



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:26 PM GMT

PDB ID : 1VT2
Title : Crystal structure of the E. coli ribosome bound to CEM-101. This file contains the 50S subunit of the second 70S ribosome.
Authors : Dunkle, J.A.; Zhang, W.; Cate, J.H.D.; Mankin, A.S.
Deposited on : 2010-09-06
Resolution : 3.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

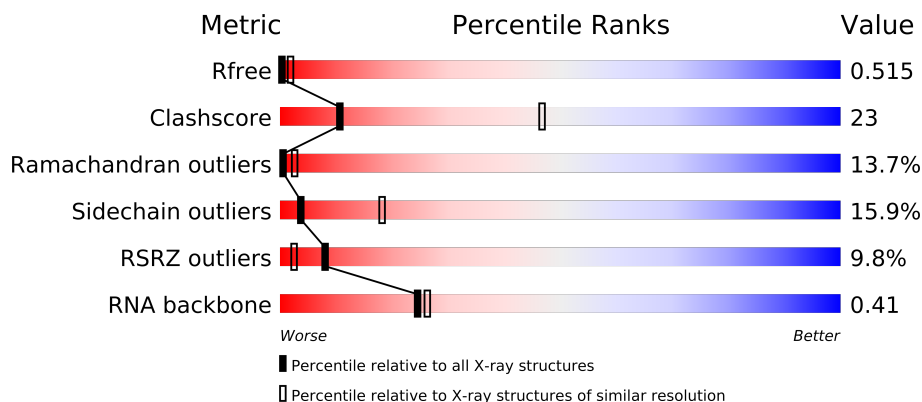
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2904	
2	B	120	
3	C	273	
4	D	209	
5	E	201	
6	F	179	
7	G	177	
8	H	149	
9	I	142	
10	J	142	
11	K	123	
12	L	144	

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Mol	Chain	Length	Quality of chain
13	M	136	
14	N	127	
15	O	117	
16	P	115	
17	Q	118	
18	R	103	
19	S	110	
20	T	100	
21	U	104	
22	V	94	
23	W	85	
24	X	78	
25	Y	63	
26	Z	59	
27	0	57	
28	1	55	
29	2	46	
30	3	65	
31	4	38	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	2906	-	X
32	MG	A	2909	-	X
32	MG	A	2913	-	X
32	MG	A	2915	-	X
32	MG	A	2917	-	X
32	MG	A	2919	-	X
32	MG	A	2923	-	X
32	MG	A	2925	-	X
32	MG	A	2930	-	X
32	MG	A	2933	-	X
32	MG	A	2936	-	X
32	MG	A	2937	-	X
32	MG	A	2938	-	X
32	MG	A	2942	-	X
32	MG	A	2960	-	X
32	MG	A	2961	-	X
32	MG	A	2962	-	X
32	MG	A	2964	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	2966	-	X
32	MG	A	2967	-	X
32	MG	A	2979	-	X
32	MG	A	2982	-	X
32	MG	A	2983	-	X
32	MG	A	2992	-	X
32	MG	A	2995	-	X
32	MG	A	2996	-	X
32	MG	A	3001	-	X
32	MG	A	3002	-	X
32	MG	A	3012	-	X
32	MG	A	3013	-	X
32	MG	A	3019	-	X
32	MG	A	3027	-	X
32	MG	A	3031	-	X
32	MG	A	3034	-	X
32	MG	A	3036	-	X
32	MG	C	722	-	X
32	MG	J	747	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 90428 atoms, of which 0 are hydrogen and 0 are deuterium.

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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	102	Total	C	N	O			
			779	492	146	141	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	W	79	Total	C	N	O	S		
			596	367	120	108	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Y	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	0	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	1	Total	Mg	0	0
			1	1		
32	A	133	Total	Mg	0	0
			133	133		
32	C	1	Total	Mg	0	0
			1	1		
32	J	1	Total	Mg	0	0
			1	1		
32	E	1	Total	Mg	0	0
			1	1		

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	4	1	Total	Zn	0	0
			1	1		

- Molecule 34 is water.

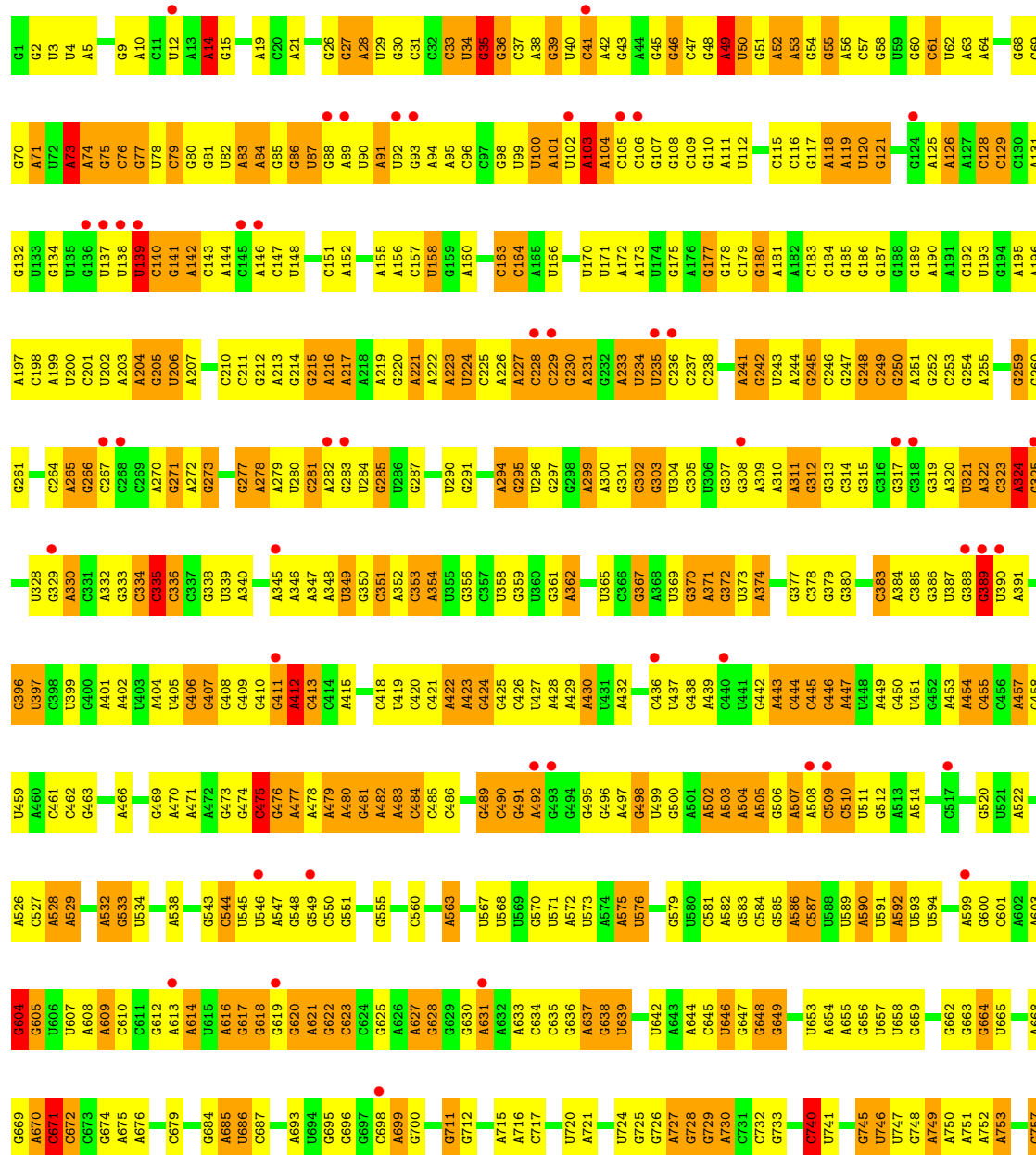
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	612	Total O 612 612	0	0
34	B	4	Total O 4 4	0	0
34	C	4	Total O 4 4	0	0
34	D	1	Total O 1 1	0	0
34	E	3	Total O 3 3	0	0
34	J	6	Total O 6 6	0	0
34	L	2	Total O 2 2	0	0
34	N	1	Total O 1 1	0	0
34	T	2	Total O 2 2	0	0
34	U	2	Total O 2 2	0	0
34	V	1	Total O 1 1	0	0
34	2	1	Total O 1 1	0	0
34	3	2	Total O 2 2	0	0
34	4	2	Total O 2 2	0	0

