checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: 2a

Bond precision: C-C = 0.0041 A Wavelength=0.71073

Cell: a=8.8009(2) b=13.7366(4) c=13.9119(5)
alpha=111.716(3) beta=93.621(2) gamma=91.141(2)
Temperature: 110 K

	Calculated	Reported
Volume	1557.69(9)	1557.69(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C31 H40 Al N3 O S), C4 H10 O	2(C31 H40 Al N3 O S), C4 H10 O
Sum formula	C66 H90 Al2 N6 O3 S2	C66 H90 Al2 N6 O3 S2
Mr	1133.54	1133.52
Dx,g cm-3	1.208	1.208
Z	1	1
Mu (mm-1)	0.164	0.164
F000	610.0	610.0
F000'	610.56	
h,k,lmax	10,16,16	10,16,16
Nref	5484	5478
Tmin,Tmax	0.952,0.977	0.965,0.985
Tmin'	0.937	

Correction method= ANALYTICAL

Data completeness= 0.999 Theta(max)= 25.000

R(reflections)= 0.0489(3770) wR2(reflections)= 0.1360(5478)

S = 1.025 Npar= 402

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 C14 -- C15 .. 8.00 su

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Alert level C
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H10 .. H8'2 .. 1.84 Ang.

Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         11
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....          9
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................          5 Perc.
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................        100 Perc.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C9     ..  C8'     ..       3.02 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C8'    ..  C8'     ..       2.82 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         13
PLAT793_ALERT_4_G The Model has Chirality at C7      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C14     (Verify) ....          R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         43
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   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
   2 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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Datablock: 2b

Bond precision: C-C = 0.0027 A Wavelength=0.71073

Cell: a=12.54209(18) b=15.8805(2) c=17.5832(3)
alpha=68.5229(14) beta=89.6375(12) gamma=73.0413(13)
Temperature: 110 K

	Calculated	Reported
Volume	3097.32(9)	3097.32(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C31 H40 Al N3 O S	C31 H40 Al N3 O S
Sum formula	C31 H40 Al N3 O S	C31 H40 Al N3 O S
Mr	529.71	529.70
Dx,g cm-3	1.136	1.136
Z	4	4
Mu (mm-1)	0.159	0.159
F000	1136.0	1136.0
F000'	1137.08	
h,k,lmax	15,19,21	15,19,21
Nref	12185	12182
Tmin,Tmax	0.935,0.967	0.948,0.974
Tmin'	0.935	

Correction method= ANALYTICAL

Data completeness= 1.000 **Theta(max)= 26.000**

R(reflections)= 0.0423(9655) **wR2(reflections)= 0.1240(12182)**

S = 1.076 **Npar= 679**

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

PLAT411_ALERT_2_C Short Inter H...H Contact H10B .. H22B .. 2.02 Ang.

Alert level G

PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure !
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6
PLAT793_ALERT_4_G The Model has Chirality at C7A (Verify) .... S
PLAT793_ALERT_4_G The Model has Chirality at C7B (Verify) .... R
PLAT793_ALERT_4_G The Model has Chirality at C14A (Verify) .... S
PLAT793_ALERT_4_G The Model has Chirality at C14B (Verify) .... R
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Al1 (III) 3.50
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Al2 (III) 3.49

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8 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
6 ALERT type 4 Improvement, methodology, query or suggestion
2 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

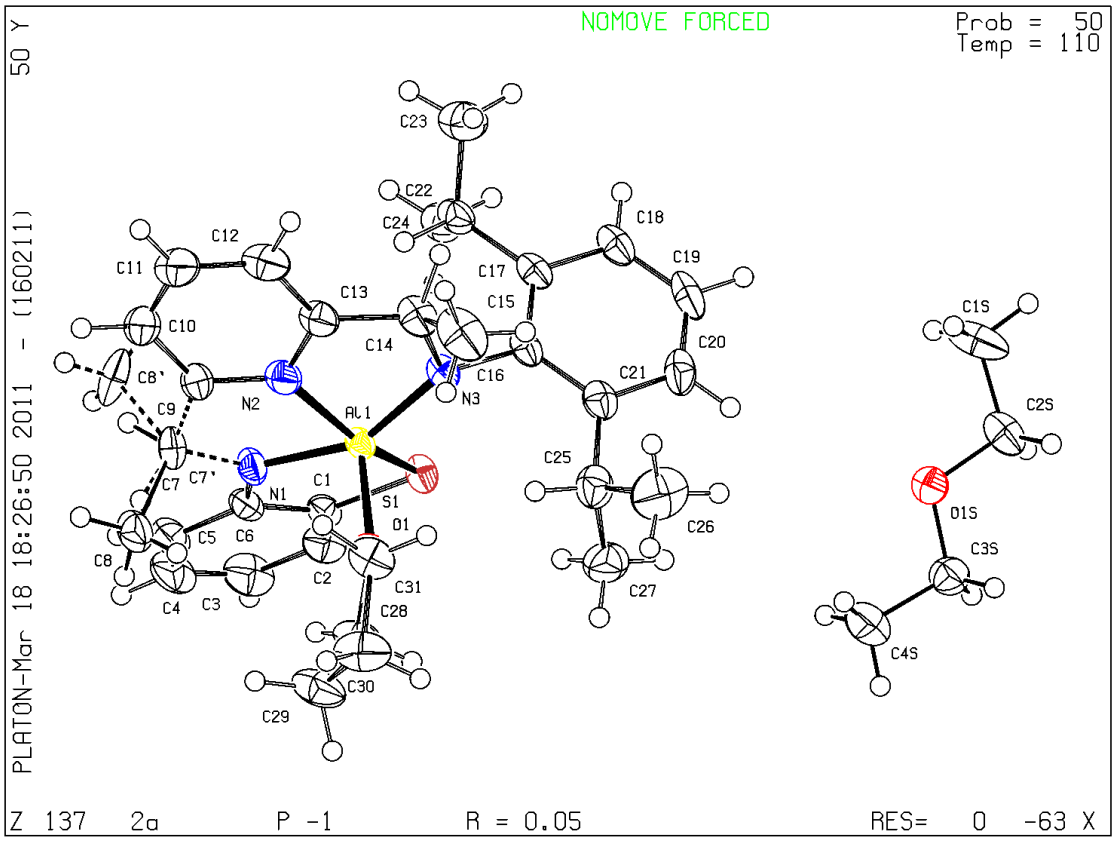
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 16/02/2011; check.def file version of 16/02/2011

Datablock 2a - ellipsoid plot



Datablock 2b - ellipsoid plot