

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) JRL2-145, JRL3-014, JRL3-015, jrl1-205, jrl1-208\_auto, jrl2-223\_auto1, jrl2-227\_1\_auto, jrl2-229\_full\_auto, jrl2-230\_auto, jrl2-234\_1\_auto, jrl2-235\_auto\_recollect\_best, jrl3-011\_auto, rmg3-209

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: jrl2-223\_auto1

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Bond precision:    C-C = 0.0031 A                      Wavelength=1.54184

Cell:                      a=12.7220 (2)              b=19.5785 (3)              c=49.9964 (7)  
                                    alpha=90                      beta=90                      gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	12453.0 (3)	12453.0 (3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C33 H49 N3 O	C33 H49 N3 O
Sum formula	C33 H49 N3 O	C33 H49 N3 O
Mr	503.75	503.75
Dx, g cm <sup>-3</sup>	1.075	1.075
Z	16	16
Mu (mm <sup>-1</sup> )	0.491	0.491
F000	4416.0	4416.0
F000'	4427.11	
h, k, lmax	15, 24, 61	15, 24, 61
Nref	12381	12294
Tmin, Tmax	0.952, 0.952	0.987, 1.000
Tmin'	0.952	

Correction method= # Reported T Limits: Tmin=0.987 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.993

Theta (max)= 72.681

R(reflections)= 0.0591( 10044)

wR2(reflections)=  
0.1488( 12294)

S = 1.053

Npar= 807

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**

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	4.2	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 2	C	Ueq(max)/Ueq(min) Range	3.8	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	4.1	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 2	H	Uiso(max)/Uiso(min) Range	6.6	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	C31	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....			9.394	Check

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				30	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms				28	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large			7.01	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				7	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records				8	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records				8	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
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
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
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used				0.0200	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of H4	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5	Constrained at			0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	.....(Resd 1 )			16%	Note
PLAT301_ALERT_3_G	Main Residue Disorder	.....(Resd 2 )			16%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H12	..H20F	.	2.08	Ang.
			x,y,z =		1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H50A	..H66D	.	1.78	Ang.
			x,y,z =		1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H17B	..H42F	.	1.92	Ang.
			x,y,z =		1_555	Check
PLAT414_ALERT_2_G	Short Intra D-H..H-X	H2	..H28A	.	2.11	Ang.
			x,y,z =		1_555	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....			217	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			86	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	.....			4.6	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				10	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  
28 **ALERT level G** = General information/check it is not something unexpected

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

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## Datablock: jrl2-229\_full\_auto

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Bond precision: C-C = 0.0018 A Wavelength=1.54184  
Cell: a=10.3763(1) b=15.5437(2) c=20.5455(2)  
alpha=106.822(1) beta=102.634(1) gamma=92.543(1)  
Temperature: 100 K

	Calculated	Reported
Volume	3074.47(6)	3074.47(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H47 N3 O	C32 H47 N3 O
Sum formula	C32 H47 N3 O	C32 H47 N3 O
Mr	489.73	489.72
Dx, g cm <sup>-3</sup>	1.058	1.058
Z	4	4
Mu (mm <sup>-1</sup> )	0.485	0.485
F000	1072.0	1072.0
F000'	1074.71	
h, k, lmax	12, 19, 25	12, 19, 25
Nref	12255	12186
Tmin, Tmax	0.908, 0.908	0.954, 1.000
Tmin'	0.908	

Correction method= # Reported T Limits: Tmin=0.954 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 72.834

R(reflections)= 0.0407( 10779) wR2(reflections)=  
0.1102( 12186)  
S = 1.043 Npar= 735

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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

PLAT220_ALERT_2_C	NonSolvent	Resd 2	C	Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	C59	Check
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of	.			61	Ang**3
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....			2.004	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				7	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				2	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
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )			8%	Note
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 2 )			8%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H25		..H28A	2.04	Ang.
				x,y,z =	1_555	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....				54	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			67	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....				4.1	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				13	Info

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

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

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## Datablock: jrl3-011\_auto