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 errors 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.

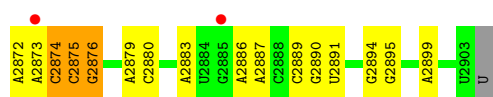
• Molecule 1: 23S rRNA

Chain A: 



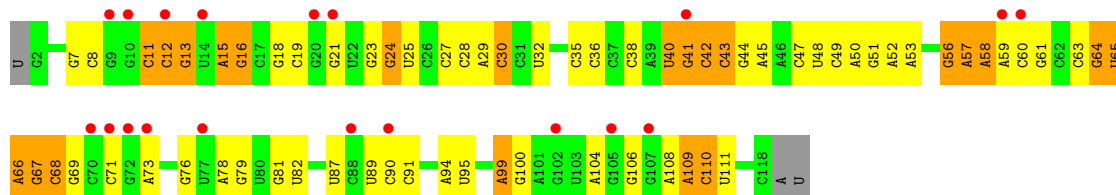


A2778	U2707	C2619	G2445	U2384	G2307	U2333	C	U2098	C1942	G1846	C1774
A2781	G2708	C2620	G2446	C2385	G2308	G2234	C	G2029	U1943	A1847	U1775
U2784	A2711	U2621	A2447	A2386	G2310	U2235	U	A2030	G1945	A1848	G1776
C2785	C2712	G2623	A2448	A2387	C2311	U2236	U	A2031	U1856	U1779	
	C2713	G2624	G2454	A2388	A2311	G2237	G	A2108	G1857	A1780	
C2788	G2714	G2625		A2389	U2312	G2238	A	U2109	U1858	U1781	
		G2626		U2390	C2313	G2239	A	G2110	U1859	U1782	
G2718		U2627	G2458	G2391	A2314		A	U	U1865	A1783	
G2719	G2719	G2628	A2459	G2392	A2315	U2243	U	G	A1866	A1784	
U2720	G2720	G2629	U2460	U2393	G2316	G2250	A	U	U1867		
A2721	A2721	C2630	A2461	C2394	A2317		C	A	G1868		
		G2631	C2462		G2318	G2251	C	G	U1869		
U2798	G2725	G2632	C2463	G2397	G2319	G2252	C	U	C1870		
A2799	A2726	U2633		U2398	U2320	G2253	C	A	U1963		
A2800	G2727	A2634		G2399	U2321	G2254	A	U	G1964		
	U2807	G2635	C2466	G2400	A2322	G2255	C	A	C1965		
U2808	U2728	G2636	U2467	U2401	A2323	G2256	C	U	U1966		
A2809	G2729	U2637	A2468	U2402	U2324	G2257	C	A	G1967		
	C2730	G2638	A2469	C2403	U2325	G2258	C	U	C1968		
G2812	G2731	G2639	U2474	U2404	G2326	U2259	C	A	U1969		
C2815	G2732	G2640	C2475	G2405	G2330	G2260	C	A	G1873		
G2816	A2733	C2641	C2476	G2406	G2331	G2261	C	U	C1874		
	A2736	U2650	U2477	A2407	G2332	C2262	C	A	U1970		
A2820	G2737	G2651	A2478	G2408	A2333	G2263	C	U	U1971		
A2821	A2738	G2652	G2488	G2410	A2334	G2264	C	U	G1875		
G2822	U2739	U2653	U2489	A2411	A2335	A2267	C	U	A1876		
A2823	A2740	G2654	G2490	A2412	A2336	A2268	C	U	U1796		
G2824	G2741	G2655	U2491	A2413	G2337		C	U	G1797		
C2825	A2742	U2656	G2492	G2414	C2338	U2272	C	U	A1877		
	U2743	A2657	G2493	G2415	C2339	A2273	C	U	G1884		
G2831	G2744	G2664	G2494	G2416	A2340	G2274	C	U	A1889		
U2832	C2745	A2665	G2495	C2417	G2341	G2275	C	U	A1899		
G2833	U2746	C2666	A2496	G2418	G2342	G2276	C	U	U1900		
A2835	G2747	G2667	C2497	U2419	U2343	A2277	C	U	A1901		
U2836	A2748	G2668	G2498	C2420	G2344	G2279	C	U	G1902		
A2837	G2750		G2502	G2421	A2345	G2280	C	U	G1903		
G2838	C2751	G2671	A2503	C2422	G2346	A2281	C	U	G1904		
	U2752	A2675	U2504	U2423	G2347	G2282	C	U	C1905		
G2844	A2753	C2676	G2506	A2425	G2348	G2283	C	U	G1906		
G2846		C2677		A2426	G2349	G2284	C	U	G1907		
U2847	U2756	A2681	A2513	G2427	G2353	G2285	C	U	A1913		
A2850	A2757	C2682	U2514	G2428	G2357	G2286	C	U	C1914		
G2851	G2758	G2683	C2515	G2429	A2358	A2287	C	U	U1915		
	C2759	U2684	A2518	G2430	G2361	G2288	C	U	U1916		
G2857	A2761	G2685	U2519	U2431	C2362	G2289	C	U	A1917		
A2860		G2686	C2520	A2432	G2363	U2291	C	U	A1918		
U2861	A2764	U2687	G2526	A2433	G2371	G2295	C	U	G1919		
G2862	A2765	U2688	C2527	A2434	U2372	U2296	C	U	C1920		
C2863	U2766	G2689	U2528	G2435	G2373	A2297	C	U	C1924		
	G2771	U2690	G2529	U2436	C2374	A2298	C	U	A1927		
U2866		G2697	U2530	A2437	G2375	U2299	C	U	A1928		
G2867	C2772	U2698	A2531	G2438	C2376	G2300	C	U	G1929		
U2868	G2773	A2700	A2532	C2440	G2379	C2301	C	U	G1930		
G2869	G2774	U2615	G2533	U2441	G2380	U2302	C	U	U1931		
	A2775	C2616	A2534	C2442	A2381		C	U	G1935		
G2869	G2776	U2617	G2535	G2444	G2382	U2305	C	U	A1936		
	G2777	G2618			G2383	G2306	C	U	A1937		
									A1938		
									G1942		
									C1943		
									U1940		
									G1945		



