# SUPPLEMENTARY INFORMATION

# Bayesian weighing of electron cryo-microscopy data for integrative structural modeling

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## Supplementary Figures

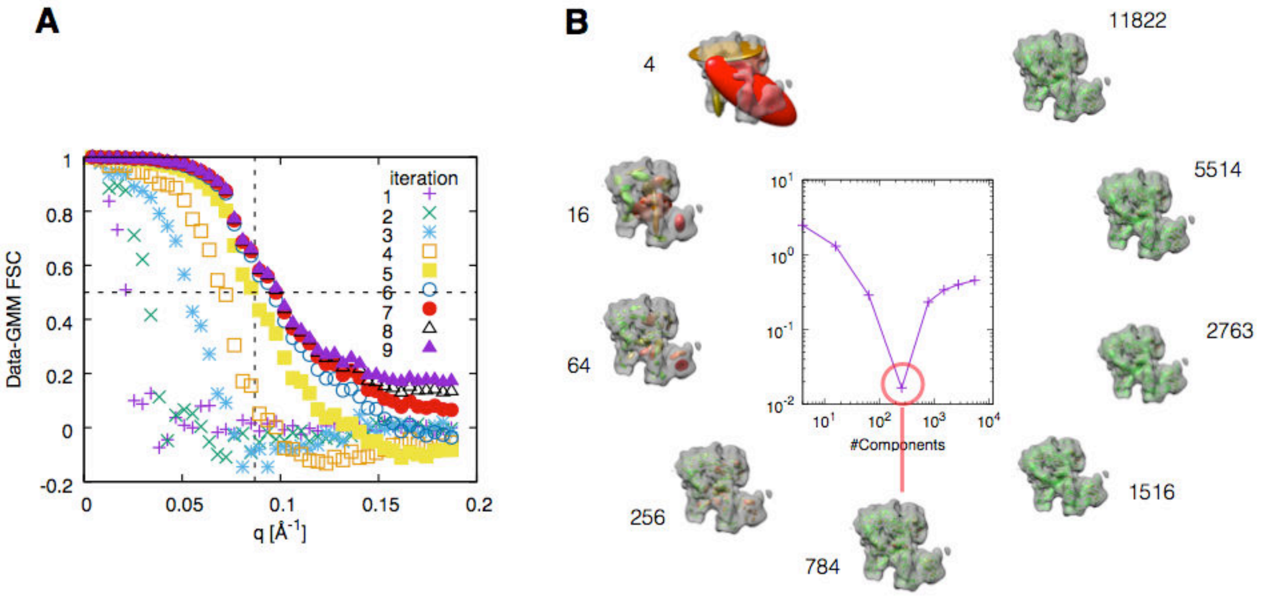


**Figure S1: Selection of the optimal data-GMM.** (A) Fourier Shell Correlation of each GMM in the series with the original map. The horizontal dotted line represents the 0.5 threshold, and the vertical dotted line marks the inverse of the resolution of the original map (11.5 Å). (B) Ellipsoid representation of the GMM series, together with the absolute relative deviation $|\Delta r|/r$ between the data-GMM resolution and the density map resolution. The optimal GMM, defined as the GMM which minimizes $|\Delta r|/r$, is highlighted.

**A**

$$p(\phi_D|M) = \prod_k p(\phi_{D,k}|M)$$

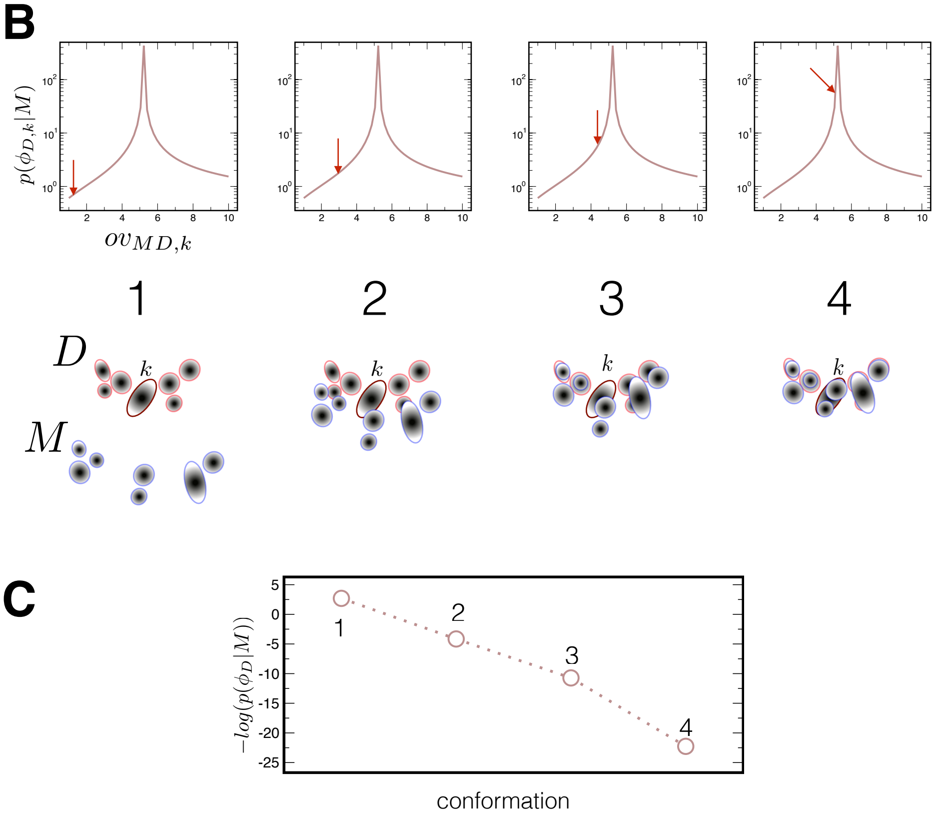


**Figure S2: Likelihood and score.** (A) Likelihood expressed as the product of individual data-component terms. (B) Representation of the evolution of the likelihood as a function of the overlap between the data- and model-GMMs. (C) Scores associated with each conformation.

