



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:50 PM GMT

PDB ID : 4A19
Title : T.THERMOPHILA 60S RIBOSOMAL SUBUNIT IN COMPLEX WITH INITIATION FACTOR 6. THIS FILE CONTAINS 26S RRNA AND PROTEINS OF MOLECULE 2.
Authors : Klinge, S.; Voigts-Hoffmann, F.; Leibundgut, M.; Arpagaus, S.; Ban, N.
Deposited on : 2011-09-14
Resolution : 3.52 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>

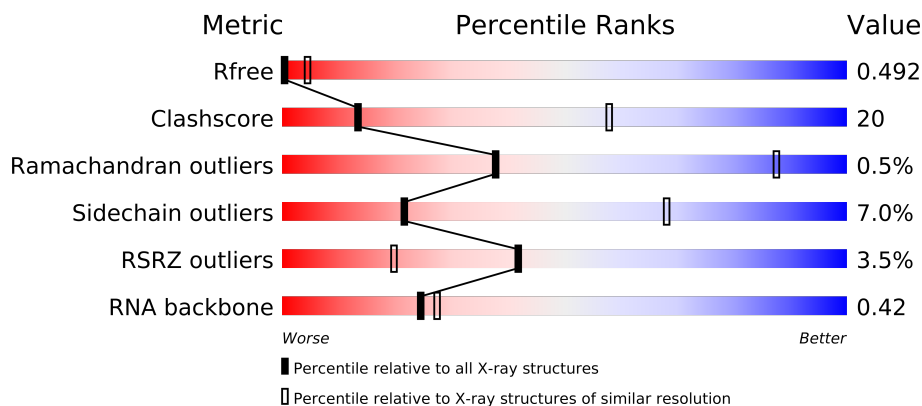
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.52 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	1256 (3.74-3.30)
Clashscore	79885	1020 (3.68-3.36)
Ramachandran outliers	78287	1082 (3.70-3.34)
Sidechain outliers	78261	1082 (3.70-3.34)
RSRZ outliers	66119	1256 (3.74-3.30)
RNA backbone	1838	1008 (4.26-2.76)

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	1	3354	
2	A	94	
3	B	52	
4	C	109	
5	E	191	
6	F	126	
7	G	104	
8	H	113	
9	J	248	
10	K	129	
11	L	123	

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Mol	Chain	Length	Quality of chain
12	M	118	
13	N	144	
14	O	134	
15	P	89	
16	Q	104	
17	T	66	
18	U	206	
19	X	189	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 83962 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 26S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3119	Total	C	N	O	P	0	0	0
			66769	29861	12195	21594	3119			

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	91	Total	C	N	O	S	0	0	0
			721	440	158	116	7			

- Molecule 3 is a protein called RPL39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	51	Total	C	N	O	S	0	0	0
			456	288	97	70	1			

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L36A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	103	Total	C	N	O	S	0	0	0
			836	526	163	140	7			

- Molecule 5 is a protein called RPL6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	190	Total	C	N	O	S	0	0	0
			1525	966	286	272	1			

- Molecule 6 is a protein called RPL14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	125	Total	C	N	O	S	0	0	0
			1021	659	192	169	1			

- Molecule 7 is a protein called RPL30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	96	Total	C	N	O	S	0	0	0
			727	455	129	138	5			

- Molecule 8 is a protein called RPL35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	107	Total	C	N	O	S	0	0	0
			850	540	167	142	1			

- Molecule 9 is a protein called TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	226	Total	C	N	O	S	0	0	0
			1716	1068	302	336	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	EXPRESSION TAG	UNP Q245F2
J	-1	THR	-	EXPRESSION TAG	UNP Q245F2
J	0	SER	-	EXPRESSION TAG	UNP Q245F2

- Molecule 10 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	52	Total	C	N	O	S	0	0	0
			415	257	83	69	6			