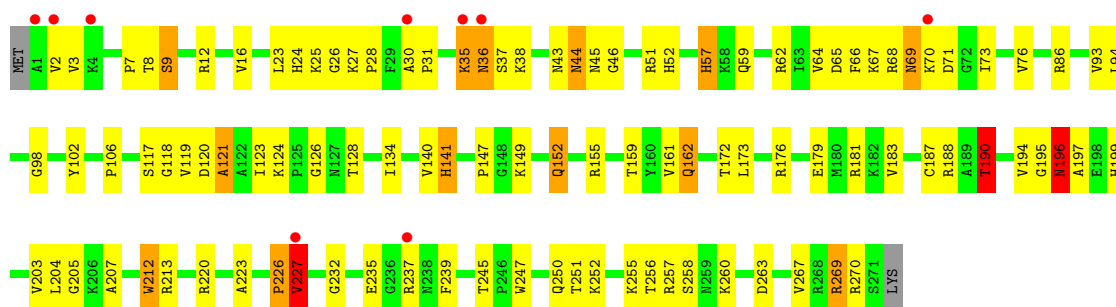
• Molecule 2: 5S rRNA

Chain B:



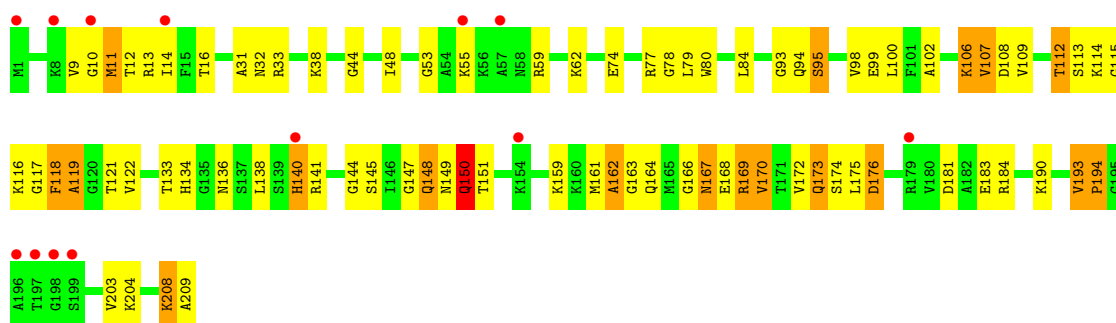
• Molecule 3: 50S ribosomal protein L2

Chain C:



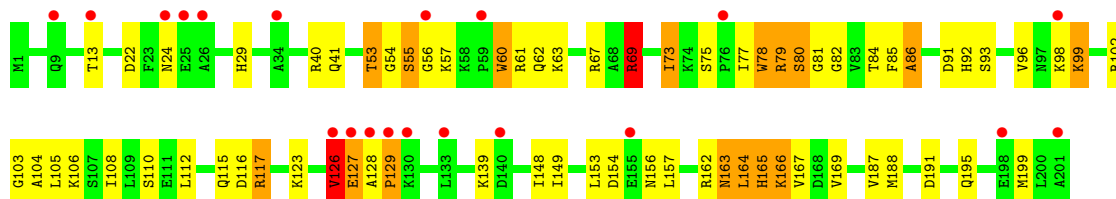
• Molecule 4: 50S ribosomal protein L3

Chain D:



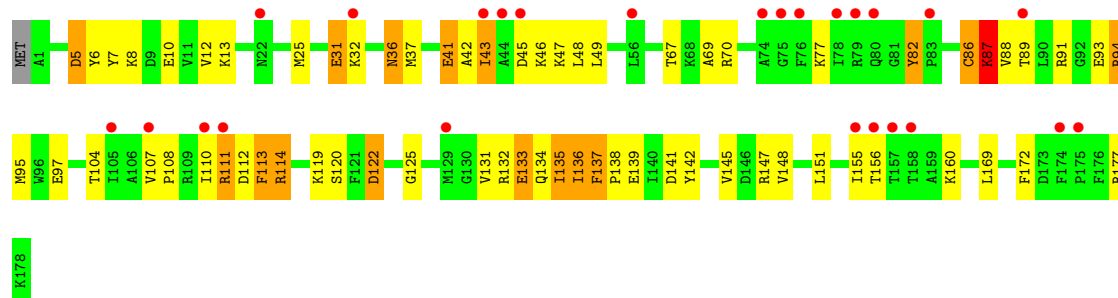
• Molecule 5: 50S ribosomal protein L4

Chain E:



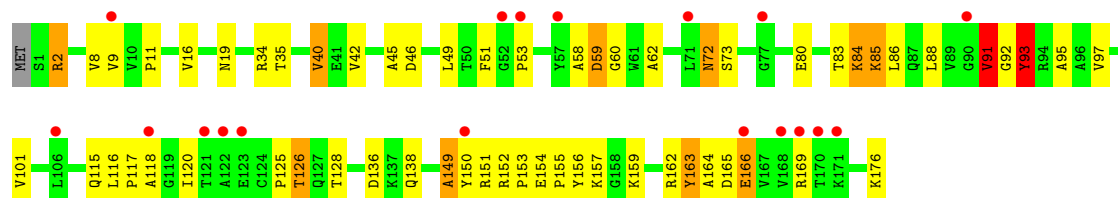
• Molecule 6: 50S ribosomal protein L5

Chain F: 



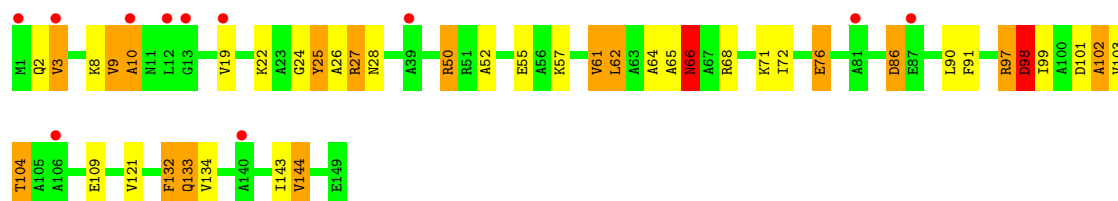
- Molecule 7: 50S ribosomal protein L6

Chain G: 



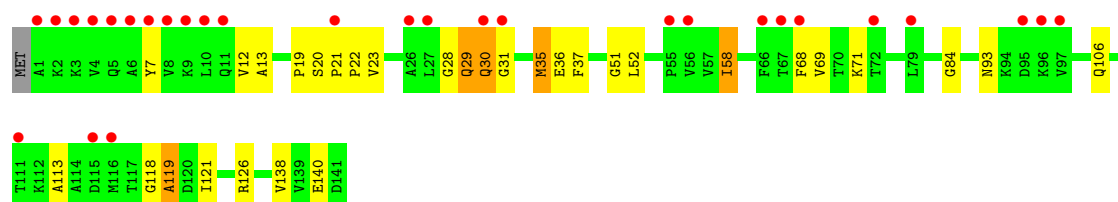
- Molecule 8: 50S ribosomal protein L9

Chain H: 



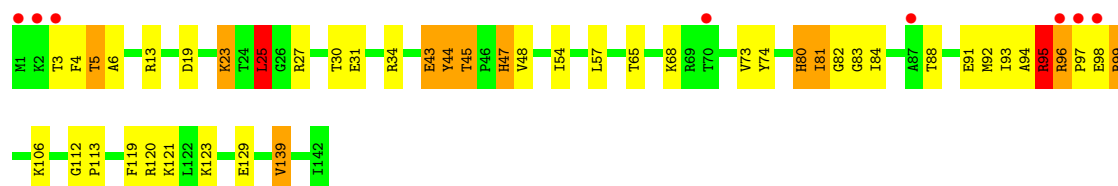
- Molecule 9: 50S ribosomal protein L11

Chain I: 



