

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lk652_a

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: lk652_a

Bond precision: C-C = 0.0211 A

Wavelength=0.71073

Cell: a=10.1614(11) b=20.487(2) c=28.789(3)
 alpha=71.352(3) beta=85.650(3) gamma=84.669(3)
Temperature: 120 K

	Calculated	Reported
Volume	5647.2(10)	5647.1(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	4(C34 H40 N2 O4), 2(C7.50 O3 S), 6(C7 O3 S), 3(C Cl3), 8(C H Cl	?
Sum formula	C204 H168 Cl33 N8 O40 S8	C51 H56.75 Cl8.25 N2 O10 S2
Mr	4797.79	1214.31
Dx,g cm-3	1.411	1.428
Z	1	4
Mu (mm-1)	0.541	0.541
F000	2457.0	2516.0
F000'	2463.83	
h,k,lmax	10,20,28	10,20,28
Nref	12033	11924
Tmin,Tmax	0.753,0.872	0.722,1.000
Tmin'	0.704	

Correction method= # Reported T Limits: Tmin=0.722 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991

Theta(max)= 20.933

R(reflections)= 0.1767(8664)

wR2(reflections)= 0.4891(11924)

S = 1.992

Npar= 1248

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

RFACR01_ALERT_3_A The value of the weighted R factor is > 0.45
Weighted R factor given 0.489

THETM01_ALERT_3_A The value of $\sin(\theta_{\max})/\lambda$ is less than 0.550
Calculated $\sin(\theta_{\max})/\lambda = 0.5027$

PLAT084_ALERT_3_A High wR_2 Value (i.e. > 0.25) 0.49 Report

PLAT213_ALERT_2_A Atom C22A has ADP max/min Ratio 8.9 prolat

PLAT213_ALERT_2_A Atom C4B has ADP max/min Ratio 9.6 prolat

PLAT213_ALERT_2_A Atom O7 has ADP max/min Ratio 7.0 prolat

Alert level B

DIFMX01_ALERT_2_B The maximum difference density is > $0.1 \times Z_{\max} \times 1.00$
_refine_diff_density_max given = 1.988
Test value = 1.700

RFACG01_ALERT_3_B The value of the R factor is > 0.15
R factor given 0.177

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 59.45 Check

PLAT082_ALERT_2_B High R_1 Value 0.18 Report

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.99 eA⁻³

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 8 Report

PLAT213_ALERT_2_B Atom C3A has ADP max/min Ratio 4.3 prolat

PLAT213_ALERT_2_B Atom C6A has ADP max/min Ratio 4.2 oblate

PLAT213_ALERT_2_B Atom O1B has ADP max/min Ratio 4.2 prolat

PLAT213_ALERT_2_B Atom C5B has ADP max/min Ratio 4.1 prolat

PLAT213_ALERT_2_B Atom C15B has ADP max/min Ratio 4.7 prolat

PLAT213_ALERT_2_B Atom C17B has ADP max/min Ratio 4.3 prolat

PLAT213_ALERT_2_B Atom O6 has ADP max/min Ratio 4.4 prolat

PLAT216_ALERT_3_B Disordered C152 (An/Solv) ADP max/min Ratio 7.1 Note

PLAT220_ALERT_2_B Non-Solvent Resd 4 C Ueq(max)/Ueq(min) Range 10.0 Ratio

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C1D Check

PLAT327_ALERT_2_B Possible Missing H on sp³? Carbon C6S Check

PLAT327_ALERT_2_B Possible Missing H on sp³? Carbon *C5S Check

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.02112 Ang.

PLAT420_ALERT_2_B D-H Without Acceptor O4A -- H4OA ... Please Check

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers 3 Check

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.99 <> 1.01

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_weight 1214.31

TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	51.00	612.56
H	1.01	42.00	42.34
N	14.01	2.00	28.01
O	16.00	10.00	159.99
S	32.07	2.00	64.13