- Molecule 11 is a protein called RPL34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	108	Total	C	N	O	S	0	0	0
			852	529	170	147	6			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	100	Total	C	N	O	S	0	0	0
			819	530	137	151	1			

- Molecule 13 is a protein called RPL27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	143	Total	C	N	O	S	0	0	0
			1170	755	213	199	3			

- Molecule 14 is a protein called RPL28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	O	134	Total	C	N	O	S	0	0	0
			1034	650	204	179	1			

- Molecule 15 is a protein called RPL38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	66	Total	C	N	O	S	0	0	0
			551	367	93	90	1			

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	102	Total	C	N	O		0	0	0
			803	506	165	132				

- Molecule 17 is a protein called RPL29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	T	65	Total	C	N	O		0	0	0
			533	324	117	92				

- Molecule 18 is a protein called RPL13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	U	203	Total	C	N	O	S	0	0	0
			1624	1015	328	279	2			

- Molecule 19 is a protein called RPL18A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	X	188	Total	C	N	O	S	0	0	0
			1536	972	287	271	6			

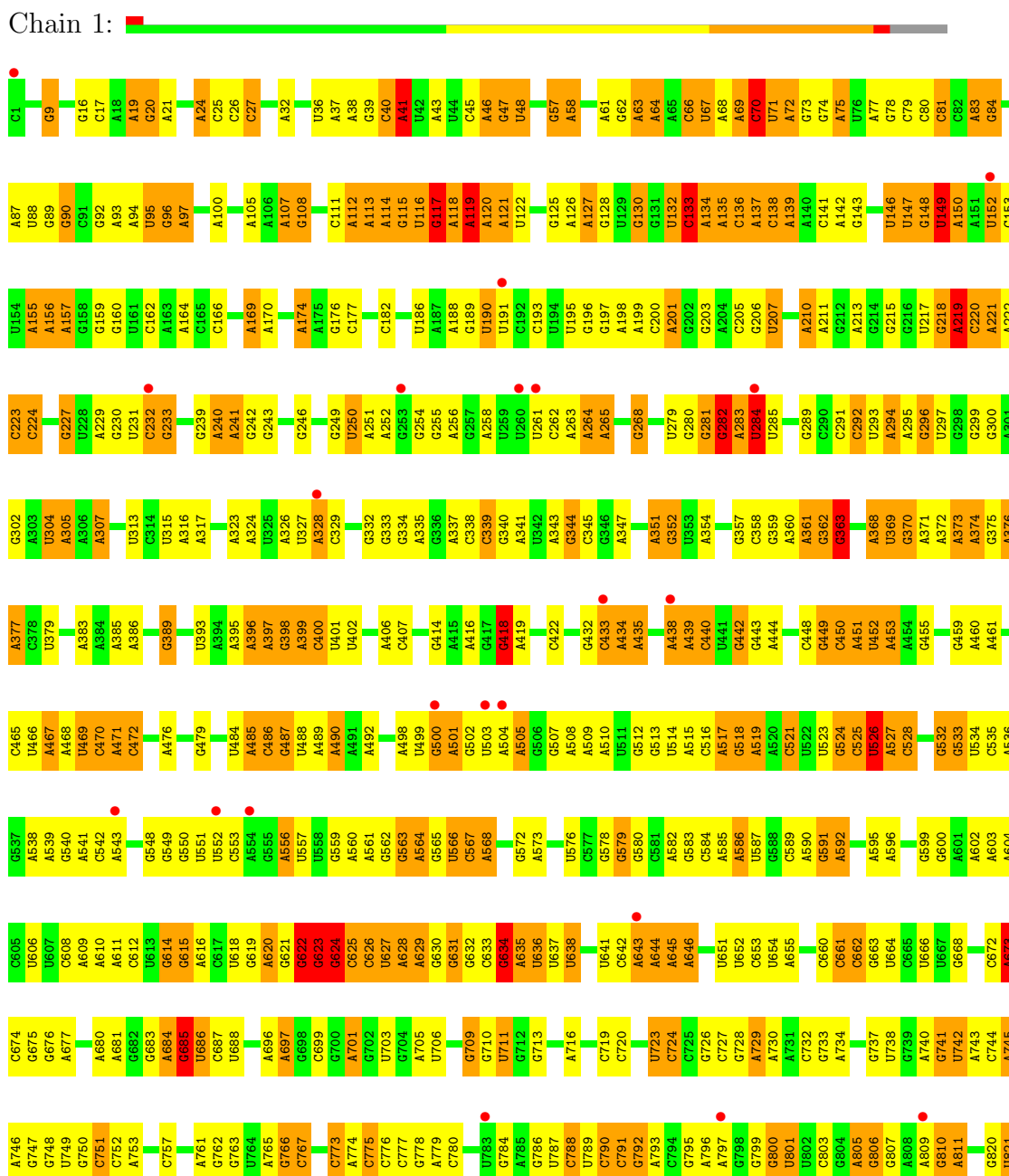
- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total 1	Zn 1	0	0
20	L	1	Total 1	Zn 1	0	0
20	C	1	Total 1	Zn 1	0	0
20	K	1	Total 1	Zn 1	0	0

