

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0061 Å

Wavelength=0.71073

Cell: a=8.813(3) b=11.082(3) c=12.620(4)
 alpha=88.805(5) beta=80.440(5) gamma=75.680(5)
Temperature: 293 K

	Calculated	Reported
Volume	1177.4(6)	1177.3(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H15 N S8	C21 H15 N S8
Sum formula	C21 H15 N S8	C21 H15 N S8
Mr	537.90	537.90
Dx, g cm-3	1.517	1.517
Z	2	2
Mu (mm-1)	0.769	0.769
F000	552.0	552.0
F000'	554.10	
h, k, lmax	10, 13, 14	10, 13, 14
Nref	4145	4051
Tmin, Tmax	0.905, 0.926	0.907, 0.927
Tmin'	0.905	

Correction method= ?

Data completeness= 0.977

Theta(max)= 25.000

R(reflections)= 0.0484(3063)

wR2(reflections)= 0.1245(4051)

S = 1.017

Npar= Npar = 290

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

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full Low	0.977 Note
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given .	Please Do !
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for	C13 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for	C10 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.0061 Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	10	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	11	Why ?
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF		Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .		mixed
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal	0.00500	Degree
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3	
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder Percentage =	7	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	33	Check
	S7' -C4 -S7 1.555 1.555 1.555	11.40	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	79	Note

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

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

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. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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

