

Summary of integrative structure determination of Integrative spatiotemporal modeling of biomolecular processes: application to the assembly of the Nuclear Pore Complex (PDB ID: 9A8T)

1. Model Composition	
<p>Entry composition</p>	<ul style="list-style-type: none"> - Nup133_spoke_1_yc_inner_cr: chain(s) A, J, S, AB, BK, BT, CC, CL, DU, ED, EM, EV, GE, GN, GW, HF, IO, IX, JG, JP, KY, LH, LQ, LZ, NI, NR, OA, OJ, PS, QB, QK, QT (639 residues) - Nup93_spoke_1_ir_core_1: chain(s) AK, AN, AQ, AT, CU, CX, DA, DD, FE, FH, FK, FN, HO, HR, HU, HX, JY, KB, KE, KH, MI, ML, MO, MR, OS, OV, OY, PB, RC, RF, RI, RL (815 residues) - Nup205_spoke_1_ir_core_1: chain(s) AL, AR, CV, DB, FF, FL, HP, HV, JZ, KF, MJ, MP, OT, OZ, RD, RJ (1684 residues) - Nup155_spoke_1_ir_core_1: chain(s) AM, AP, AS, AV, BI, BJ, CW, CZ, DC, DF, DS, DT, FG, FJ, FM, FP, GC, GD, HQ, HT, HW, HZ, IM, IN, KA, KD, KG, KJ, KW, KX, MK, MN, MQ, MT, NG, NH, OU, OX, PA, PD, PQ, PR, RE, RH, RK, RN, SA, SB (1356 residues) - Nup188_spoke_1_ir_core_2: chain(s) AO, AU, CY, DE, FI, FO, HS, HY, KC, KI, MM, MS, OW, PC, RG, RM (1564 residues) - p54_spoke_1_ir_chan_1: chain(s) AW, AZ, BC, BF, DG, DJ, DM, DP, FQ, FT, FW, FZ, IA, ID, IG, IJ, KK, KN, KQ, KT, MU, MX, NA, ND, PE, PH, PK, PN, RO, RR, RU, RX (366 residues) - p58_spoke_1_ir_chan_1: chain(s) AX, BA, BD, BG, DH, DK, DN, DQ, FR, FU, FX, GA, IB, IE, IH, IK, KL, KO, KR, KU, MV, MY, NB, NE, PF, PI, PL, PO, RP, RS, RV, RY (171 residues) - p62_spoke_1_ir_chan_1: chain(s) AY, BB, BE, BH, DI, DL, DO, DR, FS, FV, FY, GB, IC, IF, II, IL, KM, KP, KS, KV, MW, MZ, NC, NF, PG, PJ, PM, PP, RQ, RT, RW, RZ (169 residues) - Nup107_spoke_1_yc_inner_cr: chain(s) B, K, T, AC, BL, BU, CD, CM, DV, EE, EN, EW, GF, GO, GX, HG, IP, IY, JH, JQ, KZ, LI, LR, MA, NJ, NS, OB, OK, PT, QC, QL, QU (775 residues) - Nup96_spoke_1_yc_inner_cr: chain(s) C, L, U, AD, BM, BV, CE, CN, DW, EF, EO, EX, GG, GP, GY, HH, IQ, IZ, JI, JR, LA, LJ, LS, MB, NK, NT, OC, OL, PU, QD, QM, QV (475 residues) - SEC13_spoke_1_yc_inner_cr: chain(s) D, M, V, AE, BN, BW, CF, CO, DX, EG, EP, EY, GH, GQ, GZ, HI, IR, JA, JJ, JS, LB, LK, LT, MC, NL, NU, OD, OM, PV, QE, QN, QW (291 residues) - SEH1_spoke_1_yc_inner_cr: chain(s) E, N, W, AF, BO, BX, CG, CP, DY, EH, EQ, EZ, GI, GR, HA, HJ, IS, JB, JK, JT, LC, LL, LU, MD, NM, NV, OE, ON, PW, QF, QO, QX (322 residues) - Nup85_spoke_1_yc_inner_cr: chain(s) F, O, X, AG, BP, BY, CH, CQ, DZ, EI, ER, FA, GJ, GS, HB, HK, IT, JC, JL, JU, LD, LM, LV, ME, NN, NW, OF, OO, PX, QG, QP, QY (467 residues) - Nup43_spoke_1_yc_inner_cr: chain(s) G, P, Y, AH, BQ, BZ, CI, CR, EA, EJ, ES, FB, GK, GT, HC, HL, IU, JD, JM, JV, LE, LN, LW, MF, NO, NX, OG,