3 Residue-property plots

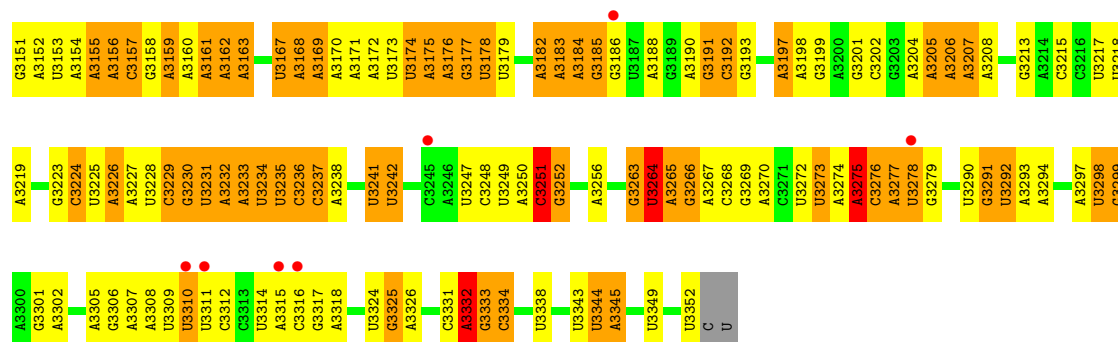
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 26S rRNA



