

Structure factors have been supplied for datablock(s) MB-10_a, MB-11_a, MB120_a, MB149B-2_a, MB149E-2_a, MB15_a, mb-01_a, mb-100_a, mb-69_a, mb-77_a, mb-80_a

Structure factors have been supplied for datablock(s) MB-10_a, MB-11_a, MB120_a, MB149B-2_a, MB149E-2_a, MB15_a, mb-01_a, mb-100_a, mb-69_a, mb-77_a, mb-80_a

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: mb-01_a

Bond precision: C-C = 0.0047 Å Wavelength=1.54184

Cell: a=6.4358 (2) b=8.0804 (3) c=16.4380 (6)
alpha=90 beta=98.198 (3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	846.10 (5)	846.10 (5)
Space group	C 2	C 2
Hall group	C 2y	C 2y
Moiety formula	C16 H20 N2 O6	C16 H20 N2 O6
Sum formula	C16 H20 N2 O6	C16 H20 N2 O6
Mr	336.34	336.34
Dx, g cm ⁻³	1.320	1.320
Z	2	2
Mu (mm ⁻¹)	0.856	0.856
F000	356.0	356.0
F000'	357.24	
h, k, lmax	7, 9, 19	7, 9, 19
Nref	1626 [871]	994
Tmin, Tmax	0.931, 0.958	0.675, 1.000
Tmin'	0.918	

```
Correction method= # Reported T Limits: Tmin=0.675 Tmax=1.000
AbsCorr = MULTI-SCAN
```

Data completeness= $1.14/0.61$ Theta (max)= 70.186

```
R(reflections)= 0.0483( 980)      wR2(reflections)=
S = 1.165                        0.1483( 994)
Npar= 116
```

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 . 0.938 Why?

Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 49 Report
PLAT915_ALERT_3_B No Flack x Check Done: Low Friedel Pair Coverage 26 %
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check

Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 6.84 Note
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.6 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2A Check
PLAT245_ALERT_2_C U(iso) Ha Smaller than U(eq) Na by 0.012 Ang**2
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00471 Ang.
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 8 Note

Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.300 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 11 Note
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). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 27 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.7 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
6 **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

- 2 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
10 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
-

Datablock: MB-10_a

Bond precision: C-C = 0.0117 A

Wavelength=1.54184

```
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

PLAT234_ALERT_4_C	Large Hirshfeld Difference C40	--C70	.	0.18	Ang.
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C1A Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C2A Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C40 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		3.377	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.507		10	Report
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage			53	%



Alert level G

PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High	.	0.400	Report
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
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1O	.	105.1	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	19	Note
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL		2019/3	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		44%	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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

Datablock: MB-11_a

Bond precision: C-C = 0.0051 A Wavelength=1.54184

Cell: a=6.5044(4) b=8.0195(6) c=18.7137(12)
 alpha=90 beta=95.141(6) gamma=90

Temperature: 293 K

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full value Low .	0.973	Why?
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	7.07	Note
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.7	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C2A	Check
PLAT245_ALERT_2_C	U(iso) Ha Smaller than U(eq) Na by	0.016	Ang**2
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00511	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	25	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	3	Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	22.49	Check

● Alert level G

PLAT012_ALERT_1_G	N.O.K. _shelx_res_checksum Found in CIF	Please Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	11 Note
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 with s.u.	0.20 Check
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	25 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	3 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.9 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

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3 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
12 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

Datablock: mb-69_a

Bond precision: C-C = 0.0086 A Wavelength=1.54184

Cell: a=4.8579(1) b=21.1948(4) c=15.9374(3)
alpha=90 beta=91.905(2) gamma=90

Temperature: 293 K

PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0010	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1O	106.9	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	30	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	11	Note
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	54	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.3	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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 2 **ALERT level B** = A potentially serious problem, consider carefully
 6 **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

2 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
 8 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

Datablock: mb-77_a

Bond precision:	C-C = 0.0084 A	Wavelength=1.54184
Cell:	a=20.892(2)	b=4.9926(3)
	alpha=90	beta=111.246(12)
		gamma=90
Temperature:	293 K	

	Calculated	Reported
Volume	2091.8(4)	2091.8(4)
Space group	C 2	C 2
Hall group	C 2y	C 2y
Moiety formula	C24 H24 N2 O4	C24 H24 N2 O4
Sum formula	C24 H24 N2 O4	C24 H24 N2 O4
Mr	404.45	404.45
Dx, g cm ⁻³	1.284	1.284
Z	4	4
Mu (mm ⁻¹)	0.714	0.714
F000	856.0	856.0
F000'	858.64	
h, k, lmax	26, 6, 27	26, 6, 27
Nref	4446[2488]	3874
Tmin, Tmax	0.942, 0.965	0.306, 1.000
Tmin'	0.867	

Correction method= # Reported T Limits: Tmin=0.306 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.56/0.87 Theta (max)= 77.035

