

S3 Text: Three additional test cases

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Here, we report three additional test cases extracted from a recent SAXS benchmark¹

- ATG7: Ubiquitin-like modifier-activating enzyme, ATG7 C-terminal domain²
- PYR1P: Abscisic acid receptor PYR1³
- SOD: Superoxide dismutase⁴

References

- Nishimura, Noriyuki, Kenichi Hitomi, Andrew S. Arvai, Robert P. Rambo, Chiharu Hitomi, Sean R. Cutler, Julian I. Schroeder, and Elizabeth D. Getzoff (2009). "Structural Mechanism of Abscisic Acid Binding and Signaling by Dimeric PYR1". In: *Science* 326.5958, pp. 1373–1379. doi: [10.1126/science.1181829](https://doi.org/10.1126/science.1181829) (cit. on p. 1).
- Schneidman-Duhovny, Dina, Michal Hammel, John A. Tainer, and Andrej Sali (2013). "Accurate SAXS Profile Computation and its Assessment by Contrast Variation Experiments". In: *Biophys. J.* 105.4, pp. 962–974. doi: [10.1016/j.bpj.2013.07.020](https://doi.org/10.1016/j.bpj.2013.07.020) (cit. on p. 1).
- Shin, David S., Michael DiDonato, David P. Barondeau, Greg L. Hura, Chiharu Hitomi, J. Andrew Berglund, Elizabeth D. Getzoff, S. Craig Cary, and John A. Tainer (2009). "Superoxide Dismutase from the Eukaryotic Thermophile Alvinella pompejana: Structures, Stability, Mechanism, and Insights into Amyotrophic Lateral Sclerosis". In: *J. Mol. Biol.* 385.5, pp. 1534–1555. doi: [10.1016/j.jmb.2008.11.031](https://doi.org/10.1016/j.jmb.2008.11.031) (cit. on p. 1).
- Taherbhoy, Asad M., Stephen W. Tait, Stephen E. Kaiser, Allison H. Williams, Alan Deng, Amanda Nourse, Michal Hammel, Igor Kurinov, Charles O. Rock, Douglas R. Green, and Brenda A. Schulman (2011). "Atg8 Transfer from Atg7 to Atg3: A Distinctive E1-E2 Architecture and Mechanism in the Autophagy Pathway". In: *Mol. Cell* 44.3, pp. 451–461. doi: [10.1016/j.molcel.2011.08.034](https://doi.org/10.1016/j.molcel.2011.08.034) (cit. on p. 1).

¹Schneidman-Duhovny et al. 2013.

²Taherbhoy et al. 2011.

³Nishimura et al. 2009.

⁴Shin et al. 2009.