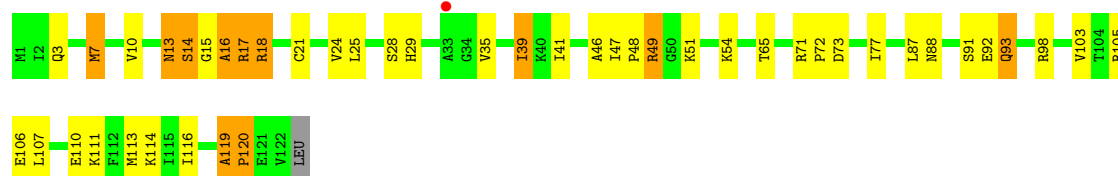
- Molecule 10: 50S ribosomal protein L13

Chain J: 



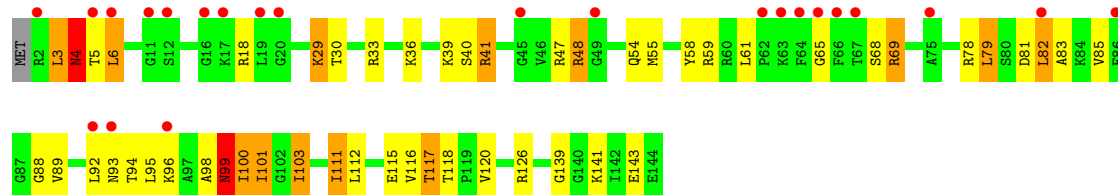
- Molecule 11: 50S ribosomal protein L14

Chain K: 



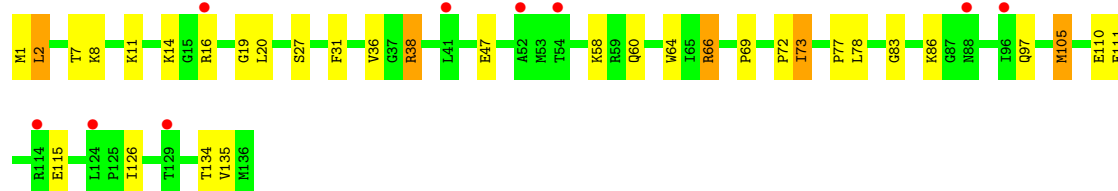
- Molecule 12: 50S ribosomal protein L15

Chain L: 



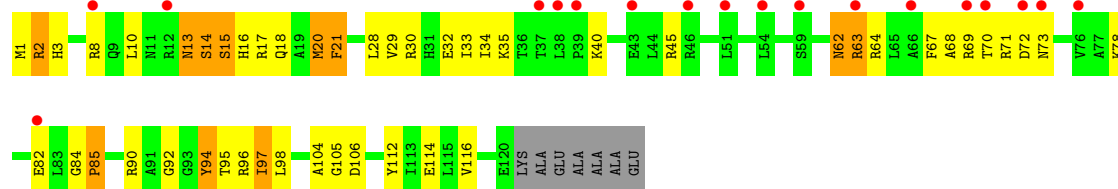
- Molecule 13: 50S ribosomal protein L16

Chain M: 



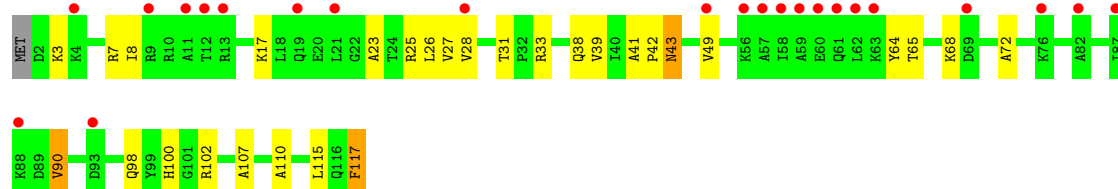
- Molecule 14: 50S ribosomal protein L17

Chain N: 



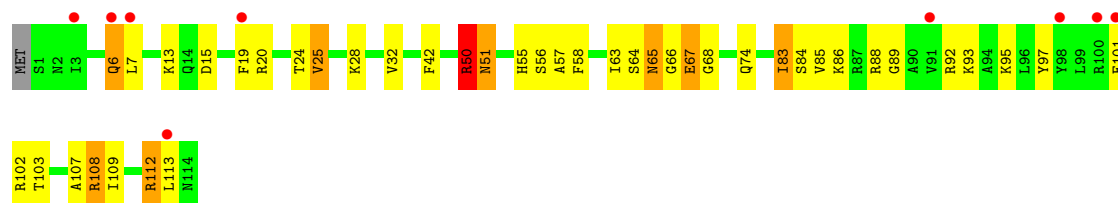
- Molecule 15: 50S ribosomal protein L18

Chain O: 



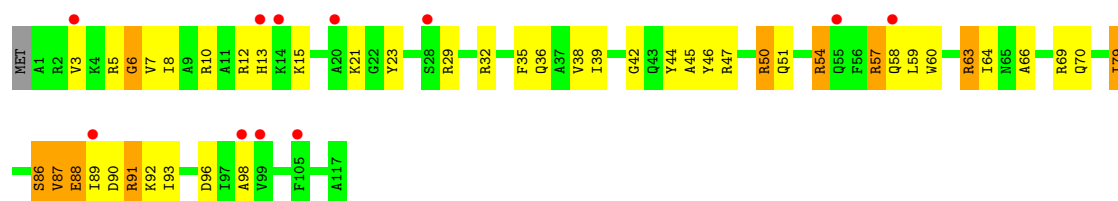
- Molecule 16: 50S ribosomal protein L19

Chain P:



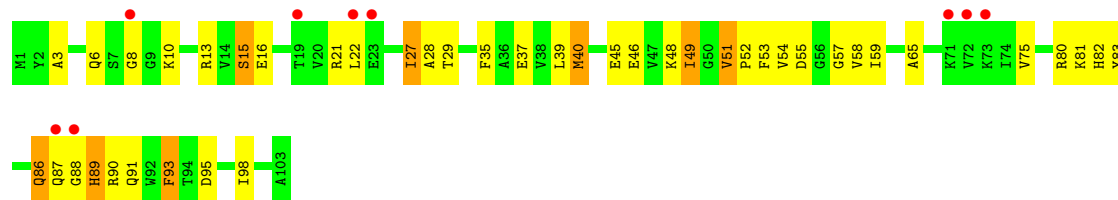
- Molecule 17: 50S ribosomal protein L20

Chain Q:



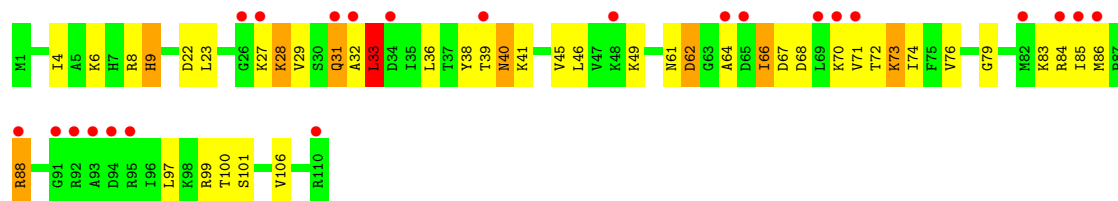
- Molecule 18: 50S ribosomal protein L21

