

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1Dy, 1Er, 2Dy

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: 1Dy

| | | |
|-----------------|------------------|-------------------------------------|
| Bond precision: | C-C = 0.0061 A | Wavelength=0.71073 |
| Cell: | a=10.8822(15) | b=11.4229(15) c=20.823(3) |
| | alpha=89.735(3) | beta=88.681(3) gamma=76.170(2) |
| Temperature: | 293 K | |
| | Calculated | Reported |
| Volume | 2512.7(6) | 2512.7(6) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C57 H66 Dy N3 O3 | C57 H66 Dy N3 O3 |
| Sum formula | C57 H66 Dy N3 O3 | C57 H66 Dy N3 O3 |
| Mr | 1003.63 | 1003.62 |
| Dx,g cm-3 | 1.327 | 0.000 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.532 | 1.532 |
| F000 | 1038.0 | 1038.0 |
| F000' | 1037.94 | |
| h,k,lmax | 13,14,25 | 13,14,25 |
| Nref | 10087 | 10012 |
| Tmin,Tmax | 0.484,0.682 | 0.484,0.682 |
| Tmin' | 0.460 | |

Correction method= # Reported T Limits: Tmin=0.484 Tmax=0.682
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 26.190

R(reflections)= 0.0381(8630) wR2(reflections)= 0.0822(10012)

S = 1.036 Npar= 589

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 | Non-Solvent Resd 1 C | Ueq(max)/Ueq(min) Range | 6.2 | Ratio |
| PLAT919_ALERT_3_B | Reflection # Likely Affected by the Beamstop ... | | 1 | Check |

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.

Absorption correction given as multi-scan

| | | | | |
|-------------------|--|---------------------------|------|--------|
| PLAT222_ALERT_3_C | Non-Solv. Resd 1 H | Uiso(max)/Uiso(min) Range | 6.9 | Ratio |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | | 01 | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | | C36 | Check |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= | 0.600 | 48 | Report |
| PLAT918_ALERT_3_C | Reflection(s) with I(obs) much Smaller I(calc) . | | 1 | Check |
| PLAT934_ALERT_3_C | Number of (Iobs-Icalc)/SigmaW > 10 Outliers | | 1 | Check |
| PLAT975_ALERT_2_C | Check Calcd Resid. Dens. 0.74A From N1 | | 0.42 | eA-3 |
| PLAT978_ALERT_2_C | Number C-C Bonds with Positive Residual Density. | | 0 | Info |

Alert level G

| | | | | |
|-------------------|--|-------|-----|-------|
| PLAT066_ALERT_1_G | Predicted and Reported Tmin&Tmax Range Identical | | ? | Check |
| PLAT199_ALERT_1_G | Reported _cell_measurement_temperature (K) | | 293 | Check |
| PLAT200_ALERT_1_G | Reported _diffrn_ambient_temperature (K) | | 293 | Check |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= | 0.600 | 26 | Note |

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

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

Datablock: 1Er

Bond precision: C-C = 0.0109 A

Wavelength=0.71073

| | | | |
|--------------|-----------------|----------------|------------------|
| Cell: | a=10.9407(11) | b=11.4509(11) | c=20.735(2) |
| | alpha=90.066(2) | beta=91.458(2) | gamma=103.853(2) |
| Temperature: | 293 K | | |

| | Calculated | Reported |
|----------------|------------------|------------------|
| Volume | 2521.3(4) | 2521.3(4) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C57 H66 Er N3 O3 | C57 H66 Er N3 O3 |
| Sum formula | C57 H66 Er N3 O3 | C57 H66 Er N3 O3 |
| Mr | 1008.39 | 1008.38 |
| Dx,g cm-3 | 1.328 | 1.328 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.710 | 1.710 |
| F000 | 1042.0 | 1042.0 |
| F000' | 1041.81 | |
| h,k,lmax | 13,14,25 | 13,14,25 |
| Nref | 9856 | 9686 |
| Tmin,Tmax | 0.605,0.710 | 0.605,0.710 |
| Tmin' | 0.593 | |

Correction method= # Reported T Limits: Tmin=0.605 Tmax=0.710
AbsCorr = MULTI-SCAN