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Bond precision: C-C = 0.0034 A

Wavelength=1.54184

Cell: a=12.5415(4) b=12.5602(4) c=14.4976(4)  
 alpha=106.503(2) beta=101.638(3) gamma=112.001(3)  
 Temperature: 100 K

	Calculated	Reported
Volume	1904.32(13)	1904.32(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C72 H108 Li2 N6 O4, 2(C4 H8 O)	C72 H108 Li2 N6 O4, 2(C4 H8 O)
Sum formula	C80 H124 Li2 N6 O6	C80 H124 Li2 N6 O6
Mr	1279.73	1279.72
Dx, g cm <sup>-3</sup>	1.116	1.116
Z	1	1
Mu (mm <sup>-1</sup> )	0.533	0.533
F000	700.0	700.0
F000'	701.82	
h, k, lmax	15, 15, 17	15, 15, 17
Nref	7631	7605
Tmin, Tmax	0.880, 0.948	0.740, 1.000
Tmin'	0.852	

Correction method= # Reported T Limits: Tmin=0.740 Tmax=1.000  
 AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 73.209

R(reflections)= 0.0621( 6401) wR2(reflections)= 0.1908( 7605)  
 S = 1.040 Npar= 450

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**

PLAT934\_ALERT\_3\_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 3 Check

**Alert level C**

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

The relevant atom site should be identified.

PLAT097\_ALERT\_2\_C Large Reported Max. (Positive) Residual Density 0.63 eA-3

PLAT353\_ALERT\_3\_C Long N-H (N0.87, N1.01A) N3 - H3 . 1.02 Ang.

PLAT790\_ALERT\_4\_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note

C72 H108 Li2 N6 O4

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	5.472	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	13.996	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	17.003	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600		2 Report

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**Alert level G**

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11	Report
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	2	Units
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	1	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	5%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3	102.5	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	10	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	41.10	Deg.
	O1 -C6 -LI1 1_555 1_555 1_555 .....	# 53	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	C4 H8 O		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	25	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	12	Info

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

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## Datablock: jrl2-227\_1\_auto

Bond precision:	C-C = 0.0039 A	Wavelength=1.54184	
Cell:	a=36.168 (1)	b=9.3438 (1)	c=29.3254 (8)
	alpha=90	beta=126.404 (4)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	7976.4(5)	7976.4(5)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C45 H56 N4 O4	C45 H56 N4 O4
Sum formula	C45 H56 N4 O4	C45 H56 N4 O4
Mr	716.94	716.93
Dx, g cm <sup>-3</sup>	1.194	1.194
Z	8	8
Mu (mm <sup>-1</sup> )	0.601	0.601
F000	3088.0	3088.0
F000'	3096.59	
h, k, lmax	44, 11, 36	44, 11, 36
Nref	8017	7981
Tmin, Tmax	0.805, 0.887	0.689, 1.000
Tmin'	0.740	

Correction method= # Reported T Limits: Tmin=0.689 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.996                      Theta(max)= 73.264

R(reflections)= 0.0686( 7221)                      wR2(reflections)=  
0.2000( 7981)  
S = 1.064                      Npar= 544

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

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C29	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C41	Check
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance .....	6.530	Check



#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	18	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	14	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.10	Report
PLAT073_ALERT_1_G	H-atoms ref, but _hydrogen_treatment Reported as	constr	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	8.58	Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a	Note
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	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	4	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	4	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report

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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
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 )                  11% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C2 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H37      ..H46A      .    2.11 Ang.
                                                              x,y,z =      1_555 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....              110 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      35 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      2 Info

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9 ALERT type 2 Indicator that the structure model may be wrong or deficient
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0 ALERT type 5 Informative message, check

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## Datablock: JRL2-145

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Bond precision: C-C = 0.0065 A

Wavelength=1.54184

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Cell:          a=10.7157(3)          b=11.1222(3)          c=16.6424(6)
               alpha=83.814(3)      beta=73.808(3)       gamma=61.632(3)
Temperature:   100 K