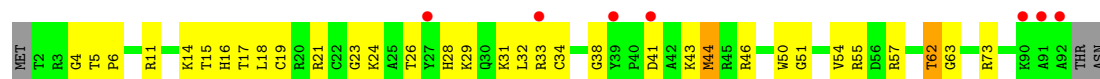


C3078	G2992	U2901	A2807	C2730	C2642	A2557	A	G2421	G2350	G2278	C2199	C2110	U
U3079	C2993	G2902	G2812	C2731	C2643	U2558	C	U2421	A2351	C2279	U2200	G2111	U
A3080	G2994	U2903	G2812	G2732	U2559	U2560	C	A2424	C2352	U2281	G2201	A2112	U
A2995	C2904	C2904	G2815	C2733	A2645	A2561	C		C2353		A2202	A2113	U
C3082	C2996	G2905	G2816	G2734	A2646	U2562	U		A2356	C2282	U2204	A2116	A
A3083	G2906	G2906	G2817	G2735	U2648	U2563	C	U2427	C2357	U2284	U2205	G2117	U
	A2907	U2817		G2736	G2649	U2564	A	U2428	A2358	C2285	G2208	G2118	U
G3087	A3000	A2821	A2821	G2737	G2650	A2565	C	U2429	U2361	C2286	A2209	G2119	U
U3088	A3001	G2822	G2822	C2738	U2655	C2566	C	U2431	G2430	A2290			A
U3096	U3004	U2911	U2912	C2739	U2656	U2567	C	U2432		A2291			U
G3097		C2913	G2827	U2741	U2658	G2568	C	A2433	G2365	U2292	G2216	C2125	U
A3098	U3008	G2828	G2828	G2742	U2659	A2569	U	A2434	G2366	U2293	G2217	A2126	U
C3099	U3009	G2829	G2829	G2743	G2661			A2435	A2367	U2294	A2218	A2127	C
U3100	A3010	U2830	G2865	G2744	G2665	U2574	A		U2368	A2299	U2220	G2130	A
U3101	G3011	U2831	G2666		G2666	G2575		G2438	G2369	A2298			U
G3104	U2920	U2831	A2667	U2748	A2676	C2576		C2439	G2370	U2299			G
G3105	A2921	A2833	A2668	G2750	A2669	G2577	U2503	A2440	G2371	U2300			U
C3106	C3014	U2834	U2670	G2751	U2672	A2579	U2504		G2372	U2301			U
C3107	A2924	A2835	U2671	U2761	U2672	G2580	U2505		U2375	C2302			U
U3108	G2925	G2838	U2672	U2762	U2672	G2581	U2506		A2376	G2303			U
C3109	A2929	U2843	G2678	C2765	A2678	A2582	U2507		G2377	U2304			U
U3110	C2930	U2843	A2679	A2766	A2680	G2583	U2508		A2378	U2305			U
A3111	C2931	U2846	U2855	A2767	U2856	A2584	U2510		A2379	U2306			U
A3112	U2932	U2847	U2855	A2768	U2857	U2585			U2380	A2307			U
U3113	G2933	U2848	A2863	A2769	U2858	G2595	U2515		U2383	U2308			U
C3114	A2934	U2849	A2864	U2770	A2885	G2596	U2516		G2384	U2309			A
A3115	C2935	U2850	U2885	U2771	U2885	G2597	A2518		A2385	G2310			U
G3117	A3035	U2855	U2888	U2772	U2888	G2597	A2519		G2386	G2311			U
A3118	U3036	C2855	U2858	U2773	U2889	U2602	U2520		C2387	U2312			U
A3119	A3037	U2856	U2857	U2774	U2889	G2603	U2521		U2314	U2313			U
U3120	G2949	U2857	A2693	G2775	U2894	A2522	A2522		G2388	U2314			U
		U2858	A2694	C2776	U2894	A2523	A2524		G2389	A2315			U
A3123	G3042	U2952	U2702	G2779	U2702	G2530	U2530		G2391	U2317			U
U3124	U3043	U2953	G2703		G2703	U2531	U2531		A2392	G2318			U
G3125	A3044	G2954	A2704	G2782	A2704	A2614	G2532		A2393	A2319			A
C3126	A3045	U2955	U2705	U2783	U2705	U2615	G2533		A2394	G2320			U
U3127	U3046	G2956	U2706	G2784	U2706	G2617			A2396	U2255			U
G3128	A3047	A2957	U2707	G2784	U2707	G2618	C2537		A2397	U2256			U
G3129	A3048	C2958	U2708	G2787	U2708	U2618	U2538		G2398	U2257			U
A3130	C3049	U2959	U2709	A2787	U2709	U2622	A2539		A2399	A2257			U
A3131	G3060	G2960	C2869	U2788	U2788	U2622	G2540		C2400	C2260			A
A3132	U3053	G2961	C2873	G2788	U2788	U2622	U2541			A2178			U
G3133	C3056	U2962	U2874	A2789	U2789	U2623	U2542			U2179			U
C3134	U3057	U2966	A2875	A2790	A2790	A2624	U2543			G2180			U
A3135	U3057	U2966	U2876	A2791	A2791	A2625	C2544			A2181			A
G3136	G3063	U2967	U2883	G2793	U2718	C2627	U2545			G2182			U
U3137			G2883		U2718		A2546			U2184			C
G3138			A2884	C2797	A2719	C2633	A2547						U
U3139	A3066	C2971	A2884	C2798	A2719	G2634	U2548						U
A3142	U3067	C2972	G2885	C2798	G2720	G2635	U2549						U
A3143	G3069	G2978	G2886	A2801	G2721	A2636	U2550						C
G3144	G3070	A2887	A2888	A2802	A2725	G2637	A2551						U
U3145	G3071	G2889	G2889	G2803	C2726	G2638	A2552						A
G3146	G3072	C2899	A2728	G2804	A2727	G2639	U2553						A
U3147	G3077	G2900	A2729	U2806	A2729	G2641	G2554						C