	<p>OP, PY, QH, QQ, QZ (377 residues)</p> <ul style="list-style-type: none"> - Nup160_spoke_1_yc_inner_cr: chain(s) H, Q, Z, AI, BR, CA, CJ, CS, EB, EK, ET, FC, GL, GU, HD, HM, IV, JE, JN, JW, LF, LO, LX, MG, NP, NY, OH, OQ, PZ, QI, QR, RA (1161 residues) - Nup37_spoke_1_yc_inner_cr: chain(s) I, R, AA, AJ, BS, CB, CK, CT, EC, EL, EU, FD, GM, GV, HE, HN, IW, JF, JO, JX, LG, LP, LY, MH, NQ, NZ, OI, OR, QA, QJ, QS, RB (318 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - 3DEM volume, Zenodo: 10.5281/zenodo.11129725 - 3DEM volume, Zenodo: 10.5281/zenodo.11129725 - 3DEM volume, Zenodo: 10.5281/zenodo.11129725 - 3DEM volume, Zenodo: 10.5281/zenodo.11129725 - 3DEM volume, Zenodo: 10.5281/zenodo.11129725 - 3DEM volume, Zenodo: 10.5281/zenodo.11129725 - Other, Zenodo: 10.5281/zenodo.11129725 - 3DEM volume, EMDB: EMD-3820 - Other, Other: idr0115 - Experimental model, PDB: 5a9q - Experimental model, PDB: 5ijo
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
Number of <i>rigid</i> and <i>flexible</i> segments	496, 0
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 6 unique EM3DRestraint: None
4. Validation	
Number of ensembles	6
Number of models in ensembles	1121, 881, 801, 801, 1121, 801
Number of deposited models	6
Model precision (uncertainty of models)	<ul style="list-style-type: none"> - 232.55, Å - 144.08, Å - 104.58, Å - 99.89, Å - 100.83, Å - 104.26, Å

<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.94-99.99%
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Name</i>	Monte Carlo sampling step 1. Repeated for each snapshot model.
<i>Method</i>	MC sampling
<i>Number of computed models</i>	1600000
2. <i>Name</i>	Choose the lowest scoring structure from each simulation.
<i>Method</i>	Filtering
<i>Number of computed models</i>	200
3. <i>Name</i>	Monte Carlo sampling step 2. Repeated for each snapshot model.
<i>Method</i>	MC sampling
<i>Number of computed models</i>	320000
4. <i>Name</i>	Choose the lowest scoring structure from each simulation.
<i>Method</i>	Filtering
<i>Number of computed models</i>	200
5. <i>Name</i>	Monte Carlo sampling step 3. Repeated for each snapshot model.
<i>Method</i>	MC sampling
<i>Number of computed models</i>	320000
6. <i>Name</i>	Choose the lowest scoring structure from each replica, and further filter by the median score.
<i>Method</i>	Filtering
<i>Number of computed models</i>	801

7. <u>Name</u>	Score trajectories based on the scores of snapshot models and the transitions between them.
8. <u>Name</u>	Monte Carlo sampling step 1. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	1600000
9. <u>Name</u>	Choose the lowest scoring structure from each simulation.
<u>Method</u>	Filtering
<u>Number of computed models</u>	200
10. <u>Name</u>	Monte Carlo sampling step 2. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	320000
11. <u>Name</u>	Choose the lowest scoring structure from each simulation.
<u>Method</u>	Filtering
<u>Number of computed models</u>	200
12. <u>Name</u>	Monte Carlo sampling step 3. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	320000
13. <u>Name</u>	Choose the lowest scoring structure from each replica, and further filter by the median score.
<u>Method</u>	Filtering
<u>Number of computed models</u>	801
14. <u>Name</u>	Score trajectories based on the scores of snapshot models and the transitions between them.
15. <u>Name</u>	Monte Carlo sampling step 1. Repeated for each snapshot model.
<u>Method</u>	MC sampling