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	Calculated	Reported
Volume	1675.34(10)	1675.34(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C37 H49 N3 S	?
Sum formula	C37 H49 N3 S	C37 H49 N3 S
Mr	567.85	567.85
Dx, g cm-3	1.126	1.126
Z	2	2
Mu (mm-1)	1.056	1.056
F000	616.0	616.0
F000'	618.10	
h, k, lmax	13, 13, 20	13, 13, 20
Nref	6351	6343
Tmin, Tmax	0.827, 0.969	0.721, 1.000
Tmin'	0.827	



Correction method= # Reported T Limits: Tmin=0.721 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.999                      Theta(max)= 69.997

R(reflections)= 0.0994( 6054)

wR2(reflections)=  
0.2723( 6343)

S = 1.133

Npar= 411

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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) .....	0.27	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.47	Report
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C23	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.0065	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	7.447	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.098	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	6	Report

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**Alert level G**

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree
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
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	5%	Note
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C26 - C29 .	1.51	Ang.
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H26 ..H28E .	1.89	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H26 ..H28F .	1.77	Ang.
	x,y,z =	1_555	Check
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	3	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.0	Low
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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4 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## Datablock: jrl1-205

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Bond precision: C-C = 0.0032 A Wavelength=1.54184  
Cell: a=17.3623(1) b=16.3139(1) c=29.6995(2)  
alpha=90 beta=96.708(1) gamma=90  
Temperature: 100 K

	Calculated	Reported
Volume	8354.70(9)	8354.70(9)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C41 H56 Li N3 O S, C4 H8 O	?
Sum formula	C45 H64 Li N3 O2 S	C45 H64 Li N3 O2 S
Mr	717.99	717.99
Dx, g cm <sup>-3</sup>	1.142	1.142
Z	8	8
Mu (mm <sup>-1</sup> )	0.976	0.976
F000	3120.0	3120.0
F000'	3130.27	
h, k, lmax	21, 20, 36	21, 20, 36
Nref	8316	8300
Tmin, Tmax	0.823, 0.971	0.157, 1.000
Tmin'	0.823	

Correction method= # Reported T Limits: Tmin=0.157 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 72.697

R(reflections)= 0.0677( 7998) wR2(reflections)=  
0.1915( 8300)  
S = 1.060 Npar= 484

---

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	5.1	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	5.1	Ratio
PLAT230_ALERT_2_C	Hirshfeld	Test Diff	for	S1	--C6	.	5.1 s.u.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq	as Compared to Neighbors of			C39 Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq	as Compared to Neighbors of			C40 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared to Neighbors of			C38 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared to Neighbors of			C41 Check
PLAT243_ALERT_4_C	High	'Solvent'	Ueq	as Compared to Neighbors of			O2 Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq	as Compared to Neighbors of			C44 Check
PLAT906_ALERT_3_C	Large K Value	in the Analysis of Variance	.....			3.299	Check

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					4	Note
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large				13.07	Why ?
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as						mixed Check
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 .....					0.00020	Ang.
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records					1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records					2	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )					20%	Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....					C2	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....					C5	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O2					102.9	Degree
PLAT410_ALERT_2_G	Short Intra H...H Contact	H42B	..H45B	.		1.79	Ang.
			x,y,z =			1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact	H45A	..H42D	.		2.14	Ang.
			x,y,z =			1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact	H45B	..H42C	.		2.13	Ang.
			x,y,z =			1_555	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact	H28	..H42D	.		2.01	Ang.
			-x,y,3/2-z =			2_556	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...					44.50	Deg.
	N2 -C4 -LI1	1_555	1_555	1_555	.....	#	49 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....					4	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				16	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File					1	Note
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.					8	Info

- 
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
23 **ALERT level G** = General information/check it is not something unexpected
- 2 **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  
12 **ALERT type 4** Improvement, methodology, query or suggestion  
0 **ALERT type 5** Informative message, check
-

## Datablock: jrl2-235\_auto\_recollect\_best

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Bond precision: C-C = 0.0031 A Wavelength=1.54184  
 Cell: a=10.5704 (1) b=24.5114 (4) c=12.5262 (2)  
       alpha=90 beta=94.375 (1) gamma=90  
 Temperature: 100 K