Data completeness= 0.983 Theta(max)= 25.946

R(reflections)= 0.0584(6697) wR2(reflections)= 0.1212(9686)

S = 0.996 Npar= 589

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 Non-Solvent Resd 1 C | Ueq(max)/Ueq(min) Range | 6.2 Ratio |
| PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... | | 1 Check |



Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

| | | |
|--|-----------------------------|--------------|
| PLAT213_ALERT_2_C Atom C37 | has ADP max/min Ratio | 3.2 prolat |
| PLAT222_ALERT_3_C Non-Solv. Resd 1 H | Uiso(max)/Uiso(min) Range | 7.7 Ratio |
| PLAT234_ALERT_4_C Large Hirshfeld Difference C1 | -- C6 | 0.17 Ang. |
| PLAT234_ALERT_4_C Large Hirshfeld Difference C30 | -- C31 | 0.18 Ang. |
| PLAT234_ALERT_4_C Large Hirshfeld Difference C36 | -- C38 | 0.19 Ang. |
| PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of | | 01 Check |
| PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of | | 03 Check |
| PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of | | C36 Check |
| PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds | | 0.01086 Ang. |
| PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= | 0.600 | 40 Report |
| PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . | | 1 Check |
| PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers | | 1 Check |

**Alert level G**

| | | | |
|-------------------|--|-------|--------|
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 1 | Report |
| PLAT066_ALERT_1_G | Predicted and Reported Tmin&Tmax Range Identical | ? | Check |
| PLAT154_ALERT_1_G | The s.u.'s on the Cell Angles are Equal ..(Note) | 0.002 | Degree |
| PLAT186_ALERT_4_G | The CIF-Embedded .res File Contains ISOR Records | 1 | Report |
| PLAT199_ALERT_1_G | Reported _cell_measurement_temperature (K) | 293 | Check |
| PLAT200_ALERT_1_G | Reported _diffrn_ambient_temperature (K) | 293 | Check |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 6 | Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 131 | Note |

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- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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 7 ALERT type 3 Indicator that the structure quality may be low
 5 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check

Datablock: 2Dy

Bond precision: C-C = 0.0072 A

Wavelength=0.71073

Cell: a=13.7983(12) b=16.6655(15) c=18.6715(17)
 alpha=70.722(1) beta=77.406(2) gamma=86.857(2)
 Temperature: 293 K

| | Calculated | Reported |
|----------------|----------------------------------|-------------------|
| Volume | 3954.7(6) | 3954.7(6) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C68 H109 Dy N4 O4 [+ solvent] | ? |
| Sum formula | C68 H109 Dy N4 O4 [+ solvent] | C68 H109 Dy N4 O4 |
| Mr | 1209.10 | 1209.09 |
| Dx,g cm-3 | 1.015 | 1.015 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.984 | 0.984 |
| F000 | 1286.0 | 1286.0 |
| F000' | 1286.00 | |
| h,k,lmax | 17,20,23 | 17,20,23 |
| Nref | 15860 | 15601 |
| Tmin,Tmax | 0.744,0.821 | 0.746,0.822 |
| Tmin' | 0.744 | |

Correction method= # Reported T Limits: Tmin=0.746 Tmax=0.822
AbsCorr = MULTI-SCAN

Data completeness= 0.984

Theta(max)= 26.183

R(reflections)= 0.0607(11672)

wR2(reflections)= 0.1875(15601)

S = 1.050

Npar= 726

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

SHFSU01_ALERT_2_B The absolute value of parameter shift to su ratio > 0.10

Absolute value of the parameter shift to su ratio given 0.144

Additional refinement cycles may be required.