<i>Number of computed models</i>	1600000
16. <i>Name</i>	Choose the lowest scoring structure from each simulation.
<i>Method</i>	Filtering
<i>Number of computed models</i>	200
17. <i>Name</i>	Monte Carlo sampling step 2. Repeated for each snapshot model.
<i>Method</i>	MC sampling
<i>Number of computed models</i>	320000
18. <i>Name</i>	Choose the lowest scoring structure from each simulation.
<i>Method</i>	Filtering
<i>Number of computed models</i>	200
19. <i>Name</i>	Monte Carlo sampling step 3. Repeated for each snapshot model.
<i>Method</i>	MC sampling
<i>Number of computed models</i>	320000
20. <i>Name</i>	Choose the lowest scoring structure from each replica, and further filter by the median score.
<i>Method</i>	Filtering
<i>Number of computed models</i>	801
21. <i>Name</i>	Score trajectories based on the scores of snapshot models and the transitions between them.
22. <i>Name</i>	Monte Carlo sampling step 1. Repeated for each snapshot model.
<i>Method</i>	MC sampling
<i>Number of computed models</i>	1600000
23. <i>Name</i>	Choose the lowest scoring structure from each simulation.
<i>Method</i>	Filtering
<i>Number of computed models</i>	200

24. <u>Name</u>	Monte Carlo sampling step 2. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	320000
25. <u>Name</u>	Choose the lowest scoring structure from each simulation.
<u>Method</u>	Filtering
<u>Number of computed models</u>	200
26. <u>Name</u>	Monte Carlo sampling step 3. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	320000
27. <u>Name</u>	Choose the lowest scoring structure from each replica, and further filter by the median score.
<u>Method</u>	Filtering
<u>Number of computed models</u>	801
28. <u>Name</u>	Score trajectories based on the scores of snapshot models and the transitions between them.
29. <u>Name</u>	Monte Carlo sampling step 1. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	1600000
30. <u>Name</u>	Choose the lowest scoring structure from each simulation.
<u>Method</u>	Filtering
<u>Number of computed models</u>	200
31. <u>Name</u>	Monte Carlo sampling step 2. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	320000

32. <u>Name</u>	Choose the lowest scoring structure from each simulation.
<u>Method</u>	Filtering
<u>Number of computed models</u>	200
33. <u>Name</u>	Monte Carlo sampling step 3. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	320000
34. <u>Name</u>	Choose the lowest scoring structure from each replica, and further filter by the median score.
<u>Method</u>	Filtering
<u>Number of computed models</u>	801
35. <u>Name</u>	Score trajectories based on the scores of snapshot models and the transitions between them.
36. <u>Name</u>	Monte Carlo sampling step 1. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	1600000
37. <u>Name</u>	Choose the lowest scoring structure from each simulation.
<u>Method</u>	Filtering
<u>Number of computed models</u>	200
38. <u>Name</u>	Monte Carlo sampling step 2. Repeated for each snapshot model.
<u>Method</u>	MC sampling
<u>Number of computed models</u>	320000
39. <u>Name</u>	Choose the lowest scoring structure from each simulation.
<u>Method</u>	Filtering
<u>Number of computed models</u>	200
40. <u>Name</u>	Monte Carlo sampling step 3. Repeated for each snapshot model.

<i>Method</i>	MC sampling
<i>Number of computed models</i>	320000
41. <i>Name</i>	Choose the lowest scoring structure from each replica, and further filter by the median score.
<i>Method</i>	Filtering
<i>Number of computed models</i>	801
42. <i>Name</i>	Score trajectories based on the scores of snapshot models and the transitions between them.
<i>Software</i>	- gmconvert (version 2022/05/09) - Integrative Modeling Platform (IMP) (version 2.20)