

Table 1: Summary of the RAG-Ragular MuSIC system integrative modeling

1) Gathering information	
<i>Physical principles and statistical preferences</i>	Excluded volume
<i>Input information</i>	Sequence connectivity
	Atomic structure prediction from Alphafold2 (AF_Q96GS4, AF_Q9BY32)
	Comparative model of the SLC38A9-RagA-RagB-Ragulator complex (template PDB ID 6WJ2)
2) Representing the system	
<i>Composition (number of copies)</i>	BORCS6: 1 ITPA: 1 Lamtor1: 1 Lamtor2: 1 Lamtor3: 1 Lamtor4: 1 Lamtor5: 1 RRAGB: 1 RRAGC: 1 SLC38A9: 1
<i>Atomic (structured) components</i>	BORCS6: 199-216, 221-228, 258-295, 319-355 ITPA: 1-194 Lamtor1: 49-68, 83-146 Lamtor2: 5-125 Lamtor3: 1-124 Lamtor4: 1-99 Lamtor5: 1-91 RRAGB: 1-337, 344-374 RRAGC: 62-369 SLC38A9: 39-78, 80-96
<i>Unstructured components</i>	BORCS6: 217-220, 229-257, 296-318 Lamtor1: 69-82, 147-158 Lamtor2: 1-4 RRAGB: 338-343 SLC38A9: 79-79
<i>Resolution of structured components</i>	1 [R1] residue per bead
<i>Resolution of unstructured components</i>	None
<i>Structural coverage</i>	94.74 %

<i>Rigid body (RB) definitions</i>	RB1: Lamtor1 _{49–68} ,Lamtor1 _{83–146} ,Lamtor2 _{5–125} ,Lamtor3 _{1–124} ,Lamtor4 _{1–99} , Lamtor5 _{1–91} ,RRAGB _{1–337} ,RRAGB _{344–374} ,RRAGC _{62–369} ,SLC38A9 _{39–78} , SLC38A9 _{80–96} RB2: BORCS6 _{199–216} RB3: BORCS6 _{221–228} RB4: BORCS6 _{258–295} RB5: BORCS6 _{319–355} RB6: ITPA _{1–194}
<i>Resolution of disordered regions</i>	1 [R1] residues per bead
<i>Spatial restraints encoded into scoring function</i>	Excluded volume; applied to the R1 representation Sequence connectivity; applied to the R1 representation Bayesian binary binding Mode restraint
3) Structural Sampling	
<i>Sampling method</i>	Replica Exchange Gibbs sampling, based on Metropolis Monte Carlo
<i>Replica exchange temperature range</i>	1.0 - 4.0
<i>Number of replicas</i>	4
<i>Number of runs</i>	60
<i>Number of structures generated</i>	3000000
<i>Movers for flexible string of bead</i>	Random translation up to 4.0 Å
<i>CPU time</i>	5 hours on 80 processors
4) Validating models	
Models selected for validation	
<i>Number of models after equilibration</i>	3000000
<i>Number of models that satisfy the input information</i>	10000
<i>Number of structures in samples A/B</i>	4619/5381
<i>p-value of non-parametric Kolmogorov-Smirnov two-sample test</i>	0.063 (threshold p-value > 0.05)
<i>Kolmogorov-Smirnov two-sample test statistic, D</i>	1.0
Thoroughness of the structural sampling	
<i>Sampling precision</i>	15.18 Å
<i>Homogeneity of proportions χ^2 test (p-value)/Cramer's V value</i>	0.000/0.086 (thresholds: p-value>0.05 OR Cramer's V<0.1)
<i>Number of clusters</i>	1
<i>Cluster populations</i>	cluster 1 : 97.2 %
<i>Cluster precisions</i>	cluster 1 : 9.96 Å
<i>Average cross-correlation between localization probability densities of samples A and B</i>	cluster 1: 0.98
Validation by information used for modeling	

<i>Percent of sequence connectivity restraints satisfied per structure</i>	99 %
<i>Percent of excluded volume restraints satisfied per structure</i>	99 %
5) Software and data availability	
Software	
<i>Modeling programs</i>	IMP PMI module, version 2.19.0 Integrative Modeling Platform (IMP), version 2.19.0 MODELLER, version SVN
<i>Modeling scripts</i>	https://github.com/integrativemodeling/IM_MuSIC
<i>Structure prediction</i>	AlphaFold2 AlphaFold-Multimer
<i>Visualization and plotting</i>	UCSF Chimera