

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FPR853

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: FPR853

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Bond precision:    C-C = 0.0141 Å

Wavelength=0.71073

Cell:                a=12.2629(16)        b=16.534(2)        c=18.118(2)  
                      alpha=79.414(5)    beta=77.667(5)    gamma=87.190(5)  
Temperature:        150 K

	Calculated	Reported
Volume	3527.5(7)	3527.4(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C64 H26 Dy2 F36 N4 O12	C64 H26 Dy2 F36 N4 O12
Sum formula	C64 H26 Dy2 F36 N4 O12	C64 H26 Dy2 F36 N4 O12
Mr	2051.89	2051.89
Dx,g cm-3	1.932	1.932
Z	2	2
Mu (mm-1)	2.261	2.261
F000	1980.0	1980.0
F000'	1980.95	
h,k,lmax	15,21,23	15,21,23
Nref	16190	15733
Tmin,Tmax	0.587,0.934	0.774,0.934
Tmin'	0.334	

Correction method= # Reported T Limits: Tmin=0.774 Tmax=0.934  
AbsCorr = MULTI-SCAN

Data completeness= 0.972

Theta(max)= 27.485

R(reflections)= 0.0672( 11594)

wR2(reflections)= 0.1818( 15733)

S = 1.063

Npar= 1027

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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.

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### 🔴 Alert level B

PLAT213_ALERT_2_B	Atom F12	has ADP max/min Ratio .....	4.2	prolat
PLAT213_ALERT_2_B	Atom F13	has ADP max/min Ratio .....	4.1	prolat
PLAT213_ALERT_2_B	Atom F14	has ADP max/min Ratio .....	4.4	prolat
PLAT213_ALERT_2_B	Atom F30	has ADP max/min Ratio .....	4.9	prolat
PLAT213_ALERT_2_B	Atom C54	has ADP max/min Ratio .....	4.5	prolat
PLAT220_ALERT_2_B	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	6.5	Ratio
PLAT230_ALERT_2_B	Hirshfeld Test Diff for F16	--C49 .	19.9	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for F17	--C49 .	13.9	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for F18	--C49 .	12.6	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for F27	--C55 .	8.8	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for F29	--C59 .	10.9	s.u.
PLAT234_ALERT_4_B	Large Hirshfeld Difference F24	--C54	0.28	Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference F36	--C64	0.26	Ang.
PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Theta(Min).		20	Note
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 1.18A	From F17	2.84	eA-3
PLAT975_ALERT_2_B	Check Calcd Resid. Dens. 1.09A	From O9	1.95	eA-3

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### 🔴 Alert level C

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	value Low .	0.976	Why?
PLAT213_ALERT_2_C	Atom F10	has ADP max/min Ratio .....	4.0	prolat
PLAT213_ALERT_2_C	Atom F11	has ADP max/min Ratio .....	4.0	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1 F	Ueq(max)/Ueq(min) Range	5.9	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min) Range	4.2	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O10	--C58 .	6.8	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O11	--C61 .	6.1	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F25	--C55	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F31	--C60	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F33	--C60	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O8	--C53	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O9	--C56	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O12	--C63	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C63	--C64	0.19	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C58	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C61	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C62	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	O9	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	O10	Check	
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....		0.01411	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	289	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....		1	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.35A	From O12	2.46	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 2.08A	From F36	2.25	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.11A	From C63	2.18	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.44A	From C59	2.07	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.09A	From O9	1.95	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.95A	From F17	1.92	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.04A	From C51	1.89	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.76A	From Dy2	1.84	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.85A	From C58	1.79	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 2.03A	From C51	1.75	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.84A	From Dy2	1.53	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.70A	From Dy1	-2.15	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.85A	From Dy2	-1.93	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.53A	From F17	-1.73	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.76A	From Dy2	-1.58	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.73A	From C49	-1.51	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on	Dy1	1.37	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on	Dy2	1.34	eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.		0	Info

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● **Alert level G**

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	45.17	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.005	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		2	Report
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C35	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C39	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C40	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C44	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C45	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C49	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C50	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C54	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C55	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C59	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C60	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C64	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3	..F13	2.81	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F6	..F29	2.82	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Dy1	(II)	1.87	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Dy2	(II)	1.89	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	148	Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
57 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 ALERT type 3 Indicator that the structure quality may be low  
11 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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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.

