
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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report
0 0 4, 0 0 6, 0 0 8, 0 0 18, 0 0 20, 1 0 21,
0 0 22,
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 67 %



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.49225 Ang.
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing 0.00006 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00013 Ang.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
0 0 2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 399 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
-1 1 22, -1 1 2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.2 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 2 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 5 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 5 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info
PLAT984_ALERT_1_G The C-f' = -0.0004 Deviates from the B&C-Value 0.0006 Check
PLAT984_ALERT_1_G The O-f' = 0.0008 Deviates from the B&C-Value 0.0038 Check
PLAT984_ALERT_1_G The S-f' = 0.0506 Deviates from the B&C-Value 0.0646 Check

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

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

Datablock: Ylid_0p12

Bond precision: C-C = 0.0038 A

Wavelength=0.49225

Cell: a=5.9332(1) b=8.9956(4) c=18.3448(3)
 alpha=90 beta=90 gamma=90
 Temperature: 293 K

	Calculated	Reported
Volume	979.11(5)	979.11(5)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C11 H10 O2 S	C11 H10 O2 S
Sum formula	C11 H10 O2 S	C11 H10 O2 S
Mr	206.25	206.25
Dx, g cm ⁻³	1.399	1.399
Z	4	4
Mu (mm ⁻¹)	0.116	0.116
F000	432.0	432.0
F000'	432.27	
h, k, lmax	9, 14, 30	8, 8, 25
Nref	4492[2576]	1559
Tmin, Tmax	0.989, 0.994	0.848, 1.000
Tmin'	0.986	

Correction method= # Reported T Limits: Tmin=0.848 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.61/0.35 Theta(max)= 23.746

R(reflections)= 0.0285(1475) wR2(reflections)=
 0.0805(1559)
 S = 1.072 Npar= 129

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
 Click on the hyperlinks for more details of the test.

Alert level A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.564 Why?

Author Response: Our experiment was done using a diamond-anvil cell rotated about one axis by 76 deg. Hence, due to the strategy and a limited access to the sample in a high-pressure cell no complete data was collected.

Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 392 Report

0	2	0,	1	2	0,	1	3	0,	2	3	0,	0	4	0,	1	4	0,
2	4	0,	3	4	0,	4	4	0,	1	5	0,	2	5	0,	3	5	0,
4	5	0,	5	5	0,	6	5	0,	0	6	0,	1	6	0,	2	6	0,
3	6	0,	4	6	0,	5	6	0,	1	7	0,	2	7	0,	3	7	0,
4	7	0,	5	7	0,	0	8	0,	1	8	0,	2	8	0,	3	8	0,
4	8	0,	0	2	1,	1	2	1,	0	3	1,	1	3	1,	2	3	1,
0	4	1,	1	4	1,	2	4	1,	3	4	1,	0	5	1,	1	5	1,
2	5	1,	3	5	1,	4	5	1,	5	5	1,	6	5	1,	0	6	1,
1	6	1,	2	6	1,	3	6	1,	4	6	1,	5	6	1,	0	7	1,
1	7	1,	2	7	1,	3	7	1,	4	7	1,	5	7	1,	0	8	1,
1	8	1,	2	8	1,	3	8	1,	4	8	1,	0	2	2,	1	2	2,
0	3	2,	1	3	2,	2	3	2,	0	4	2,	1	4	2,	2	4	2,
3	4	2,	0	5	2,	1	5	2,	2	5	2,	3	5	2,	4	5	2,
5	5	2,	0	6	2,	1	6	2,	2	6	2,	3	6	2,	4	6	2,
5	6	2,	0	7	2,	1	7	2,	2	7	2,	3	7	2,	4	7	2,
5	7	2,	0	8	2,	1	8	2,	2	8	2,	3	8	2,	4	8	2,

PLAT915_ALERT_3_B No Flack x Check Done: Low Friedel Pair Coverage 27 %

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.

PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.49225 Ang.