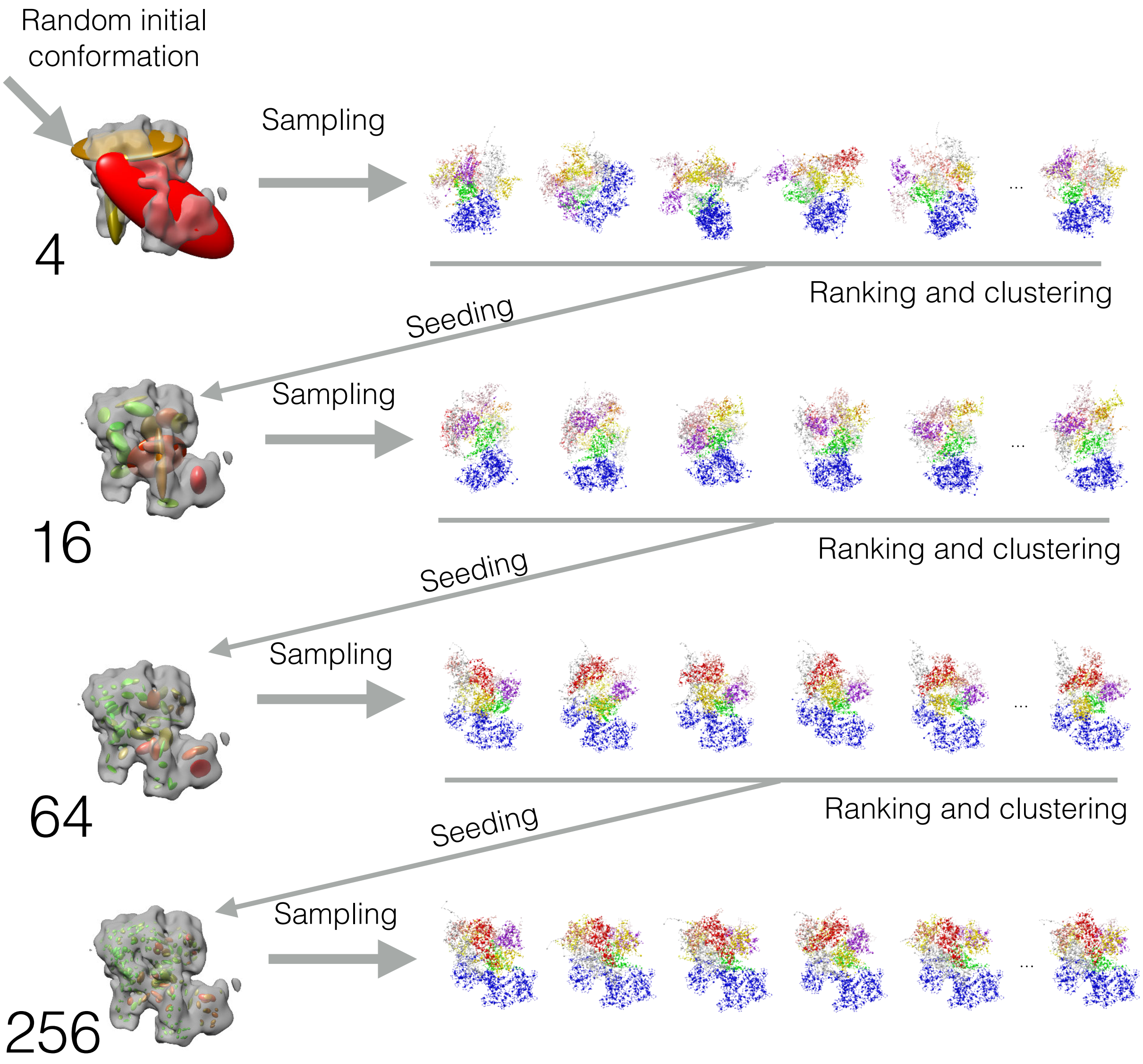


**Figure S3: Schematic representation of the iterative sampling protocol.** For the four iterations of the exosome modeling, the data-GMM is represented as a set of ellipsoids along with resulting models that were selected as seed for the next iteration. A subset of models as structurally diverse as possible is selected from the 100 best scoring models produced at every iteration and used as starting configurations for the following iteration.

