	G1818	U1819	A1820	A1821	C1824	G1825	U1826	G1827	A1831	G1832					
U1768	U1769	U1770	C1773	A1774	A1775	A1776	U1777	U1778	U1779	A1780	C1781	A1782	A1785	C1786	U1787	G1788	U1789	G1790	C1791	G1792	A1793	A1794	C1795	A1796	C1797	G1798	A1799	A1800	C1801	A1802	G1803	U1804	G1805	G1806	A1807	C1808	G1809	A1810	A1811	A1812	A1813	G1814	G1815	U1816	U1817	G1818	U1819	A1820	A1821	C1824	G1825	U1826	G1827	A1831	G1832		
U1688	C1691	C1692	A1693	A1694	C1698	A1699	C1703	G1704	U1705	U1710	U1711	U1712	U1713	U1714	U1715	G1716	C1717	A1718	U1723	C1724	C1725	G1726	C1727	A1728	C1731	U1732	U1733	C1734	G1735	G1740	G1741	G1744	U1747	U1748	G1749	A1750	U1751	U1752	U1753	G1754	G1755	G1760	G1761	C1762	G1763	A1764	G1765	C1766	G1767								



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.72Å 412.59Å 696.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.65 19.99 – 3.65	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.99-3.65) 95.3 (19.99-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.226 , 0.270 0.227 , 0.268	Depositor DCC
R_{free} test set	13171 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	108.4	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83768	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.61	1/2025 (0.0%)	1.25	33/2726 (1.2%)
2	B	0.69	0/1567	1.18	8/2105 (0.4%)
3	C	0.58	0/1504	1.15	13/2036 (0.6%)
4	D	0.37	0/1419	0.86	2/1903 (0.1%)
5	E	0.40	0/1308	0.94	5/1771 (0.3%)
6	G	0.61	0/1138	1.29	15/1539 (1.0%)
7	H	0.75	1/1007 (0.1%)	1.17	6/1352 (0.4%)
8	I	0.63	0/1022	1.21	9/1366 (0.7%)
9	J	0.64	0/1113	1.29	22/1486 (1.5%)
10	K	0.79	0/886	1.26	8/1188 (0.7%)
11	L	0.45	0/785	0.95	1/1048 (0.1%)
12	M	0.79	2/884 (0.2%)	1.28	10/1186 (0.8%)
13	N	0.56	0/994	1.03	2/1323 (0.2%)
14	O	0.50	0/750	1.11	5/1000 (0.5%)
15	P	0.74	0/1052	1.27	9/1409 (0.6%)
16	Q	0.54	0/737	1.18	7/988 (0.7%)
17	R	0.60	0/835	1.16	10/1121 (0.9%)
18	S	0.43	0/1370	0.91	2/1862 (0.1%)
19	T	0.54	0/563	1.14	7/747 (0.9%)
20	U	0.59	0/556	1.07	2/741 (0.3%)
21	V	0.39	0/529	0.99	4/704 (0.6%)
22	W	0.48	0/426	0.93	2/568 (0.4%)
23	Z	0.66	0/455	1.20	4/611 (0.7%)
24	1	0.56	0/438	1.27	5/583 (0.9%)
25	2	0.56	0/387	1.22	6/509 (1.2%)
26	3	0.63	0/468	1.36	8/614 (1.3%)
27	X	0.32	0/64113	0.52	5/99999 (0.0%)
28	Y	0.22	0/2907	0.40	0/4529
All	All	0.41	4/91238 (0.0%)	0.72	210/137014 (0.2%)

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	A	0	1
2	B	0	2
6	G	0	4
7	H	0	1
8	I	0	2
10	K	0	1
17	R	0	2
20	U	0	1
26	3	0	1
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	29	PRO	CA-C	6.04	1.60	1.52
7	H	2	ILE	CA-CB	-5.23	1.48	1.54
1	A	20	ASP	CA-C	5.21	1.58	1.52
12	M	35	VAL	CA-CB	5.13	1.59	1.53

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	69	ILE	N-CA-C	12.65	124.19	112.29
16	Q	61	LYS	N-CA-C	12.42	125.44	110.91
8	I	52	GLY	N-CA-C	11.67	123.94	112.04
15	P	60	ILE	CA-C-N	10.65	130.32	119.56
15	P	60	ILE	C-N-CA	10.65	130.32	119.56

