

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) JRL2-002, JRL2-159, JRL2-490, jrl1-165, jrl2-003\_auto, jrl2-009\_auto, jrl2-224\_auto, jrl2-225\_1\_monop, jrl2-226\_1\_auto, jrl2-228\_auto, jrl2-511, jrl3-026\_auto

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: jrl1-165

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Bond precision:    C-C = 0.0026 A                      Wavelength=0.71073

Cell:                      a=10.6772 (3)              b=23.2998 (7)              c=12.8824 (4)  
                                    alpha=90                      beta=96.187 (3)              gamma=90

Temperature:              123 K

	Calculated	Reported
Volume	3186.17 (17)	3186.17 (17)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C34 H51 N3 O	C34 H51 N3 O
Sum formula	C34 H51 N3 O	C34 H51 N3 O
Mr	517.78	517.77
Dx, g cm <sup>-3</sup>	1.079	1.079
Z	4	4
Mu (mm <sup>-1</sup> )	0.065	0.065
F000	1136.0	1136.0
F000'	1136.38	
h, k, lmax	14, 30, 17	13, 30, 17
Nref	7675	7616
Tmin, Tmax	0.992, 0.994	0.828, 1.000
Tmin'	0.987	

Correction method= # Reported T Limits: Tmin=0.828 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.992

Theta (max)= 27.997

R(reflections)= 0.0606( 5223)

wR2(reflections)=  
0.1493( 7616)

S = 1.022

Npar= 368

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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**

PLAT910\_ALERT\_3\_B Missing # of FCF Reflection(s) Below Theta(Min). 15 Note

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**Alert level C**

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.2 Ratio  
PLAT222\_ALERT\_3\_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.6 Ratio  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C3 --C6 . 6.3 s.u.  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C32 Check  
PLAT420\_ALERT\_2\_C D-H Bond Without Acceptor N3 --H3 . Please Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 10.905 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.238 Check

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**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 4 Note  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H1 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H2 Constrained at 0.5 Check  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 2 Note  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 32 Note  
PLAT967\_ALERT\_5\_G Note: Two-Theta Cutoff Value in Embedded .res .. 56.0 Degree  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 6 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 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  
4 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## Datablock: jrl3-026\_auto

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Bond precision: C-C = 0.0019 A

Wavelength=1.54184

Cell: a=9.3798(1) b=12.7676(2) c=17.6482(2)  
 alpha=90.791(1) beta=100.797(1) gamma=103.777(1)  
 Temperature: 100 K

	Calculated	Reported
Volume	2012.58(5)	2012.58(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H66 Li N3 O3	C42 H66 Li N3 O3
Sum formula	C42 H66 Li N3 O3	C42 H66 Li N3 O3
Mr	667.92	667.91
Dx, g cm <sup>-3</sup>	1.102	1.102
Z	2	2
Mu (mm <sup>-1</sup> )	0.522	0.522
F000	732.0	732.0
F000'	733.89	
h, k, lmax	11, 15, 21	11, 15, 21
Nref	8080	8047
Tmin, Tmax		0.864, 1.000
Tmin'	0.987	

Correction method= # Reported T Limits: Tmin=0.864 Tmax=1.000  
 AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 73.240

R(reflections)= 0.0467( 6927) wR2(reflections)=  
 0.1371( 8047)  
 S = 1.064 Npar= 459

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**

PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. # C42 H66 Li N3 O3	1 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3 Report

**Alert level G**

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001 Degree
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	35.75 Deg.

O1 -C6 -LI1 1\_555 1\_555 1\_555 ..... # 46 Check  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 31 Note  
 PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 2 Note  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 14 Info

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

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

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## Datablock: jrl2-009\_auto

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Bond precision: C-C = 0.0016 A Wavelength=1.54184  
 Cell: a=8.9764(1) b=11.6785(1) c=20.1645(2)  
 alpha=94.861(1) beta=94.332(1) gamma=102.153(1)  
 Temperature: 100 K

	Calculated	Reported
Volume	2049.57(4)	2049.57(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C45 H64 Li N3 O4	C45 H64 Li N3 O4
Sum formula	C45 H64 Li N3 O4	C45 H64 Li N3 O4
Mr	717.93	717.93
Dx, g cm <sup>-3</sup>	1.163	1.163
Z	2	2
Mu (mm <sup>-1</sup> )	0.569	0.569
F000	780.0	780.0
F000'	782.10	
h, k, lmax	11, 14, 24	11, 14, 24
Nref	8136	8122
Tmin, Tmax	0.945, 0.945	0.315, 1.000
Tmin'	0.945	