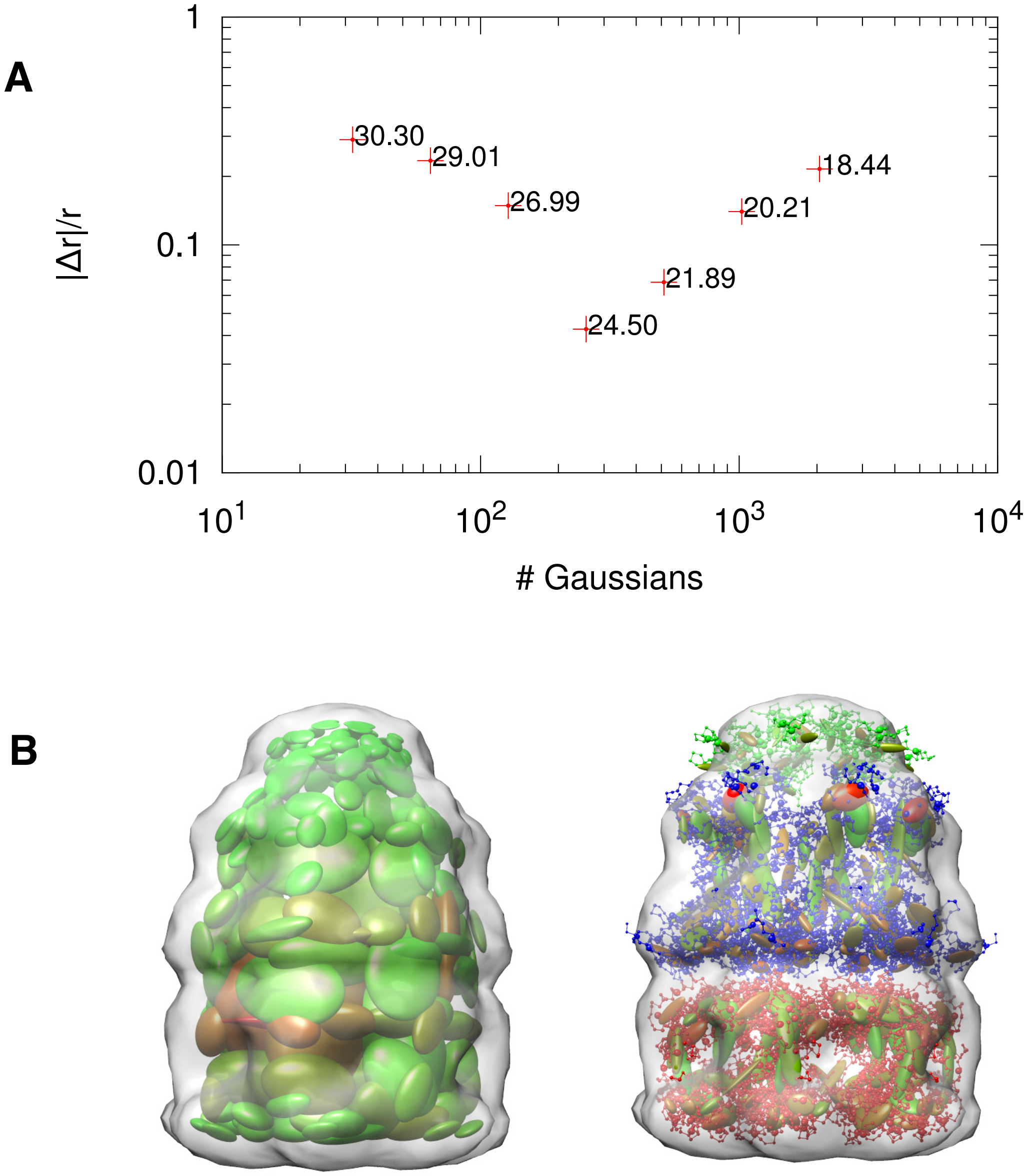
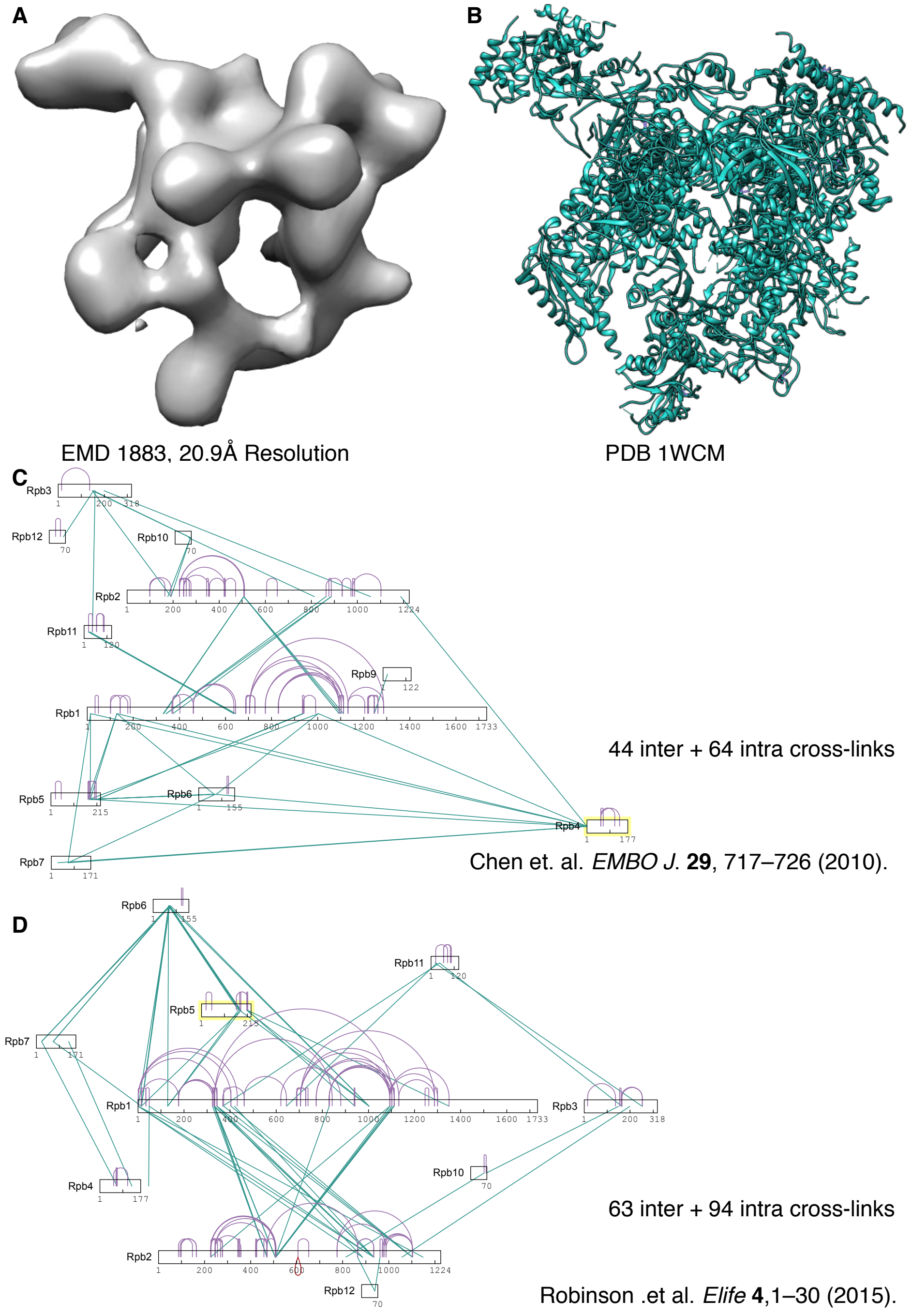


**Figure S4: Modeling of the GroEL/ES complex.** (A) Absolute relative deviation $|\Delta r|/r$ between the data-GMM resolution and the density map resolution as a function of the number of Gaussians of the data-GMM; (B) The model-GMM is represented as a set of ellipsoids (left) and representation of the best scoring model (right). Each subunit is represented as a string of connected beads, where the diameter of the beads defines the coarse-graining resolution.



