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 = 0.0038 A Wavelength=0.71073
Cell: a=11.7604(4) b=14.9847(7) c=15.1844(8)
alpha=90 beta=90 gamma=90

	Calculated	Reported
Volume	2675.9(2)	2675.9(2)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C13 H16 N2 O3 S	C13 H16 N2 O3 S
Sum formula	C13 H16 N2 O3 S	C13 H16 N2 O3 S
Mr	280.35	280.34
Dx,g cm-3	1.392	1.392
Z	8	8
Mu (mm-1)	0.248	0.248
F000	1184.0	1184.0
F000'	1185.50	
h,k,lmax	15,19,19	15,19,19
Nref	3436(6129)	6032
Tmin,Tmax	0.959,0.993	0.944,0.993
Tmin'	0.933	

Correction method= AbsCorr=MULTI-SCAN
Data completeness= 1.76(0.98) Theta(max)= 27.460
R(reflections)= 0.0464(4005) wR2(reflections)= 0.0831(6032)
S = 0.985 Npar= 347

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

PLAT035_ALERT_1_A No _chemical_absolute_configuration info given . ?

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for N32A - C32A .. 5.64 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for O4B - C4B .. 5.35 su

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 27.46
From the CIF: _reflns_number_total 6032
Count of symmetry unique reflns 3436
Completeness (_total/calc) 175.55%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 2596
Fraction of Friedel pairs measured 0.756
Are heavy atom types Z>Si present yes
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C2A ... S
PLAT791_ALERT_1_G Confirm the Absolute Configuration of C2B ... R

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 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

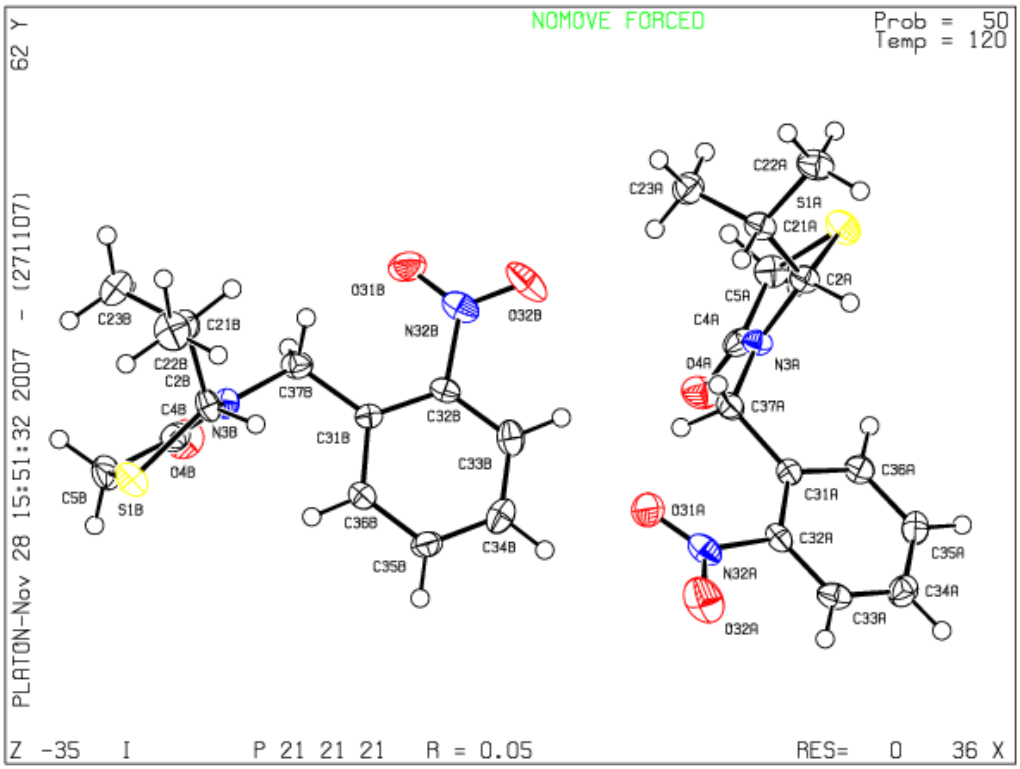
These full checks give an indication of potential problems with your CIF. Please note that if you intend to submit your CIF for publication in Acta Crystallographica Section C or E, you must make sure that full publication checks are run on the final version of the CIF prior to submission.

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.

PLATON version of 27/11/2007; check.def file version of 27/11/2007

Datablock I - ellipsoid plot



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