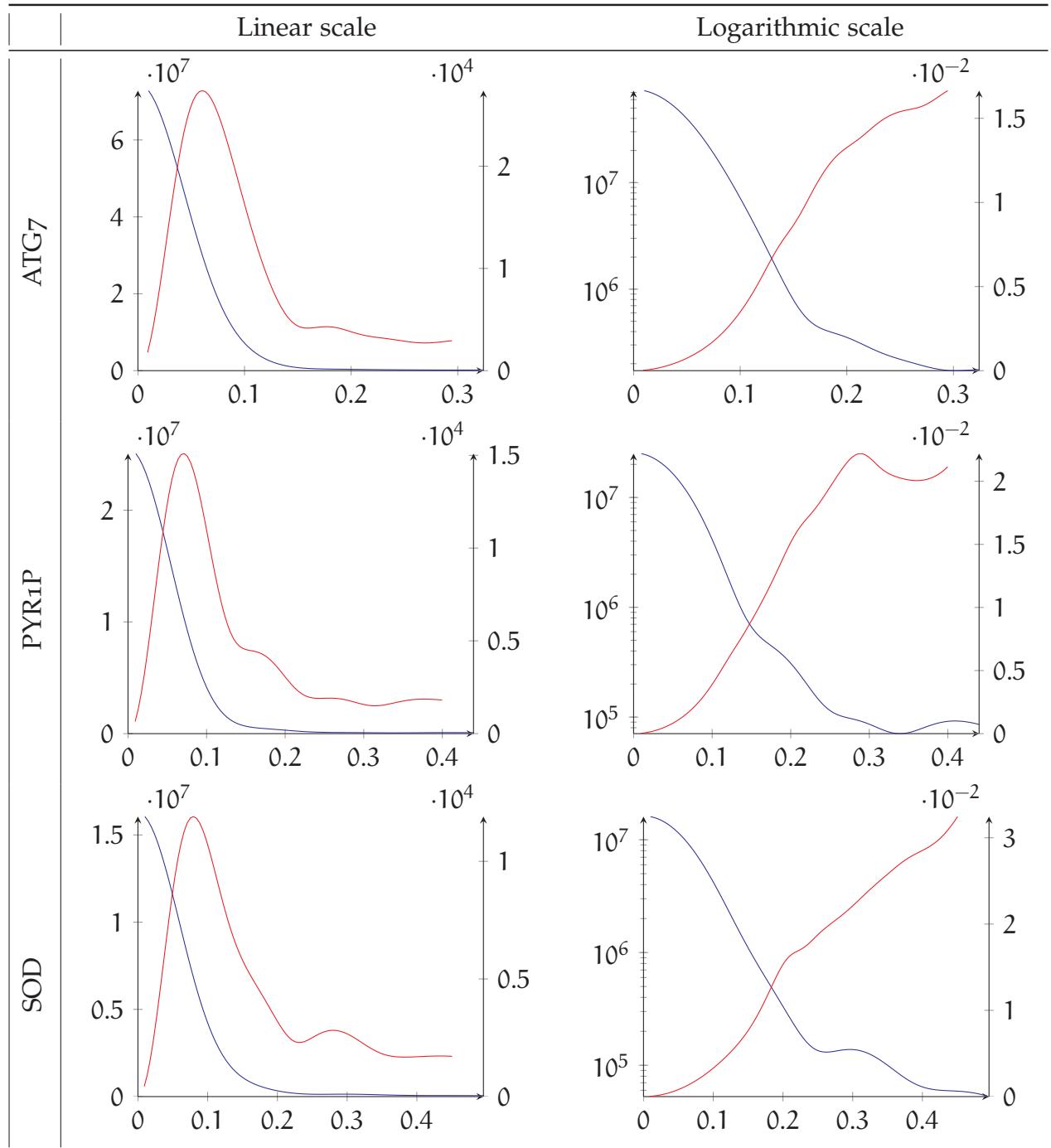


Figure 1: Mean (blue) and standard deviation (red) of the SAXS profile of three different protein systems. X-axis is $q(\text{\AA}^{-1})$. Left y-axis is SAXS intensity (A.U.), right y-axis is standard deviation (left panel, A.U.) or coefficient of variation $V \equiv \sigma/\mu$ (right panel).

