

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dymnt\_031121\_nbb\_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: dymnt\_031121\_nbb\_0m

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Bond precision:      C-C = 0.0073 Å      Wavelength=0.71073

Cell:                      a=13.6517(5)      b=18.3713(7)      c=17.5608(7)  
                                alpha=90                  beta=92.063(1)      gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	4401.4(3)	4401.4(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C32 Dy2 N16 S16, 12(C2 N), 10(Na)	C28 Dy N14 Na5 S8
Sum formula	C56 Dy2 N28 Na10 S16	C28 Dy N14 Na5 S8
Mr	2132.70	1066.35
Dx, g cm <sup>-3</sup>	1.609	1.609
Z	2	4
Mu (mm <sup>-1</sup> )	2.166	2.166
F000	2060.0	2060.0
F000'	2064.11	
h,k,lmax	20,27,25	20,27,25
Nref	14698	14672
Tmin,Tmax	0.771,0.805	0.572,0.746
Tmin'	0.648	

Correction method= # Reported T Limits: Tmin=0.572 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.998      Theta(max)= 31.545

R(reflections)= 0.0377( 12711)

wR2(reflections)=  
0.1099( 14672)

S = 1.177

Npar= 506

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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

PLAT919_ALERT_3_B	Reflection # Likely Affected by the Beamstop ...	1	Check
	1 1 1,		
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	6	Check
	3 1 0, 3 2 0, 1 1 1, -3 3 1, -1 2 2,	13 5 18,	
PLAT939_ALERT_3_B	Large Value of Not (SHELXL) Weight Optimized S .	233.76	Check

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### Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please	Check
	Calc: C32 Dy2 N16 S16, 12(C2 N), 10(Na)		
	Rep.: C28 Dy N14 Na5 S8		
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C01A	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C01G	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C01H	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C22	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including N01C	0.101	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including N14	0.117	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	6	Note
	1 1 0, 0 2 0, -1 0 1, 1 0 1, -1 1 1,	0 1 1,	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	14	Report
	1 2 0, -1 2 1, 0 2 1, 0 0 2, 0 1 2,	-2 5 2,	
	-2 0 4, -2 1 4, 2 1 4, 3 1 4, -3 1 5,	3 1 5,	
	7 0 9, 1 0 11,		
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....	8	Note
	-1 0 1, 1 0 1, -2 5 2, -2 0 4, 2 1 4,	3 1 4,	
	-3 1 5, 3 1 5,		
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	5	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.40Ang From Na3	1.61	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.48Ang From Na5	1.54	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.22Ang From Na5	1.54	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.09Ang From N01B .	1.38	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.95Ang From C018 .	0.68	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.55Ang From C18 .	-0.67	eA-3

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### Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	16.14	Why ?
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	15	Note
	Dy01 N00J C00Y N00Z N013 C015 C018	C019	
	C01A N01B N01C C01E C01G C01H C01I		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	5	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	4	Note
	0 2 0, -1 1 1, 0 0 2, -1 2 1,		
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....	5.067	Note
	Predicted wr2: Based on SigI**2 2.17 or SHELX Weight	9.33	

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
10 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  
6 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.

```
# start Validation Reply Form
_vrf_PLAT919_dymnt_031121_nbb_0m
;
PROBLEM: Reflection # Likely Affected by the Beamstop ...          1 Check
RESPONSE: ...
;
_vrf_PLAT934_dymnt_031121_nbb_0m
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..        6 Check
RESPONSE: ...
;
_vrf_PLAT939_dymnt_031121_nbb_0m
;
PROBLEM: Large Value of Not (SHELXL) Weight Optimized S .        233.76 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.