Chain R:



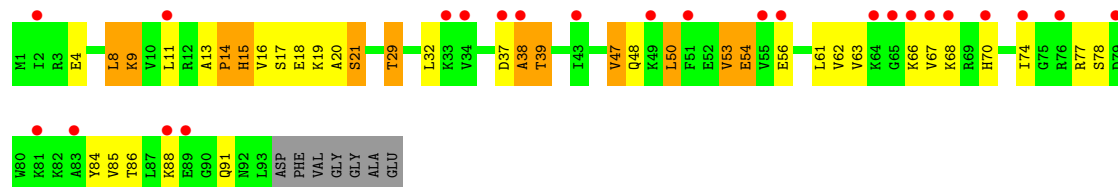
- Molecule 19: 50S ribosomal protein L22

Chain S:



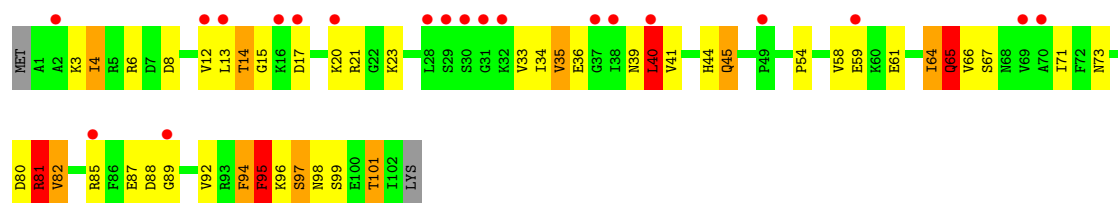
- Molecule 20: 50S ribosomal protein L23

Chain T:



- Molecule 21: 50S ribosomal protein L24

Chain U:



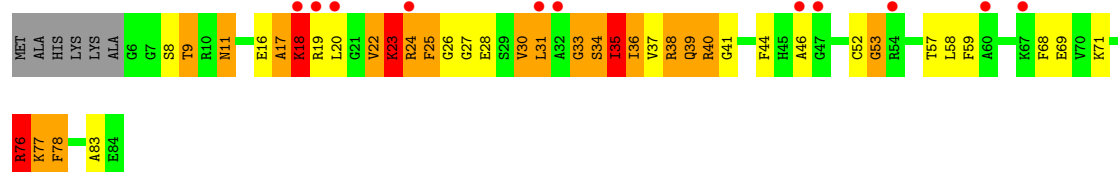
- Molecule 22: 50S ribosomal protein L25

Chain V:



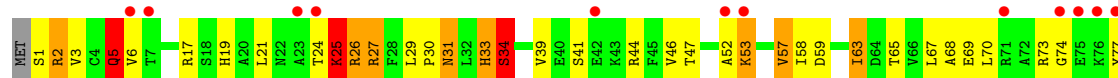
- Molecule 23: 50S ribosomal protein L27

Chain W:



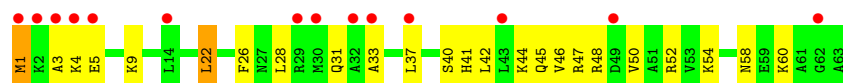
- Molecule 24: 50S ribosomal protein L28

Chain X:



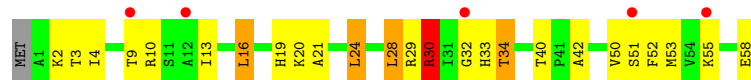
- Molecule 25: 50S ribosomal protein L29

Chain Y:



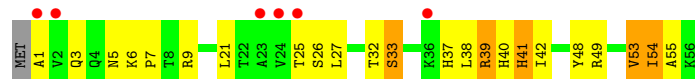
- Molecule 26: 50S ribosomal protein L30

Chain Z:



- Molecule 27: 50S ribosomal protein L32

Chain 0:



- Molecule 28: 50S ribosomal protein L33

Chain 1: 



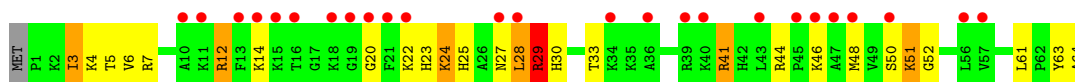
- Molecule 29: 50S ribosomal protein L34

Chain 2: 



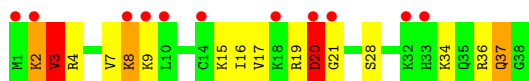
- Molecule 30: 50S ribosomal protein L35

Chain 3: 



- Molecule 31: 50S ribosomal protein L36

Chain 4: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.76Å 433.27Å 618.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.78 – 3.30 69.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (69.78-3.30) 95.9 (69.78-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_501)	Depositor
R, R_{free}	0.187 , 0.244 0.515 , 0.515	Depositor DCC
R_{free} test set	19610 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 72.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 971020 reflections	Xtriage
F_o, F_c correlation	0.53	EDS
Total number of atoms	90428	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.38	0/68314	0.83	60/106569 (0.1%)
2	B	0.30	0/2803	0.76	1/4371 (0.0%)
3	C	0.32	0/2121	0.55	0/2852
4	D	0.31	0/1586	0.57	0/2134
5	E	0.27	0/1571	0.51	0/2113
6	F	0.24	0/1444	0.50	0/1937
7	G	0.24	0/1343	0.50	0/1816
8	H	0.29	0/1122	0.52	0/1515
9	I	0.22	0/1046	0.47	0/1410
10	J	0.29	0/1152	0.60	1/1551 (0.1%)
11	K	0.34	0/947	0.58	0/1268
12	L	0.28	0/1054	0.56	0/1403
13	M	0.29	0/1093	0.50	0/1460
14	N	0.30	0/973	0.53	0/1301
15	O	0.24	0/902	0.45	0/1209
16	P	0.32	0/929	0.52	0/1242
17	Q	0.30	0/960	0.47	0/1278
18	R	0.30	0/829	0.52	0/1107
19	S	0.29	0/864	0.54	1/1156 (0.1%)
20	T	0.26	0/744	0.54	0/994
21	U	0.26	0/787	0.51	0/1051
22	V	0.24	0/766	0.44	0/1025
23	W	0.29	0/603	0.54	0/797
24	X	0.28	0/635	0.58	0/848
25	Y	0.23	0/510	0.50	0/677
26	Z	0.28	0/453	0.53	0/605
27	0	0.30	0/450	0.52	0/599
28	1	0.27	0/416	0.49	0/554
29	2	0.30	0/380	0.54	0/498
30	3	0.29	0/513	0.56	0/676
31	4	0.33	0/303	0.53	0/397
All	All	0.35	0/97613	0.76	63/146413 (0.0%)

There are no bond length outliers.