```
R(reflections)= 0.0671( 2974)      wR2(reflections)=
S = 1.060                        0.1950( 3874)
Npar= 281
```

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

PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00842 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.438 Check
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	73 %

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High .	0.400	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	44	Note
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	51	Note
PLAT916_ALERT_2_G	Hooft y and Flack x Parameter Values Differ by .	0.40	Check
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.7	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

2 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
 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

Datablock: mb-80_a

Bond precision: C-C = 0.0110 A Wavelength=1.54184
 Cell: a=18.8640(2) b=18.8640(2) c=19.6976(4)
 alpha=90 beta=90 gamma=90
 Temperature: 293 K

	Calculated	Reported
Volume	7009.4(2)	7009.4(2)
Space group	P 43 21 2	P 43 21 2
Hall group	P 4nw 2abw	P 4nw 2abw
Moiety formula	C37 H37 N3 O8	C37 H37 N3 O8
Sum formula	C37 H37 N3 O8	C37 H37 N3 O8
Mr	651.70	651.69
Dx, g cm ⁻³	1.235	1.235
Z	8	8
Mu (mm ⁻¹)	0.719	0.719
F000	2752.0	2752.0
F000'	2760.84	
h, k, lmax	23, 23, 24	21, 23, 24
Nref	7311[4144]	7226
Tmin, Tmax	0.842, 0.931	0.763, 1.000
Tmin'	0.806	

Correction method= # Reported T Limits: Tmin=0.763 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 1.74/0.99 Theta(max)= 75.839

R(reflections)= 0.0852(4601) wR2(reflections)=
 0.2762(7226)
 S = 1.053 Npar= 443

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

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01096 Ang.



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 3.9 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.4 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C4B Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7B Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C6P2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8P2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2P1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3B Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2P2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4P2 Check
PLAT245_ALERT_2_C U(iso) Hp1 Smaller than U(eq) Np1 by 0.011 Ang**2
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Ocl 0.138 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.597 Check



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 12 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 2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 4 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 13% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 73 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 219 Note
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 30 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 3 Check

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

14 **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

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

14 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
3 ALERT type 5 Informative message, check

Datablock: mb-100_a

Bond precision: C-C = 0.0059 A Wavelength=1.54184

Cell: a=18.8070(2) b=18.8070(2) c=19.0641(5)
alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	6743.0(2)	6743.0(2)
Space group	P 41 21 2	P 41 21 2
Hall group	P 4abw 2nw	P 4abw 2nw
Moiety formula	C37 H35 N3 O7	C37 H35 N3 O7
Sum formula	C37 H35 N3 O7	C37 H35 N3 O7
Mr	633.68	633.68
Dx, g cm ⁻³	1.248	1.248
Z	8	8
Mu (mm ⁻¹)	0.711	0.711
F000	2672.0	2672.0
F000'	2680.45	
h, k, lmax	22, 22, 23	20, 22, 23
Nref	6235[3554]	5899
Tmin, Tmax	0.880, 0.965	0.295, 1.000
Tmin'	0.867	

Correction method= # Reported T Limits: Tmin=0.295 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.66/0.95 Theta(max)= 68.589

R(reflections)= 0.0419(4958) wR2(reflections)=
0.1103(5899)

S = 1.038 Npar= 434

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

STRVA01_ALERT_4_C Flack parameter is too small
From the CIF: _refine_ls_abs_structure_Flack -0.260
From the CIF: _refine_ls_abs_structure_Flack_su 0.110
PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.964 Why?
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.2 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C6P2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2P2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4P2 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C4P1 --C9P1 . 1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00586 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 123 Report

● 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
