

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ga601

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: ga601

Bond precision: C-C = 0.0046 A

Wavelength=0.71073

Cell: a=11.6732 (5) b=16.7232 (7) c=17.6214 (8)
 alpha=98.987 (1) beta=96.472 (2) gamma=109.408 (1)
Temperature: 150 K

	Calculated	Reported
Volume	3154.2 (2)	3154.2 (2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C80 H96 O4	C80 H96 O4
Sum formula	C80 H96 O4	C80 H96 O4
Mr	1121.57	1121.56
Dx, g cm ⁻³	1.181	1.181
Z	2	2
Mu (mm ⁻¹)	0.070	0.070
F000	1216.0	1216.0
F000'	1216.47	
h, k, lmax	14, 20, 22	14, 20, 22
Nref	12942	12821
Tmin, Tmax	0.982, 0.996	0.628, 0.745
Tmin'	0.982	

Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.991

Theta(max)= 26.416

R(reflections)= 0.0846 (8352)

wR2(reflections)=
0.2170 (12821)

S = 1.057

Npar= 801

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	6.3	Ratio											
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds			0.00457	Ang.											
PLAT411_ALERT_2_C	Short Inter H...H Contact	H01T	..H01T	.		2.12	Ang.											
				1-x,-y,1-z =		2_656	Check											
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance				13.241	Check											
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance				3.022	Check											
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=			0.600		77	Report											
	11	5	0,	9	9	0,	5	10	0,	3	16	0,	-8	-11	1,	-5	-10	1,
	11	-7	1,	-7	-5	1,	-12	-3	1,	-1	-2	1,	-3	5	1,	-6	-14	2,
	-8	-11	2,	-5	-10	2,	-8	-5	2,	-6	-14	3,	-5	-10	3,	-7	-7	3,
	-7	-7	4,	-11	-6	4,	-3	-17	5,	-5	-15	5,	-2	-13	5,	-3	-12	5,
	-4	-11	5,	-8	-9	5,	-7	-7	5,	-11	-6	5,	9	7	5,	-4	-16	6,
	-8	-11	6,	-7	-7	6,	-11	-6	6,	-8	-11	7,	-7	11	7,	-8	17	7,
	-8	-11	8,	-11	-6	8,	-6	11	8,	-9	15	8,	-7	-12	9,	-4	-10	9,
	7	-10	9,	-5	-9	9,	-6	10	9,	-4	-15	10,	-5	-14	10,	-6	-13	10,
	-6	9	10,	-11	12	10,	-9	14	10,	-4	9	11,	-8	14	11,	10	-10	12,
	-7	6	12,	-2	8	12,	-8	13	12,	-4	-14	13,	-5	-13	13,	-7	-11	13,
	-4	6	13,	-8	12	13,	9	-8	14,	-5	4	14,	-8	11	14,	-6	12	14,
	-4	-13	15,	-9	9	15,	4	-2	16,	-7	9	16,	-4	10	16,	-3	10	16,
	-2	10	16,	-8	7	17,	-6	8	17,	-1	8	17,	-2	2	20,			

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					33	Note
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					12	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records					7	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
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
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C8	--C015	.		7.0	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C9	--C01K	.		7.5	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C14	--C01Q	.		7.0	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C15	--C015	.		5.5	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C01K	--C023	.		6.0	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of	C1	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C7	Constrained at			0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C8	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C9	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C14	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C15	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C16	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C01S	Constrained at			0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C01U	Constrained at			0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C01V	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C01W	Constrained at			0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C01X	Constrained at			0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C01Z	Constrained at			0.75	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H020	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02A	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02B	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02E	Constrained at	0.7	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02F	Constrained at	0.7	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02G	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02H	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H026	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02I	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02J	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02K	Constrained at	0.7	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02L	Constrained at	0.7	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02M	Constrained at	0.7	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H029	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02N	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02O	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02P	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02Q	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02R	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02S	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02T	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3A	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11A	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11C	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of He	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Hf	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Hl	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Hm	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H021	Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder (Resd 1)		23%	Note
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C00G - C015 .		1.53	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C015 - C01C .		1.53	Ang.
PLAT410_ALERT_2_G	Short Intra H...H Contact H00L ..H8B .		2.08	Ang.
	x, y, z =		1_555	Check

PLAT410_ALERT_2_G Short Intra H...H Contact H000 ..H15B . 2.07 Ang.
x,y,z = 1_555 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 170 Note

O001	O002	O003	O004	C005	C006	C007	H007
C008	H008	C009	C00A	C00B	H00B	C00C	C00D
C00E	C00F	C00G	C00H	C00I	H00I	C00J	C00K
H00A	H00C	C00L	H00L	C00M	C00N	C00O	H00O
C00P	C00Q	C00R	C00S	H00S	C00T	H00T	C00U
C00V	C00W	H00D	H00E	C00X	H00F	H00G	C00Y
C00Z	H00H	H00J	C010	H01A	H01B	C011	H01C
H01D	C012	H01E	H01F	C013	H01G	H01H	C014
H014	C015	C016	C017	H01I	H01J	C018	H018
C019	H01K	H01L	C01A	H01M	C01B	H01N	H01O
C01C	H01P	H01Q	C01D	H01R	H01S	C01E	H01T
H01U	C01F	H01V	C01G	H01W	H01X	C01H	H01Y
C01I	H01Z	C01J	H01	C01K	Ha	C01L	Hb
C01M	Hc	C01N	Hd	He	Hf	C01O	C01P
Hg	C01Q	Hh	Hi	Hj	C01R	C01S	C01T
Hk	Hl	Hm	C01U	Hn	C01V	Ho	C01W
Hp	C01X	Hq	C01Y	C01Z	C020	H020	C021
H021	C022	H02A	H02B	C023	H02C	H02D	C024
H02E	H02F	C025	H02G	H02H	C026	H026	C027
H02I	H02J	C028	H02K	H02L	H02M	C029	H029
C02A	H02N	H02O	C02B	H02P	H02Q	C02C	H02R
H02S	H02T						

PLAT860_ALERT_3_G Number of Least-Squares Restraints 41 Note

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

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

0 1 0, 0 -1 1, 0 0 1,

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 2 Note

0 -1 1, -3 5 1,

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.3 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.04 Note

Predicted wR2: Based on SigI**2 7.14 or SHELX Weight 21.21

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 5 Check

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

1 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
13 ALERT type 3 Indicator that the structure quality may be low
127 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.