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	C	C2-N1-C1'	6.54	125.99	118.80
1	A	1428	C	C2-N1-C1'	-6.53	111.62	118.80
10	J	25	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	740	C	C6-N1-C2	6.25	122.80	120.30
1	A	2405	G	C4-N9-C1'	6.17	134.53	126.50

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60995	0	0	1547	0
2	B	2507	0	0	67	0
3	C	2082	0	0	41	0
4	D	1565	0	0	39	0
5	E	1552	0	0	26	0
6	F	1420	0	12	17	0
7	G	1323	0	0	19	0
8	H	1111	0	0	15	0
9	I	1032	0	0	7	0
10	J	1129	0	0	26	0
11	K	938	0	0	12	0
12	L	1045	0	0	26	0
13	M	1074	0	0	9	0
14	N	960	0	0	24	0
15	O	892	0	0	11	0
16	P	917	0	0	21	0
17	Q	947	0	0	28	0
18	R	816	0	0	15	0
19	S	857	0	0	16	0
20	T	738	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	779	0	0	16	0
22	V	753	0	0	10	0
23	W	596	0	0	31	0
24	X	625	0	0	21	0
25	Y	509	0	0	12	0
26	Z	449	0	0	8	0
27	0	444	0	0	9	0
28	1	409	0	0	6	0
29	2	377	0	0	16	0
30	3	504	0	0	13	0
31	4	302	0	0	7	0
32	A	133	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	E	1	0	0	0	0
32	J	1	0	0	0	0
33	4	1	0	0	0	0
34	2	1	0	0	1	0
34	3	2	0	0	0	0
34	4	2	0	0	0	0
34	A	612	0	0	23	0
34	B	4	0	0	1	0
34	C	4	0	0	0	0
34	D	1	0	0	0	0
34	E	3	0	0	0	0
34	J	6	0	0	0	0
34	L	2	0	0	0	0
34	N	1	0	0	0	0
34	T	2	0	0	0	0
34	U	2	0	0	0	0
34	V	1	0	0	0	0
All	All	90428	0	12	1981	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

The worst 5 of 1981 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:216:A:O2'	1:A:217:A:C8	2.20	0.94
2:B:57:A:O2'	2:B:58:A:C8	2.24	0.91
1:A:1809:A:O2'	1:A:1810:A:C8	2.26	0.88
1:A:1135:C:N4	1:A:1139:G:C6	2.45	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:975:A:O2'	1:A:976:G:C8	2.30	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	C	269/273 (98%)	180 (67%)	60 (22%)	29 (11%)	1	6
4	D	207/209 (99%)	128 (62%)	45 (22%)	34 (16%)	0	1
5	E	199/201 (99%)	117 (59%)	55 (28%)	27 (14%)	0	3
6	F	176/179 (98%)	102 (58%)	42 (24%)	32 (18%)	0	1
7	G	174/177 (98%)	104 (60%)	36 (21%)	34 (20%)	0	1
8	H	147/149 (99%)	73 (50%)	59 (40%)	15 (10%)	1	7
9	I	139/142 (98%)	85 (61%)	37 (27%)	17 (12%)	1	4
10	J	140/142 (99%)	98 (70%)	28 (20%)	14 (10%)	1	8
11	K	120/123 (98%)	83 (69%)	20 (17%)	17 (14%)	0	2
12	L	141/144 (98%)	77 (55%)	45 (32%)	19 (14%)	0	3
13	M	134/136 (98%)	92 (69%)	28 (21%)	14 (10%)	1	7
14	N	118/127 (93%)	72 (61%)	30 (25%)	16 (14%)	0	3
15	O	114/117 (97%)	74 (65%)	29 (25%)	11 (10%)	1	9
16	P	112/115 (97%)	70 (62%)	25 (22%)	17 (15%)	0	1
17	Q	115/118 (98%)	77 (67%)	27 (24%)	11 (10%)	1	9
18	R	101/103 (98%)	66 (65%)	22 (22%)	13 (13%)	0	3
19	S	108/110 (98%)	75 (69%)	22 (20%)	11 (10%)	1	7
20	T	91/100 (91%)	42 (46%)	27 (30%)	22 (24%)	0	0
21	U	100/104 (96%)	53 (53%)	23 (23%)	24 (24%)	0	0
22	V	92/94 (98%)	61 (66%)	23 (25%)	8 (9%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	W	77/85 (91%)	30 (39%)	27 (35%)	20 (26%)	0	0
24	X	75/78 (96%)	45 (60%)	22 (29%)	8 (11%)	1	6
25	Y	61/63 (97%)	37 (61%)	20 (33%)	4 (7%)	2	19
26	Z	56/59 (95%)	34 (61%)	16 (29%)	6 (11%)	1	6
27	0	54/57 (95%)	38 (70%)	7 (13%)	9 (17%)	0	1
28	1	48/55 (87%)	33 (69%)	10 (21%)	5 (10%)	1	7
29	2	44/46 (96%)	29 (66%)	9 (20%)	6 (14%)	0	3
30	3	62/65 (95%)	43 (69%)	13 (21%)	6 (10%)	1	8
31	4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	1
All	All	3310/3409 (97%)	2040 (62%)	815 (25%)	455 (14%)	0	2

5 of 455 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	9	SER
3	C	28	PRO
3	C	69	ASN
3	C	140	VAL
3	C	141	HIS

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	C	216/218 (99%)	181 (84%)	35 (16%)	3	17
4	D	164/164 (100%)	142 (87%)	22 (13%)	6	27
5	E	165/165 (100%)	140 (85%)	25 (15%)	4	20
6	F	149/150 (99%)	120 (80%)	29 (20%)	2	9
7	G	137/138 (99%)	119 (87%)	18 (13%)	6	28
8	H	114/114 (100%)	91 (80%)	23 (20%)	2	8
9	I	109/110 (99%)	102 (94%)	7 (6%)	25	69
10	J	116/116 (100%)	99 (85%)	17 (15%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	103/104 (99%)	84 (82%)	19 (18%)	2	12
12	L	102/103 (99%)	85 (83%)	17 (17%)	3	16
13	M	109/109 (100%)	98 (90%)	11 (10%)	11	42
14	N	100/103 (97%)	85 (85%)	15 (15%)	4	21
15	O	86/87 (99%)	79 (92%)	7 (8%)	17	58
16	P	99/100 (99%)	89 (90%)	10 (10%)	11	42
17	Q	89/90 (99%)	75 (84%)	14 (16%)	4	19
18	R	84/84 (100%)	67 (80%)	17 (20%)	2	8
19	S	93/93 (100%)	73 (78%)	20 (22%)	1	7
20	T	80/84 (95%)	71 (89%)	9 (11%)	9	36
21	U	83/85 (98%)	68 (82%)	15 (18%)	2	12
22	V	78/78 (100%)	67 (86%)	11 (14%)	5	24
23	W	59/63 (94%)	41 (70%)	18 (30%)	0	1
24	X	67/68 (98%)	52 (78%)	15 (22%)	1	6
25	Y	55/55 (100%)	51 (93%)	4 (7%)	20	63
26	Z	48/49 (98%)	37 (77%)	11 (23%)	1	5
27	0	47/48 (98%)	34 (72%)	13 (28%)	0	2
28	1	45/49 (92%)	41 (91%)	4 (9%)	14	51
29	2	38/38 (100%)	32 (84%)	6 (16%)	4	18
30	3	51/52 (98%)	38 (74%)	13 (26%)	1	3
31	4	34/34 (100%)	27 (79%)	7 (21%)	2	8
All	All	2720/2751 (99%)	2288 (84%)	432 (16%)	4	18

5 of 432 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	3	LEU
15	O	68	LYS
27	0	49	ARG
12	L	69	ARG
13	M	97	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2837/2904 (97%)	870 (30%)	153 (5%)
2	B	116/120 (96%)	31 (26%)	6 (5%)
All	All	2953/3024 (97%)	901 (30%)	159 (5%)

5 of 901 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	14	A
1	A	15	G
1	A	27	G
1	A	28	A

5 of 159 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1275	A
1	A	1635	A
1	A	2776	A
1	A	1339	G
1	A	1417	C

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 138 ligands modelled in this entry, 138 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.