EMD 1883, 20.9Å Resolution

PDB 1WCM

Chen et. al. *EMBO J*. **29**, 717–726 (2010).

Robinson .et al. *Elife* **4**,1–30 (2015).

**Figure S5: Modeling of the RNA polymerase II.** (A) The cryo-EM map (EMDB code 1883) used in the modeling. (B) The prior structure (PDB code 1WCM) used to initialize the coordinates of the beads. (C, D) Visual representation of the two XL-MS datasets used. The sequence of each subunit is represented as a rectangle, with numbers indicating the residue indexes in the sequence. Cross-links between two residues are represented as a line connecting the two residues. The intra-molecular and inter-molecular cross-links are represented as curved purple lines and straight green lines, respectively.

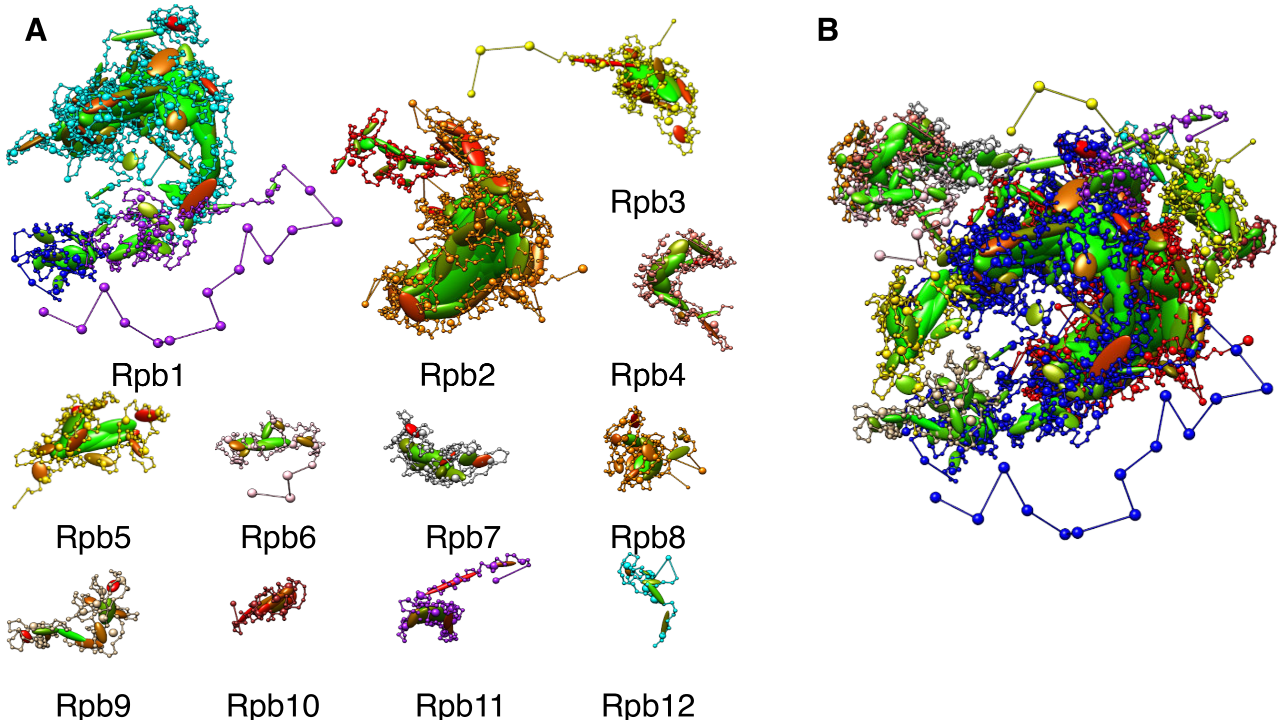
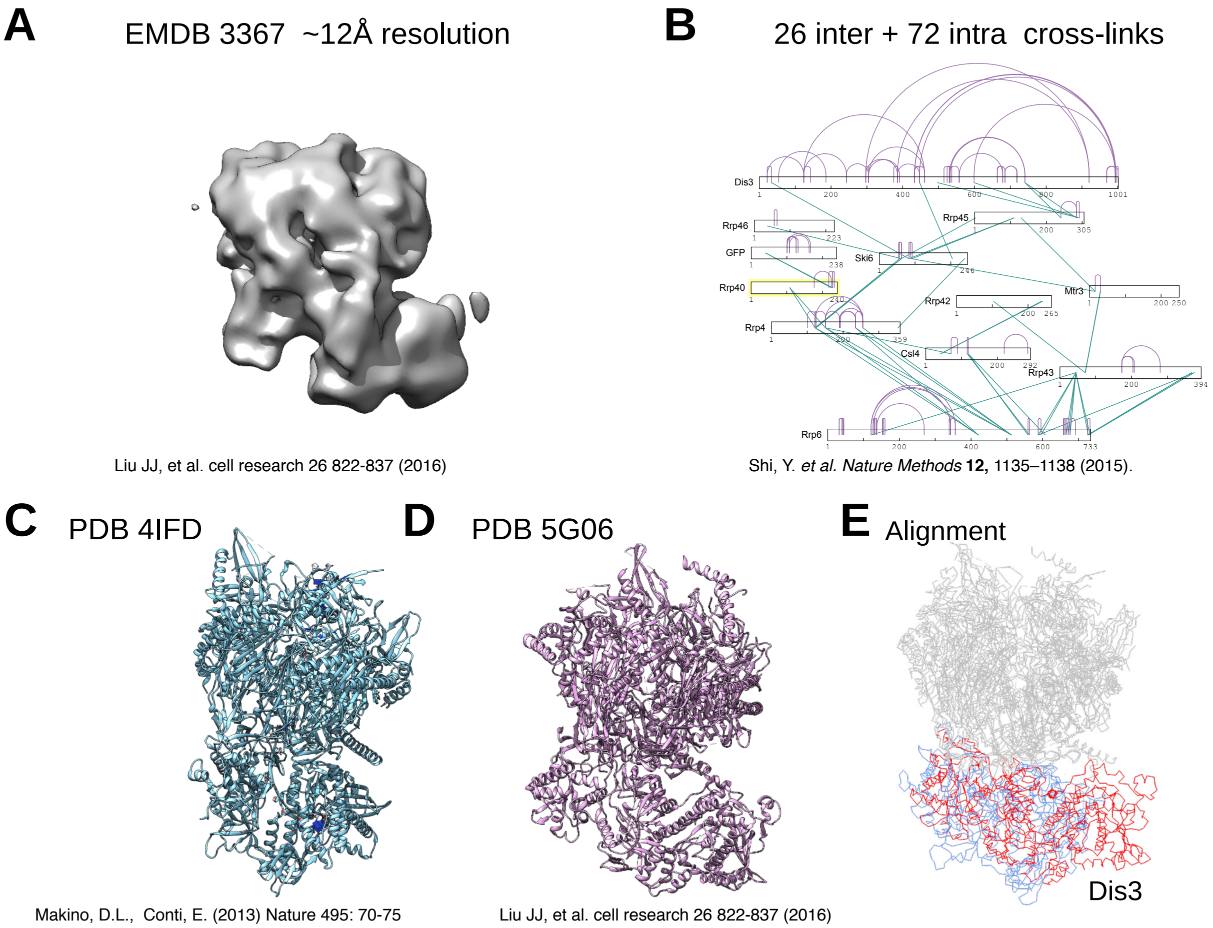