Correction method= # Reported T Limits: Tmin=0.315 Tmax=1.000  
 AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 72.565

R(reflections)= 0.0370( 7791)

wR2(reflections)=  
0.0946( 8122)

S = 1.039

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 C

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.225	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report

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### Alert level G

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 ...	5	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	8% Note
PLAT410_ALERT_2_G	Short Intra H...H Contact H32 ..H40D	2.07	Ang.
	x,y,z =	1_555	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	39.82	Deg.
	O1 -C6 -LI1 1_555 1_555 1_555 .....	# 50	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	50	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	12	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	23	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2	Check

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

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

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## Datablock: JRL2-159

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Bond precision: C-C = 0.0026 A

Wavelength=1.54184

Cell: a=10.6807(1) b=18.1547(2) c=19.0465(2)  
 alpha=62.273(1) beta=85.797(1) gamma=84.539(1)  
 Temperature: 100 K

	Calculated	Reported
Volume	3252.53(7)	3252.53(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C37 H49 N3 O	?
Sum formula	C37 H49 N3 O	C37 H49 N3 O
Mr	551.79	551.79
Dx, g cm <sup>-3</sup>	1.127	1.127
Z	4	4
Mu (mm <sup>-1</sup> )	0.514	0.514
F000	1200.0	1200.0
F000'	1203.05	
h, k, lmax	13, 22, 23	13, 22, 23
Nref	12942	12909
Tmin, Tmax	0.940, 0.950	0.923, 1.000
Tmin'	0.926	

Correction method= # Reported T Limits: Tmin=0.923 Tmax=1.000  
 AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 72.702

R(reflections)= 0.0592( 11425) wR2(reflections)=  
 0.1617( 12909)  
 S = 1.089 Npar= 791

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**

PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem	I	94 %Fit
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range		3.1 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....		6.081 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=	0.600	2 Report

**Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite		10 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...		8 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)		0.001 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records		4 Report

PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C24A --C25B .	5.4	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	10%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H5A ..H31B .	2.14	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H24A ..H25E .	1.89	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H24A ..H25F .	2.10	Ang.
	x,y,z =	1_555	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	56	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	32	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	11	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2	Check

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 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  
1 ALERT type 5 Informative message, check

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## Datablock: jrl2-003\_auto

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Bond precision: C-C = 0.0019 A

Wavelength=1.54184

Cell: a=8.8114(1) b=11.7153(1) c=20.2669(2)  
alpha=94.871(1) beta=92.921(1) gamma=102.488(1)  
Temperature: 100 K





PLAT411\_ALERT\_2\_G Short Inter H...H Contact H11 ..H40A . 2.13 Ang.  
 1-x,1-y,-z = 2\_665 Check  
 PLAT779\_ALERT\_4\_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 40.08 Deg.  
 O1 -C6 -LI1 1\_555 1\_555 1\_555 ..... # 49 Check  
 PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 50 Note  
 PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 36 Note  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 18 Info

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- 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
  - 18 **ALERT level G** = General information/check it is not something unexpected
- 
- 1 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
  - 7 ALERT type 3 Indicator that the structure quality may be low
  - 6 ALERT type 4 Improvement, methodology, query or suggestion
  - 0 ALERT type 5 Informative message, check
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## Datablock: jrl2-226\_1\_auto

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Bond precision: C-C = 0.0062 A Wavelength=1.54184

Cell: a=13.9795(1) b=8.7269(1) c=27.0841(3)  
 alpha=90 beta=101.962(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	3232.45(6)	3232.45(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C37 H49 N3 O	C37 H49 N3 O
Sum formula	C37 H49 N3 O	C37 H49 N3 O
Mr	551.79	551.79
Dx, g cm-3	1.134	1.134
Z	4	4
Mu (mm-1)	0.517	0.517
F000	1200.0	1200.0
F000'	1203.05	
h, k, lmax	17, 10, 33	17, 10, 33
Nref	6499	65209
Tmin, Tmax	0.830, 0.856	0.807, 1.000
Tmin'	0.813	

Correction method= # Reported T Limits: Tmin=0.807 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 10.034                      Theta(max)= 73.387

R(reflections)= 0.0860( 54816)

wR2(reflections)=  
0.2767( 65209)

S = 1.100

Npar= 390

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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 C**

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) .....	0.28	Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.6	Ratio
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds .....	0.00625	Ang.
PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N2 - H2 .	1.03	Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	10.617	Check