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	2841/2904 (97%)	0.58	204 (7%) 15 4	64, 141, 260, 408	0
2	B	117/120 (97%)	0.89	19 (16%) 2 1	111, 185, 242, 277	0
3	C	271/273 (99%)	0.42	9 (3%) 44 10	64, 107, 154, 181	0
4	D	209/209 (100%)	0.33	13 (6%) 20 5	71, 122, 174, 236	0
5	E	201/201 (100%)	0.68	20 (9%) 8 2	91, 214, 335, 378	0
6	F	178/179 (99%)	0.79	25 (14%) 3 1	154, 229, 270, 299	0
7	G	176/177 (99%)	0.74	18 (10%) 7 2	129, 198, 270, 312	0
8	H	149/149 (100%)	0.36	11 (7%) 14 4	100, 197, 252, 272	0
9	I	141/142 (99%)	1.27	29 (20%) 1 1	231, 317, 353, 360	0
10	J	142/142 (100%)	0.40	8 (5%) 24 5	75, 127, 168, 193	0
11	K	122/123 (99%)	0.28	1 (0%) 83 39	66, 107, 155, 228	0
12	L	143/144 (99%)	0.98	23 (16%) 2 1	86, 169, 242, 284	0
13	M	136/136 (100%)	0.55	9 (6%) 18 4	78, 131, 175, 208	0
14	N	120/127 (94%)	0.92	18 (15%) 3 1	88, 136, 190, 237	0
15	O	116/117 (99%)	1.07	23 (19%) 2 1	134, 182, 227, 252	0
16	P	114/115 (99%)	0.51	9 (7%) 13 4	82, 121, 160, 197	0
17	Q	117/118 (99%)	0.83	11 (9%) 9 3	88, 126, 203, 287	0
18	R	103/103 (100%)	0.47	9 (8%) 10 3	98, 154, 219, 274	0
19	S	110/110 (100%)	1.10	23 (20%) 1 1	86, 141, 208, 266	0
20	T	93/100 (93%)	1.39	24 (25%) 1 1	133, 215, 282, 315	0
21	U	102/104 (98%)	1.10	20 (19%) 2 1	151, 251, 347, 416	0
22	V	94/94 (100%)	0.38	6 (6%) 19 5	107, 157, 199, 222	0
23	W	79/85 (92%)	1.02	11 (13%) 4 1	108, 163, 232, 250	0
24	X	77/78 (98%)	1.00	12 (15%) 3 1	88, 134, 182, 237	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	63/63 (100%)	1.22	14 (22%) 1 1	167, 286, 366, 383	0
26	Z	58/59 (98%)	0.61	5 (8%) 11 3	104, 143, 200, 247	0
27	0	56/57 (98%)	0.63	6 (10%) 6 2	87, 161, 210, 255	0
28	1	50/55 (90%)	0.16	0 100 100	106, 161, 203, 255	0
29	2	46/46 (100%)	1.15	7 (15%) 3 1	95, 128, 162, 176	0
30	3	64/65 (98%)	2.10	25 (39%) 1 0	96, 140, 173, 212	0
31	4	38/38 (100%)	1.50	11 (28%) 1 1	94, 155, 195, 203	0
All	All	6326/6433 (98%)	0.67	623 (9%) 8 2	64, 149, 286, 416	0