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O10 . 105.5 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 56 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 2 Note
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 26 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.4 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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2 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
8 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

Datablock: MB120_a

Bond precision: C-C = 0.0034 A Wavelength=1.54184

Cell: a=7.3061(1) b=7.3061(1) c=29.5083(6)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	(K)	293	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1O	.	105.3	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		19	Note
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	23	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.3	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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

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

Datablock: MB149B-2_a

Bond precision: C-C = 0.0022 A Wavelength=1.54184
 Cell: a=14.4335(2) b=13.2892(2) c=9.4990(2)
 alpha=90 beta=105.099(2) gamma=90
 Temperature: 293 K

	Calculated	Reported
Volume	1759.10(5)	1759.10(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C19 H20 N2 O4	C19 H20 N2 O4
Sum formula	C19 H20 N2 O4	C19 H20 N2 O4
Mr	340.37	340.37
Dx, g cm ⁻³	1.285	1.285
Z	4	4
Mu (mm ⁻¹)	0.747	0.747
F000	720.0	720.0
F000'	722.30	
h, k, lmax	18, 16, 12	18, 16, 12
Nref	3821	3615
Tmin, Tmax	0.799, 0.861	0.856, 1.000
Tmin'	0.799	

Correction method= # Reported T Limits: Tmin=0.856 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.946 Theta(max)= 79.704

R(reflections)= 0.0528(3143) wR2(reflections)=
 0.1550(3615)
 S = 1.063 Npar= 233

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

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C50	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C40	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		3.216	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	4	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..		1	Check



Alert level G

PLAT153_ALERT_1_G	The s.u.'s on the Cell Axes	are Equal ..(Note)	0.0002	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	(K)	293	Check
PLAT398_ALERT_2_G	Deviating C-O-C	Angle From 120 for O1O	106.3	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		18	Note
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	202	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.5	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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0 ALERT type 5 Informative message, check

Datablock: MB149E-2_a

Bond precision: C-C = 0.0039 A

Wavelength=1.54184

Cell:	a=13.2430(4)	b=20.7980(6)	c=7.7513(2)
	alpha=90	beta=90	gamma=90

Temperature: 293 K

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1O	.	105.2	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	19	Note
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	165	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		3.5	Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		2	Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by		2	Check

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Datablock: MB15_a

Bond precision: C-C = 0.0071 A Wavelength=1.54184

Cell: a=5.1830 (1) b=5.5120 (1) c=64.5994 (13)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	1845.52 (6)	1845.52 (6)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C20 H22 N2 O4	C20 H22 N2 O4
Sum formula	C20 H22 N2 O4	C20 H22 N2 O4
Mr	354.40	354.39
Dx, g cm ⁻³	1.276	1.275
Z	4	4
Mu (mm ⁻¹)	0.731	0.731
F000	752.0	752.0
F000'	754.36	
h, k, lmax	6, 7, 82	6, 6, 81
Nref	4008 [2439]	3887
Tmin, Tmax	0.839, 0.964	0.735, 1.000
Tmin'	0.803	

Correction method= # Reported T Limits: Tmin=0.735 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 1.59/0.97

Theta(max)= 79.716

R(reflections)= 0.0867(3813)

wR2(reflections)=
0.2865(3887)

S = 1.161

Npar= 243

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

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.29 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.2 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2A Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00706 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.775 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report



Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.400 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O1O . 105.8 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 19 Note
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 37 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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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.





















