# checkCIF/PLATON report (full structural check)

No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

## Datablock: I

Bond precision: C-C = 0.0160 A Wavelength=0.71073
Cell: a=8.304(2) b=5.534(1) c=8.237(2)
alpha=90 beta=111.36(3) gamma=90

| | Calculated | Reported |
|---|---|---|
| Volume | 352.53(15) | 352.52(15) |
| Space group | P c | P c |
| Hall group | P -2yc | P -2yc |
| Moiety formula | C6 H7 N O2 S | C6 H7 N O2 S |
| Sum formula | C6 H7 N O2 S | C6 H7 N O2 S |
| Mr | 157.20 | 157.19 |
| Dx,g cm-3 | 1.481 | 1.481 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.391 | 0.391 |
| F000 | 164.0 | 164.0 |
| F000' | 164.32 | |
| h,k,lmax | 10,6,10 | 10,6,10 |
| Nref | 668( 1330) | 1003 |
| Tmin,Tmax | 0.816,0.965 | 0.812,0.956 |
| Tmin' | 0.816 | |

Correction method= AbsCorr=ANALYTICAL
Data completeness= 1.50(0.75) Theta(max)= 25.660
R(reflections)= 0.0739( 621) wR2(reflections)= 0.2598( 1003)
S = 1.006 Npar= 93

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 B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds (x 1000) Ang ... 16

### Alert level C

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.260
PLAT032_ALERT_4_C Std. Uncertainty in Flack Parameter too High ... 0.30
PLAT084_ALERT_2_C High R2 Value ..... 0.26
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for S1
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist. C1 -C6 1.37 Ang.

### Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
correct. If it is not, please give the correct count in the
_publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 25.66
From the CIF: _reflns_number_total 1003
Count of symmetry unique reflns 668
Completeness (_total/calc) 150.15%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 335
Fraction of Friedel pairs measured 0.501
Are heavy atom types Z>Si present yes
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints ..... 5

0 **ALERT level A** = In general: serious problem
1 **ALERT level B** = Potentially serious problem
5 **ALERT level C** = Check and explain
2 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

**Publication of your CIF**

A full structural check has been run on your CIF. This includes checks on:

- CIF syntax and construction
- Cell and geometry details
- Space-group symmetry
- Anisotropic displacement parameters

These full checks give an indication of potential problems with your CIF. Please note that if you intend to submit your CIF for publication in Acta Crystallographica Section C or E, you must make sure that full publication checks are run on the final version of the CIF prior to submission.

If you intend to submit to another section of Acta Crystallographica, Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least basic structural checks are run on the final version of your CIF prior to submission.

To submit your CIF for publication in an IUCr journal click here.

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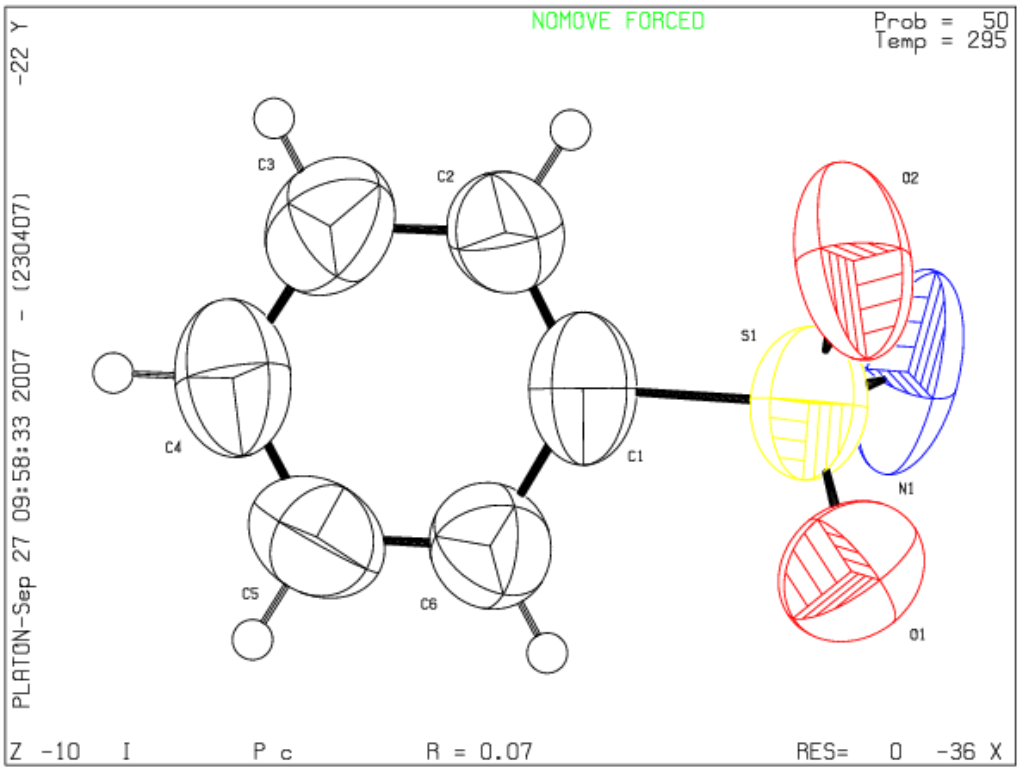
**PLATON version of 23/04/2007; check.def file version of 23/04/2007**

# **Datablock I** - ellipsoid plot

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Test a new CIF entry