



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 19090503

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: 19090503

Bond precision:	C-C = 0.0023 Å		Wavelength=1.54184
Cell:	a=8.6894 (2)	b=35.8672 (5)	c=8.1002 (1)
	alpha=90	beta=107.351 (2)	gamma=90
Temperature:	220 K		
	Calculated	Reported	
Volume	2409.67 (8)	2409.67 (8)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C33 H22 N2 O2	C33 H22 N2 O2	
Sum formula	C33 H22 N2 O2	C33 H22 N2 O2	
Mr	478.53	478.52	
Dx, g cm-3	1.319	1.319	
Z	4	4	
Mu (mm-1)	0.653	0.653	
F000	1000.0	1000.0	
F000'	1002.87		
h, k, lmax	10, 44, 10	10, 43, 9	
Nref	4831	4617	
Tmin, Tmax	0.889, 0.974	0.297, 1.000	
Tmin'	0.861		

Correction method= # Reported T Limits: Tmin=0.297 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.956

Theta(max)= 73.323

R(reflections)= 0.0489(4070)

wR2(reflections)=
0.1427(4617)

S = 0.997

Npar= 335

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 2.116 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 48 Report

1	0	0,	2	0	0,	3	0	0,	0	20	0,	0	22	0,	0	24	0,
6	34	0,	2	1	1,	0	22	1,	-1	23	1,	0	23	1,	-1	24	1,
0	24	1,	0	0	2,	1	0	2,	2	0	2,	0	1	2,	0	22	2,
-10	1	5,	-10	2	5,	4	0	6,	5	0	6,	5	1	6,	5	2	6,
5	3	6,	-9	11	6,	-9	12	6,	-9	13	6,	-9	14	6,	-8	21	6,

(18 More Missing: see the .ckf listing file)

● Alert level G

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 59 Note

O001	O002	N003	N004	C005	C006	C007	C008
C009	H009	C00A	C00B	C00C	C00D	H00D	C00E
C00F	H00F	C00G	H00G	C00H	C00I	H00I	C00J
H00J	C00K	H00K	C00L	H00L	C00M	H00M	C00N
C00O	C00P	H00P	C00Q	C00R	C00S	H00S	C00T
H00T	C00U	H00U	C00V	H00V	C00W	H00W	C00X
H00X	C00Y	H00Y	C00Z	H00A	H00B	H00C	C010
H010	C011	H011					

PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.93 Note
0 2 0,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 152 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.7 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.785 Note
Predicted wR2: Based on SigI**2 5.13 or SHELX Weight 14.32

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 16 Info

PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 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
7 **ALERT level G** = General information/check it is not something unexpected

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

PLATON version of 26/09/2025; check.def file version of 20/09/2025

No duplication found

PLATON-Oct 1 9:25:03 2025 - (VERSION=260925)

40 Y

NOMOVE FORCED

Prob = 50%
Temp = 220K

ORTEP diagram of a complex organic molecule, likely a carboxylate salt or a complex organic acid derivative. The structure features a central core with a nitrogen atom (N004) and a disordered region (N003). The molecule is shown in a stick representation with thermal ellipsoids at the 50% probability level. The structure includes several carboxylate groups (COO) and a central core with a nitrogen atom (N004) and a disordered region (N003). The labels for the atoms are: COO1, COO2, COO3, COO4, COO5, COO6, COO7, COO8, COO9, COO10, COO11, COO12, COO13, COO14, COO15, COO16, COO17, COO18, COO19, COO20, COO21, COO22, COO23, COO24, COO25, COO26, COO27, COO28, COO29, COO30, COO31, COO32, COO33, COO34, COO35, COO36, COO37, COO38, COO39, COO40, COO41, COO42, COO43, COO44, COO45, COO46, COO47, COO48, COO49, COO50, COO51, COO52, COO53, COO54, COO55, COO56, COO57, COO58, COO59, COO60, COO61, COO62, COO63, COO64, COO65, COO66, COO67, COO68, COO69, COO70, COO71, COO72, COO73, COO74, COO75, COO76, COO77, COO78, COO79, COO80, COO81, COO82, COO83, COO84, COO85, COO86, COO87, COO88, COO89, COO90, COO91, COO92, COO93, COO94, COO95, COO96, COO97, COO98, COO99, COO100, COO101, COO102, COO103, COO104, COO105, COO106, COO107, COO108, COO109, COO110, COO111, COO112, COO113, COO114, COO115, COO116, COO117, COO118, COO119, COO120, COO121, COO122, COO123, COO124, COO125, COO126, COO127, COO128, COO129, COO130, COO131, COO132, COO133, COO134, 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