Structure Validation

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Structure Validation

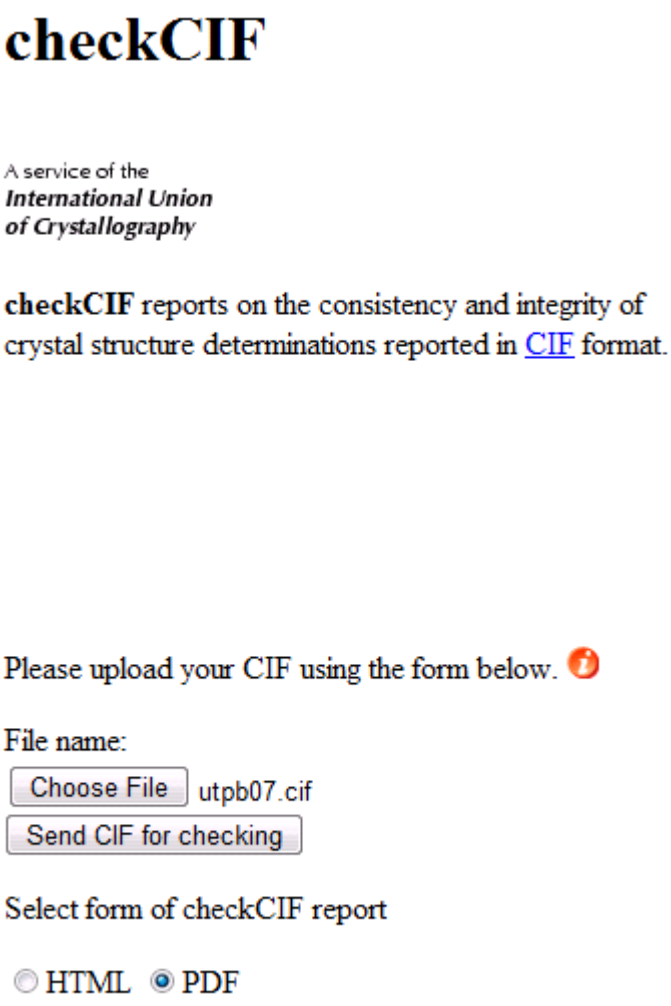
✓Is the unit cell/lattice correct?
✓Is the space group correct?
✓Is the structure correct?

The warning signs

•The Unit Cell
–Relationships in lattice parameters
•e.g. a = b a = b probably centered cell
•Unpopular space group
–The most popular space groups
•5 space groups (P-1, $P2_1$, $P2_1/c$, C2/c and $P2_12_12_1$) account for over 75% of all structures.
•Two (or more) molecules in the asymmetric unit.

IUCR CheckCIF

http://checkcif.iucr.org/



checkCIF

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No syntax errors have been found. A PDF version of the **checkCIF** report may be downloaded from the link that will appear below shortly.

Download checkCIF report

Example Alert

```
Alert level C
PLAT342 ALERT 3 C Low Bond Precision on  C-C Bonds (x 1000) Ang ..          9
```

PLAT342

PLAT342 Type_3 Check Bond Precision for C-C in Structures (Z(max) > 39)

```
The average su for X-Y bonds is tested (named bond-precision). X-Y will
generally be C-C bonds, unless there are none. In the last case the su's of
the lowest element numbers are considered (excluding hydrogen). There are
three test ranges: one for structures with the largest element Z < 20, one
for the largest Z in the range 20 to 39 and one for structures with Z(max) 40
or higher (_340, _341 and _342 respectively)
```

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Common Alert A.

```
The following ALERTS were generated. Each ALERT has the format
       test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
```

```
Alert level A
DENSX01 ALERT 1 A  The ratio of the calculated to measured crystal density
           lies outside the range 0.80 <> 1.20
           Calculated density =      1.766
           Measured density   =      0.000
```

D = 0?
Replace 0 with ?

_exptl_crystal_size_max	0.32
_exptl_crystal_size_mid	0.17
_exptl_crystal_size_min	0.13
_exptl_crystal_density_meas	0
_exptl_crystal_density_diffrn	1.766