**Supplementary file 2.** Out-of-plane distortions in the PbRC protein environment of the dark structure for dataset b (Å).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **saddling** | **ruffling** | **doming** | **waving** |  | **propellering** |
|  | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| PL | 0.11 | -0.68 | -0.05 | -0.03 | 0.11 | -0.18 |
| PM | -0.08 | -0.91 | -0.10 | 0.01 | 0.22 | -0.28 |
| BL | -0.10 | 0.14 | -0.02 | 0.19 | 0.12 | 0.06 |
| BM | -0.09 | 0.05 | 0.04 | 0.14 | 0.10 | 0.09 |
| HL | 0.13 | 0.35 | -0.13 | 0.07 | 0.09 | 0.20 |
| HM | 0.08 | 0.57 | -0.11 | 0.16 | 0.20 | 0.32 |