

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pmterpytry1

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: pmterpytry1

Bond precision: C-C = 0.0082 Å

Wavelength=0.71073

Cell: a=11.1738 (4) b=15.9791 (6) c=16.2596 (6)
 alpha=105.8847 (18) beta=95.6780 (19) gamma=95.970 (2)
Temperature: 300 K

	Calculated	Reported
Volume	2752.37 (18)	2752.37 (18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H22 N8 O6 Pm, C15 H11 N7 O12 Pm, 2 (C2 H3 N)	C30 H22 N8 O6 Pm, C15 H11 N7 O12 Pm, 2 (C2 H3 N)
Sum formula	C49 H39 N17 O18 Pm2	C49 H39 N17 O18 Pm2
Mr	1447.81	1447.81
Dx, g cm ⁻³	1.747	1.747
Z	2	2
Mu (mm ⁻¹)	2.071	2.071
F000	1436.0	1436.0
F000'	1435.90	
h, k, lmax	14, 21, 21	14, 21, 21
Nref	13742	13384
Tmin, Tmax	0.513, 0.615	0.590, 0.707
Tmin'	0.503	

Correction method= # Reported T Limits: Tmin=0.590 Tmax=0.707
AbsCorr = MULTI-SCAN

Data completeness= 0.974

Theta (max)= 28.334

R(reflections)= 0.0387 (9890)

wR2(reflections)=
0.1034 (13384)

S = 1.041

Npar= 786

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

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N15 Check



Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O18B --N15 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 09 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O10 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O16 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Pm2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O17 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N12 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N13 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C46 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C48 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N16 0.107 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N17 0.130 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00825 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.370 Report
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note
1 0 0, 0 1 0, 0 -1 1, -1 0 1, 0 0 1, 0 1 1,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 276 Report
2 0 0, 3 0 0, 5 0 0, -4 1 0, 1 1 0, 2 1 0,
4 1 0, -2 2 0, 0 2 0, 1 2 0, 5 2 0, -3 3 0,
-2 3 0, -1 3 0, -6 4 0, -1 4 0, 0 4 0, 1 4 0,
3 4 0, -6 5 0, -3 5 0, 0 5 0, 2 5 0, -2 6 0,
-1 7 0, 0 7 0, 1 8 0, -1 -8 1, -2 -7 1, 3 -7 1,
-3 -6 1, -1 -6 1, 0 -6 1, -4 -5 1, -2 -5 1, 1 -5 1,
4 -5 1, -3 -4 1, -1 -4 1, 1 -4 1, 2 -4 1, -4 -3 1,
-1 -3 1, 0 -3 1, 2 -3 1, 4 -3 1, -5 -2 1, -3 -2 1,
-2 -2 1, -1 -2 1, 0 -2 1, 1 -2 1, 5 -2 1, -4 -1 1,
-3 -1 1, -2 -1 1, -1 -1 1, 1 -1 1, -5 0 1, -3 0 1,
-2 0 1, 1 0 1, 2 0 1, 3 0 1, -4 1 1, -3 1 1,
-1 1 1, 1 1 1, 4 1 1, -2 2 1, 0 2 1, 1 2 1,
3 2 1, 4 2 1, -2 3 1, 0 3 1, 1 3 1, -5 4 1,
-2 4 1, 0 4 1, 1 4 1, -1 5 1, 0 5 1, -4 6 1,
1 6 1, -3 7 1, 2 7 1, 0 -8 2, -2 -7 2, 1 -7 2,
2 -6 2, 3 -5 2, 4 -5 2, -3 -4 2, 5 -4 2, -3 -3 2,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 78 Note
1 1 0, 5 2 0, -2 3 0, -1 3 0, 0 4 0, 1 4 0,
-3 5 0, 0 5 0, 2 5 0, -2 6 0, -1 7 0, 0 7 0,
1 8 0, 3 -7 1, -1 -6 1, -1 -4 1, 2 -4 1, -4 -3 1,
0 -2 1, -3 -1 1, 1 -1 1, -3 0 1, -2 0 1, 3 0 1,
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
-2 0 2,
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.01Ang From O14 . 0.83 eA-3

● Alert level G

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Pm2	--O10	.	6.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Pm2	--O13	.	5.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Pm2	--O14	.	10.5 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O18B		Constrained at		0.62 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O18A		Constrained at		0.38 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)				3% Note
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O18A			.	44.0 Degree
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...				43.90 Deg.
	N15 -O17 -O18A 1_555 1_555 1_555			#	198 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...				44.00 Deg.
	N15 -O18A -O17 1_555 1_555 1_555			#	199 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.			#	2 Note
	C15 H11 N7 O12 Pm				
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.			#	3 Note
	C2 H3 N				
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.			#	4 Note
	C2 H3 N				
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			76 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity				2.1 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value				2.069 Note
	Predicted wR2: Based on SigI**2	5.00	or SHELX Weight	9.93	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				2 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
 12 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.