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note

0 1 1, 0 0 2, 0 1 2,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 411 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note

0 2 2,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.9 Low

PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 6 Units

PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 5 Units

PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 6 Units

PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 5 Units

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

PLAT984_ALERT_1_G The C-f' = -0.0004 Deviates from the B&C-Value 0.0006 Check

PLAT984_ALERT_1_G The O-f' = 0.0008 Deviates from the B&C-Value 0.0038 Check

PLAT984_ALERT_1_G The S-f' = 0.0506 Deviates from the B&C-Value 0.0646 Check

1 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully

0 **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

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

1 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

2 ALERT type 4 Improvement, methodology, query or suggestion

2 ALERT type 5 Informative message, check

Datablock: Ylid_0p59

Bond precision: C-C = 0.0038 Å Wavelength=0.49225

Cell: a=5.83702 (5) b=8.8449 (3) c=18.1582 (2)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	937.47 (3)	937.47 (4)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C11 H10 O2 S	C11 H10 O2 S
Sum formula	C11 H10 O2 S	C11 H10 O2 S
Mr	206.25	206.25
Dx, g cm ⁻³	1.461	1.461
Z	4	4
Mu (mm ⁻¹)	0.121	0.121
F000	432.0	432.0
F000'	432.27	
h, k, lmax	9, 14, 29	8, 8, 25
Nref	4274 [2457]	1543
Tmin, Tmax	0.988, 0.994	0.871, 1.000
Tmin'	0.986	

Correction method= # Reported T Limits: Tmin=0.871 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.63/0.36 Theta(max)= 23.676

R(reflections)= 0.0304 (1466) wR2(reflections)=
 0.0828 (1543)

S = 1.006 Npar= 129

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
 Click on the hyperlinks for more details of the test.

Alert level A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.592 Why?

Author Response: Our experiment was done using a diamond-anvil cell rotated about one axis by 76 deg. Hence, due to the strategy and a limited access to the sample in a high-pressure cell no complete data was collected.

Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 350 Report
0 2 0, 1 2 0, 1 3 0, 2 3 0, 3 3 0, 0 4 0,
1 4 0, 2 4 0, 3 4 0, 4 4 0, 1 5 0, 2 5 0,
3 5 0, 4 5 0, 5 5 0, 6 5 0, 0 6 0, 1 6 0,
2 6 0, 3 6 0, 4 6 0, 5 6 0, 1 7 0, 2 7 0,
3 7 0, 4 7 0, 5 7 0, 0 8 0, 1 8 0, 2 8 0,
3 8 0, 4 8 0, 0 2 1, 1 2 1, 0 3 1, 1 3 1,
2 3 1, 0 4 1, 1 4 1, 2 4 1, 3 4 1, 4 4 1,
0 5 1, 1 5 1, 2 5 1, 3 5 1, 4 5 1, 5 5 1,
6 5 1, 0 6 1, 1 6 1, 2 6 1, 3 6 1, 4 6 1,
5 6 1, 0 7 1, 1 7 1, 2 7 1, 3 7 1, 4 7 1,
5 7 1, 0 8 1, 1 8 1, 2 8 1, 3 8 1, 4 8 1,
0 2 2, 0 3 2, 1 3 2, 2 3 2, 0 4 2, 1 4 2,
2 4 2, 3 4 2, 0 5 2, 1 5 2, 2 5 2, 3 5 2,
4 5 2, 5 5 2, 6 5 2, 0 6 2, 1 6 2, 2 6 2,
3 6 2, 4 6 2, 5 6 2, 0 7 2, 1 7 2, 2 7 2,
3 7 2, 4 7 2, 5 7 2, 0 8 2, 1 8 2, 2 8 2,
PLAT915_ALERT_3_B No Flack x Check Done: Low Friedel Pair Coverage 28 %

