

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0046 Å

Wavelength=0.71073

Cell: a=7.7322(17) b=7.9076(17) c=15.664(3)
 alpha=79.857(3) beta=81.807(2) gamma=74.309(3)
Temperature: 291 K

	Calculated	Reported
Volume	903.1(3)	903.1(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H16 N6 O2 S	C18 H16 N6 O2 S
Sum formula	C18 H16 N6 O2 S	C18 H16 N6 O2 S
Mr	380.44	380.43
Dx, g cm-3	1.399	1.399
Z	2	2
Mu (mm-1)	0.206	0.206
F000	396.0	396.0
F000'	396.39	
h, k, lmax	9, 9, 18	9, 9, 18
Nref	3183	3141
Tmin, Tmax	0.976, 0.984	0.976, 0.984
Tmin'	0.976	

Correction method= MULTI-SCAN

Data completeness= 0.987

Theta(max)= 25.010

R(reflections)= 0.0600(2328)

wR2(reflections)= 0.1805(3141)

S = 1.088

Npar= 245

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for N5 -- C17 .. 10.25 su

Alert level C

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.43 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C17 -- C18 .. 5.36 su

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C16
 PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 5
 PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C17 - C18 ... 1.35 Ang.

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 5 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
 0 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check

Datablock: 2

Bond precision: C-C = 0.0113 A **Wavelength=0.71073**

Cell: a=28.332(6) b=5.7844(14) c=24.118(6)
 alpha=90 beta=95.131(3) gamma=90

Temperature: 291 K

	Calculated	Reported
Volume	3936.7(16)	3936.7(16)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C19 H17 Cl2 N5 S	C19 H17 Cl2 N5 S
Sum formula	C19 H17 Cl2 N5 S	C19 H17 Cl2 N5 S
Mr	418.35	418.34
Dx, g cm-3	1.412	1.412
Z	8	8
Mu (mm-1)	0.450	0.450
F000	1728.0	1728.0
F000'	1731.78	
h, k, lmax	33, 6, 28	33, 6, 28
Nref	3467	3447
Tmin, Tmax	0.956, 0.956	0.932, 0.956
Tmin'	0.956	

Correction method= MULTI-SCAN

Data completeness= 0.994 **Theta(max)= 25.000**

R(reflections)= 0.0890(1135) **wR2(reflections)= 0.1949(3447)**

S = 0.999 **Npar= 246**

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

PLAT026_ALERT_3_B	Ratio Observed / Unique Reflections too Low	33 Perc.
PLAT340_ALERT_3_B	Low Bond Precision on C-C Bonds (x 1000) Ang ..	11

🟢 Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.85
PLAT230_ALERT_2_C	Hirshfeld Test Diff for S1 -- C1 ..	5.55 su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C2 -- C3 ..	6.88 su
PLAT241_ALERT_2_C	Check High Ueq as Compared to Neighbors for	C4
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	C5
PLAT410_ALERT_2_C	Short Intra H...H Contact H12 .. H15A ..	1.92 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Cl2 -- C6 ..	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N1 -- C7 ..	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C1 -- C6 ..	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C3 -- C4 ..	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C5 -- C6 ..	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C18 -- C19 ..	0.18 Ang.

🟠 Alert level G

PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	8
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0 ALERT level A = In general: serious problem

2 ALERT level B = Potentially serious problem

12 ALERT level C = Check and explain

1 ALERT level G = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

6 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

6 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

Datablock: 3

Bond precision: C-C = 0.0038 A

Wavelength=0.71073

Cell: a=7.421(4)

b=12.245(6)

c=20.593(11)

alpha=90

beta=90

gamma=90

Temperature: 291 K

	Calculated	Reported
Volume	1871.3(17)	1871.1(16)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C18 H15 Cl2 N5 S	C18 H15 Cl2 N5 S
Sum formula	C18 H15 Cl2 N5 S	C18 H15 Cl2 N5 S
Mr	404.32	404.31
Dx, g cm-3	1.435	1.435
Z	4	4
Mu (mm-1)	0.471	0.471
F000	832.0	832.0
F000'	833.88	
h, k, lmax	8, 14, 24	8, 14, 24
Nref	1732	1715
Tmin, Tmax	0.945, 0.954	0.946, 0.954
Tmin'	0.945	

Correction method= MULTI-SCAN

Data completeness= 0.990

Theta(max)= 25.000

R(reflections)= 0.0488(929)

wR2(reflections)= 0.1359(1715)

S = 0.946

Npar= 199

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

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	8.62
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for C7	
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for C10	
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for C13	
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for C14	
PLAT245_ALERT_2_C	U(iso) H6A Smaller than U(eq) C16 by ...	0.01 AngSq
PLAT245_ALERT_2_C	U(iso) H6B Smaller than U(eq) C16 by ...	0.01 AngSq

Alert level G

PLAT301_ALERT_3_G	Note: Main Residue Disorder	38.00 Perc.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	24
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!

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

Datablock: 4

Bond precision: C-C = 0.0122 Å

Wavelength=0.71073

Cell: a=8.011(5) b=12.238(7) c=22.350(13)
alpha=90 beta=90 gamma=90
Temperature: 291 K

	Calculated	Reported
Volume	2191(2)	2191(2)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C23 H20 Cl2 N4 S	C23 H20 Cl2 N4 S
Sum formula	C23 H20 Cl2 N4 S	C23 H20 Cl2 N4 S
Mr	455.40	455.39
Dx, g cm ⁻³	1.381	1.380
Z	4	4
Mu (mm ⁻¹)	0.410	0.410
F000	944.0	944.0
F000'	945.93	
h, k, lmax	9, 14, 26	9, 14, 26
Nref	2227[3866]	3838
Tmin, Tmax	0.943, 0.960	0.937, 0.960
Tmin'	0.937	

Correction method= MULTI-SCAN

Data completeness= 1.72/0.99 Theta(max)= 25.010

R(reflections)= 0.0694(1642) wR2(reflections)= 0.1461(3838)

S = 0.909 Npar= 283

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
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Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for N4 -- C15 .. 11.88 su
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds (x 1000) Ang .. 12



Alert level C

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections too Low	43 Perc.
PLAT241_ALERT_2_C	Check High Ueq as Compared to Neighbors for C15	
PLAT241_ALERT_2_C	Check High Ueq as Compared to Neighbors for C22	
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for C18	
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C15 - C16 ...	1.36 Ang.
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond C3 - C4 ...	1.37 Ang.
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond C4 - C5 ...	1.38 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C4 -- C5 ..	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C9 -- C14 ..	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C11 -- C12 ..	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C12 -- C13 ..	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C21 -- C22 ..	0.19 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_reflms_theta_max	25.01
From the CIF: _reflns_number_total	3838
Count of symmetry unique reflns	2227
Completeness (_total/calc)	172.34%
TEST3: Check Friedels for noncentro structure	
Estimate of Friedel pairs measured	1611
Fraction of Friedel pairs measured	0.723
Are heavy atom types Z>Si present	yes

PLAT301_ALERT_3_G Note: Main Residue Disorder 3.00 Perc.

PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 6

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Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Datablock 1 - ellipsoid plot