| | | | | |
|-------------------|--|---------------------------|-------|--------|
| PLAT080_ALERT_2_B | Maximum Shift/Error | | 0.14 | Why ? |
| PLAT220_ALERT_2_B | Non-Solvent Resd 1 | C Ueq(max)/Ueq(min) Range | 10.0 | Ratio |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | N2 --C17 .. | 19.0 | s.u. |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | N2 --C18 .. | 86.0 | s.u. |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | N2 --C19 .. | 82.5 | s.u. |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | C27 --C30 .. | 18.3 | s.u. |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | C31 --C32 .. | 19.7 | s.u. |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | C31 --C33 .. | 14.0 | s.u. |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | C45 --C48 .. | 19.7 | s.u. |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | C61 --C62 .. | 22.3 | s.u. |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | C61 --C63 .. | 18.0 | s.u. |
| PLAT242_ALERT_2_B | Low 'MainMol' Ueq as Compared to Neighbors of | N2 | Check | |
| PLAT936_ALERT_2_B | The Embedded .res File Includes a DAMP Command | . | 800.0 | Report |
| PLAT990_ALERT_1_B | Deprecated .res/.hkl Input Style SQUEEZE Job | ... | | ! Note |

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

| | | | | |
|-------------------|--|-----------------------------|--------|--------|
| PLAT220_ALERT_2_C | Non-Solvent Resd 1 | N Ueq(max)/Ueq(min) Range | 5.1 | Ratio |
| PLAT222_ALERT_3_C | Non-Solv. Resd 1 | H Uiso(max)/Uiso(min) Range | 10.0 | Ratio |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for | C16 --C17 .. | 7.0 | s.u. |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C11 | Check | |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C31 | Check | |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C45 | Check | |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C61 | Check | |
| PLAT353_ALERT_3_C | Long N-H (N0.87,N1.01A) | N1 - H70 | 1.01 | Ang. |
| PLAT361_ALERT_2_C | Long C(sp3)-C(sp3) Bond | C16 - C17 .. | 1.65 | Ang. |
| PLAT412_ALERT_2_C | Short Intra XH3 .. XHn | H17A ..H18A .. | 1.84 | Ang. |
| PLAT412_ALERT_2_C | Short Intra XH3 .. XHn | H17B ..H19A .. | 1.81 | Ang. |
| PLAT905_ALERT_3_C | Negative K value in the Analysis of Variance | ... | -0.759 | Report |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= | 0.600 | 142 | Report |
| PLAT918_ALERT_3_C | Reflection(s) with I(obs) much Smaller I(calc) | . | 1 | Check |
| PLAT934_ALERT_3_C | Number of (Iobs-Icalc)/SigmaW > 10 Outliers | | 1 | Check |
| PLAT973_ALERT_2_C | Check Calcd Positive Resid. Density on | Dy1 | 1.48 | eA-3 |
| PLAT977_ALERT_2_C | Check Negative Difference Density on | H47C | -0.46 | eA-3 |
| PLAT977_ALERT_2_C | Check Negative Difference Density on | H48A | -0.32 | eA-3 |
| PLAT977_ALERT_2_C | Check Negative Difference Density on | H64A | -0.31 | eA-3 |

| | | |
|-------------------|--|------------|
| PLAT977_ALERT_2_C | Check Negative Difference Density on H64C | -0.32 eA-3 |
| PLAT978_ALERT_2_C | Number C-C Bonds with Positive Residual Density. | 0 Info |

Alert level G

| | | |
|-------------------|--|-------------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 6 Note |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 9 Report |
| PLAT066_ALERT_1_G | Predicted and Reported Tmin&Tmax Range Identical | ? Check |
| PLAT072_ALERT_2_G | SHELXL First Parameter in WGHT Unusually Large | 0.11 Report |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records | 4 Report |
| PLAT177_ALERT_4_G | The CIF-Embedded .res File Contains DELU Records | 2 Report |
| PLAT186_ALERT_4_G | The CIF-Embedded .res File Contains ISOR Records | 3 Report |
| PLAT199_ALERT_1_G | Reported _cell_measurement_temperature (K) | 293 Check |
| PLAT200_ALERT_1_G | Reported _diffrn_ambient_temperature (K) | 293 Check |
| PLAT606_ALERT_4_G | VERY LARGE Solvent Accessible VOID(S) in Structure | ! Info |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 58 Note |
| PLAT869_ALERT_4_G | ALERTS Related to the Use of SQUEEZE Suppressed | ! Info |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min). | 2 Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 112 Note |
| PLAT933_ALERT_2_G | Number of OMIT Records in Embedded .res File ... | 21 Note |

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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 09/11/2017; check.def file version of 08/11/2017





