Comparison of B-factors for cluster modeled as exclusively FeS vs FeSe forms.

|  |  |  |  |
| --- | --- | --- | --- |
| All S Cluster Form | | All Se Cluster Form | |
| Rwork | 16.87 | Rwork | 16.75 |
| Rfree | 19.28 | Rfree | 19.02 |
| Atom | **B-factor** | **Atom** | **B-factor** |
| S3 | 11.07 | Se3 | 19.90 |
| S4 | 11.40 | Se4 | 20.18 |
| Fe1 | 16.02 | Fe1 | 15.53 |
| Fe2 | 16.41 | Fe2 | 15.89 |