

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: L3_02967

Bond precision:	C-C = 0.0028 A	Wavelength=0.71073	
Cell:	a=10.9930(11)	b=11.8907(10)	c=9.4100(7)
	alpha=90	beta=93.034(4)	gamma=90
Temperature:	200 K		
	Calculated	Reported	
Volume	1228.30(18)	1228.30(18)	
Space group	C 2/c	C 1 2/c 1	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C13 H9 N5 O4	?	
Sum formula	C13 H9 N5 O4	C13 H9 N5 O4	
Mr	299.25	299.25	
Dx,g cm-3	1.618	1.618	
Z	4	4	
Mu (mm-1)	0.125	0.125	
F000	616.0	616.0	
F000'	616.30		
h,k,lmax	13,14,11	13,14,11	
Nref	1127	1127	
Tmin,Tmax	0.996,0.998	0.920,1.000	
Tmin'	0.995		

Correction method= # Reported T Limits: Tmin=0.920 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.340

R(reflections)= 0.0386(784) wR2(reflections)= 0.0977(1127)

S = 1.014 Npar= 105

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

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.1 Note

● Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints 1 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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1 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: L4_02811

Bond precision: C-C = 0.0109 A

Wavelength=0.71073

Cell: a=12.1706(12) b=6.5022(7) c=20.4013(19)
alpha=90 beta=90 gamma=90

Temperature: 250 K

	Calculated	Reported
Volume	1614.5(3)	1614.5(3)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	2(C13 H9 N5 O4), C2 N	?
Sum formula	C28 H18 N11 O8	C14 H9 N5.50 O4
Mr	636.53	318.27
Dx,g cm-3	1.309	1.309
Z	2	4
Mu (mm-1)	0.100	0.100
F000	654.0	654.0
F000'	654.31	
h,k,lmax	14,7,24	14,7,24
Nref	1617	1619
Tmin,Tmax	0.997,0.998	0.850,1.000
Tmin'	0.984	

Correction method= # Reported T Limits: Tmin=0.850 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.001

Theta(max)= 25.330

R(reflections)= 0.1017(847)

wR2(reflections)= 0.3585(1619)

S = 1.105

Npar= 147

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

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25)	0.36 Report
PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density	1.13 eA-3
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing).	C15 Check
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds	0.0109 Ang.



Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75	
The relevant atom site should be identified.	
RINTA01_ALERT_3_C The value of Rint is greater than 0.12	
Rint given 0.121	
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12	0.121 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density	2.18 Report
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.2 Note



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	3 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	2 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.20 Report
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	1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of N6 Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14 Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15 Constrained at	0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 1)	15.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2)	0.75 Check
PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder	! Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints	3 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !

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-

Datablock: YbL3_02349

Bond precision: C-C = 0.0092 A Wavelength=0.71073

Cell: a=20.2374(7) b=6.8593(3) c=29.4468(13)
alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	4087.6(3)	4087.6(3)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	2(C13 H7 N6 O9 Yb), C2 N, 2(H2 O), 2(H O)	?
Sum formula	C28 H20 N13 O22 Yb2	C14 H10 N6.50 O11 Yb
Mr	1236.65	618.32
Dx,g cm-3	2.010	2.009
Z	4	8
Mu (mm-1)	4.649	4.649
F000	2380.0	2380.0
F000'	2378.25	
h,k,lmax	24,8,35	24,8,35
Nref	3744	3741
Tmin,Tmax	0.818,0.995	0.840,0.990
Tmin'	0.370	

Correction method= # Reported T Limits: Tmin=0.840 Tmax=0.990

AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.350

R(reflections)= 0.0314(2867) wR2(reflections)= 0.0714(3741)

S = 1.101 Npar= 307

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

PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing).

C15 Check



Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.124

PLAT213_ALERT_2_C Atom N5

has ADP max/min Ratio

3.3 oblate

PLAT214_ALERT_2_C Atom C15

(Anion/Solvent) ADP max/min Ratio

4.6 prolat

PLAT223_ALERT_4_C	Solv./Anion Resd 3 H	Ueq(max)/Ueq(min) Range	4.5 Ratio
PLAT244_ALERT_4_C	Low Solvent Ueq as Compared to Neighbors of	C14 Check	
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00918 Ang.	



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	5 Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12	0.124 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	17.62 Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2 Report
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for	C15 Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C14 - C15 .	1.51 Ang.
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.16 Ratio
PLAT794_ALERT_5_G	Tentative Bond Valency for Yb1 (III) .	3.27 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	3 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3 Note

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 4 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

Datablock: YbL4_02351

Bond precision: C-C = 0.0380 A

Wavelength=0.71073

Cell:	a=4.7056(17)	b=9.193(3)	c=15.322(6)
	alpha=72.711(9)	beta=88.774(11)	gamma=86.788(9)
Temperature:	296 K		

	Calculated	Reported
Volume	631.9(4)	631.9(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H15 N10 O8 Yb	?
Sum formula	C26 H15 N10 O8 Yb	C26 H15 N10 O8 Yb
Mr	768.52	768.52
Dx,g cm-3	2.020	2.020
Z	1	1
Mu (mm-1)	3.777	3.777
F000	375.0	375.0
F000'	374.77	
h,k,lmax	5,11,18	5,11,18
Nref	2321	2304
Tmin,Tmax	0.873,0.945	0.750,0.950
Tmin'	0.530	

Correction method= # Reported T Limits: Tmin=0.750 Tmax=0.950
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 25.350

R(reflections)= 0.0901(1861) wR2(reflections)= 0.2669(2304)

S = 1.090 Npar= 177

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

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.038 Ang.



Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.137

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.137 Report

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.27 Report

PLAT234_ALERT_4_C Large Hirshfeld Difference N1 --C1 . 0.17 Ang.

PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of O1 Check

PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of C13 Check



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.17 Report

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.51 Why ?

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Yb1 --O1 . 5.1 s.u.

PLAT300_ALERT_4_G Atom Site Occupancy of H2O Constrained at 0.5 Check

PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder ! Report

PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.17 Ratio
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 68 Check
 O4 -C13 -Yb1 1.555 1.555 1.345 39.30 Deg.
 PLAT794_ALERT_5_G Tentative Bond Valency for Yb1 (III) . 3.33 Info
 PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON 28 Info
 PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

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 4 ALERT type 3 Indicator that the structure quality may be low
 6 ALERT type 4 Improvement, methodology, query or suggestion
 3 ALERT type 5 Informative message, check

Datablock: TbYbL3_02366

Bond precision: C-C = 0.0223 A

Wavelength=0.71073

Cell: a=18.0063(9) b=12.3925(7) c=24.4944(13)
 alpha=90 beta=106.133(4) gamma=90
 Temperature: 296 K

	Calculated	Reported
Volume	5250.5(5)	5250.5(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C39 H21 N15 O15 Tb0.98 Yb1.02), 6(O0.50)	?
Sum formula	C78 H42 N30 O35 Tb1.96 Yb2.04	C39 H21 N15 O17.50 Tb0.98 Yb1.02
Mr	2623.92	1311.95
Dx,g cm-3	1.660	1.660
Z	2	4
Mu (mm-1)	3.195	3.195
F000	2540.4	2540.0
F000'	2539.33	
h,k,lmax	21,14,29	21,14,29
Nref	9610	9574
Tmin,Tmax	0.851,0.906	0.770,0.910
Tmin'	0.463	

Correction method= # Reported T Limits: Tmin=0.770 Tmax=0.910
 AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 25.350

R(reflections)= 0.0597(5783)

wR2(reflections)= 0.2051(9574)

S = 1.020

Npar= 669

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 A

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Author Response: There are disordered solvent molecules in the voids that could not be included in the model.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18

Rint given 0.187

PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	016W	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	017W	Check
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.02233	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	O8 ..017W .	2.78	Ang.
		1+x,1+y,z =	1_665	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O9 ..018W .	2.83	Ang.
		1/2-x,1/2+y,3/2-z =	2_556	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O15T ..017W .	2.80	Ang.
		1-x,1-y,1-z =	3_666	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O15T ..016W .	2.82	Ang.
		x,1+y,z =	1_565	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O17W ..018W .	2.74	Ang.
		x,y,z =	1_555	Check

Alert level C

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms	..	Please	Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range		3.9	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O5 --C22 .	0.17	Ang.
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of		014T	Check
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of		015T	Check
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of		C17	Check
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of		C30	Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of		C27	Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	O11 ..016W .	2.87	Ang.
		3/2-x,1/2+y,3/2-z =	2_656	Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	O14T ..017W .	2.89	Ang.
		1-x,1-y,1-z =	3_666	Check
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H7 ..05 .	2.66	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H24 ..017W .	2.64	Ang.

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1	Info
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12	0.187	Report

PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Yb2 --O12 .	5.4	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Tb2 --O12 .	5.4	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of Yb1 Constrained at	0.51	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Yb2 Constrained at	0.51	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Tb1 Constrained at	0.49	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Tb2 Constrained at	0.49	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O18W Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	3%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	O18W	Check
PLAT650_ALERT_4_G	SWAT Instruction Used to Model Solvent Disorder		! Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1	Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.19	Ratio
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !

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 1 ALERT type 5 Informative message, check

Datablock: TbYbL402367

Bond precision: C-C = 0.0076 A

Wavelength=0.71073

Cell:	a=8.6338(18)	b=15.998(2)	c=12.721(3)
	alpha=90	beta=90.686(11)	gamma=90
Temperature:	296 K		

	Calculated	Reported
Volume	1756.9(6)	1756.9(6)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C13 H8 N7 O10 Tb0.38 Yb0.62	?
Sum formula	C13 H8 N7 O10 Tb0.38 Yb0.62	C13 H8 N7 O10 Tb0.38 Yb0.62
Mr	589.94	589.94
Dx,g cm-3	2.230	2.230
Z	4	4
Mu (mm-1)	4.907	4.906
F000	1132.4	1132.0
F000'	1131.78	
h,k,lmax	10,19,15	10,19,15
Nref	1612	1611
Tmin,Tmax	0.843,0.925	0.780,0.930
Tmin'	0.563	

Correction method= # Reported T Limits: Tmin=0.780 Tmax=0.930
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.350

R(reflections)= 0.0332(1384) wR2(reflections)= 0.0642(1611)

S = 1.057 Npar= 142

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.140

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..

Please Check

PLAT213_ALERT_2_C Atom O2 has ADP max/min Ratio

3.8 prolat



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	1 Report
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12	0.140 Report
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	8.98 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Yb1 Constrained at	0.62 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Tb1 Constrained at	0.38 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2O Constrained at	0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1)	6% Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .	1.26 Ratio
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !

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6 **ALERT type 4** Improvement, methodology, query or suggestion
2 **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.