**Figure S6: Model representation of the RNA polymerase II. (**A) Representation of each subunit, with different colors for each individual rigid body. (B) Representation of the best scoring model. Each subunit is represented as a string of connected beads, where the diameter of the beads defines the coarse-graining resolution. The model-GMM is represented as a set of ellipsoids.



EMDB 3367 ~12Å resolution

Liu JJ, et al. cell research 26 822-837 (2016)

26 inter + 72 intra cross-links

Shi, Y. *et al. Nature Methods* **12,** 1135–1138 (2015).

PDB 4IFD

Makino, D.L., Conti, E. (2013) Nature 495: 70-75

PDB 5G06

Liu JJ, et al. cell research 26 822-837 (2016)

Alignment

**Figure S7: Modeling of the exosome.** (A) The cryo-EM map (EMDB code 3367) and (B) a visualization of the XL-MS dataset used in the modeling. (C) Prior structure (PDB code 4IFD), (D) reference structure (PDB code 5G06), and (E) an alignment of the two, in which the conformational change between RNA-bound (blue) and RNA-free (red) structures is highlighted.

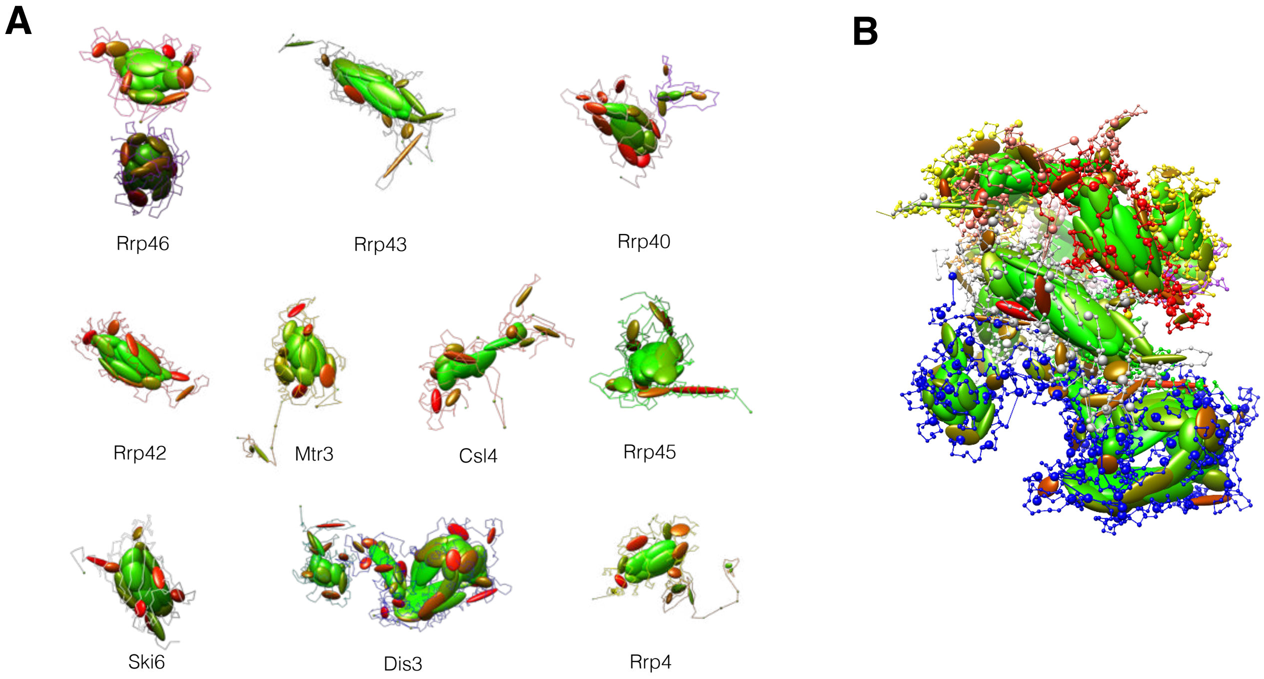


**Figure S8: Model representation of the exosome. (**A) Representation of each subunit, with different colors for each individual rigid body. (B) Representation of the best scoring model. Each subunit is represented as a string of connected beads, where the diameter of the beads defines the coarse-graining resolution. The model-GMM is represented as a set of ellipsoids.