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	THR	Peptide
2	B	122	PHE	Peptide
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
6	G	34	PRO	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	A	1987	0	2056	130	0
2	B	1539	0	1600	107	0
3	C	1481	0	1504	102	0
4	D	1400	0	1481	61	0
5	E	1286	0	1336	36	0
6	G	1114	0	1144	66	0
7	H	997	0	1046	64	0
8	I	1011	0	1047	55	0
9	J	1090	0	1125	57	0
10	K	878	0	930	40	0
11	L	779	0	820	40	0
12	M	871	0	894	50	0
13	N	978	0	1020	71	0
14	O	741	0	756	47	0
15	P	1038	0	1125	81	0
16	Q	726	0	753	37	0
17	R	825	0	881	52	0
18	S	1345	0	1372	44	0
19	T	556	0	579	28	0
20	U	552	0	604	30	0
21	V	525	0	546	16	0
22	W	424	0	470	16	0
23	Z	443	0	444	28	0
24	1	431	0	456	30	0
25	2	383	0	414	28	0
26	3	462	0	506	49	0
27	X	57254	0	28850	1335	0
28	Y	2601	0	1327	54	0
29	K	1	0	0	0	0
29	X	50	0	0	0	0
All	All	83768	0	55086	2395	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 18.

The worst 5 of 2395 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)
1:A:55:GLY:H	1:A:217:ARG:HB2	1.20	1.04
2:B:136:ARG:HB3	27:X:1673:C:H5'	1.36	1.04
27:X:571:U:HO2'	27:X:581:A:H8	1.12	0.98
27:X:517:A:H5''	27:X:518:A:H5'	1.45	0.95
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.49	0.95

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	
1	A	258/275 (94%)	223 (86%)	34 (13%)	1 (0%)	30	58
2	B	203/211 (96%)	182 (90%)	20 (10%)	1 (0%)	24	55
3	C	192/205 (94%)	165 (86%)	25 (13%)	2 (1%)	12	41
4	D	175/180 (97%)	153 (87%)	21 (12%)	1 (1%)	21	51
5	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	21	51
6	G	140/174 (80%)	126 (90%)	14 (10%)	0	100	100
7	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	16	45
8	I	132/156 (85%)	101 (76%)	28 (21%)	3 (2%)	5	26
9	J	134/141 (95%)	115 (86%)	19 (14%)	0	100	100
10	K	111/116 (96%)	102 (92%)	9 (8%)	0	100	100
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100	100
12	M	106/166 (64%)	101 (95%)	5 (5%)	0	100	100
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	7	31
14	O	92/100 (92%)	81 (88%)	11 (12%)	0	100	100
15	P	128/137 (93%)	109 (85%)	17 (13%)	2 (2%)	7	32
16	Q	91/95 (96%)	78 (86%)	11 (12%)	2 (2%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	108/114 (95%)	86 (80%)	22 (20%)	0	100	100
18	S	173/237 (73%)	152 (88%)	21 (12%)	0	100	100
19	T	72/91 (79%)	61 (85%)	9 (12%)	2 (3%)	4	23
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	1	12
21	V	63/67 (94%)	59 (94%)	4 (6%)	0	100	100
22	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	37 (72%)	11 (22%)	3 (6%)	1	12
25	2	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
26	3	57/66 (86%)	46 (81%)	11 (19%)	0	100	100
All	All	3025/3380 (90%)	2633 (87%)	367 (12%)	25 (1%)	16	45

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	6	ILE
13	N	94	VAL
15	P	127	ILE
24	1	9	ILE
24	1	10	VAL

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	
1	A	202/216 (94%)	157 (78%)	45 (22%)	1	6
2	B	155/157 (99%)	130 (84%)	25 (16%)	2	13
3	C	154/163 (94%)	121 (79%)	33 (21%)	1	7
4	D	153/156 (98%)	140 (92%)	13 (8%)	10	32
5	E	136/144 (94%)	120 (88%)	16 (12%)	5	22
6	G	118/146 (81%)	95 (80%)	23 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	103/103 (100%)	84 (82%)	19 (18%)	1	10
8	I	101/121 (84%)	79 (78%)	22 (22%)	1	6
9	J	110/115 (96%)	87 (79%)	23 (21%)	1	7
10	K	90/93 (97%)	74 (82%)	16 (18%)	2	11
11	L	74/82 (90%)	54 (73%)	20 (27%)	0	3
12	M	94/134 (70%)	66 (70%)	28 (30%)	0	2
13	N	96/97 (99%)	79 (82%)	17 (18%)	2	11
14	O	75/79 (95%)	65 (87%)	10 (13%)	4	19
15	P	112/118 (95%)	87 (78%)	25 (22%)	1	6
16	Q	75/76 (99%)	55 (73%)	20 (27%)	0	3
17	R	91/95 (96%)	80 (88%)	11 (12%)	5	21
18	S	149/192 (78%)	125 (84%)	24 (16%)	2	13
19	T	55/67 (82%)	48 (87%)	7 (13%)	4	20
20	U	57/66 (86%)	41 (72%)	16 (28%)	0	2
21	V	53/55 (96%)	49 (92%)	4 (8%)	12	37
22	W	48/48 (100%)	45 (94%)	3 (6%)	16	41
23	Z	50/53 (94%)	43 (86%)	7 (14%)	3	17
24	1	46/48 (96%)	31 (67%)	15 (33%)	0	1
25	2	39/40 (98%)	30 (77%)	9 (23%)	1	5
26	3	46/52 (88%)	39 (85%)	7 (15%)	3	15
All	All	2482/2716 (91%)	2024 (82%)	458 (18%)	1	10