• Molecule 2: RIBOSOMAL PROTEIN L37

Chain A:



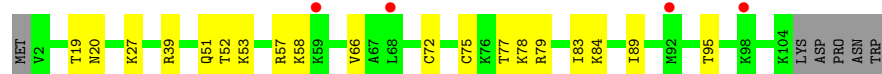
• Molecule 3: RPL39

Chain B:



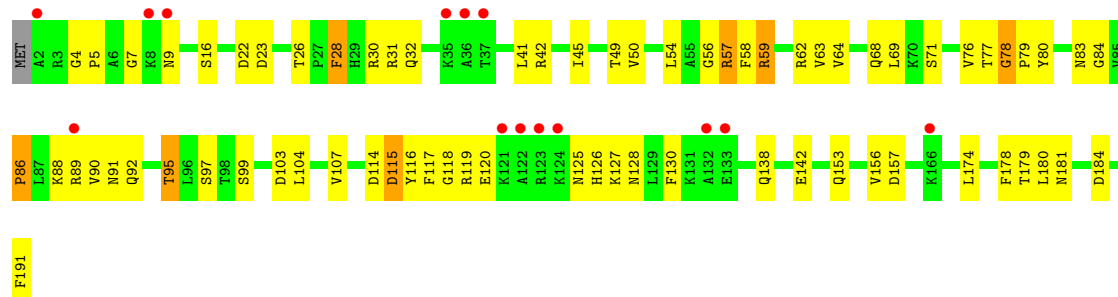
• Molecule 4: 60S RIBOSOMAL PROTEIN L36A

Chain C:



• Molecule 5: RPL6

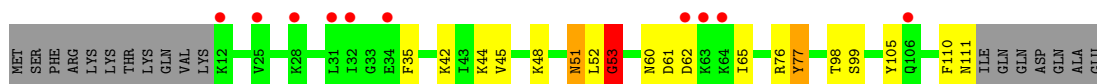
Chain E:



• Molecule 6: RPL14

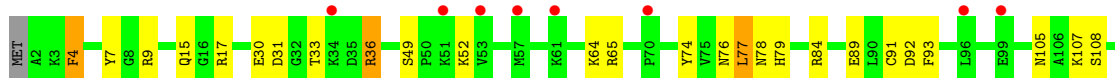
Chain F:





• Molecule 13: RPL27

Chain N:



• Molecule 14: RPL28

Chain O:



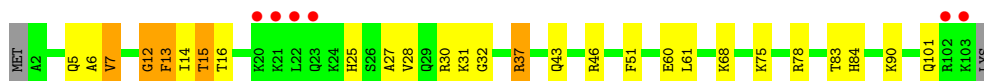
• Molecule 15: RPL38

Chain P:



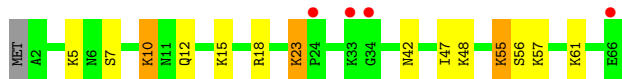
• Molecule 16: 60S RIBOSOMAL PROTEIN L36

Chain Q:



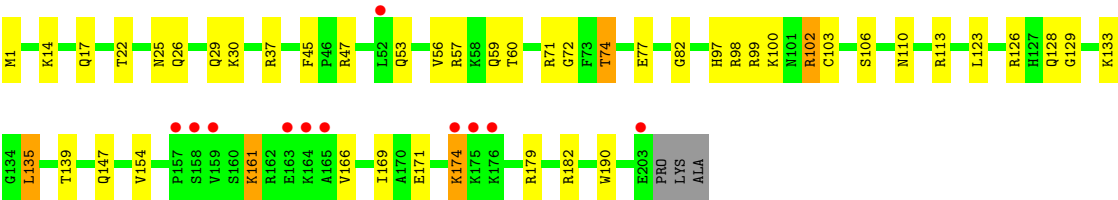
• Molecule 17: RPL29

Chain T:



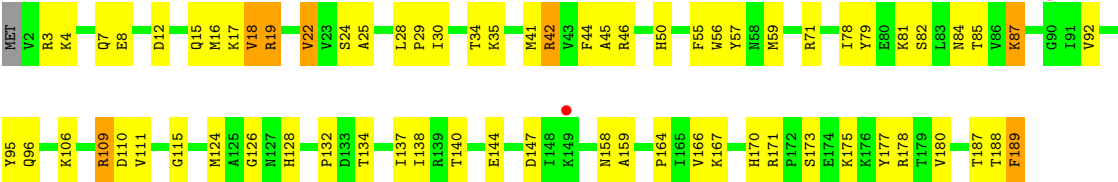
• Molecule 18: RPL13

Chain U:



• Molecule 19: RPL18A

Chain X:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	320.19Å 289.25Å 535.04Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	20.00 – 3.52 39.96 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.52) 99.4 (39.96-3.52)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.216 , 0.244 0.489 , 0.492	Depositor DCC
R_{free} test set	10000 reflections (0.85%)	DCC
Wilson B-factor (Å ²)	96.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.1	EDS
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 1192534 reflections	Xtriage
F_o, F_c correlation	0.53	EDS
Total number of atoms	83962	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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

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	1	0.82	60/74792 (0.1%)	1.14	368/116594 (0.3%)
2	A	0.63	0/734	0.76	0/972
3	B	0.46	0/466	0.62	0/619
4	C	0.53	0/848	0.69	0/1123
5	E	0.47	0/1550	0.74	2/2077 (0.1%)
6	F	0.51	0/1033	0.71	0/1380
7	G	0.47	0/736	0.73	0/990
8	H	0.62	0/870	0.82	0/1175
9	J	0.49	0/1739	0.70	0/2368
10	K	0.45	0/421	0.70	0/558
11	L	0.57	0/861	0.72	0/1154
12	M	0.41	0/832	0.67	0/1113
13	N	0.38	0/1190	0.58	0/1582
14	O	0.47	0/1047	0.77	1/1400 (0.1%)
15	P	0.38	0/561	0.62	0/745
16	Q	0.48	0/808	0.69	0/1068
17	T	0.48	0/539	0.72	0/711
18	U	0.51	0/1647	0.74	1/2201 (0.0%)
19	X	0.50	0/1563	0.75	1/2104 (0.0%)
All	All	0.76	60/92237 (0.1%)	1.08	373/139934 (0.3%)

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
2	A	0	1
12	M	0	1
16	Q	0	1
All	All	0	3

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2254	A	C5-C4	17.31	1.50	1.38
1	1	2254	A	N7-C5	15.90	1.48	1.39
1	1	2254	A	N3-C4	15.68	1.44	1.34
1	1	2251	A	N7-C5	15.41	1.48	1.39
1	1	2251	A	N3-C4	15.05	1.43	1.34