The worst 5 of 623 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	9	LYS	16.9
5	E	128	ALA	12.3
1	A	1537	G	11.7
25	Y	1	MET	11.6
9	I	8	VAL	11.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	3036	1/1	0.32	181.00	240,240,240,240	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2962	1/1	0.81	68.56	249,249,249,249	0
32	MG	A	2961	1/1	1.29	55.32	205,205,205,205	0
32	MG	J	747	1/1	1.29	35.40	319,319,319,319	0
32	MG	A	2967	1/1	0.97	32.68	273,273,273,273	0
32	MG	A	3031	1/1	1.07	29.05	248,248,248,248	0
32	MG	A	3001	1/1	0.94	20.74	159,159,159,159	0
32	MG	A	2966	1/1	1.06	20.69	190,190,190,190	0
32	MG	A	2923	1/1	0.77	19.47	278,278,278,278	0
32	MG	A	2919	1/1	0.70	17.02	219,219,219,219	0
32	MG	A	2983	1/1	1.23	15.54	225,225,225,225	0
32	MG	A	2937	1/1	1.10	12.85	151,151,151,151	0
32	MG	A	2930	1/1	1.24	12.62	242,242,242,242	0
32	MG	A	3013	1/1	0.39	12.30	227,227,227,227	0
32	MG	A	2992	1/1	0.44	11.94	222,222,222,222	0
32	MG	A	2979	1/1	0.58	10.75	209,209,209,209	0
32	MG	A	2909	1/1	1.02	7.80	282,282,282,282	0
32	MG	A	3012	1/1	0.80	6.70	217,217,217,217	0
32	MG	C	722	1/1	0.89	6.30	201,201,201,201	0
32	MG	A	2995	1/1	0.72	6.18	184,184,184,184	0
32	MG	A	2964	1/1	0.58	6.00	235,235,235,235	0
32	MG	A	2933	1/1	0.44	5.95	178,178,178,178	0
32	MG	A	3002	1/1	0.39	5.23	183,183,183,183	0
32	MG	A	2996	1/1	0.40	5.07	169,169,169,169	0
32	MG	A	3027	1/1	0.60	5.06	217,217,217,217	0
32	MG	A	3034	1/1	1.06	3.98	271,271,271,271	0
32	MG	A	2942	1/1	0.69	3.93	234,234,234,234	0
32	MG	A	2915	1/1	0.45	3.91	150,150,150,150	0
32	MG	A	2925	1/1	0.30	3.78	183,183,183,183	0
32	MG	A	2913	1/1	0.33	3.50	157,157,157,157	0
32	MG	A	3019	1/1	0.25	3.46	176,176,176,176	0
32	MG	A	2982	1/1	0.36	3.41	214,214,214,214	0
32	MG	A	2906	1/1	0.31	3.17	231,231,231,231	0
32	MG	A	2960	1/1	0.31	3.04	85,85,85,85	0
32	MG	A	2917	1/1	0.54	2.24	241,241,241,241	0
32	MG	A	2936	1/1	0.28	2.17	162,162,162,162	0
32	MG	A	2938	1/1	0.43	2.15	88,88,88,88	0
32	MG	A	2968	1/1	0.31	1.93	256,256,256,256	0
32	MG	A	2991	1/1	0.25	1.88	199,199,199,199	0
32	MG	A	2973	1/1	0.39	1.55	267,267,267,267	0
32	MG	A	2949	1/1	0.34	1.54	206,206,206,206	0
32	MG	A	3003	1/1	0.25	1.51	188,188,188,188	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2986	1/1	0.32	1.45	164,164,164,164	0
32	MG	A	2990	1/1	0.31	1.38	109,109,109,109	0
32	MG	A	3026	1/1	0.28	1.38	104,104,104,104	0
32	MG	A	2912	1/1	0.25	1.30	147,147,147,147	0
32	MG	A	3029	1/1	0.44	1.27	200,200,200,200	0
32	MG	A	2932	1/1	0.38	1.27	222,222,222,222	0
32	MG	A	3018	1/1	0.43	1.13	182,182,182,182	0
32	MG	A	3015	1/1	0.33	1.04	202,202,202,202	0
32	MG	A	2998	1/1	0.41	1.01	145,145,145,145	0
32	MG	A	3025	1/1	0.23	0.93	168,168,168,168	0
32	MG	A	2907	1/1	0.35	0.79	238,238,238,238	0
32	MG	A	3033	1/1	0.28	0.70	261,261,261,261	0
32	MG	A	2954	1/1	0.25	0.55	154,154,154,154	0
32	MG	A	3032	1/1	0.37	0.34	163,163,163,163	0
32	MG	B	590	1/1	0.24	0.34	111,111,111,111	0
32	MG	A	2987	1/1	0.23	0.32	214,214,214,214	0
32	MG	A	2963	1/1	0.20	0.30	233,233,233,233	0
32	MG	A	2934	1/1	0.31	0.25	130,130,130,130	0
32	MG	A	2945	1/1	0.26	0.23	119,119,119,119	0
32	MG	A	3009	1/1	0.25	0.16	97,97,97,97	0
32	MG	A	2918	1/1	0.27	0.11	113,113,113,113	0
32	MG	A	2988	1/1	0.25	0.10	168,168,168,168	0
32	MG	A	2929	1/1	0.29	0.07	162,162,162,162	0
32	MG	A	2953	1/1	0.27	0.05	243,243,243,243	0
32	MG	A	3020	1/1	0.24	0.04	84,84,84,84	0
32	MG	A	2997	1/1	0.26	0.01	189,189,189,189	0
32	MG	A	2989	1/1	0.30	-0.01	158,158,158,158	0
32	MG	A	3037	1/1	0.36	-0.02	220,220,220,220	0
32	MG	A	2978	1/1	0.20	-0.32	260,260,260,260	0
32	MG	A	2952	1/1	0.26	-0.34	103,103,103,103	0
32	MG	A	2921	1/1	0.25	-0.34	185,185,185,185	0
32	MG	A	2928	1/1	0.24	-0.36	102,102,102,102	0
32	MG	A	2985	1/1	0.25	-0.60	83,83,83,83	0
32	MG	A	3006	1/1	0.25	-0.68	118,118,118,118	0
32	MG	A	3005	1/1	0.21	-0.75	96,96,96,96	0
32	MG	A	3010	1/1	0.18	-0.81	218,218,218,218	0
32	MG	A	2940	1/1	0.18	-0.84	205,205,205,205	0
32	MG	A	2999	1/1	0.18	-0.84	138,138,138,138	0
32	MG	A	2984	1/1	0.24	-0.88	154,154,154,154	0
32	MG	A	3000	1/1	0.17	-0.91	127,127,127,127	0
32	MG	A	3004	1/1	0.22	-1.00	124,124,124,124	0
32	MG	A	2972	1/1	0.17	-1.08	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2905	1/1	0.15	-1.10	141,141,141,141	0
32	MG	A	3024	1/1	0.18	-1.11	124,124,124,124	0
32	MG	A	2947	1/1	0.19	-1.12	155,155,155,155	0
32	MG	A	2935	1/1	0.14	-1.18	80,80,80,80	0
32	MG	A	2951	1/1	0.17	-1.19	174,174,174,174	0
32	MG	A	2975	1/1	0.22	-1.19	102,102,102,102	0
32	MG	A	2922	1/1	0.18	-1.23	185,185,185,185	0
32	MG	A	2977	1/1	0.12	-1.32	193,193,193,193	0
32	MG	A	2910	1/1	0.14	-1.35	237,237,237,237	0
32	MG	A	2911	1/1	0.16	-1.41	232,232,232,232	0
32	MG	A	3016	1/1	0.14	-1.74	79,79,79,79	0
32	MG	A	2971	1/1	0.10	-1.82	72,72,72,72	0
32	MG	A	2927	1/1	0.13	-1.83	130,130,130,130	0
32	MG	A	3030	1/1	0.18	-1.85	120,120,120,120	0
32	MG	A	3035	1/1	0.05	-1.87	94,94,94,94	0
32	MG	A	3014	1/1	0.07	-1.92	120,120,120,120	0
32	MG	A	2931	1/1	0.17	-1.97	194,194,194,194	0
32	MG	A	3011	1/1	0.17	-1.98	91,91,91,91	0
32	MG	A	2957	1/1	0.16	-1.98	127,127,127,127	0
32	MG	A	2969	1/1	0.16	-2.06	88,88,88,88	0
33	ZN	4	781	1/1	0.07	-2.09	169,169,169,169	0
32	MG	A	2976	1/1	0.16	-2.15	183,183,183,183	0
32	MG	A	2994	1/1	0.14	-2.17	112,112,112,112	0
32	MG	A	2956	1/1	0.10	-2.18	72,72,72,72	0
32	MG	A	3028	1/1	0.12	-2.18	82,82,82,82	0
32	MG	A	2944	1/1	0.16	-2.27	72,72,72,72	0
32	MG	A	2981	1/1	0.14	-2.42	109,109,109,109	0
32	MG	A	2943	1/1	0.11	-2.57	105,105,105,105	0
32	MG	A	2941	1/1	0.07	-2.64	81,81,81,81	0
32	MG	A	3022	1/1	0.12	-2.95	100,100,100,100	0
32	MG	A	2974	1/1	0.13	-2.96	91,91,91,91	0
32	MG	A	2908	1/1	0.14	-3.07	134,134,134,134	0
32	MG	A	2993	1/1	0.09	-3.12	101,101,101,101	0
32	MG	A	2916	1/1	0.15	-3.13	72,72,72,72	0
32	MG	A	3021	1/1	0.14	-3.18	73,73,73,73	0
32	MG	A	3008	1/1	0.16	-3.35	52,52,52,52	0
32	MG	A	2920	1/1	0.11	-3.38	60,60,60,60	0
32	MG	E	202	1/1	0.17	-3.40	199,199,199,199	0
32	MG	A	2939	1/1	0.10	-3.47	90,90,90,90	0
32	MG	A	2948	1/1	0.07	-3.59	87,87,87,87	0
32	MG	A	3023	1/1	0.11	-3.63	60,60,60,60	0
32	MG	A	2959	1/1	0.12	-3.71	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2980	1/1	0.14	-3.82	195,195,195,195	0
32	MG	A	2924	1/1	0.12	-3.94	53,53,53,53	0
32	MG	A	2970	1/1	0.10	-4.24	105,105,105,105	0
32	MG	A	2926	1/1	0.12	-4.40	149,149,149,149	0
32	MG	A	2950	1/1	0.08	-4.92	73,73,73,73	0
32	MG	A	3007	1/1	0.14	-5.08	86,86,86,86	0
32	MG	A	3017	1/1	0.09	-5.60	128,128,128,128	0
32	MG	A	2965	1/1	0.07	-6.44	110,110,110,110	0
32	MG	A	2955	1/1	0.13	-9.11	88,88,88,88	0
32	MG	A	2946	1/1	0.08	-12.79	81,81,81,81	0
32	MG	A	2958	1/1	0.08	-21.80	86,86,86,86	0
32	MG	A	2914	1/1	1.12	-	272,272,272,272	0

6.5 Other polymers ⓘ

There are no such residues in this entry.