5 of 458 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	K	95	THR
25	2	10	ARG
13	N	18	LEU
24	1	43	VAL
20	U	17	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
21	V	54	ASN
23	Z	35	GLN
26	3	31	HIS
6	G	140	GLN
6	G	129	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2657/2880 (92%)	612 (23%)	39 (1%)
28	Y	121/123 (98%)	31 (25%)	2 (1%)
All	All	2778/3003 (92%)	643 (23%)	41 (1%)

5 of 643 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	4	C
27	X	13	A
27	X	14	A
27	X	15	G
27	X	17	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	1923	U
27	X	2409	A
27	X	1975	G
27	X	2299	A
27	X	2756	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 51 ligands modelled in this entry, 51 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	260/275 (94%)	0.57	30 (11%) 9 9	45, 101, 165, 255	0
2	B	205/211 (97%)	0.05	7 (3%) 48 29	26, 43, 97, 208	0
3	C	194/205 (94%)	0.26	11 (5%) 29 19	38, 101, 172, 256	0
4	D	177/180 (98%)	0.47	13 (7%) 21 15	108, 173, 225, 261	0
5	E	171/185 (92%)	0.07	9 (5%) 32 20	51, 120, 177, 236	0
6	G	142/174 (81%)	0.41	13 (9%) 14 11	35, 72, 151, 204	0
7	H	134/134 (100%)	-0.07	3 (2%) 62 37	31, 42, 85, 136	0
8	I	134/156 (85%)	0.84	22 (16%) 4 5	53, 125, 199, 245	0
9	J	136/141 (96%)	0.46	15 (11%) 10 10	56, 88, 168, 221	0
10	K	113/116 (97%)	-0.03	3 (2%) 56 33	25, 30, 61, 99	0
11	L	104/114 (91%)	0.81	12 (11%) 9 9	128, 160, 197, 232	0
12	M	108/166 (65%)	-0.05	2 (1%) 66 40	29, 37, 93, 143	0
13	N	117/118 (99%)	0.27	9 (7%) 19 13	40, 78, 123, 213	0
14	O	94/100 (94%)	0.43	8 (8%) 16 12	51, 96, 164, 191	0
15	P	130/137 (94%)	0.03	3 (2%) 61 36	31, 51, 149, 168	0
16	Q	93/95 (97%)	-0.05	2 (2%) 62 37	45, 83, 145, 192	0
17	R	110/114 (96%)	0.51	9 (8%) 17 13	66, 97, 187, 238	0
18	S	175/237 (73%)	0.28	9 (5%) 33 21	89, 141, 204, 258	0
19	T	74/91 (81%)	0.56	6 (8%) 18 13	70, 110, 148, 231	0
20	U	72/81 (88%)	0.78	9 (12%) 8 8	73, 123, 178, 252	0
21	V	65/67 (97%)	-0.09	0 100 100	67, 111, 168, 222	0
22	W	55/55 (100%)	-0.16	1 (1%) 67 41	72, 94, 147, 177	0
23	Z	56/60 (93%)	0.00	1 (1%) 67 41	30, 36, 87, 100	0
24	1	53/55 (96%)	1.09	12 (22%) 2 3	98, 127, 189, 275	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	46/47 (97%)	0.50	4 (8%) 16 12	39, 69, 102, 127	0
26	3	59/66 (89%)	1.19	14 (23%) 2 2	79, 99, 176, 252	0
27	X	2667/2880 (92%)	0.09	71 (2%) 56 33	25, 73, 176, 304	0
28	Y	122/123 (99%)	0.56	8 (6%) 24 16	74, 150, 189, 279	0
All	All	5866/6383 (91%)	0.23	306 (5%) 33 21	25, 87, 182, 304	0