| | 2UZX:A<br>289 | | 2UZX:B<br>727 | |
|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.5 | 0.5, 3.3 | 0.3 | 0.5, 0.6 |
| C1 | 0.8 | 0.9, 6.7 | 0.5 | 0.6, 0.8 |

| | 3R5D:A<br>347 | | 3R5D:B<br>347 | | 3R5D:C<br>347 | |
|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.7 | 0.9, 2.0 | 0.9 | 1.6, 0.4 | 0.6 | 0.8, 2.8 |
| C1 | 0.8 | 1.2, 1.5 | 0.9 | 1.4, 2.4 | 0.7 | 0.6, 3.8 |

| | 1CS4:A<br>225 | | 1CS4:B<br>212 | | 1CS4:C<br>394 | |
|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 1.3 | 2.0, 1.6 | 1.1 | 0.7, 1.3 | 0.4 | 0.2, 0.3 |
| C1 | 1.3 | 1.0, 2.9 | 0.9 | 0.8, 0.3 | 0.9 | 0.7, 0.4 |

| | 2WVY:A<br>737 | | 2WVY:B<br>737 | | 2WVY:C<br>737 | |
|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.4 | 0.5, 1.1 | 0.3 | 0.3, 0.0 | 0.5 | 0.4, 0.4 |
| C1 | 0.6 | 0.9, 1.0 | 0.3 | 0.2, 0.4 | 0.4 | 0.4, 0.4 |

| | 2DQJ:H<br>114 | | 2DQJ:L<br>107 | | 2DQJ:Y<br>129 | |
|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.7 | 1.2, 0.2 | 1.4 | 0.8, 6.3 | 1.2 | 1.1, 2.0 |
| C1 | 0.9 | 1.2, 1.2 | 2.0 | 2.3, 6.5 | 1.3 | 1.5, 1.7 |
| C2 | 13.6 | 1.0, 179.0 | 3.6 | 3.0, 14.3 | 1.1 | 1.0, 1.7 |
| C3 | 1.6 | 1.0, 5.8 | 12.6 | 3.7, 169.7 | 1.4 | 1.1, 2.2 |

|  | 1VCB:C 160 |  | 1VCB:A 118 |  | 1VCB:B 112 |  |
|---|---|---|---|---|---|---|
|  | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.7 | 0.4, 5.3 | 0.6 | 0.9, 1.5 | 0.8 | 1.1, 1.0 |
| C1 | 0.6 | 0.6, 4.5 | 0.7 | 0.9, 1.8 | 1.1 | 1.7, 0.8 |

|  | 2GC7:C 105 |  | 2GC7:D 147 |  | 2GC7:A 386 |  | 2GC7:B 131 |  |
|---|---|---|---|---|---|---|---|---|
|  | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 1.1 | 0.9, 0.8 | 0.5 | 0.6, 0.5 | 0.7 | 0.8, 1.2 | 0.6 | 0.5, 1.0 |
| C1 | 1.6 | 1.5, 0.9 | 0.6 | 0.2, 0.8 | 1.1 | 0.9, 2.9 | 0.5 | 0.8, 0.3 |

|  | 2BO9:A 308 |  | 2BO9:C 308 |  | 2BO9:B 222 |  | 2BO9:D 222 |  |
|---|---|---|---|---|---|---|---|---|
|  | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.8 | 0.9, 0.3 | 0.2 | 0.2, 0.2 | 0.8 | 1.0, 2.5 | 0.7 | 0.8, 1.3 |
| C1 | 0.9 | 0.8, 0.5 | 0.7 | 1.1, 0.1 | 1 | 0.6, 4.0 | 0.7 | 0.9, 1.9 |

|  | 2BBK:H 355 |  | 2BBK:J 355 |  | 2BBK:L 125 |  | 2BBK:M 125 |  |
|---|---|---|---|---|---|---|---|---|
|  | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.9 | 1.2, 0.7 | 1.3 | 1.9, 1.0 | 1.4 | 1.8, 0.7 | 1.4 | 2.1, 1.4 |
| C1 | 1.2 | 1.2, 0.8 | 1.2 | 1.7, 0.9 | 1.1 | 1.5, 0.6 | 2.2 | 3.2, 1.9 |

|  | 1GPQ:A 135 |  | 1GPQ:B 135 |  | 1GPQ:C 129 |  | 1GPQ:D 129 |  |
|---|---|---|---|---|---|---|---|---|
|  | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.9 | 1.4, 1.0 | 1.0 | 1.7, 0.4 | 1.0 | 0.4, 1.4 | 1.1 | 1.0, 2.0 |
| C1 | 0.9 | 1.0, 1.4 | 1.2 | 2.0, 0.5 | 1.2 | 1.0, 1.8 | 1.3 | 1.6, 2.4 |

| | 3V6D:A 556 | | 3V6D:B 428 | | 3V6D:P 21 | | 3V6D:T 27 | |
|---|---|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.7 | 1.0, 1.6 | 0.6 | 1.0, 0.7 | 2.9 | 1.9, 32.6 | 2.2 | 1.7, 8.8 |
| C1 | 1.0 | 1.2, 3.9 | 0.7 | 0.6, 2.4 | 4.0 | 2.0, 70.4 | 3.4 | 1.7, 23.8 |
| C2 | 22.2 | 38.5, 1.1 | 16.1 | 27.9, 1.6 | 19.5 | 32.4, 90.0 | 19.7 | 32.7, 51.2 |

