Outline of a Typical Crystal Structure Report

**data collection**
- source of sample and conditions of crystallization
- habit, color, and dimensions of crystal
- formula and formula weight
- unit cell parameters and volume with esds; number of data and $\theta$ range used to determine cell parameters
- crystal type and space group
- $Z$, density, and linear absorption coefficient
- instrument and temperature of data collection and cell parameter determination
- # of data collected, unique [R(int)]
- absorption correction details

**structure solution**
method and program used for structure solution

**structure refinement**
- method and program for refinement
- # of data refined, # restraints, # parameters
- weighting scheme
- $R_1$(observed data), $wR_2$(all data), and $S$ values
- final maximum shift/error
- final maximum and minimum of difference electron density map

**tables and figures**
- positional parameters and isotropic or equivalent displacement parameters
- bond distances and angles
- anisotropic displacement parameters
- structure factor tables (often required for review but discarded by the journal)
- torsion angles (optional)
- least-squares planes (optional)
- hydrogen bond geometry (optional)
- labeled figure showing the displacement ellipsoids
- packing diagram showing relevant IM interactions

Summary

Outline of a Typical Crystal Structure Report

- data collection
- structure solution
- structure refinement
- tables and figures