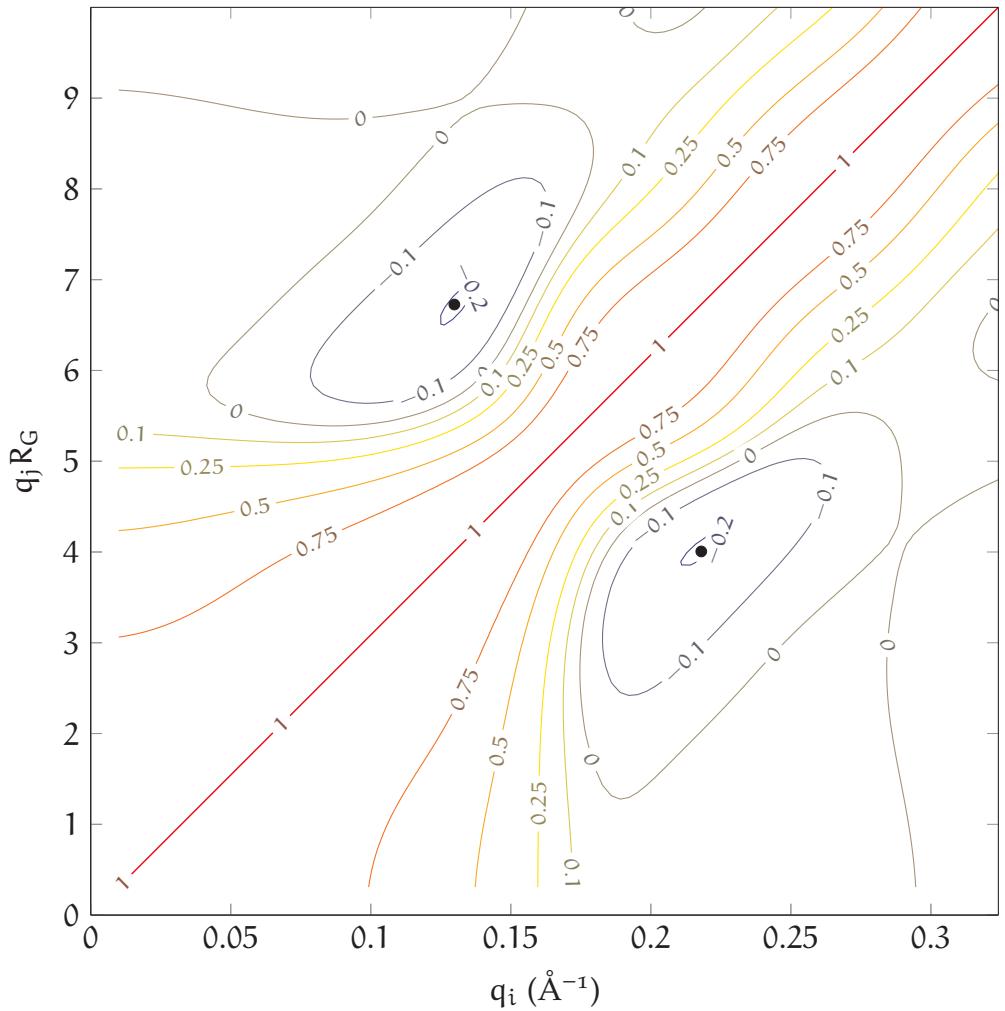


Figure 2: ATG7

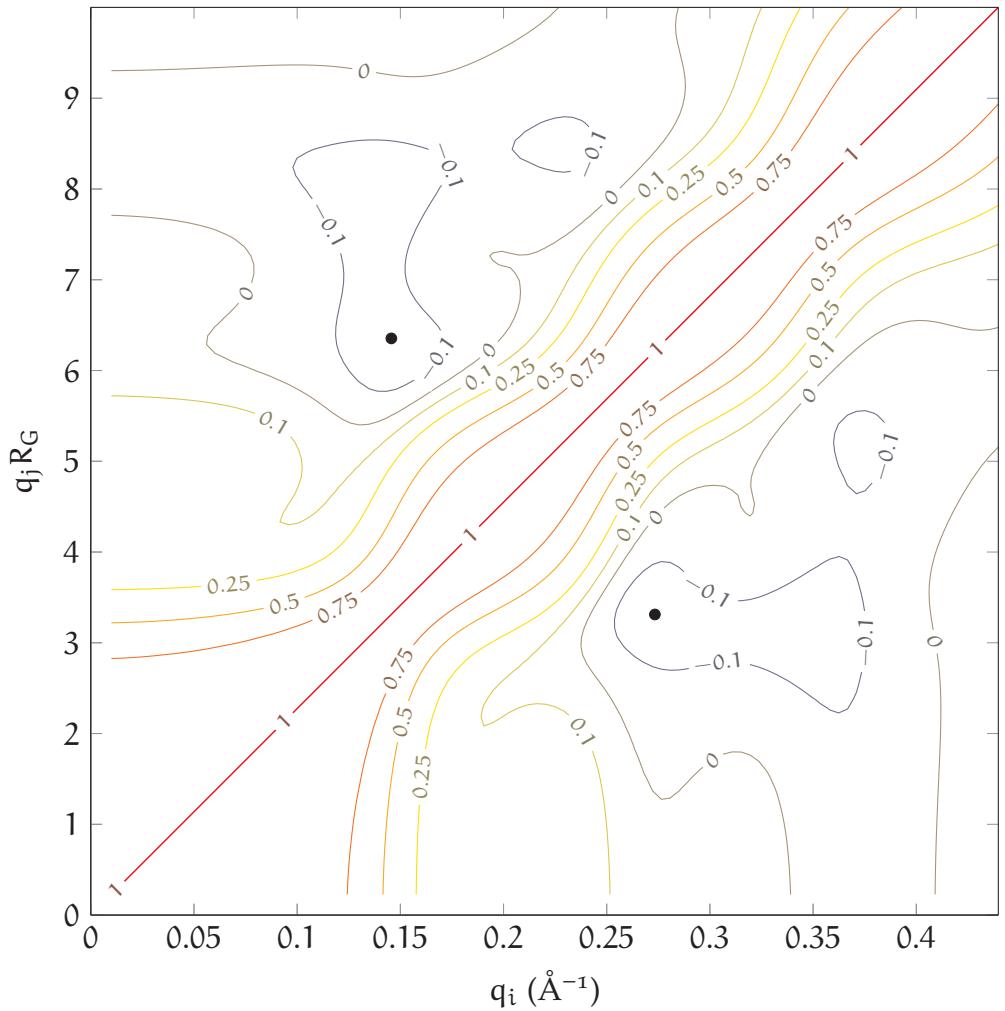


