checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SB1_autored

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: SB1_autored

Bond precision: C-C = 0.0074 A Wavelength=1.54184

Cell: a=22.7557(3) b=10.3435(2) c=8.1124(1)
alpha=90 beta=91.147(1) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1909.06(5)	1909.06(5)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C21 H15 B F2 N2 O2 S	C21 H15 B F2 N2 O2 S
Sum formula	C21 H15 B F2 N2 O2 S	C21 H15 B F2 N2 O2 S
Mr	408.22	408.22
Dx,g cm-3	1.420	1.420
Z	4	4
Mu (mm-1)	1.856	1.856
F000	840.0	840.0
F000'	843.99	
h,k,lmax	28,12,10	28,12,10
Nref	3766[1886]	2958
Tmin,Tmax	0.752,0.757	0.584,1.000
Tmin'	0.657	

Correction method= # Reported T Limits: Tmin=0.584 Tmax=1.000
AbsCorr = MULTI-SCAN

```
Data completeness= 1.57/0.79        Theta(max)= 72.114

R(reflections)= 0.0452( 2731)                    wR2(reflections)=
                                                 0.1234( 2958)
S = 1.129                    Npar= 263
```

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 C

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00743 Ang.
```

Alert level G

```
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 with s.u.       0.02 Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          6 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage         57 %
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         10 Note
              -12   8   4, -12 10   3,   -8   2   6,   -8 10   1,   -6 10   1,   11   5   6,
               12   4   5,   13   5   4,   13   5   5,   14   4   4,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.087 Note
              Predicted wR2: Based on SigI**2  5.91 or SHELX Weight 10.93
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

   2 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
   2 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT340_SB1_autored
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.00743 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

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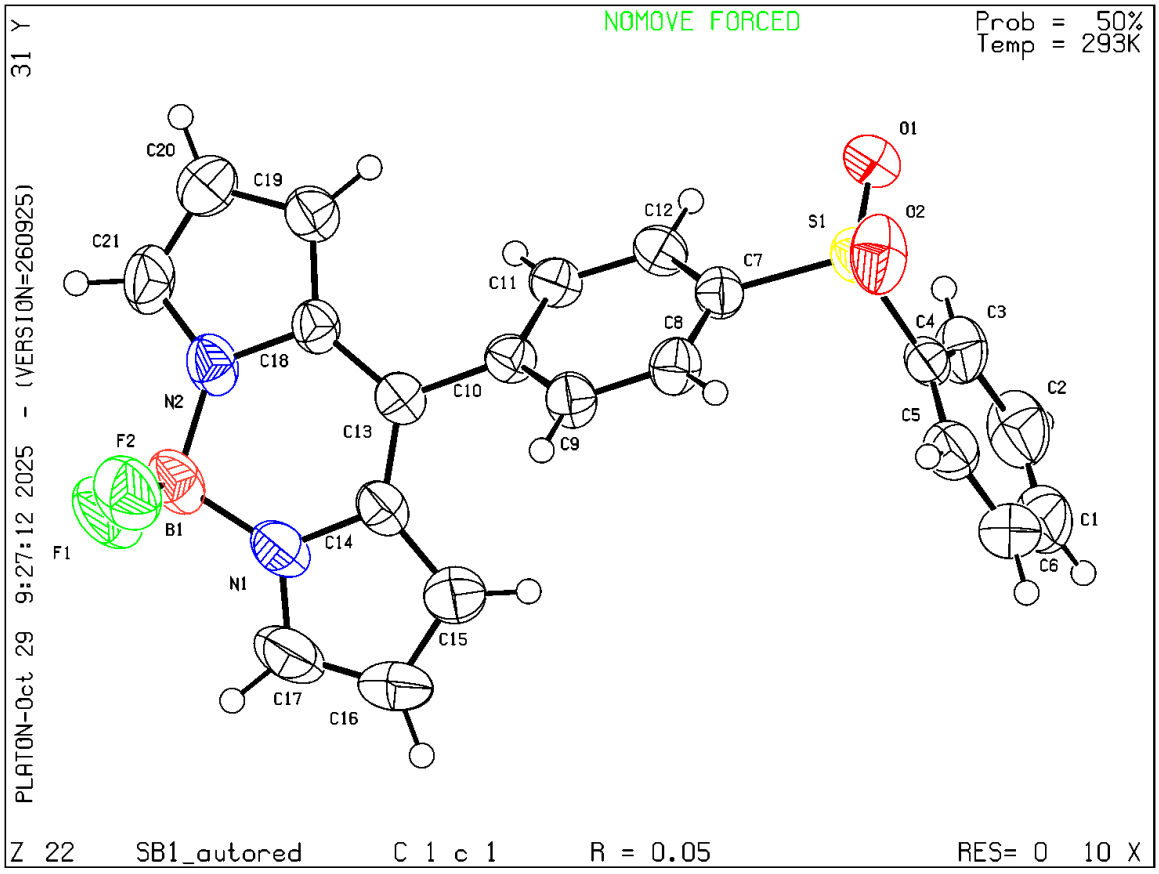
duplicate check

No duplication found

Datablock SB1_autored - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SB2_auto

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: SB2_auto

```
Bond precision:   C-C = 0.0037 A          Wavelength=1.54184

Cell:             a=23.4041(2)     b=10.5262(1)        c=8.3998(1)
                  alpha=90         beta=96.483(1)      gamma=90
Temperature:      293 K

                Calculated                Reported
Volume          2056.11(4)                2056.11(4)
Space group     C c                       C 1 c 1
Hall group      C -2yc                    C -2yc
Moiety formula  C22 H17 B F2 N2 O2 S      C22 H17 B F2 N2 O2 S
Sum formula     C22 H17 B F2 N2 O2 S      C22 H17 B F2 N2 O2 S
Mr              422.25                    422.24
Dx,g cm-3       1.364                     1.364
Z               4                         4
Mu (mm-1)       1.741                     1.741
F000            872.0                     872.0
F000'           876.06
h,k,lmax        28,12,10                  28,12,10
Nref            4046[ 2026]               3168
Tmin,Tmax       0.677,0.718               0.826,1.000
Tmin'           0.606

Correction method= # Reported T Limits: Tmin=0.826 Tmax=1.000
AbsCorr = MULTI-SCAN
```

Data completeness= 1.56/0.78 Theta(max)= 72.028

R(reflections)= 0.0257(3093) wR2(reflections)= 0.0676(3168)

S = 1.018 Npar= 274

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 C

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C21 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT987_ALERT_1_C The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

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Alert level G

PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..... 0.00010 Ang.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder ! Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 1 Note
S01
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage 57 %
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.457 Note
Predicted wR2: Based on SigI**2 1.96 or SHELX Weight 6.64
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

3 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
1 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT241_SB2_auto
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of        C21 Check
RESPONSE: ...
;
_vrf_PLAT242_SB2_auto
```

```
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of         C2 Check
RESPONSE: ...
;
_vrf_PLAT987_SB2_auto
;
PROBLEM: The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

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duplicate check

No duplication found

Datablock SB2_auto - ellipsoid plot