

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: a028a12

Bond precision: C-C = 0.0081 Å

Wavelength=0.71073

Cell: a=8.3147(6) b=19.2037(13) c=14.1567(10)
 alpha=90 beta=102.128(2) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	2210.0(3)	2210.0(3)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C28 H28 N4 O8, C3 H7 O, 2(C6 H16 N)	C28 H28 N4 O8, 2(C6 H16 N), C3 H7 O
Sum formula	C43 H67 N6 O9	C43 H68 N6 O9
Mr	812.03	813.03
Dx,g cm-3	1.220	1.222
Z	2	2
Mu (mm-1)	0.086	0.086
F000	878.0	880.0
F000'	878.40	
h,k,lmax	9,21,15	9,21,15
Nref	6138[3179]	6058
Tmin,Tmax	0.978,0.987	0.526,0.732
Tmin'	0.978	

Correction method= # Reported T Limits: Tmin=0.526 Tmax=0.732
AbsCorr = MULTI-SCAN

Data completeness= 1.91/0.99 Theta(max)= 22.985

R(reflections)= 0.0572(5189) wR2(reflections)= 0.1492(6058)

S = 1.029 Npar= 540

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5494

🟡 Alert level B

PLAT018_ALERT_1_B _diffn_measured_fraction_theta_max .NE. _full ! Check

🟢 Alert level C

STRVA01_ALERT_4_C Flack test results are meaningless.
From the CIF: _refine_ls_abs_structure_Flack 0.100
From the CIF: _refine_ls_abs_structure_Flack_su 0.900
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 1.00 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 5.89 Note
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) 09 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0081 Ang.

🟠 Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C43 H68 N6 O9
Atom count from _chemical_formula_moiety: C43 H67 N6 O9
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: C43 H68 N6 O9
Atom count from the _atom_site data: C43 H67 N6 O9
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 2
From the CIF: _chemical_formula_sum C43 H68 N6 O9
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	86.00	86.00	0.00
H	136.00	134.00	2.00
N	12.00	12.00	0.00
O	18.00	18.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 9 Note
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 8 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.900 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C41 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C42 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C43 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C44 is Constrained at 0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C45 is Constrained at 0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C46 is Constrained at 0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C47 is Constrained at 0.200 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C48 is Constrained at 0.200 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C49 is Constrained at 0.200 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H41A is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H41B is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H42A is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H42B is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H43A is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H43B is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H43C is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H44A is Constrained at 0.300 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H44B is Constrained at 0.300 Check

PLAT300_ALERT_4_G Atom Site Occupancy of <H45A	is Constrained at	0.300	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H45B	is Constrained at	0.300	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H46A	is Constrained at	0.300	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H46B	is Constrained at	0.300	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H46C	is Constrained at	0.300	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H47A	is Constrained at	0.200	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H47B	is Constrained at	0.200	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H48A	is Constrained at	0.200	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H48B	is Constrained at	0.200	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H49A	is Constrained at	0.200	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H49B	is Constrained at	0.200	Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H49C	is Constrained at	0.200	Check
PLAT302_ALERT_4_G Anion/Solvent Disorder	Percentage =	17	Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #		2	Note
C3 H7 O			
PLAT860_ALERT_3_G Number of Least-Squares Restraints		7	Note

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

8 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
5 ALERT type 3 Indicator that the structure quality may be low
34 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.

Datablock a028a12 - ellipsoid plot