Figure 3: PYR1P

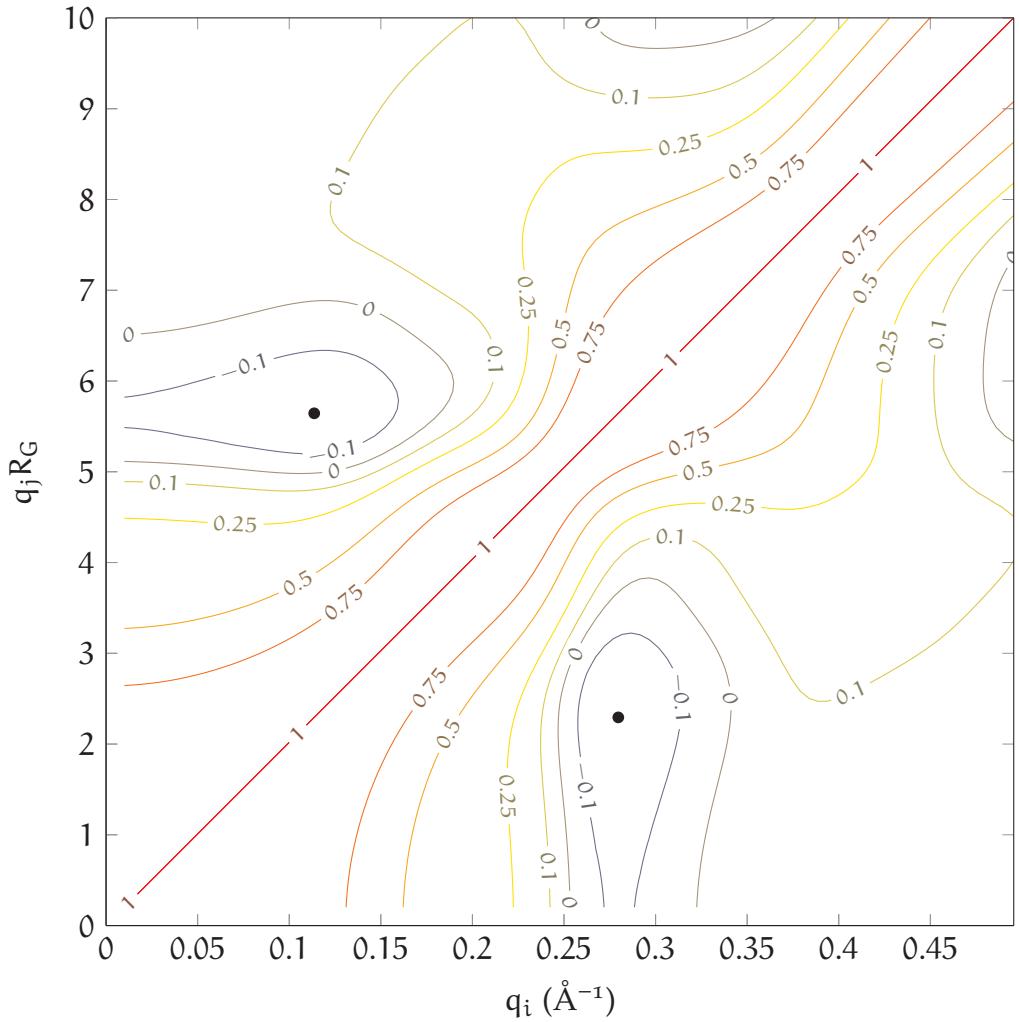


Figure 4: *sod*