

Atomic accuracy models from 4.5 Å cryo-electron microscopy data with density-guided local rebuilding

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Supplementary Information

Supplementary Table 1. A comparison to previously published methods. For a series of comparative models of 20S, our refinement was compared to two previously developed methods combining Rosetta refinement with experimental density data, comparing the fraction of C α atoms within 1 Å using the same starting models. *DiMaio 2009*¹ as well as *RosettaCM*² augmented with fit-to-density-energy are both outperformed by the *IterativeBuild* method reported here. Results are reported for 20S maps at 3.3 and 4.4Å resolution.

	20S proteasome (3.3Å)			20S proteasome (4.4Å)		
	DiMaio 2009	Rosetta CM	Iterative Build	DiMaio 2009	Rosetta CM	Iterative Build
1yar	0.90	0.96	0.94	0.93	0.94	0.88
3h4p	0.86	0.85	0.93	0.75	0.79	0.81
1iru	0.86	0.90	0.92	0.83	0.83	0.88
3unf	0.77	0.83	0.87	0.67	0.70	0.78
3nzj	0.85	0.86	0.92	0.83	0.78	0.81
1ryp	0.79	0.87	0.92	0.80	0.80	0.87
1q5q	0.61	0.78	0.94	0.61	0.58	0.68
1g0u	0.58	0.62	0.78	0.49	0.50	0.76
4hnz	0.29	0.69	0.79	0.46	0.61	0.68
2x3b	0.42	0.58	0.75	0.41	0.48	0.61
1g3k	0.42	0.63	0.73	0.42	0.45	0.58
1m4y	0.37	0.66	0.78	0.37	0.55	0.72
Average	0.64	0.77	0.86	0.63	0.67	0.76

Supplementary References

- 1 DiMaio, F., Tyka, M. D., Baker, M. L., Chiu, W. & Baker, D. Refinement of protein structures into low-resolution density maps using rosetta. *Journal of molecular biology* **392**, 181-190 (2009).
- 2 Song, Y. *et al.* High-Resolution Comparative Modeling with RosettaCM. *Structure* **21**, 1735-1742 (2013).