

# 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: el643b

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Bond precision:    C-C = 0.0054 Å                      Wavelength=1.54184

Cell:                      a=14.6954(4)              b=14.3307(6)              c=18.2161(4)  
                            alpha=90                      beta=90                      gamma=90  
Temperature:              173 K

	Calculated	Reported
Volume	3836.2(2)	3836.2(2)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C14.63 H14.27 N4 O7 Y, 0.683(C2 H6 O)	C14.63 H14.27 N4 O7 Y, 0.68(C2 H6 O)
Sum formula	C16 H18.37 N4 O7.68 Y	C16 H18.37 N4 O7.68 Y
Mr	478.55	478.56
Dx,g cm-3	1.657	1.657
Z	8	8
Mu (mm-1)	4.750	4.750
F000	1942.6	1943.0
F000'	1946.42	
h,k,lmax	18,17,22	17,17,22
Nref	3746	3721
Tmin,Tmax	0.653,0.867	0.778,1.000
Tmin'	0.592	

Correction method= # Reported T Limits: Tmin=0.778 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.993                      Theta(max)= 71.620

R(reflections)= 0.0447( 2838)              wR2(reflections)= 0.1183( 3721)

S = 1.054                      Npar= 287

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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**

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s) .....	1 Report
PLAT415_ALERT_2_B	Short Inter D-H..H-X           H00B_A .. H00L ..	2.06 Ang.
PLAT420_ALERT_2_B	D-H Without Acceptor           >O005_A - >H00B_A ..	Please Check

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**Alert level C**

PLAT241_ALERT_2_C	High           Ueq as Compared to Neighbors for .....	0009 Check
PLAT241_ALERT_2_C	High           Ueq as Compared to Neighbors for .....	000A Check

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**Alert level G**

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C16 H18.37 N4 O7.68 Y1  
Atom count from \_chemical\_formula\_moiety:C15.99 H18.35 N4 O7.68 Y1

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G ALERT: check formula stoichiometry or atom site occupancies.

From the CIF: \_cell\_formula\_units\_Z 8

From the CIF: \_chemical\_formula\_sum C16 H18.37 N4 O7.68 Y

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	128.00	128.00	0.00
H	146.96	146.93	0.03
N	32.00	32.00	0.00
O	61.44	61.47	-0.03
Y	8.00	8.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	9 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	6 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	3 Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Y001 -- O00A ..	14.4 su
PLAT300_ALERT_4_G	Atom Site Occupancy of >O005_A is Constrained at	0.683 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <O0_B is Constrained at	0.317 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1A_B is Constrained at	0.317 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C0AA_B is Constrained at	0.317 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H00A_A is Constrained at	0.683 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H00B_A is Constrained at	0.683 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H1AA_B is Constrained at	0.317 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H1AB_B is Constrained at	0.317 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H0AA_B is Constrained at	0.317 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H0AB_B is Constrained at	0.317 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H0AC_B is Constrained at	0.317 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <H0_B is Constrained at	0.317 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >O1_A is Constrained at	0.683 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C1_A is Constrained at	0.683 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C2_A is Constrained at	0.683 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H1_A is Constrained at	0.683 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H1A_A is Constrained at	0.683 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H1B_A is Constrained at	0.683 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H2A_A is Constrained at	0.683 Check

PLAT300_ALERT_4_G Atom Site Occupancy of >H2B_A is Constrained at	0.683	Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H2C_A is Constrained at	0.683	Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage =	6	Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =	100	Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....	57	Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .	1.13	Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....	32	Note

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 37 **ALERT level G** = General information/check it is not something unexpected

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

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## Datablock: el508b

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Bond precision: C-C = 0.0093 A

Wavelength=0.71073

Cell: a=14.2871(3) b=19.9839(6) c=20.0637(7)  
 alpha=90 beta=101.857(3) gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	5606.2(3)	5606.2(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C42 H36 Cl2 Dy2 N9 O9, Cl	C42 H36 Cl2 Dy2 N9 O9, Cl
Sum formula	C42 H36 Cl3 Dy2 N9 O9	C42 H36 Cl3 Dy2 N9 O9
Mr	1242.15	1242.15
Dx,g cm-3	1.472	1.472
Z	4	4
Mu (mm-1)	2.840	2.840
F000	2424.0	2424.0
F000'	2425.11	
h,k,lmax	17,24,25	19,27,26
Nref	11460	11177
Tmin,Tmax	0.718,0.797	0.674,1.000
Tmin'	0.647	