	Calculated	Reported
Volume	3236.02 (8)	3236.02 (8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C34 H51 N3 S	?
Sum formula	C34 H51 N3 S	C34 H51 N3 S
Mr	533.84	533.83
Dx, g cm <sup>-3</sup>	1.096	1.096
Z	4	4
Mu (mm <sup>-1</sup> )	1.060	1.060
F000	1168.0	1168.0
F000'	1171.99	
h, k, lmax	13, 30, 15	13, 30, 15
Nref	6515	6473
Tmin, Tmax	0.826, 0.909	0.738, 1.000
Tmin'	0.759	

Correction method= # Reported T Limits: Tmin=0.738 Tmax=1.000  
 AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 73.424

R(reflections)= 0.0719 ( 5861) wR2(reflections)=  
 0.2064 ( 6473)  
 S = 1.075 Npar= 501

---

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	3.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C13 --C14 .	0.17 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C25 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N3 --H3N .	Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	6.586 Check

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	28	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	43	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	12	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	5	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	7	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	8	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
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
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
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 )	58%	Note
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C3 - C6 .	1.51	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C20 - C28 .	1.52	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C24 - C25 .	1.52	Ang.
PLAT410_ALERT_2_G	Short Intra H...H Contact H16 ..H25 .	2.13	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H21 ..H30D .	2.10	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H23 ..H26A .	2.12	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H25 ..H26E .	1.43	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H25 ..H26F .	1.85	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H28 ..H29D .	2.05	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H28 ..H29E .	1.89	Ang.
	x,y,z =	1_555	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....		! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	328	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	41	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
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.	7	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  
34 **ALERT level G** = General information/check it is not something unexpected

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

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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	6.81	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 .....	0.00020	Ang.
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
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O1 --C37A .	8.5	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	9%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O2 .	104.7	Degree
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	44.61	Deg.
	N2 -C4 -LI1 1_555 1_555 1_555 .....	#	52 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	C4 H8 O		
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
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	29	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	12	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  
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

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

---

## Datablock: jrl2-230\_auto

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Bond precision: C-C = 0.0023 A

Wavelength=1.54184

Cell: a=10.7566(1)

b=14.9826(2)

c=20.4206(2)

alpha=104.718(1)

beta=102.225(1)

gamma=92.800(1)

Temperature: 100 K

	Calculated	Reported
Volume	3092.46(6)	3092.46(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H47 N3 S	C32 H47 N3 S
Sum formula	C32 H47 N3 S	C32 H47 N3 S
Mr	505.79	505.78
Dx,g cm-3	1.086	1.086
Z	4	4
Mu (mm-1)	1.086	1.086
F000	1104.0	1104.0
F000'	1107.85	
h,k,lmax	13,18,25	13,18,25
Nref	12290	12239
Tmin,Tmax	0.897,0.897	0.847,1.000
Tmin'	0.897	

Correction method= # Reported T Limits: Tmin=0.847 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.996                      Theta(max)= 72.657

R(reflections)= 0.0494( 11023)

wR2(reflections)=  
0.1469( 12239)

S = 1.048

Npar= 735

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

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C18	Check
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of .	33	Ang**3
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3	Report

#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	14	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	14	Report
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF .....		Please Check
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	2	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	4	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	4	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







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

1 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  
3 ALERT type 3 Indicator that the structure quality may be low  
5 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

---

## Datablock: jrl2-234\_1\_auto

---

Bond precision: C-C = 0.0031 A Wavelength=1.54184  
Cell: a=19.1031(3) b=13.1154(2) c=17.1154(2)  
alpha=90 beta=95.202(1) gamma=90  
Temperature: 100 K

