

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: c__~1__dyop~3_sl248

Bond precision: C-C = 0.0104 A Wavelength=0.71073

Cell: a=16.0038(8) b=16.5124(8) c=26.6249(10)
 alpha=90 beta=90 gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	7035.9(6)	7035.9(6)
Space group	P c c n	Pccn
Hall group	-P 2ab 2ac	?
Moiety formula	C72 H60 Dy N2 O10 P4, N O3 ?	
Sum formula	C72 H60 Dy N3 O13 P4	C72 H60 Dy N3 O13 P4
Mr	1461.61	1461.61
Dx,g cm-3	1.380	1.380
Z	4	4
Mu (mm-1)	1.216	1.216
F000	2972.0	2972.0
F000'	2974.04	
h,k,lmax	20,21,34	20,21,34
Nref	8088	8081
Tmin,Tmax	0.652,0.784	0.652,0.784
Tmin'	0.539	

Correction method= # Reported T Limits: Tmin=0.652 Tmax=0.784
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.500

R(reflections)= 0.0637(6095) wR2(reflections)= 0.1853(8081)

S = 1.124 Npar= 457

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

PLAT430_ALERT_2_A	Short Inter D...A Contact	O4S	..05S	2.00	Ang.
PLAT430_ALERT_2_A	Short Inter D...A Contact	O5S	..05S	2.20	Ang.

Alert level B

PLAT216_ALERT_3_B	Disordered	O4S	(An/Solv) ADP max/min Ratio	7.9	Note
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Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.06	Report
PLAT221_ALERT_2_C	Solv./Anion Resd 2 O Ueq(max)/Ueq(min) Range	4.6	Ratio
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01044	Ang.

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	5	Report
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	48.91	Why ?
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1S Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2S Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3S Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1S Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4S Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O5S Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2S Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	4	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	N O3		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	38	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018	Note

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

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

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_PLAT430_c__~1__dyop~3_sl248
;
PROBLEM: Short Inter D...A Contact  O4S      ..05S      2.00 Ang.
RESPONSE: ...
;
# end Validation Reply Form
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PLATON version of 30/01/2018; check.def file version of 30/01/2018