| | 3SFD:A 622 | | 3SFD:B 252 | | 3SFD:C 140 | | 3SFD:D 103 | |
|---|---|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.3 | 0.2, 0.1 | 1.0 | 1.3, 1.9 | 1.6 | 1.9, 1.3 | 1.1 | 1.7, 4.1 |
| C1 | 0.3 | 0.2, 0.1 | 1.0 | 1.3, 1.9 | 1.6 | 1.8, 1.1 | 1.1 | 1.7, 4.1 |

| | 3PDU:A 287 | | 3PDU:B 287 | | 3PDU:C 287 | | 3PDU:D 287 | |
|---|---|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.5 | 0.7, 0.5 | 0.9 | 1.1, 1.2 | 0.7 | 1.2, 0.4 | 0.7 | 1.1, 0.4 |
| C1 | 0.6 | 0.7, 0.7 | 1.2 | 1.6, 2.0 | 0.9 | 1.5, 0.3 | 0.8 | 1.3, 0.5 |

| | 3NVQ:A 590 | | 3NVQ:E 590 | | 3NVQ:B 476 | | 3NVQ:F 476 | |
|---|---|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 0.5 | 0.7, 0.2 | 0.5 | 0.7, 1.3 | 0.3 | 0.2, 0.2 | 0.7 | 0.8, 0.4 |
| C1 | 0.6 | 0.8, 0.4 | 0.8 | 0.7, 1.8 | 0.2 | 0.2, 0.2 | 0.5 | 0.7, 0.2 |

| | 2Y7H:A 464 | | 2Y7H:B 529 | | 2Y7H:C 529 | | 2Y7H:D 20 | | 2Y7H:E 20 | |
|---|---|---|---|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 1.0 | 1.5, 0.7 | 1.1 | 1.4, 1.9 | 0.8 | 1.0, 1.4 | 2.0 | 3.1, 9.7 | 2.0 | 3.0, 10.6 |
| C1 | 1.5 | 2.6, 1.0 | 1.3 | 2.0, 1.3 | 0.7 | 1.1, 1.2 | 3.1 | 3.4, 17.5 | 3.1 | 2.7, 14.2 |

|  | 1SUV:A<br>639 |  | 1SUV:B<br>639 |  | 1SUV:C<br>329 |  | 1SUV:D<br>329 |  | 1SUV:E<br>345 |  | 1SUV:F<br>345 |  |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
|  | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 2.9 | 4.9, 0.6 | 2.8 | 4.8, 0.1 | 3.3 | 5.6, 0.6 | 3.4 | 5.8, 0.5 | 2.9 | 5.0, 0.2 | 3.0 | 5.2, 0.1 |
| C1 | 2.9 | 4.9, 0.6 | 3 | 5.2, 0.1 | 3.3 | 5.6, 0.6 | 3.4 | 5.8, 0.5 | 2.9 | 5.0, 0.2 | 3.0 | 5.2, 0.1 |

|  | 1Z5S:A<br>156 |  | 1Z5S:B<br>82 |  | 1Z5S:C<br>172 |  | 1Z5S:D<br>83 |  |
|---|---|---|---|---|---|---|---|---|
|  | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 1.0 | 1.6, 1.0 | 12.0 | 1.2, 171.0 | 0.7 | 0.9, 0.7 | 1.4 | 2.3, 1.4 |
| C1 | 1.3 | 2.0, 1.7 | 12.3 | 2.2, 178.9 | 1.0 | 1.4, 0.9 | 1.3 | 1.9, 4.1 |

|  | 3LU0:A<br>329 |  | 3LU0:B<br>329 |  | 3LU0:C<br>1342 |  | 3LU0:D<br>1407 |  | 3LU0:E<br>91 |  |
|---|---|---|---|---|---|---|---|---|---|---|
|  | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 10.1 | 10.2, 35.5 | 9.6 | 7.5, 30.5 | 4.8 | 3.6, 1.1 | 2.6 | 3.1, 0.3 | 5.5 | 7.4, 20.7 |
| C1 | 10.3 | 10.9, 33.7 | 9.8 | 7.3, 24.1 | 4.2 | 3.2, 0.8 | 2.8 | 3.1, 0.4 | 11.3 | 13.5, 34.6 |
| C2 | 9.9 | 11.0, 30.3 | 27.3 | 21.2, 50.4 | 5.5 | 3.2, 1.6 | 2.3 | 3.5, 0.3 | 43.5 | 72.6, 151.7 |

|  | 1MDA:A<br>103 |  | 1MDA:B<br>103 |  | 1MDA:H<br>368 |  | 1MDA:J<br>368 |  | 1MDA:L<br>121 |  | 1MDA:M<br>121 |  |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
|  | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 10.3 | 2.0, 178.4 | 10 | 3.1, 172.0 | 1.4 | 2.2, 0.4 | 2.1 | 2.7, 2.5 | 2.4 | 0.8, 2.3 | 1.7 | 2.3, 2.8 |
| C1 | 10.4 | 3.6, 176.1 | 1.8 | 2.4, 1.2 | 1.9 | 2.8, 1.4 | 2.1 | 3.4, 0.3 | 2.0 | 3.4, 3.0 | 9.4 | 4.0, 174.0 |

| | 3PUV:A 381 | | 3PUV:B 381 | | 3PUV:E 378 | | 3PUV:F 514 | | 3PUV:G 296 | |
|---|---|---|---|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 15.7 | 17.3, 14.6 | 24.7 | 16.9, 134.1 | 0.6 | 0.7, 1.9 | 1.3 | 1.7, 1.2 | 1.3 | 2.1, 0.4 |
| C1 | 16.1 | 17.6, 17.7 | 25.1 | 18.1, 136.7 | 1.1 | 0.9, 2.7 | 1.7 | 2.0, 0.7 | 1.5 | 2.2, 1.4 |

