

Structure factors have been supplied for datablock(s) comp_luz1_x3301fin, comp_luz2_x3302fin, comp_luz4_x3594fin, comp_luz5_x3531fin, comp_luz6_x3609fin, comp_luz7_x3551fin

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0030 A	Wavelength=0.71073	
Cell:	a=15.3336(8)	b=7.3247(3)	c=18.8973(9)
	alpha=90	beta=105.003(5)	gamma=90
Temperature:	130 K		

	Calculated	Reported
Volume	2050.08(17)	2050.08(17)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C15 H24 B10 F N3 O2	C15 H24 B10 F N3 O2
Sum formula	C15 H24 B10 F N3 O2	C15 H24 B10 F N3 O2
Mr	405.47	405.47
Dx, g cm-3	1.314	1.314
Z	4	4
Mu (mm-1)	0.084	0.084
F000	840.0	840.0
F000'	840.30	
h, k, lmax	20, 9, 25	20, 9, 24
Nref	5078	4476
Tmin, Tmax	0.997, 0.998	0.715, 1.000
Tmin'	0.967	

Data completeness= 0.881 Theta (max)= 28.262

R(reflections)= 0.0565(2702)	wR2(reflections)= 0.1427(4476)
S = 1.011	Npar= 401

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	3.8	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 1	O	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	7.1	Ratio
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance				4.634	Check

 Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				39	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				19	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms				2	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				4	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records				1	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records				1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records				2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records				1	Report
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)			61%	Note
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for			C1	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1		- C2		1.68	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				2	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms				!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				80	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				596	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity				3.8	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				4	Info

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

0 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
6 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

Datablock: comp_luz2_x3302fin

Bond precision: C-C = 0.0026 A

Wavelength=0.71073

Cell: a=7.2038(2)

b=24.2149(6)

c=10.9508(3)

alpha=90

beta=93.956(2)

gamma=90

Temperature: 130 K

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C2	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C2	1.63	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C2 - C3	1.52	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	531	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

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 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

 0 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
 4 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: comp_luz4_x3594fin

Bond precision: C-C = 0.0016 A Wavelength=0.71073

 Cell: a=6.9499(2) b=12.2343(5) c=13.0166(5)
 alpha=109.825(4) beta=94.822(3) gamma=92.968(3)
 Temperature: 130 K

	Calculated	Reported
Volume	1033.67(7)	1033.67(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C15 H24 B10 F N3 O2	C15 H24 B10 F N3 O2
Sum formula	C15 H24 B10 F N3 O2	C15 H24 B10 F N3 O2
Mr	405.47	405.47
Dx, g cm-3	1.303	1.303
Z	2	2
Mu (mm-1)	0.083	0.083
F000	420.0	420.0
F000'	420.15	
h, k, lmax	10, 18, 19	10, 18, 19
Nref	7481	6887
Tmin, Tmax	0.964, 0.993	0.993, 1.000
Tmin'	0.964	

Correction method= # Reported T Limits: Tmin=0.993 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.921 Theta(max)= 32.473

R(reflections)= 0.0489(5493) wR2(reflections)=
 0.1370(6887)
 S = 1.024 Npar= 376

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 3.141 Check



Alert level G

PLAT343_ALERT_2_G Unusual sp?	Angle Range in Main Residue for	C1 Check
PLAT343_ALERT_2_G Unusual sp?	Angle Range in Main Residue for	C2 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels		1 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).		3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		592 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		3.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		12 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by		3 Check

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- 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
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
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Datablock: comp_luz5_x3531fin

Bond precision: C-C = 0.0030 A

Wavelength=0.71073

Cell: a=13.2567(4) b=7.4299(2) c=20.6105(6)

alpha=90 beta=104.120(3) gamma=90

Temperature: 293 K

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	10	Report
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	5	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	6	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	4	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	0.0100	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT230_ALERT_2_G	Hirshfeld Test Diff for B0 --B6 .	5.5	s.u.

PLAT300_ALERT_4_G	Atom Site Occupancy of B0	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of B3	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of B5	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of B7	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of B10	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1F	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1G	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1H	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1I	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H0X	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3X	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5X	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7X	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10X	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1F	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1G	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1H	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1I	Constrained at	0.2	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		37%	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C2	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C2 - C3		1.52	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		2	Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1F --C1H		1.75	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1G --C1I		1.73	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1H --C1I		1.73	Ang.
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		71	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		472	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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 58 **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
 9 ALERT type 3 Indicator that the structure quality may be low
 38 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

Datablock: comp_luz6_x3609fin

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=22.6667(7) b=7.4977(2) c=24.4845(7)
alpha=90 beta=97.632(3) gamma=90

Temperature: 130 K

	Calculated	Reported
Volume	4124.2(2)	4124.2(2)
Space group	I 2/a	I 2/a
Hall group	-I 2ya	-I 2ya
Moiety formula	C15 H24 B10 F N3 O2	C15 H24 B10 F N3 O2
Sum formula	C15 H24 B10 F N3 O2	C15 H24 B10 F N3 O2
Mr	405.47	405.47
Dx, g cm ⁻³	1.306	1.306
Z	8	8
Mu (mm ⁻¹)	0.083	0.083
F000	1680.0	1680.0
F000'	1680.59	
h, k, lmax	30, 9, 32	29, 9, 31
Nref	5092	4617
Tmin, Tmax	0.985, 0.992	0.947, 1.000
Tmin'	0.963	

Correction method= # Reported T Limits: Tmin=0.947 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.907 Theta(max)= 28.237

R(reflections)= 0.0557(3112) wR2(reflections)=
0.1453(4617)

S = 1.016 Npar= 372

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

PLAT213_ALERT_2_C Atom C12	has ADP max/min Ratio	3.8 oblate
PLAT213_ALERT_2_C Atom C12F	has ADP max/min Ratio	3.8 oblate
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance		2.448 Check

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11	Note
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	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0030	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0030	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0030	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	16%	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C2	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	14	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	460	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

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3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: comp_luz7_x3551fin

Bond precision: C-C = 0.0019 A

Wavelength=1.54184

Cell: a=6.8918(2) b=10.4396(3) c=14.0592(3)
alpha=99.793(2) beta=100.469(2) gamma=92.309(2)
Temperature: 130 K

- ```
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
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8 **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

3 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

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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.

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