The worst 5 of 373 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	284	U	C6-N1-C2	-15.54	111.67	121.00
1	1	119	A	N1-C6-N6	13.39	126.63	118.60
1	1	2253	U	C5-C6-N1	-11.75	116.83	122.70
1	1	2606	U	N3-C4-C5	-11.50	107.70	114.60
1	1	2273	C	N1-C2-O2	10.79	125.37	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	51	GLY	Peptide
12	M	53	GLY	Peptide
16	Q	12	GLY	Peptide

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	1	66769	0	0	1333	0
2	A	721	0	0	20	0
3	B	456	0	0	14	0
4	C	836	0	0	12	0
5	E	1525	0	0	62	0
6	F	1021	0	0	35	0
7	G	727	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	850	0	0	44	0
9	J	1716	0	0	27	0
10	K	415	0	0	12	0
11	L	852	0	0	19	0
12	M	819	0	0	13	0
13	N	1170	0	0	26	0
14	O	1034	0	0	29	0
15	P	551	0	0	16	0
16	Q	803	0	0	25	0
17	T	533	0	0	13	0
18	U	1624	0	0	36	0
19	X	1536	0	0	49	0
20	A	1	0	0	0	0
20	C	1	0	0	0	0
20	K	1	0	0	0	0
20	L	1	0	0	0	0
All	All	83962	0	0	1626	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 20.

The worst 5 of 1626 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:3044:A:O2'	1:1:3046:A:OP2	1.54	1.23
1:1:451:A:O2'	14:O:56:GLN:NE2	1.75	1.18
1:1:1207:A:O2'	1:1:1208:U:OP1	1.56	1.18
1:1:265:A:N6	16:Q:30:ARG:O	1.78	1.17
1:1:1909:C:O2'	1:1:1910:A:OP2	1.62	1.15

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	
2	A	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	B	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
4	C	101/109 (93%)	99 (98%)	2 (2%)	0	100	100
5	E	188/191 (98%)	176 (94%)	11 (6%)	1 (0%)	38	87
6	F	123/126 (98%)	116 (94%)	7 (6%)	0	100	100
7	G	94/104 (90%)	90 (96%)	4 (4%)	0	100	100
8	H	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
9	J	224/248 (90%)	211 (94%)	11 (5%)	2 (1%)	25	80
10	K	50/129 (39%)	44 (88%)	6 (12%)	0	100	100
11	L	106/123 (86%)	98 (92%)	8 (8%)	0	100	100
12	M	98/118 (83%)	94 (96%)	3 (3%)	1 (1%)	22	78
13	N	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	30	83
14	O	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
15	P	62/89 (70%)	58 (94%)	4 (6%)	0	100	100
16	Q	100/104 (96%)	89 (89%)	9 (9%)	2 (2%)	11	63
17	T	63/66 (96%)	60 (95%)	2 (3%)	1 (2%)	14	68
18	U	201/206 (98%)	187 (93%)	13 (6%)	1 (0%)	38	87
19	X	186/189 (98%)	178 (96%)	6 (3%)	2 (1%)	21	77
All	All	2112/2339 (90%)	1989 (94%)	112 (5%)	11 (0%)	38	87

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	7	VAL
5	E	86	PRO
17	T	10	LYS
18	U	135	LEU
9	J	13	ILE