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.49225 Ang.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
0 1 1, 0 0 2, 0 1 2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 411 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
0 2 2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
8 2 2, 0 2 8,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.6 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 6 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 4 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 6 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 4 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info
PLAT984_ALERT_1_G The C-f'= -0.0004 Deviates from the B&C-Value 0.0006 Check
PLAT984_ALERT_1_G The O-f'= 0.0008 Deviates from the B&C-Value 0.0038 Check
PLAT984_ALERT_1_G The S-f'= 0.0506 Deviates from the B&C-Value 0.0646 Check

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

- 8 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: Ylid_2p12

Bond precision: C-C = 0.0061 Å Wavelength=0.49225
Cell: a=5.65687(7) b=8.5142(6) c=17.8238(4)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	858.46(6)	858.46(6)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C11 H10 O2 S	C11 H10 O2 S
Sum formula	C11 H10 O2 S	C11 H10 O2 S
Mr	206.25	206.25
Dx, g cm ⁻³	1.596	1.596
Z	4	4
Mu (mm ⁻¹)	0.133	0.132
F000	432.0	432.0
F000'	432.27	
h, k, lmax	9, 13, 29	8, 7, 24
Nref	3869[2235]	1314
Tmin, Tmax	0.987, 0.993	0.559, 1.000
Tmin'	0.984	

Correction method= # Reported T Limits: Tmin=0.559 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.59/0.34 Theta(max)= 23.617

R(reflections)= 0.0441(1246) wR2(reflections)=
0.1337(1314)
S = 1.151 Npar= 129

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.574 Why?

Author Response: Our experiment was done using a diamond-anvil cell rotated about one axis by 76 deg. Hence, due to the strategy and a limited access to the sample in a high-pressure cell no complete data was collected.

● Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 303 Report
 0 2 0, 0 4 0, 0 6 0, 1 2 0, 1 3 0, 1 4 0,
 1 5 0, 1 6 0, 1 7 0, 2 3 0, 2 4 0, 2 5 0,
 2 6 0, 2 7 0, 3 3 0, 3 4 0, 3 5 0, 3 6 0,
 3 7 0, 4 4 0, 4 5 0, 4 6 0, 4 7 0, 5 5 0,
 5 6 0, 0 2 1, 0 3 1, 0 4 1, 0 5 1, 0 6 1,
 0 7 1, 1 2 1, 1 3 1, 1 4 1, 1 5 1, 1 6 1,
 1 7 1, 2 3 1, 2 4 1, 2 5 1, 2 6 1, 2 7 1,
 3 4 1, 3 5 1, 3 6 1, 3 7 1, 4 4 1, 4 5 1,
 4 6 1, 4 7 1, 5 5 1, 5 6 1, 0 2 2, 0 3 2,
 0 4 2, 0 5 2, 0 6 2, 0 7 2, 1 2 2, 1 3 2,
 1 4 2, 1 5 2, 1 6 2, 1 7 2, 2 3 2, 2 4 2,
 2 5 2, 2 6 2, 2 7 2, 3 4 2, 3 5 2, 3 6 2,
 3 7 2, 4 5 2, 4 6 2, 4 7 2, 5 5 2, 5 6 2,
 0 1 3, 0 2 3, 0 3 3, 0 4 3, 0 5 3, 0 6 3,
 0 7 3, 1 2 3, 1 3 3, 1 4 3, 1 5 3, 1 6 3,
 1 7 3, 2 3 3, 2 4 3, 2 5 3, 2 6 3, 2 7 3,
 PLAT915_ALERT_3_B No Flack x Check Done: Low Friedel Pair Coverage 26 %

● Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 6.89 Note
 PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0061 Ang.

● Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
 not performed for this radiation type.
 PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.300 Report
 PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
 PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.49225 Ang.
 PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
 PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
 PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 with s.u. 0.30 Check
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
 0 1 1, 0 0 2, 0 1 2,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 349 Note
 PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
 0 2 2,
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
 2 1 19, 2 1 18,
 PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 6 Units
 PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 5 Units
 PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 6 Units
 PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 5 Units
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 10 Info
 PLAT984_ALERT_1_G The C-f' = -0.0004 Deviates from the B&C-Value 0.0006 Check
 PLAT984_ALERT_1_G The O-f' = 0.0008 Deviates from the B&C-Value 0.0038 Check

PLAT984_ALERT_1_G The S-f' = 0.0506 Deviates from the B&C-Value 0.0646 Check

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

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

Datablock: Ylid_2p82

Bond precision: C-C = 0.0125 A Wavelength=0.49225

Cell: a=5.6326(2) b=8.3700(15) c=17.6601(13)
alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	832.58(16)	832.58(16)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C11 H10 O2 S	C11 H10 O2 S
Sum formula	C11 H10 O2 S	C11 H10 O2 S
Mr	206.25	206.25
Dx, g cm ⁻³	1.645	1.645
Z	4	4
Mu (mm ⁻¹)	0.137	0.136
F000	432.0	432.0
F000'	432.27	
h, k, lmax	9, 13, 28	8, 7, 24
Nref	3696[2138]	1284
Tmin, Tmax	0.987, 0.993	0.239, 1.000
Tmin'	0.984	

Correction method= # Reported T Limits: Tmin=0.239 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.60/0.35 Theta(max)= 23.460

R(reflections)= 0.0893(1122)

wR2(reflections)=
0.2478(1284)

S = 1.130

Npar= 129

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

 Alert level A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.573 Why?

Author Response: Our experiment was done using a diamond-anvil cell rotated about one axis by 76 deg. Hence, due to the strategy and a limited access to the sample in a high-pressure cell no complete data was collected.

 Alert level B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.0125 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 304 Report

0	2	0,	0	4	0,	0	6	0,	1	2	0,	1	3	0,	1	4	0,
1	5	0,	1	6	0,	1	7	0,	2	3	0,	2	4	0,	2	5	0,
2	6	0,	2	7	0,	3	3	0,	3	4	0,	3	5	0,	3	6	0,
3	7	0,	4	4	0,	4	5	0,	4	6	0,	4	7	0,	5	5	0,
5	6	0,	0	2	1,	0	3	1,	0	4	1,	0	5	1,	0	6	1,
0	7	1,	1	2	1,	1	3	1,	1	4	1,	1	5	1,	1	6	1,
1	7	1,	2	3	1,	2	4	1,	2	5	1,	2	6	1,	2	7	1,
3	4	1,	3	5	1,	3	6	1,	3	7	1,	4	4	1,	4	5	1,
4	6	1,	4	7	1,	5	5	1,	5	6	1,	0	2	2,	0	3	2,
0	4	2,	0	5	2,	0	6	2,	0	7	2,	1	2	2,	1	3	2,
1	4	2,	1	5	2,	1	6	2,	1	7	2,	2	3	2,	2	4	2,
2	5	2,	2	6	2,	2	7	2,	3	4	2,	3	5	2,	3	6	2,
3	7	2,	4	4	2,	4	5	2,	4	6	2,	4	7	2,	5	5	2,
5	6	2,	0	1	3,	0	2	3,	0	3	3,	0	4	3,	0	5	3,
0	6	3,	0	7	3,	1	2	3,	1	3	3,	1	4	3,	1	5	3,
1	6	3,	1	7	3,	2	3	3,	2	4	3,	2	5	3,	2	6	3,

PLAT915_ALERT_3_B No Flack x Check Done: Low Friedel Pair Coverage 27 %

 Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 6.71 Note
PLAT234_ALERT_4_C Large Hirshfeld Difference S1 --C11 . 0.17 Ang.

 Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.300 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.49225 Ang.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact	S1	..C11	.	3.28 Ang.
		-x,-1/2+y,3/2-z	=	4_546 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	O2	..C4	.	2.99 Ang.
		-1+x,y,z	=	1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C4	..C9	.	3.18 Ang.
		1+x,y,z	=	1_655 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).				3 Note
	0	1	1,	0
	0	0	2,	0
	0	1	2,	
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600			349 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF				1 Note
	0	2	2,	
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity				4.7 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ				6 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.				4 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ				6 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.				4 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.				3 Info
PLAT984_ALERT_1_G The C-f' =	-0.0004	Deviates from the B&C-Value		0.0006 Check
PLAT984_ALERT_1_G The O-f' =	0.0008	Deviates from the B&C-Value		0.0038 Check
PLAT984_ALERT_1_G The S-f' =	0.0506	Deviates from the B&C-Value		0.0646 Check

1 **ALERT level A** = Most likely a serious problem - resolve or explain
 3 **ALERT level B** = A potentially serious problem, consider carefully
 2 **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

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

Datablock: Ylid_3p23

Bond precision:	C-C = 0.0135 A	Wavelength=0.49255
Cell:	a=5.6203(3)	b=8.346(2)
	alpha=90	beta=90
		gamma=90
Temperature:	293 K	

Alert level B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.0135 Ang.

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 309 Report

0	2	0,	0	4	0,	0	6	0,	1	2	0,	1	3	0,	1	4	0,
1	5	0,	1	6	0,	1	7	0,	2	3	0,	2	4	0,	2	5	0,
2	6	0,	2	7	0,	3	3	0,	3	4	0,	3	5	0,	3	6	0,
3	7	0,	4	4	0,	4	5	0,	4	6	0,	4	7	0,	5	4	0,

5	5	0,	5	6	0,	0	2	1,	0	3	1,	0	4	1,	0	5	1,
0	6	1,	0	7	1,	1	2	1,	1	3	1,	1	4	1,	1	5	1,
1	6	1,	1	7	1,	2	3	1,	2	4	1,	2	5	1,	2	6	1,
2	7	1,	3	4	1,	3	5	1,	3	6	1,	3	7	1,	4	4	1,
4	5	1,	4	6	1,	4	7	1,	5	5	1,	5	6	1,	0	2	2,
0	3	2,	0	4	2,	0	5	2,	0	6	2,	0	7	2,	1	2	2,
1	3	2,	1	4	2,	1	5	2,	1	6	2,	1	7	2,	2	3	2,
2	4	2,	2	5	2,	2	6	2,	2	7	2,	3	4	2,	3	5	2,
3	6	2,	3	7	2,	4	4	2,	4	5	2,	4	6	2,	4	7	2,
5	5	2,	5	6	2,	0	1	3,	0	2	3,	0	3	3,	0	4	3,
0	5	3,	0	6	3,	0	7	3,	1	3	3,	1	4	3,	1	5	3,
1	6	3,	1	7	3,	2	3	3,	2	4	3,	2	5	3,	2	6	3,

PLAT915_ALERT_3_B No Flack x Check Done: Low Friedel Pair Coverage 25 %

Alert level C

STRVA01_ALERT_4_C Flack parameter is too small
 From the CIF: `_refine_ls_abs_structure_Flack` -0.500
 From the CIF: `_refine_ls_abs_structure_Flack_su` 0.300

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)		0.26	Report
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)		6.64	Note
PLAT234_ALERT_4_C	Large Hirshfeld Difference S1	--C11	0.19	Ang.
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.87Ang From O2	0.40	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.05Ang From O1	0.40	eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of `_exptl_absorpt_correction_mu`
 not performed for this radiation type.

PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High	.	0.300	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.20	Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka		0.49255	Ang.
PLAT199_ALERT_1_G	Reported <code>_cell_measurement_temperature</code>	 (K)	293	Check
PLAT200_ALERT_1_G	Reported <code>_diffrn_ambient_temperature</code>	 (K)	293	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact S1	..C11	3.28	Ang.
		-x,-1/2+y,3/2-z =	4_546	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2	..C4	2.96	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C4	..C9	3.16	Ang.
		1+x,y,z =	1_655	Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3	Note
	0 1 1, 0 0 2, 0 1 2,			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	362	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
	0 2 2,			
PLAT930_ALERT_2_G	FCF-based Twin Law	[0 5 1] Est.d BASF	0.60	Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law	[0 5 1] Est.d BASF	0.60	Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.8	Low
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ		6	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.		4	Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ		6	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.		4	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	Info
PLAT984_ALERT_1_G	The C-f' =	-0.0004 Deviates from the B&C-Value	0.0006	Check
PLAT984_ALERT_1_G	The O-f' =	0.0008 Deviates from the B&C-Value	0.0038	Check
PLAT984_ALERT_1_G	The S-f' =	0.0507 Deviates from the B&C-Value	0.0647	Check

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.547 Why?