| | 1TYQ:A 418 | | 1TYQ:B 394 | | 1TYQ:C 372 | | 1TYQ:D 300 | | 1TYQ:E 178 | | 1TYQ:F 168 | | 1TYQ:G 151 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 1.0 | 0.7, 3.8 | 3.1 | 2.6, 4.9 | 1.2 | 0.6, 2.3 | 21.0 | 7.7, 144.5 | 14.7 | 1.6, 175.7 | 12.1 | 14.1, 154.7 | 2.4 | 2.9, 5.0 |
| C1 | 0.9 | 1.0, 0.9 | 3.6 | 3.3, 5.4 | 1.1 | 1.2, 1.2 | 21.3 | 7.9, 144.8 | 14.9 | 1.5, 178.4 | 13.1 | 16.0, 154.5 | 2.6 | 3.4, 8.1 |
| C2 | 28.3 | 36.0, 147.4 | 3.3 | 2.7, 5.3 | 1.4 | 1.0, 2.7 | 32.2 | 49.0, 140.7 | 0.6 | 0.6, 1.0 | 10.2 | 12.4, 30.6 | 3.3 | 4.7, 9.7 |
| C3 | 28.5 | 36.5, 148.6 | 1.6 | 2.3, 3.6 | 0.8 | 1.0, 1.0 | 31.9 | 48.9, 141.0 | 1.0 | 1.5, 0.4 | 10.1 | 12.8, 30.5 | 3.0 | 2.9, 10.8 |

**Table S1: Detailed results of the benchmark.** Rmsd (in Ångstrom) and Placement scores (PS, in Ångstrom and angular degrees) of every subunit for the best-rmsd model and the best scoring model of each structural cluster. By construction, cluster C1 contains the absolute best scoring model, whose properties are reported in **Table 2**. Each column is titled with the PDB code, chain id, and number of residues. For instance, 2B09:A 308 refers to chain A of PDB id 2B09, which is composed of 308 residues.

| rank | rank | rmsd [Å] | p(10) | CC | PS [Å,°] |
|---|---|---|---|---|---|
| best rsmd | 99 | 8.6 | 0.98 | 0.85 | 4.4, 18.2 |
| C1 | 0 | 9 | 0.98 | 0.85 | 5.4, 18.1 |
| C2 | 1 | 30.9 | 0.53 | 0.82 | 5.2, 103.3 |
| C3 | 84 | 25 | 0.55 | 0.82 | 5.3, 94 |

| | groEL-trans (524) | | groEL-cis (524) | | groES (97) | |
|---|---|---|---|---|---|---|
| | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] | rmsd [Å] | PS [Å,°] |
| best rsmd | 4.4 | 2.9, 0.3 | 9 | 5.7, 11.8 | 18.3 | 4.8, 148.9 |
| C1 | 6.2 | 5.6, 2.9 | 9.1 | 4.6, 12.4 | 17.4 | 7.9, 130.7 |
| C2 | 43.2 | 2.9, 177.5 | 11.1 | 6.4, 19.7 | 21.8 | 10.6, 153.3 |
| C3 | 33.4 | 3.1, 178.6 | 13.3 | 5.4, 19.7 | 20.4 | 16.3, 38.3 |

**Table S2: Results for the GroEL/GroES modeling.** (Top) Rmsd (in Ångstrom) Placement scores (PS, in Ångstrom and angular degrees) p(10) and cross-correlation (CC) for the best-rmsd structure, and the best scoring structures of clusters C1, C2 and C3. (Bottom) rmsd and PS contributions for the three subunits.

| | | rmsd [Å] | | | | PS [Å,°] | | | |
|---|---|---|---|---|---|---|---|---|---|
| | Reference | Total | GroEL-cis | GroEL-trans | GroES | Total | GroEL-cis | GroEL-trans | GroES |
| This Work | | 9.0 | 9.1 | 6.2 | 17.4 | 5.4, 18.1 | 4.6, 12.4 | 5.6, 2.9 | 7.9, 130.7 |
| gmfit | Kawabata 2008 | 14.7 | | | | | | | |
| Attract-EM[1] | de Vries 2012 | 11.1 | 5.7 | 12.7 | 19.7 | | | | |
| IQP[2] | Zhang 2010 | (best) 8.6 | | | | 5.7,17.7 | | | |
| MultiFit[3] | Lasker 2009 | | | | | 11.0,84 | | | |
| ISD | Habeck 2017 | | 3.5 (both GroEL rings) | | 2.0-20.0[4] | | | | |
| y-TEMPy[5] | Pandurangan 2015 | | | 11.7 | | | | 8.9,21.0 | |
| PowerFit | Zundert 2015 | | 3.8-7.3 | 2.9-5.5 | 4.2-4.6 | | | | |
| gEMfitter | Hoang 2013 | | 4.0-4.5 | 2.5-2.8 | 5.3-6.1 | | | | |
| COLORES[6] | Chacon 2002 | Failed | | | | | | | |
| ADP_EM | Garzon 2006 | | <1.3 (both GroEL rings) | | Failed | | | | |
| Segger | Pintilie 2012 | | 5.07 | 3.06 | 6.03 | | | | |

**Table S3: Comparison of GroEL/ES modeling with other software.** Rmsd (in Ångstrom) and Placement scores (PS, in Ångstrom and angular degrees) for the whole complex (Total) or its subunits.

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[1] Before refinement.

[2] Fit into a manual segmentation of GroEL-trans ring. Only best-rmsd is reported.

[3] Fine grained search.

[4] GroES was found to have two clusters with similar scores.

[5] Only GroEL-trans fitted.

[6] In the gEMfitter article it is reported that COLORES was not able to model the heptameric double-ring by fitting GroEL-cis and -trans separately.