

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pu_mnt_082322_0m

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: pu_mnt_082322_0m

Bond precision:	C-C = 0.0106 Å	Wavelength=0.71073		
Cell:	a=14.1718(10)	b=18.5779(11)	c=18.0434(11)	
	alpha=90	beta=91.772(2)	gamma=90	
Temperature:	100 K			

	Calculated	Reported
Volume	4748.2(5)	4748.2(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H18 K5 N14 Pu S8	C28 H18 K5 N14 Pu S8
Sum formula	C28 H18 K5 N14 Pu S8	C28 H18 K5 N14 Pu S8
Mr	1244.55	1244.54
Dx, g cm ⁻³	1.741	1.741
Z	4	4
Mu (mm ⁻¹)	2.217	2.217
F000	2404.0	2404.0
F000'	2374.66	
h, k, lmax	19, 25, 24	19, 25, 24
Nref	12340	12305
Tmin, Tmax	0.643, 0.845	0.609, 0.746
Tmin'	0.532	

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Correction method= # Reported T Limits: Tmin=0.609 Tmax=0.746
AbsCorr = MULTI-SCAN
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Data completeness= 0.997 Theta (max)= 28.750

R(reflections)= 0.0456(10564)	wR2(reflections)= 0.1080(12305)
S = 1.132	Npar= 539

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

PLAT220_ALERT_2_B	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	7.4	Ratio
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	N20	Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	K4	Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	C18	Check	

Alert level C

CHEMW01_ALERT_1_C The difference between the given and expected weight for compound is greater 1 mass unit. Check that all hydrogen atoms have been taken into account.

PLAT220_ALERT_2_C	NonSolvent	Resd 1	N	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	5.1	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N00Z	Check	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N3	Check	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N018	Check	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N8	Check	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N10	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	K3	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	K5	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C01C	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C01I	Check	
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds		0.01059	Ang.	
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4			Please	Check	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			3.048	Check	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		2	Report	
	1 0 1, 2 0 4,					
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.74Ang	From C20	1.82	eA-3	
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.94Ang	From K2	1.74	eA-3	
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.47Ang	From C01F	1.73	eA-3	
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.52Ang	From K5	1.56	eA-3	
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.48Ang	From N10	1.52	eA-3	
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.65Ang	From K2	-1.93	eA-3	
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.78Ang	From Pu01	-1.64	eA-3	
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.26Ang	From K2	-1.61	eA-3	

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			4	Note	
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H Atoms			7	Report	
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension			3	Info	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large			37.57	Why ?	
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records			3	Report	
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records			3	Report	
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records			3	Report	
PLAT300_ALERT_4_G	Atom Site Occupancy of N11	Constrained at		0.6667	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of C016	Constrained at		0.6667	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of C017	Constrained at		0.6667	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of N9	Constrained at		0.3333	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of C0	Constrained at		0.3333	Check	

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PLAT300_ALERT_4_G Atom Site Occupancy of C21          Constrained at      0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H01A          Constrained at      0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H01B          Constrained at      0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H01C          Constrained at      0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21A          Constrained at      0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21B          Constrained at      0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21C          Constrained at      0.3333 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd  1)      5% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  S5      ..S7      .      3.16 Ang.
                                     5/2-x,-1/2+y,3/2-z =      2_746 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....      25 Note
      Pu01      N00Z      N012      C014      C016      C017      H01A      H01B
      H01C      N018      C01A      H01D      H01E      H01F      C01C      C01E
      H01G      H01H      H01I      C01F      H01J      H01K      H01L      C01I
      CO
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.12 Ratio
PLAT774_ALERT_1_G Check  X-Y Bond in CIF: Pu01      --K3      ..      4.25 Ang.
PLAT774_ALERT_1_G Check  X-Y Bond in CIF: Pu01      --K1      ..      4.10 Ang.
PLAT774_ALERT_1_G Check  X-Y Bond in CIF: K3      --K2      ..      4.19 Ang.
PLAT774_ALERT_1_G Check  X-Y Bond in CIF: K5      --K2      ..      4.44 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      38.70 Deg.
      N20      -C18      -K4      1_555      1_555      1_555      .....      #      274 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      36.20 Deg.
      N9      -C0      -K1      1_555      1_555      1_555      .....      #      339 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....      45 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).      2 Note
      -1      0      1,      0      1      1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      29 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      2 Note
      1      0      1,      2      0      4,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      4.829 Note
      Predicted wR2: Based on SigI**2 2.24 or SHELX Weight 9.55
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      0 Info

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 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
21 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

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# start Validation Reply Form
_vrf_PLAT220_pu_mnt_082322_0m
;
PROBLEM: NonSolvent      Resd 1      C      Ueq(max)/Ueq(min) Range      7.4 Ratio
RESPONSE: ...
;

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_vrf_PLAT241_pu_mnt_082322_0m
;
PROBLEM: High      'MainMol' Ueq as Compared to Neighbors of      N20 Check
RESPONSE: ...
;
_vrf_PLAT242_pu_mnt_082322_0m
;
PROBLEM: Low       'MainMol' Ueq as Compared to Neighbors of      K4 Check
RESPONSE: ...
;
# end Validation Reply Form

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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.

PLATON version of 15/07/2024; check.def file version of 15/07/2024