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**Alert level G**

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	6.90	Why ?
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	21	Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law ( 0 0 1) Est.d BASF	0.39	Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	4	Note
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by	7	Check

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

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

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## Datablock: jrl2-228\_auto

Bond precision: C-C = 0.0036 A

Wavelength=1.54184

Cell: a=23.9798(2)

b=12.1099(1)

c=24.9659(3)

alpha=90

beta=90

gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	7249.92(12)	7249.92(12)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C38 H51 N3 O, C H4 O	C38 H51 N3 O, C H4 O
Sum formula	C39 H55 N3 O2	C39 H55 N3 O2
Mr	597.86	597.86
Dx, g cm <sup>-3</sup>	1.095	1.095
Z	8	8
Mu (mm <sup>-1</sup> )	0.515	0.515
F000	2608.0	2608.0
F000'	2614.77	
h, k, lmax	29, 15, 30	29, 15, 30
Nref	14450[ 7403]	13878
Tmin, Tmax		0.940, 1.000
Tmin'	0.813	

Correction method= # Reported T Limits: Tmin=0.940 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.87/0.96          Theta(max)= 72.832

R(reflections)= 0.0368( 13529)          wR2(reflections)=  
0.1027( 13878)  
S = 1.023          Npar= 844

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

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.3 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range	3.3 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C55 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C64 Check

### ● Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	2 Note
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing .....	0.00010 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp <sup>2</sup> )-Methyl Moiety .....	C44 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....	2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	46 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	7 Info

---

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

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

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## Datablock: jrl2-225\_1\_monop

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Bond precision: C-C = 0.0117 A Wavelength=1.54184

Cell: a=12.1188(3) b=24.4511(4) c=24.1015(4)  
alpha=90 beta=90.980(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	7140.7(2)	7140.7(2)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C36 H53 N3 O, C H4 O	C36 H53 N3 O, 1(C1 H4 O1)
Sum formula	C37 H57 N3 O2	C37 H57 N3 O2
Mr	575.86	575.85
Dx, g cm <sup>-3</sup>	1.071	1.071
Z	8	8
Mu (mm <sup>-1</sup> )	0.503	0.503
F000	2528.0	2528.0
F000'	2534.50	
h, k, lmax	14, 29, 29	14, 29, 29
Nref	27089[ 13884]	75133
Tmin, Tmax	0.941, 0.951	0.940, 1.000
Tmin'	0.904	

Correction method= # Reported T Limits: Tmin=0.940 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 5.41/2.77 Theta(max)= 69.997

R(reflections)= 0.0795( 59408)

wR2(reflections)=  
0.2409( 75133)

S = 1.026

Npar= 1618

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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**

PLAT414\_ALERT\_2\_A Short Intra D-H..H-X H6A ..H11M . 1.74 Ang.  
x,y,z = 1\_555 Check

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**Alert level B**

PLAT340\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.01168 Ang.  
PLAT417\_ALERT\_2\_B Short Inter D-H..H-D H6A ..H12 . 1.84 Ang.  
-x,-1/2+y,-z = 2\_545 Check

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**Alert level C**

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT213\_ALERT\_2\_C Atom C84 has ADP max/min Ratio ..... 3.5 prolat  
PLAT213\_ALERT\_2\_C Atom C84A has ADP max/min Ratio ..... 3.5 prolat  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio  
PLAT220\_ALERT\_2\_C NonSolvent Resd 4 C Ueq(max)/Ueq(min) Range 3.2 Ratio  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for N8 --C78 . 6.0 s.u.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C122 --C123 . 0.23 Ang.  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C121 Check  
PLAT414\_ALERT\_2\_C Short Intra D-H..H-X H12 ..H119 . 1.96 Ang.  
x,y,z = 1\_555 Check  
PLAT601\_ALERT\_2\_C Unit Cell Contains Solvent Accessible VOIDS of . 34 Ang\*\*3  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & Sth/L= 0.600 30 Report

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**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 33 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 14 Report  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 5 Report  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.14 Report  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 8 Report  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 6 Report  
PLAT177\_ALERT\_4\_G The CIF-Embedded .res File Contains DELU Records 3 Report  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 3 Report  
PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0100 Report  
PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0200 Report  
PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0200 Report  
PLAT192\_ALERT\_3\_G A Non-default DELU Restraint Value for First Par 0.0050 Report  
PLAT192\_ALERT\_3\_G A Non-default DELU Restraint Value for SecondPar 0.0050 Report  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 15% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 5 ) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 9 ) 100% Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 5 ) 5.14 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 9 ) 0.86 Check  
PLAT415\_ALERT\_2\_G Short Inter D-H..H-X H6 ..H38F . 1.67 Ang.  
2-x,1/2+y,1-z = 2\_756 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O1 ..C38A . 2.68 Ang.  
x,y,z = 1\_555 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 1 Note