Correction method= # Reported T Limits: Tmin=0.674 Tmax=1.000  
 AbsCorr = MULTI-SCAN

Data completeness= 0.975

Theta(max)= 26.371

R(reflections)= 0.0452( 9122)      wR2(reflections)= 0.1221( 11177)

S = 1.077      Npar= 589

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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 B

PLAT213_ALERT_2_B Atom C27	has ADP max/min Ratio .....	4.3	prolat
PLAT213_ALERT_2_B Atom C40	has ADP max/min Ratio .....	4.8	prolat
PLAT241_ALERT_2_B High	Ueq as Compared to Neighbors for .....	C27	Check
PLAT241_ALERT_2_B High	Ueq as Compared to Neighbors for .....	C40	Check



#### Alert level C

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full Low .....	0.976	Note
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range	5.9	Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) ...	5.5	Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C38 -- C39 ..	0.16	Ang.
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for .....	Dy1	Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for .....	Dy2	Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for .....	N6	Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for .....	N9	Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for .....	C38	Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .....	0.0093	Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N2 - H2 ..	Please	Check
PLAT420_ALERT_2_C D-H Without Acceptor N5 - H5 ..	Please	Check
PLAT420_ALERT_2_C D-H Without Acceptor N8 - H8 ..	Please	Check



#### Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....	3	Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.	6.80	Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Dy1 -- Cl2 ..	25.0	su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Dy2 -- Cl1 ..	33.7	su
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT868_ALERT_4_G ALERTS Due to the use of _smtbx_masks Suppressed	!	Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ	-2	Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ	-3	Units

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0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
16 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  
3 ALERT type 4 Improvement, methodology, query or suggestion  
4 ALERT type 5 Informative message, check

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**Datablock: el529**

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Bond precision: C-C = 0.0184 Å

Wavelength=0.71073

Cell: a=14.218(3) b=20.386(4) c=20.455(4)  
alpha=90 beta=101.982(16) gamma=90  
Temperature: 173 K

	Calculated	Reported
Volume	5800(2)	5799.5(18)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C42 H35 Cl2 Gd2 N9 O9, Cl	C42 H35 Cl2 Gd2 N9 O9, Cl
Sum formula	C42 H35 Cl3 Gd2 N9 O9	C42 H35 Cl3 Gd2 N9 O9
Mr	1230.64	1230.64
Dx, g cm <sup>-3</sup>	1.409	1.409
Z	4	4
Mu (mm <sup>-1</sup> )	2.456	2.456
F000	2404.0	2404.0
F000'	2405.24	
h,k,lmax	16,24,24	16,28,25
Nref	10231	7486
Tmin,Tmax	0.745,0.822	0.487,1.000
Tmin'	0.659	

Correction method= # Reported T Limits: Tmin=0.487 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.732

Theta(max)= 24.999

R(reflections)= 0.0608( 4625)

wR2(reflections)= 0.1576( 7486)

S = 0.937

Npar= 589

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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 B

PLAT018\_ALERT\_1\_B \_diffrn\_measured\_fraction\_theta\_max .NE. \_full ! Check  
PLAT241\_ALERT\_2\_B High Ueq as Compared to Neighbors for ..... C33 Check



#### Alert level C

SHFSU01\_ALERT\_2\_C The absolute value of parameter shift to su ratio > 0.05  
Absolute value of the parameter shift to su ratio given 0.098  
Additional refinement cycles may be required.  
PLAT080\_ALERT\_2\_C Maximum Shift/Error ..... 0.10 Why ?  
PLAT213\_ALERT\_2\_C Atom C35 has ADP max/min Ratio ..... 3.3 prolat  
PLAT220\_ALERT\_2\_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.1 Ratio  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C35 -- C36 .. 5.4 su  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N1 -- C7 .. 0.21 Ang.

