

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3-Y

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: 3-Y

Bond precision:	C-C = 0.0044 Å	Wavelength=1.54178	
Cell:	a=63.711(4)	b=11.8813(7)	c=23.5145(14)
	alpha=90	beta=104.577(2)	gamma=90
Temperature:	120 K		

	Calculated	Reported
Volume	17226.8(18)	17226.8(17)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C56 H89 O4 P4 Y	C56 H89 O4 P4 Y
Sum formula	C56 H89 O4 P4 Y	C56 H89 O4 P4 Y
Mr	1039.06	1039.06
Dx, g cm-3	1.202	1.202
Z	12	12
Mu (mm-1)	2.795	2.795
F000	6672.0	6672.0
F000'	6696.76	
h, k, lmax	78, 14, 29	78, 14, 29
Nref	17021	16874
Tmin, Tmax	0.239, 0.353	0.482, 0.754
Tmin'	0.106	

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Correction method= # Reported T Limits: Tmin=0.482 Tmax=0.754
AbsCorr = MULTI-SCAN
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Data completeness= 0.991 Theta(max)= 72.283

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R(reflections)= 0.0457( 16230)      wR2(reflections)=
S = 1.059                          0.1066( 16874)
Npar= 1002
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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 C

PLAT220_ALERT_2_C	NonSolvent	Resd 2	C	Ueq(max)/Ueq(min)	Range	3.3	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 2	H	Uiso(max)/Uiso(min)	Range	4.3	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C63	--C65	.		5.5	s.u.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd.	#				1	Note
	C56	H89	O4	P4	Y		
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance				2.185	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600				72	Report
	0	2	0,	1	1	0,	3
	1	0,	67	3	0,	-7	1
	1	1,	3	1	1,	5	1
	1	1,	3	1	1,	-46	0
	-10	0	2,	-6	0	2,	-5
	0	0	2,	1	1	2,	2
	4	0	4,	-6	2	5,	0
	4	0	8,	8	4	8,	-9
	4	0	10,	10	0	10,	-19
	-2	0	12,	10	0	12,	16
	-30	0	14,	-10	2	14,	16
	19	9	17,	-22	0	20,	38
	24	0	22,	26	2	22,	19
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF				4	Note
	6	0	0,	-10	0	2,	0
PLAT977_ALERT_2_C	Check Negative Difference Density on H4	.				-0.63	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	19	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H Atoms	18	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
	H6	H4	
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	0.66	mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	80.14	Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	C2/c	I2/a Note
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0080	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	P6	--C72
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Y2	--P5
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at	0.5	Check
	P6	P6A	C77
	C80	C80A	C81
	C84	C84A	H6
	H78F	H79A	H79B
	H80B	H80C	H80D
	H82D	H82E	H82F
	H83F	H84A	H84B
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd	1)
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H66A	..H78F
		x,y,z	=
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H73	..H79F

PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H73	x,y,z = ..H84D	.	1_555 Check	2.13 Ang.
			x,y,z =		1_555 Check	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#			2	Note
	C56 H89 O4 P4 Y					
PLAT794_ALERT_5_G	Tentative Bond Valency for Y1	(III)		.	3.17	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters				1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				262	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				1	Note
	2 0 0,					
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			73	Note
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by	.			1	Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value				4.032	Note
	Predicted wR2: Based on SigI**2	2.64	or SHELX Weight	10.07		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				0	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
 8 ALERT type 3 Indicator that the structure quality may be low
 10 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.

