Supplemental Information

Large-Scale Movements of IF3 and tRNA

during Bacterial Translation Initiation

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Table S1. Refinement and model statistics, Related to Figure 1.

	PIC-1A	PIC-1B	PIC-1C	PIC-2A	PIC-2B	PIC-2C	PIC-3	PIC-4	PIC-III
Model Composition									
Non-hydrogen atoms	54057	54036	54058	55811	55695	55681	55727	55151	59482
Protein residues	4162	4160	4161	4251	4241	4234	4238	4166	4739
RNA bases	1534	1533	1534	1611	1608	1610	1611	1611	1611
Refinement									
Resolution used for refinement (Å)	3.6	4.4	5.4	4.3	4.5	5.2	4.25	4.15	5.1
Map sharpening B-factor (Å)	-87	-130	-157	-89	-101	-103	-107	-108	-180
Average B-factor (Å)	89.7	-	-	-	-	-	-	-	-
Fourier Shell Correlation (FSC)*	0.83	0.66	0.73	0.73	0.71	0.72	0.72	0.75	0.71
Rms deviations									
Bonds (Å)	0.006	0.008	0.008	0.007	0.065	0.008	0.007	0.006	0.006
Angles (°)	1.263	1.306	1.287	1.292	1.220	1.305	1.273	1.310	1.137
Validation (proteins)									
Molprobity score (Percentile in brackets)	3.36 (74th)	3.37 (75th)	3.33 (77th)	3.40 (74th)	3.25 (81st)	3.45 (71st)	3.43 (73rd)	3.53 (65th)	3.14 (84th)
Clashscore, all atoms (Percentile in brackets)	16.84 (97th)	16.05 (97th)	16.19 (97th)	17.23 (97th)	17.00 (97th)	18.85 (97th)	16.97 (97th)	19.27 (97th)	13.17 (97th)
Good rotamers (%)	60.67	61.19	62.28	60.24	64.93	60.45	59.12	55.20	66.80
Ramachandran plot									
Favored (%)	85.37	84.71	85.02	85.29	88.06	83.32	84.00	83.23	87.29
Outliers (%)	4.18	3.99	3.10	3.97	3.13	3.34	3.84	4.26	2.80
Validation (RNA)									
Correct sugar puckers(%)	96.48	96.02	96.41	96.15	96.64	96.28	96.65	96.46	95.16
Good backbone conformations(%)	70.27	68.75	70.34	71.64	71.71	69.96	72.26	69.09	72.33

* FSC= $\Sigma(N_{shell} FSC_{shell})/ \Sigma(N_{shell})$, where FSC_{shell} is the FSC in a given shell, N_{shell} is the number of "structure factors" in the shell. $FSC_{shell} = \Sigma(F_{model} F_{EM})/ (\sqrt{(\Sigma(|F|^2_{model}))} \sqrt{(\Sigma(|F|^2_{EM}))})$

Table S2. Local resolution of ligands, Related to Figure 1.

Structures	PIC-1A (Å)	PIC-1B (Å)	PIC-1C (Å)	PIC-2A (Å)	PIC-2B (Å)	PIC-2C (Å)	PIC-3 (Å)	PIC-4 (Å)	PIC-III (Å)
Overall Resolution	3.55	4.30	5.35	4.20	4.45	5.10	4.15	4.00	4.90
IF3: NTD-linker	4.55	6.10	7.00	5.10	6.20	8.30	6.70	6.95	8.50
IF3: CTD	3.90	5.20	6.00	4.90	6.20	6.95	5.10	5.25	5.80
IF1	4.05	5.20	6.45	4.65	6.20	6.55	4.85	-	5.45
IF2	-	-	-	-	-	-	-	-	6.95
tRNA	-	-	-	5.10	5.90	6.55	4.35	4.20	5.05
ASL + mRNA(-4 to +4)	-	-	-	4.85	4.60	5.45	4.10	3.95	4.95

Table S3. 30S head position in PICs, Related to Figure 2.

PICs	Degree of rotation of 30S head (degree of rotation)	Open/closed conformation of 30S
PIC-1A	Canonical position (0°)	Closed
PIC-1B	Swiveled position (~ 5°)	Closed
PIC-1C	(0°)	Open (30S head moves up)
PIC-2A	(~ 3 °)	Open (30S head moves up)
PIC-2B	Swiveled position (~ 9°)	Closed
PIC-2C	Canonical position (0°)	Closed
PIC-3	Canonical position (0°)	Closed
PIC-4	Canonical position (0°)	Closed
PIC-I	Canonical position (0°)	Closed
PIC-II	(~ 4°)	Closed
PIC-III	Canonical position (0°)	Closed