PLAT234_ALERT_4_C	Large Hirshfeld Difference N2	--	C6	..	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N7	--	N8	..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C7	--	C8	..	0.23	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C29	--	C30	..	0.19	Ang.
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	.....			C5	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	.....			Gd1	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	.....			Gd2	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	.....			N9	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	.....			0.0184	Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor N2	-	H2	..		Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor N5	-	H5	..		Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor N8	-	H8	..		Please Check



### Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms	...			6	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension				1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	.....			3	Report
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by	...			2	Units
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Gd1	--	C11	..	11.5	su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Gd2	--	C12	..	19.1	su
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for				C1	Check
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure				!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....			39	Note
PLAT868_ALERT_4_G	ALERTS Due to the use of _smtbx_masks Suppressed				!	Info
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ				-4	Units

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

## Datablock: el486c

Bond precision: C-C = 0.0069 A

Wavelength=1.54184

Cell: a=10.3419(3) b=14.5850(5) c=15.7309(5)  
 alpha=95.672(3) beta=95.377(2) gamma=109.768(3)  
 Temperature: 173 K

	Calculated	Reported
Volume	2201.46(13)	2201.47(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H20 Dy N5 O11	C16 H20 Dy N5 O11
Sum formula	C16 H20 Dy N5 O11	C16 H20 Dy N5 O11
Mr	620.87	620.87
Dx,g cm-3	1.873	1.873
Z	4	4
Mu (mm-1)	18.780	18.780
F000	1220.0	1220.0
F000'	1185.15	
h,k,lmax	11,16,17	11,16,17
Nref	6760	6718
Tmin,Tmax	0.206,0.472	0.782,1.000
Tmin'	0.084	

Correction method= # Reported T Limits: Tmin=0.782 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.994                      Theta(max)= 61.091

R(reflections)= 0.0310( 5861)              wR2(reflections)= 0.0793( 6718)

S = 1.049                                      Npar= 614

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

THETM01\_ALERT\_3\_B The value of sine(theta\_max)/wavelength is less than 0.575  
Calculated sin(theta\_max)/wavelength = 0.5678



#### Alert level C

PLAT241\_ALERT\_2\_C High              Ueq as Compared to Neighbors for .....              017 Check  
PLAT430\_ALERT\_2\_C Short Inter D...A Contact    022      ..    022      ..              2.90 Ang.



#### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite              14 Note  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms .....              2 Report  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records              4 Report  
PLAT173\_ALERT\_4\_G The CIF-Embedded .res File Contains DANG Records              8 Report  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X)    Dy1      --    09      ..              6.3 su  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X)    Dy1      --    012      ..              5.2 su  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints .....              12 Note

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1 ALERT type 5 Informative message, check

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## Datablock: 2015ncs0277

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Bond precision: C-C = 0.0050 A Wavelength=0.71075

Cell: a=12.2901(9) b=15.4666(11) c=18.7780(13)  
alpha=90 beta=100.085(6) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	3514.3(4)	3514.3(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C30 H32 N6 O8 Y, C2 H3 N, Cl	C30 H32 N6 O8 Y, Cl, C2 H3 N
Sum formula	C32 H35 Cl N7 O8 Y	C32 H35 Cl N7 O8 Y
Mr	770.03	770.03
Dx,g cm-3	1.455	1.455
Z	4	4
Mu (mm-1)	1.794	1.794
F000	1584.0	1584.0
F000'	1574.04	
h,k,lmax	15,20,24	15,20,24
Nref	8101	7924
Tmin,Tmax	0.851,0.948	
Tmin'	0.851	

Correction method= Not given

Data completeness= 0.978 Theta(max)= 27.540

R(reflections)= 0.0524( 5547) wR2(reflections)= 0.1338( 7924)

S = 1.007 Npar= 453

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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 A**



DIFF003\_ALERT\_1\_A \_diffn\_measurement\_device\_type is missing  
Diffractometer make and type. Replaces \_diffn\_measurement\_type.



### Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method Not Given .	Please Do !
PLAT057_ALERT_3_C	Correction for Absorption Required RT(exp) ...	1.11 Do !
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C31 Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.9 Note



### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7 Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	2 Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	4 Report
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	6 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*, 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.









