Transmittal Checklist for Acta C Papers

Title
Name correct w.r.t. charges and moieties
Check also solvents and stoichiometry
Clear and informative

Abstract
Formula given if not in title
Any imposed symmetry described
Main findings of study summarised
Comprehensible on its own
No “flannel” or “padding”

Comment
No duplication with entries in Tables
No included data would be better in a Table
No use of parentheses in atom labels
No “flannel” or “padding”

Crystal Data
Molecular weight, etc, includes all H atoms
Proportionate s.u.’s on cell dimensions
Crystal shape matches dimensions
Correct temperature given (in K)
Formula matches chemical and crystallographic diagrams
Data resolution and completeness adequate
Enough reflections for lattice refinement

Experimental
Adequate synthetic details
Adequate description of crystal growth
Computer programs correct and referenced

Refinement
Correct placement of H atoms
Location of H atoms adequately described
H atom restraints and constraints given
Consistent treatment of H atoms
Transmission factors not calculated values
Extinction correction refined and significant
Absolute structure details
Number of Friedels given
Friedels merged if no real anomalous effects
Special features described
Routine features deposited
SHELXL-97 used, not SHELXL-93

References
Correspondence with entries in text
All computer programs included
Reference format correct
Number of self-references acceptable

Diagrams
Appropriate content
Atoms are a connected set
Good orientation
Figure matches fractional coordinates
Correct hand shown in diagram and Scheme
Unambiguous labels
Crystal and chemical numbering match
Simplest atom labels used
No use of parentheses in atom labels
Labels must not overlap atoms or bonds
Appropriate ellipsoid level chosen
Ellipsoid probability level in caption
Caption described any atoms omitted
Ellipsoid sizes match temperature given
Packing diagrams show cell axes
Packing diagrams adequately labelled
Only relevant H atoms in packing diagrams
Scheme shows all moieties
Orientations of Scheme and Figure match
Chemical diagram suitable for Contents

Tables
Good ordering of atoms in coordinate tables
Do coordinates lie in the basic unit cell?
Agreement for equivalent parameters
Similar parameters have similar s.u.’s
Geometry parameters lie in expected ranges
Appropriate precision for parameters
Full geometry (bonds and angles) in CIF?
Good selection of geometry parameters
No missing parameters such as torsions
No duplication of geometry parameters
No duplication with entries in text
Sensible ordering of geometry parameters
H-bonding parameters if required
Sensible H-bonding geometry
H bonds correctly characterised
Correct (or no) s.u.’s for H-bonding