The worst 5 of 306 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	T	15	ASP	9.6
9	J	84	MET	9.5
1	A	220	HIS	8.6
9	J	21	ASP	7.9
6	G	129	HIS	7.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
29	MG	X	2944	1/1	0.65	0.71	55,55,55,55	0
29	MG	X	2926	1/1	0.66	0.76	32,32,32,32	0
29	MG	X	2908	1/1	0.68	0.56	31,31,31,31	0
29	MG	X	2948	1/1	0.71	0.40	48,48,48,48	0
29	MG	X	2924	1/1	0.72	0.42	77,77,77,77	0
29	MG	X	2922	1/1	0.73	0.35	30,30,30,30	0
29	MG	X	2950	1/1	0.74	0.31	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	2910	1/1	0.75	0.60	39,39,39,39	0
29	MG	X	2904	1/1	0.76	0.29	29,29,29,29	0
29	MG	X	2919	1/1	0.76	0.37	59,59,59,59	0
29	MG	X	2947	1/1	0.77	0.36	49,49,49,49	0
29	MG	X	2912	1/1	0.78	0.39	27,27,27,27	0
29	MG	X	2914	1/1	0.78	0.35	26,26,26,26	0
29	MG	K	201	1/1	0.80	0.27	25,25,25,25	0
29	MG	X	2930	1/1	0.82	0.39	30,30,30,30	0
29	MG	X	2934	1/1	0.83	0.38	42,42,42,42	0
29	MG	X	2941	1/1	0.83	0.46	115,115,115,115	0
29	MG	X	2925	1/1	0.83	0.38	32,32,32,32	0
29	MG	X	2917	1/1	0.84	1.26	55,55,55,55	0
29	MG	X	2931	1/1	0.84	0.26	25,25,25,25	0
29	MG	X	2909	1/1	0.85	0.29	51,51,51,51	0
29	MG	X	2903	1/1	0.85	0.39	30,30,30,30	0
29	MG	X	2937	1/1	0.86	0.20	36,36,36,36	0
29	MG	X	2915	1/1	0.86	0.30	28,28,28,28	0
29	MG	X	2911	1/1	0.86	0.70	40,40,40,40	0
29	MG	X	2933	1/1	0.87	0.28	55,55,55,55	0
29	MG	X	2905	1/1	0.87	0.28	27,27,27,27	0
29	MG	X	2902	1/1	0.87	0.37	33,33,33,33	0
29	MG	X	2932	1/1	0.87	0.37	39,39,39,39	0
29	MG	X	2906	1/1	0.88	0.61	27,27,27,27	0
29	MG	X	2901	1/1	0.88	0.26	37,37,37,37	0
29	MG	X	2945	1/1	0.88	0.56	61,61,61,61	0
29	MG	X	2935	1/1	0.89	0.40	74,74,74,74	0
29	MG	X	2929	1/1	0.89	0.45	37,37,37,37	0
29	MG	X	2938	1/1	0.89	0.52	27,27,27,27	0
29	MG	X	2940	1/1	0.89	0.49	54,54,54,54	0
29	MG	X	2949	1/1	0.89	0.24	32,32,32,32	0
29	MG	X	2928	1/1	0.89	0.21	36,36,36,36	0
29	MG	X	2927	1/1	0.90	0.12	69,69,69,69	0
29	MG	X	2921	1/1	0.91	0.51	51,51,51,51	0
29	MG	X	2907	1/1	0.91	0.91	42,42,42,42	0
29	MG	X	2913	1/1	0.91	0.31	27,27,27,27	0
29	MG	X	2918	1/1	0.92	0.41	36,36,36,36	0
29	MG	X	2936	1/1	0.93	0.24	33,33,33,33	0
29	MG	X	2939	1/1	0.93	0.21	32,32,32,32	0
29	MG	X	2923	1/1	0.95	0.21	33,33,33,33	0
29	MG	X	2916	1/1	0.95	0.29	26,26,26,26	0
29	MG	X	2920	1/1	0.95	0.30	41,41,41,41	0
29	MG	X	2946	1/1	0.95	0.96	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	2943	1/1	0.97	0.20	31,31,31,31	0
29	MG	X	2942	1/1	0.97	0.17	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.