The term $R$ factor in crystallography is commonly taken to refer to the 'conventional' $R$ factor

$$R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum |F_{\text{obs}}|},$$

a measure of agreement between the amplitudes of the structure factors calculated from a crystallographic model and those from the original X-ray diffraction data. The $R$ factor is calculated during each cycle of least-squares structure refinement to assess progress. The final $R$ factor is one measure of model quality.

More generally, a variety of $R$ factors may be determined to measure analogous residuals during least-squares optimization procedures. Where the refinement attempts to minimize the deviates of the squares of the structure factors (refinement against $F^2$), the $R$ factor based on $F^2$ is used to monitor the progress of refinement:

$$R(F^2) = \frac{\sum |F_{\text{obs}}^2 - F_{\text{calc}}^2|}{\sum |F_{\text{obs}}^2|}.$$

Likewise, refinement against $I$ can be tracked using the Bragg $R$ factor

$$R_B = \frac{\sum |I_{\text{obs}} - I_{\text{calc}}|}{\sum |I_{\text{obs}}|}.$$

Even for refinement against $F^2$ or $I$, the 'conventional' $R$ factor may be calculated and quoted as a measure of model quality, in order to compare the resulting quality of models calculated at different times and with different refinement strategies.

The $R$ factor is sometimes described as the discrepancy index.

---

**$R$ factor as a measure of structure quality**

Theoretical values of $R$ range from zero (perfect agreement of calculated and observed intensities) to about 0.6 for a set of measured intensities compared against a set of random intensities. $R$ factors greater than 0.5 indicate very poor agreement between observed and calculated intensities, and many models with

$$R \geq 0.5$$

will not respond to attempts at improvement. An early model with

$$R \leq 0.4$$

can usually be improved during refinement. A desirable target $R$ factor for a protein model refined with data to 2.5 Å is considered to be

$$\sim 0.2$$

. Small organic molecules commonly refine to $R < 0.05$. However, the $R$ factor must always be treated with caution, as an
indicator of precision and not accuracy. Partially incorrect structures have been reported with \( R \) values below 0.1; many imprecise but essentially correct structures have been reported with higher \( R \) values.

---

**Weighted \( R \) factors**

In practice, *weighted* \( R \) factors are more often used to track least-squares refinement, since the functions minimized are weighted according to estimates of the precision of the measured quantity \( Y \):

\[
\sum w (Y_o - Y_c)^2
\]

(\( Y \) being \( F, F^2 \) or \( I \)). The general term for a weighted residual is

\[
wR = \left( \frac{\sum w|Y_o - Y_c|^2}{\sum wY_o^2} \right)^{1/2}
\]

The sum is usually computed over all reflections measured in the experiment. However, occasionally reflections are omitted from the calculation, either because they are believed to result from a systematic experimental error or are recorded with an intensity small compared with background noise. Any such selection may introduce statistical artifacts, and must always be described when reporting \( R \) factors.

---

**Contributors**

- [Online Dictionary of Crystallography](https://www.cryst.ehu.es)