**Supplementary file 1.** Out-of-plane distortions in the PbRC protein environment of the dark structure for dataset a (Å).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **saddling** | **ruffling** | **doming** | **waving** |  | **propellering** |
|  | **B2u** | **B1u** | **A2u** | **Eg(x)** | **Eg(y)** | **A1u** |
| PL | 0.10 | -0.63 | -0.06 | -0.01 | 0.12 | -0.15 |
| PM | -0.02 | -0.94 | -0.08 | 0.01 | 0.26 | -0.28 |
| BL | -0.13 | 0.16 | -0.07 | 0.20 | 0.10 | 0.10 |
| BM | -0.18 | -0.03 | 0.10 | 0.13 | 0.04 | 0.13 |
| HL | 0.07 | 0.28 | -0.05 | 0.11 | 0.12 | 0.18 |
| HM | 0.02 | 0.69 | -0.04 | 0.14 | 0.22 | 0.37 |