PLAT722_ALERT_1_G	Angle Calc	113.00, Rep	111.80 Dev...	1.20 Degree
	C83A -C82A -H82C	1_555 1_555 1_555	# 748	Check
PLAT722_ALERT_1_G	Angle Calc	111.00, Rep	109.40 Dev...	1.60 Degree
	C82A -C83A -H83D	1_555 1_555 1_555	# 751	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell:	Resd.	#	2 Note
	C36 H53 N3 O			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell:	Resd.	#	5 Note
	C H4 O			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell:	Resd.	#	6 Note
	C H4 O			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell:	Resd.	#	9 Note
	C H4 O			
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....		127 Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed	..		! Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			1 Note
PLAT916_ALERT_2_G	Hooft y and Flack x Parameter Values Differ by	.		0.36 Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law ( 0 0 1)		Est.d BASF	0.34 Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law ( 1 0 0)		Est.d BASF	0.26 Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res	..		140.0 Degree
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by			7 Check

---

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

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

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## Datablock: jrl2-224\_auto

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Bond precision:	C-C = 0.0018 A		Wavelength=1.54184
Cell:	a=18.1209(1)	b=16.4444(1)	c=48.5140(3)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	14456.56(15)	14456.56(15)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C36 H47 N3 O, 2(C H4 O)	C36 H47 N3 O, 2(C H4 O)
Sum formula	C38 H55 N3 O3	C38 H55 N3 O3
Mr	601.85	601.85
Dx, g cm <sup>-3</sup>	1.106	1.106
Z	16	16
Mu (mm <sup>-1</sup> )	0.540	0.540
F000	5248.0	5248.0
F000'	5262.05	
h, k, lmax	22, 20, 60	22, 20, 60
Nref	14508	14411
Tmin, Tmax	0.937, 0.947	0.827, 1.000
Tmin'	0.922	

Correction method= # Reported T Limits: Tmin=0.827 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.993                      Theta(max)= 73.177

R(reflections)= 0.0423( 12832)                      wR2(reflections)=  
0.1091( 14411)  
S = 1.016                      Npar= 861

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

PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.9 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.3 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C22 --C23 .	5.7 s.u.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C22	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.168 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	8 Report

### ● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	4 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.23 Why ?
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing .....	0.00010 Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing .....	0.00030 Ang.
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2 Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1 Report

PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200 Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C31 --C32 .	6.5 s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	8% Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	4 Note
	C H4 O	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	30 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	87 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	11 Info

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

0 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  
7 ALERT type 3 Indicator that the structure quality may be low  
8 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

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## Datablock: jrl2-511

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Bond precision:	C-C = 0.0052 A	Wavelength=1.54184	
Cell:	a=17.7856(3)	b=16.5240(2)	c=48.7265(6)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	14320.2(3)	14320.2(3)	
Space group	P b c a	P b c a	
Hall group	-P 2ac 2ab	-P 2ac 2ab	
Moiety formula	C36 H47 N3 O, C4 H8 O	?	
Sum formula	C40 H55 N3 O2	C40 H55 N3 O2	
Mr	609.87	609.87	
Dx, g cm <sup>-3</sup>	1.132	1.132	
Z	16	16	
Mu (mm <sup>-1</sup> )	0.532	0.532	
F000	5312.0	5312.0	
F000'	5325.82		
h, k, lmax	21, 20, 59	21, 20, 59	
Nref	13579	13539	
Tmin, Tmax	0.938, 0.974	0.632, 1.000	
Tmin'	0.899		



Correction method= # Reported T Limits: Tmin=0.632 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.997                      Theta(max)= 69.991

R(reflections)= 0.1061( 11369)

wR2(reflections)=  
0.2779( 13539)

S = 1.055

Npar= 858


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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**

PLAT353\_ALERT\_3\_B Long    N-H (N0.87,N1.01A)    N3            - H3            .            1.11 Ang.

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 **Alert level C**

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75

The relevant atom site should be identified.