C1	35.45	8.25	292.49	
Calculated formula weight		1199.52		
DIFMX02_ALERT_1_C	The maximum difference density is > 0.1*ZMAX*0.75			
	The relevant atom site should be identified.			
REFNR01_ALERT_3_C	Ratio of reflections to parameters is < 10 for a centrosymmetric structure			
	sine(theta)/lambda	0.5027		
	Proportion of unique data used	1.0000		
	Ratio reflections to parameters	9.5545		
PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ		Please Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...			Please Check
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio		9.55	Note
PLAT213_ALERT_2_C	Atom C1A	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C	Atom C7A	has ADP max/min Ratio	4.0	oblate
PLAT213_ALERT_2_C	Atom C12A	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C26A	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C27A	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C28A	has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom C2B	has ADP max/min Ratio	3.5	prolat
PLAT213_ALERT_2_C	Atom C3B	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C9B	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C	Atom C24B	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C25B	has ADP max/min Ratio	3.2	oblate
PLAT213_ALERT_2_C	Atom C26B	has ADP max/min Ratio	4.0	prolat
PLAT213_ALERT_2_C	Atom C28B	has ADP max/min Ratio	3.8	prolat
PLAT213_ALERT_2_C	Atom C29B	has ADP max/min Ratio	3.8	prolat
PLAT213_ALERT_2_C	Atom C33B	has ADP max/min Ratio	3.3	prolat
PLAT213_ALERT_2_C	Atom O4	has ADP max/min Ratio	3.7	prolat
PLAT213_ALERT_2_C	Atom O3	has ADP max/min Ratio	3.5	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 2	C Ueq(max)/Ueq(min) Range	4.5	Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 3	C Ueq(max)/Ueq(min) Range	4.1	Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 5	C Ueq(max)/Ueq(min) Range	5.9	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C26A -- C27A ..	5.2	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	N2A -- C34A ..	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C2A -- C3A ..	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C3A -- C4A ..	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C24A -- C25A ..	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C3B -- C4B ..	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C8B -- C13B ..	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C16B -- C17B ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C17B -- C21B ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C21B -- C22B ..	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C29B -- C30B ..	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C164 -- C6S ..	0.22	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C21B	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C31B	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S2	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S4	Check	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C6S	Check	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C1S	Check	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C4S	Check	
PLAT336_ALERT_2_C	Long Bond Distance for	C6S -C161	1.890	Ang.
PLAT336_ALERT_2_C	Long Bond Distance for	C6S -C166	1.900	Ang.
PLAT336_ALERT_2_C	Long Bond Distance for	C4S -C143	1.890	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C30B - C31B ..	1.38	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	17.868	Check	
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	3.453	Check	
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min)	7	Note	
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.503	102	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check	
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.18A From O11	2.02	eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	2.00A From C5S	1.85	eA-3

PLAT971_ALERT_2_C	Check Calcd Residual Density	1.09A From	O3	1.76 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.22A From	Cl53	1.70 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.01A From	C3S	1.69 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.24A From	Cl43	1.66 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.55A From	Cl64	1.57 eA-3
PLAT975_ALERT_2_C	Check Calcd Residual Density	1.07A From	O7	1.06 eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H7A2		-0.38 eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum: C51 H56.75 Cl8.25 N2 O10 S2
 Atom count from the _atom_site data: C51 H42 Cl8.25 N2 O10 S2
 CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
 CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
 From the CIF: _cell_formula_units_Z 4
 From the CIF: _chemical_formula_sum C51 H56.75 Cl8.25 N2 O10 S2
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	204.00	204.00	0.00
H	227.00	168.00	59.00
Cl	33.00	33.00	0.00
N	8.00	8.00	0.00
O	40.00	40.00	0.00
S	8.00	8.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	97	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	16	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.25	Check
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.65	mm
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.20	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of *C2D is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C3D is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C4D is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C5D is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C6D is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *ClDA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C7D is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C2DA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C3DA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C4DA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C5DA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C6DA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C7DA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C1E is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C2E is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C3E is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C4E is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C5E is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C6E is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C7E is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C1EA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C2EA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C3EA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C4EA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C5EA is Constrained at	0.5	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of *C6EA	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C7EA	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C1F	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C2F	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C3F	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C4F	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C5F	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C6F	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C7F	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C1FA	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C2FA	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C3FA	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C4FA	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C5FA	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C6FA	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C7FA	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C161	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C162	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C163	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C164	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C165	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C166	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C151	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C152	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C153	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C5S	is Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =	21	Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =	23	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (11.50) in Resd. #		3	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Cl33 .. C7FA ..		3.09	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact O10 .. C3S ..		2.97	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl22 .. Cl64 ..		3.03	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl32 .. Cl41 ..		3.09	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl33 .. Cl43 ..		3.36	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		47	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		42	Check
	C6S -CL63 -CL65 1.555 1.555 1.555		37.70	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		274	Check
	CL65 -C6S -CL62 1.555 1.555 1.555		39.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		279	Check
	CL63 -C6S -CL61 1.555 1.555 1.555		42.30	Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C34 H40 N2 O4			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		8	Note
	C H Cl3			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		12	Note
	C Cl3			
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		584	Note
PLAT909_ALERT_3_G	Percentage of Observed Data at Theta(Max) Still		48	%
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density		1	Note

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

9 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
68 **ALERT type 2** Indicator that the structure model may be wrong or deficient
17 **ALERT type 3** Indicator that the structure quality may be low
77 **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* or *IUCrData*, 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.

