

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) nt1009_NaCl_in_capsule, nt1021_Glycine_full, nt1023_alpha-glycine_auto

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: nt1009_NaCl_in_capsule

Bond precision: = 0.0000 A Wavelength=0.71073

Cell: a=5.6357(3) b=5.6357(3) c=5.6357(3)
 alpha=90 beta=90 gamma=90

Temperature: 295 K

	Calculated	Reported
Volume	179.00(3)	179.00(3)
Space group	F m -3 m	F m -3 m
Hall group	-F 4 2 3	-F 4 2 3
Moiety formula	Cl, Na	Cl Na
Sum formula	Cl Na	Cl Na
Mr	58.44	58.44
Dx, g cm ⁻³	2.169	2.169
Z	4	4
Mu (mm ⁻¹)	1.774	1.774
F000	112.0	112.0
F000'	112.71	
h, k, lmax	8, 8, 8	8, 8, 8
Nref	26	26
Tmin, Tmax	0.775, 0.901	0.833, 0.904
Tmin'	0.766	

Correction method= # Reported T Limits: Tmin=0.833 Tmax=0.904
AbsCorr = ANALYTICAL

Data completeness= 1.000 Theta(max)= 30.295

R(reflections)= 0.0102(26)

wR2(reflections)=
0.0239(26)

S = 1.246

Npar= 4

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

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.50 Note

Author Response: Rock salt structure, limited number of reflections.

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pm-3m Check
Check Model Parameter Symmetry for Reflection Data Support

Author Response: Rock salt structure.



Alert level G

PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Translation ... ? Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem I 100 %Fit
PLAT116_ALERT_2_G ADDSYM Included (Pseudo) Lattice Translation ... Please Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 1) 0.02 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 0.02 Check
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

0 **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
6 **ALERT level G** = General information/check it is not something unexpected

0 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
1 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

Datablock: nt1023_alpha-glycine_auto

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

Cell: a=5.1018(9) b=11.9664(16) c=5.4624(9)
alpha=90 beta=111.73(2) gamma=90

Temperature: 295 K

1 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
2 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

Datablock: nt1021_Glycine_full

Bond precision: C-C = 0.0030 A Wavelength=0.71073
Cell: a=5.0947(6) b=6.2681(5) c=5.3883(6)
alpha=90 beta=113.232(14) gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	158.12(3)	158.12(3)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C2 H5 N O2	C2 H5 N O2
Sum formula	C2 H5 N O2	C2 H5 N O2
Mr	75.07	75.07
Dx, g cm ⁻³	1.577	1.577
Z	2	2
Mu (mm ⁻¹)	0.140	0.140
F000	80.0	80.0
F000'	80.05	
h, k, lmax	7, 9, 8	7, 9, 8
Nref	1176[634]	1053
Tmin, Tmax	0.985, 0.990	0.976, 0.991
Tmin'	0.966	

Correction method= # Reported T Limits: Tmin=0.976 Tmax=0.991
AbsCorr = ANALYTICAL

Data completeness= 1.66/0.90 Theta(max)= 32.752

R(reflections)= 0.0429(921) wR2(reflections)=
0.0970(1053)
S = 1.073 Npar= 66

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 G

PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT111_ALERT_2_G	ADDSYM Detects New (Pseudo) Centre of Symmetry .	80 %Fit
PLAT113_ALERT_2_G	ADDSYM Suggests Possible Pseudo/New Space Group	P21/m Check
	Check Model Parameter Symmetry for Reflection Data Support	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	47 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 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.