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	
2	A	69/72 (96%)	58 (84%)	11 (16%)	4	22
3	B	48/49 (98%)	44 (92%)	4 (8%)	16	59
4	C	95/101 (94%)	92 (97%)	3 (3%)	51	89
5	E	162/163 (99%)	152 (94%)	10 (6%)	26	73
6	F	111/112 (99%)	106 (96%)	5 (4%)	38	83
7	G	80/88 (91%)	74 (92%)	6 (8%)	19	65
8	H	87/92 (95%)	78 (90%)	9 (10%)	10	47
9	J	195/216 (90%)	176 (90%)	19 (10%)	12	50
10	K	46/113 (41%)	43 (94%)	3 (6%)	24	72
11	L	92/107 (86%)	87 (95%)	5 (5%)	31	78
12	M	93/110 (84%)	90 (97%)	3 (3%)	51	89
13	N	130/131 (99%)	122 (94%)	8 (6%)	26	73
14	O	108/108 (100%)	102 (94%)	6 (6%)	30	77
15	P	60/77 (78%)	56 (93%)	4 (7%)	23	70
16	Q	81/83 (98%)	75 (93%)	6 (7%)	20	66
17	T	61/62 (98%)	57 (93%)	4 (7%)	24	71
18	U	169/171 (99%)	161 (95%)	8 (5%)	36	82
19	X	167/168 (99%)	152 (91%)	15 (9%)	14	55
All	All	1854/2023 (92%)	1725 (93%)	129 (7%)	21	68

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	123	ARG
11	L	21	ARG
19	X	46	ARG
9	J	144	ASN
9	J	198	VAL

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	1	3114/3354 (92%)	1113 (35%)	215 (6%)

5 of 1113 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	9	G
1	1	16	G
1	1	17	C
1	1	19	A
1	1	20	G

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1495	C
1	1	1839	A
1	1	3191	G
1	1	1580	G
1	1	1738	A

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 4 ligands modelled in this entry, 4 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	1	3119/3354 (92%)	0.16	72 (2%) 57 28	40, 79, 164, 330	0
2	A	91/94 (96%)	0.69	7 (7%) 13 7	34, 66, 123, 226	0
3	B	51/52 (98%)	0.45	2 (3%) 37 17	49, 69, 111, 146	0
4	C	103/109 (94%)	0.45	4 (3%) 37 17	46, 84, 135, 194	0
5	E	190/191 (99%)	0.55	14 (7%) 14 7	74, 124, 169, 226	0
6	F	125/126 (99%)	0.49	9 (7%) 15 7	70, 106, 157, 190	0
7	G	96/104 (92%)	0.45	7 (7%) 15 7	57, 114, 179, 222	0
8	H	107/113 (94%)	0.18	1 (0%) 81 51	54, 89, 127, 138	0
9	J	226/248 (91%)	0.20	3 (1%) 74 41	51, 89, 136, 206	0
10	K	52/129 (40%)	0.65	5 (9%) 8 6	53, 79, 134, 151	0
11	L	108/123 (87%)	0.62	6 (5%) 24 10	47, 85, 144, 217	0
12	M	100/118 (84%)	0.62	10 (10%) 8 5	73, 126, 179, 199	0
13	N	143/144 (99%)	0.59	12 (8%) 11 6	73, 121, 179, 214	0
14	O	134/134 (100%)	0.43	8 (5%) 21 10	52, 99, 151, 209	0
15	P	66/89 (74%)	0.38	3 (4%) 32 14	73, 116, 176, 245	0
16	Q	102/104 (98%)	0.47	6 (5%) 22 10	63, 105, 151, 186	0
17	T	65/66 (98%)	0.62	4 (6%) 20 9	51, 87, 122, 211	0
18	U	203/206 (98%)	0.48	11 (5%) 25 11	48, 98, 158, 198	0
19	X	188/189 (99%)	0.27	2 (1%) 77 45	54, 89, 128, 170	0
All	All	5269/5693 (92%)	0.28	186 (3%) 42 20	34, 87, 163, 330	0

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	92	ALA	10.0

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Mol	Chain	Res	Type	RSRZ
1	1	2252	C	9.7
12	M	12	LYS	8.7
1	1	3311	U	8.2
2	A	91	ALA	7.9

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
20	ZN	A	1193	1/1	0.09	-1.28	69,69,69,69	0
20	ZN	C	1105	1/1	0.06	-1.57	89,89,89,89	0
20	ZN	L	1110	1/1	0.09	-1.71	86,86,86,86	0
20	ZN	K	1130	1/1	0.09	-1.92	68,68,68,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.