PLAT082_ALERT_2_C High R1 Value .....	0.11	Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) .....	0.28	Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density	0.61	eA-3
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds .....	0.00522	Ang.
PLAT353_ALERT_3_C Long    N-H (N0.87,N1.01A)    N5            - H5            .	1.01	Ang.
PLAT353_ALERT_3_C Long    N-H (N0.87,N1.01A)    N6            - H6            .	1.03	Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	14.591	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	3.299	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600	28	Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1	Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens.    1.02Ang From N6            .	0.47	eA-3

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 **Alert level G**

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 ...	5	Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT    Unusually Large	35.26	Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT300_ALERT_4_G Atom Site Occupancy of C37            Constrained at	0.5021	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C38            Constrained at	0.5021	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C39            Constrained at	0.5021	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C40            Constrained at	0.5021	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C37A            Constrained at	0.4979	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C38A            Constrained at	0.4979	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C39A            Constrained at	0.4979	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C40A            Constrained at	0.4979	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37A            Constrained at	0.5021	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37B            Constrained at	0.5021	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H38A	Constrained at	0.5021	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38B	Constrained at	0.5021	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39A	Constrained at	0.5021	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39B	Constrained at	0.5021	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40A	Constrained at	0.5021	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40B	Constrained at	0.5021	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37C	Constrained at	0.4979	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37D	Constrained at	0.4979	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38C	Constrained at	0.4979	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38D	Constrained at	0.4979	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39C	Constrained at	0.4979	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39D	Constrained at	0.4979	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40C	Constrained at	0.4979	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40D	Constrained at	0.4979	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )		80%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O2	.	103.6	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O4	.	109.6	Degree
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		50	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL		2019/3	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		12	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		2	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged			Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		140.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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

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

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## Datablock: JRL2-002

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Bond precision: C-C = 0.0055 A                      Wavelength=1.54184

Cell:                      a=11.9011(2)                      b=39.1542(5)                      c=17.6802(2)  
                                alpha=90                      beta=103.815(1)                      gamma=90

Temperature:                      100 K



PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	27.06	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	8%	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	39.60	Deg.
	O1 -C6 -LI1 1_555 1_555 1_555 ..... #	76	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	41.20	Deg.
	O4 -C50 -LI2 1_555 1_555 1_555 ..... #	277	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	50	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	125	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	15	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.1	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
6 **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  
8 ALERT type 2 Indicator that the structure model may be wrong or deficient  
10 ALERT type 3 Indicator that the structure quality may be low  
8 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

---

## Datablock: JRL2-490

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Bond precision: C-C = 0.0048 Å                      Wavelength=1.54184

Cell:                      a=17.4150(2)              b=21.3107(3)              c=19.8706(2)  
                                alpha=90                      beta=94.020(1)              gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	7356.35(15)	7356.35(15)
Space group	I 2	I 2
Hall group	I 2y	I 2y
Moiety formula	2(C152 H200 Li4 N12 O6), 4(C3 H2.50), C2 H6	?
Sum formula	C318 H416 Li8 N24 O12	C159 H208 Li4 N12 O6
Mr	4822.29	2411.12
Dx, g cm <sup>-3</sup>	1.089	1.089
Z	1	2
Mu (mm <sup>-1</sup> )	0.499	0.499
F000	2612.0	2612.0
F000'	2618.69	
h, k, lmax	21, 26, 24	21, 26, 24
Nref	14801[ 7608]	12324
Tmin, Tmax	0.877, 0.947	0.479, 1.000
Tmin'	0.848	

Correction method= # Reported T Limits: Tmin=0.479 Tmax=1.000  
AbsCorr = GAUSSIAN

Data completeness= 1.62/0.83                      Theta(max)= 73.277

R(reflections)= 0.0473( 11771)

wR2(reflections)=  
0.1304( 12324)

S = 1.051

Npar= 886

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

PLAT035_ALERT_1_B	_chemical_absolute_configuration	Info	Not Given	Please Do !
PLAT250_ALERT_2_B	Large U3/U1 Ratio for Average U(i,j) Tensor	....		6.5 Note
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers	..		2 Check

#### Alert level C

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	5.6	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	6.0	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	03	Check
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	C19	Check
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	C58	Check
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	C70	Check
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....		0.0048	Ang.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible	VOIDS of	.		58	Ang**3
PLAT911_ALERT_3_C	Missing FCF Refl Between	Thmin & STh/L=	0.600		18	Report



PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	82	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.5	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

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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
  - 10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  - 52 **ALERT level G** = General information/check it is not something unexpected
- 
- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  - 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
  - 12 ALERT type 3 Indicator that the structure quality may be low
  - 35 ALERT type 4 Improvement, methodology, query or suggestion
  - 0 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.