	Calculated	Reported
Volume	4270.51(11)	4270.51(11)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C24 H28 N2 O S	C24 H28 N2 O S
Sum formula	C24 H28 N2 O S	C24 H28 N2 O S
Mr	392.54	392.54
Dx, g cm <sup>-3</sup>	1.221	1.221
Z	8	8
Mu (mm <sup>-1</sup> )	1.460	1.460
F000	1680.0	1680.0
F000'	1686.79	
h, k, lmax	23, 16, 21	23, 16, 21
Nref	4297	4230
Tmin, Tmax	0.740, 0.864	0.674, 1.000
Tmin'	0.661	

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

Data completeness= 0.984 Theta(max)= 73.152

R(reflections)= 0.0479( 3673)

wR2(reflections)=  
0.1398( 4230)

S = 1.061

Npar= 259

---

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**

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	46.631	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	36.103	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.977	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	13	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1	Check

---

● **Alert level G**

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	54	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	4	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.6	Low
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  
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

1 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  
6 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: jrl1-208\_auto

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Bond precision:	C-C = 0.0018 A	Wavelength=1.54184	
Cell:	a=10.3476(1)	b=26.5676(3)	c=12.3488(1)
	alpha=90	beta=94.130(1)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	3386.00(6)	3386.00(6)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C36 H56 N4	C36 H56 N4
Sum formula	C36 H56 N4	C36 H56 N4
Mr	544.85	544.84
Dx, g cm <sup>-3</sup>	1.069	1.069
Z	4	4
Mu (mm <sup>-1</sup> )	0.468	0.468
F000	1200.0	1200.0
F000'	1202.89	
h, k, lmax	12, 32, 15	12, 32, 15
Nref	6750	6726
Tmin, Tmax	0.894, 0.954	0.862, 1.000
Tmin'	0.869	

Correction method= # Reported T Limits: Tmin=0.862 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.996                      Theta(max)= 72.836

R(reflections)= 0.0455( 6320)    wR2(reflections)=  
0.1188( 6726)

S = 1.037    Npar= 383

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

PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 2.31 Report  
PLAT420\_ALERT\_2\_C D-H Bond Without Acceptor N4 --H4 . Please Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.281 Check



#### Alert level G

PLAT143\_ALERT\_4\_G s.u. on c - Axis Small or Missing ..... 0.00010 Ang.  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 25 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 9 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
  - 0 **ALERT level B** = A potentially serious problem, consider carefully
  - 3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  - 3 **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  
1 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

---

## Datablock: rmg3-209

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Bond precision: C-C = 0.0022 A Wavelength=0.71073  
Cell: a=8.9017(4) b=22.600(1) c=17.5432(7)  
alpha=90 beta=98.902(4) gamma=90  
Temperature: 123 K

	Calculated	Reported
Volume	3486.8(3)	3486.8(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C36 H56 N4	C36 H56 N4
Sum formula	C36 H56 N4	C36 H56 N4
Mr	544.85	544.84
Dx, g cm <sup>-3</sup>	1.038	1.038
Z	4	4
Mu (mm <sup>-1</sup> )	0.060	0.060
F000	1200.0	1200.0
F000'	1200.36	
h, k, lmax	12, 30, 23	12, 30, 23
Nref	9255	8838
Tmin, Tmax	0.993, 0.994	0.556, 1.000
Tmin'	0.988	

Correction method= # Reported T Limits: Tmin=0.556 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.955 Theta(max)= 28.990

R(reflections)= 0.0584( 6077) wR2(reflections)=  
0.1337( 8838)  
S = 1.018 Npar= 379

---

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). 16 Note

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**Alert level C**

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.2 Ratio  
PLAT410\_ALERT\_2\_C Short Intra H...H Contact H3A ..H10 . 1.92 Ang.  
x,y,z = 1\_555 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 6.234 Check

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**Alert level G**

PLAT380\_ALERT\_4\_G Incorrectly? Oriented X(sp<sup>2</sup>)-Methyl Moiety ..... C2 Check  
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= 0.600 402 Note  
PLAT967\_ALERT\_5\_G Note: Two-Theta Cutoff Value in Embedded .res .. 58.0 Degree  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 7 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  
1 **ALERT level B** = A potentially serious problem, consider carefully  
3 **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

- 1 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  
2 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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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.





