Author Response: Our experiment was done using a diamond-anvil cell rotated about one axis by 76 deg. Hence, due to the strategy and a limited access to the sample in a high-pressure cell no complete data was collected.

Alert level B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.0151 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 262 Report

0	2	0,	0	4	0,	0	6	0,	1	2	0,	1	3	0,	1	4	0,
1	5	0,	1	6	0,	2	0	0,	2	3	0,	2	4	0,	2	5	0,
2	6	0,	3	3	0,	3	4	0,	3	5	0,	3	6	0,	4	4	0,
4	5	0,	4	6	0,	5	4	0,	5	5	0,	5	6	0,	6	0	0,
0	2	1,	0	3	1,	0	4	1,	0	5	1,	0	6	1,	1	2	1,
1	3	1,	1	4	1,	1	5	1,	1	6	1,	2	0	1,	2	3	1,
2	4	1,	2	5	1,	2	6	1,	3	3	1,	3	4	1,	3	5	1,
3	6	1,	4	4	1,	4	5	1,	4	6	1,	5	5	1,	5	6	1,
0	2	2,	0	3	2,	0	4	2,	0	5	2,	0	6	2,	1	2	2,
1	3	2,	1	4	2,	1	5	2,	1	6	2,	2	3	2,	2	4	2,
2	5	2,	2	6	2,	3	4	2,	3	5	2,	3	6	2,	4	4	2,
4	5	2,	4	6	2,	5	5	2,	5	6	2,	0	2	3,	0	3	3,
0	4	3,	0	5	3,	0	6	3,	1	2	3,	1	3	3,	1	4	3,
1	5	3,	1	6	3,	2	3	3,	2	4	3,	2	5	3,	2	6	3,
3	4	3,	3	5	3,	3	6	3,	4	4	3,	4	5	3,	4	6	3,
5	5	3,	5	6	3,	0	0	4,	0	1	4,	0	2	4,	0	3	4,

PLAT915_ALERT_3_B No Flack x Check Done: Low Friedel Pair Coverage 24 %

Alert level C

STRVA01_ALERT_4_C Flack parameter is too small
From the CIF: _refine_ls_abs_structure_Flack -0.400
From the CIF: _refine_ls_abs_structure_Flack_su 0.400

PLAT082_ALERT_2_C High R1 Value 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.29 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.04 Report
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note

0	1	1,	1	0	1,	0	0	2,	0	1	2,	0	1	3,
---	---	----	---	---	----	---	---	----	---	---	----	---	---	----

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.400 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.49225 Ang.

PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact S1 ..C11 .	3.26 Ang.
	-x,-1/2+y,3/2-z =	4_546 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C4 .	2.91 Ang.
	-1+x,y,z =	1_455 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2 ..C5 .	3.18 Ang.
	-1/2+x,3/2-y,1-z =	3_466 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C4 ..C9 .	3.10 Ang.
	1+x,y,z =	1_655 Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	281 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note
	0 2 2,	
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	4 Note
	2 0 0, 2 0 1, 5 3 15, 1 0 1,	
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	7 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	4 Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ	7 Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	4 Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	6 Info
PLAT984_ALERT_1_G	The C-f' = -0.0004 Deviates from the B&C-Value	0.0006 Check
PLAT984_ALERT_1_G	The O-f' = 0.0008 Deviates from the B&C-Value	0.0038 Check
PLAT984_ALERT_1_G	The S-f' = 0.0506 Deviates from the B&C-Value	0.0646 Check

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

8 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
 5 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.













