Table A5.7.1.1 (*cont.*).

`loop_`	
`_geom_angle_atom_site_label_1`	Labels identifying the atom sites 1, 2 and 3
`_geom_angle_atom_site_label_2`	
`_geom_angle_atom_site_label_3`	
`_geom_angle_site_symmetry_1`	Symmetry codes for atom sites 1, 2 and 3
`_geom_angle_site_symmetry_2`	
`_geom_angle_site_symmetry_3`	
`_geom_angle`	Angle between atom sites 1, 2 and 3 (°)
`_geom_angle_publ_flag`	Flag for print request (yes or no)
`loop_`	
`_geom_torsion_atom_site_label_1`	Labels identifying the atom sites 1, 2, 3 and 4
`_geom_torsion_atom_site_label_2`	
`_geom_torsion_atom_site_label_3`	
`_geom_torsion_atom_site_label_4`	
`_geom_torsion_site_symmetry_1`	Symmetry codes for atom sites 1, 2, 3 and 4
`_geom_torsion_site_symmetry_2`	
`_geom_torsion_site_symmetry_3`	
`_geom_torsion_site_symmetry_4`	
`_geom_torsion`	Torsion angle between atom sites 1, 2, 3 and 4 (°)
`_geom_torsion_publ_flag`	Flag for print request (yes or no)
`loop_`	
`_geom_hbond_atom_site_label_D`	Donor-atom label in hydrogen bond
`_geom_hbond_atom_site_label_H`	H-atom label in hydrogen bond
`_geom_hbond_atom_site_label_A`	Acceptor-atom label in hydrogen bond
`_geom_hbond_site_symmetry_D`	Symmetry code for donor site
`_geom_hbond_site_symmetry_H`	Symmetry code for H-atom site
`_geom_hbond_site_symmetry_A`	Symmetry code for acceptor site
`_geom_hbond_distance_DH`	Donor atom-to-H-atom distance (Å)
`_geom_hbond_distance_HA`	H-atom-to-acceptor atom distance (Å)
`_geom_hbond_distance_DA`	Donor atom-to-acceptor atom distance (Å)
`_geom_hbond_angle_DHA`	Donor to H to acceptor angle (°)
`_geom_hbond_publ_flag`	Flag for print request (yes or no)
(*c*) Data names for adding items to the standard request list	
`loop_`	
`_publ_manuscript_incl_extra_item`	Additional CIF item submitted for publication
`_publ_manuscript_incl_extra_defn`	Is item defined in core dictionary? (yes or no)
(*d*) Data names for structure-factor lists	
`loop_`	
`_refln_index_h`	Miller indices *h*, *k* and *l*
`_refln_index_k`	
`_refln_index_l`	
`_refln_F_meas`	Measured *F*
`_refln_F_squared_meas`‡	Measured F^2
`_refln_F_sigma`	Standard uncertainty of *F*
`_refln_F_squared_sigma`‡	Standard uncertainty of F^2
`_refln_F_calc`	Calculated *F*
`_refln_F_squared_calc`‡	Calculated F^2

‡ Alternative to the corresponding data name without 'squared'.

Appendix 5.7.2
Data validation using *checkcif*

Table A5.7.2.1 lists the *checkcif* tests concerned primarily with the completeness and self-consistency of individual or closely related data items. These tests were developed from the routines of *PREPUB* (du Boulay & Hall, 1996) and in the IUCr Editorial Office. Table A5.7.2.2 lists the tests applied specifically by the program *PLATON* (Spek, 2003), which performs a more detailed crystallographic analysis of the structure itself.

Each entry in each table has an identifying code and a numeric type. The type is used to categorize the alert messages generated when the tested values deviate from assigned norms. Type 1 refers to syntactic or other errors of construction in the CIF, or to inconsistent or missing data. Type 2 alerts indicate that the structure model may be wrong or deficient. Type 3 alerts indicate that the quality of the structure may be low, owing to limited or incomplete data coverage. Alerts of type 4 are indicative of deviations from style or suggested good practice, or may offer suggestions for improvement in presentation. The alerts within each category may be of varying levels of severity.

Full details of the tests and algorithms applied for the *checkcif* tests may be found at http://journals.iucr.org/services/cif/datavalidation.html or on the CD-ROM accompanying this volume. These include comments which provide help in interpreting the results of the tests and suggest ways in which the author can improve the data. The comments were provided by A. Linden and other members of the IUCr journal editorial boards.

The tests listed in Tables A5.7.2.1 and A5.7.2.2 are appropriate for small-unit-cell single-crystal structure determinations. More discriminating tests are being introduced for powder diffraction studies and for modulated structures.

Table A5.7.2.1. *List of data-validation tests applied by checkcif*

Test name	Type	Purpose
ABSMU01	1	Check that μ is consistent with the cell contents
ABSTM01	1	Check that T_{min} is less than T_{max}
ABSTM02	3	Check that T_{min} and T_{max} are appropriate to the crystal size and μ
ABSTY01	1	Check that `_exptl_absorpt_correction_type` is a recognized keyword
ABSTY02	1	Check that `_exptl_absorpt_correction_type` contains some reference text
CELLK01	1	Check that temperature is in Kelvin
CELLT01	1	Check that θ_{min} is less than θ_{max}
CELLV01	1	Check that the `_cell_volume` matches `_cell_length_` and `_cell_angle_` values
CELLV02	1	Check that the `_cell_volume` s.u. matches `_cell_length_` and `_cell_angle_` s.u. values
CELLZ01	1	Check consistency between formula, *Z*, atom list and symmetry
CHEMS01	1	Check that the `_chemical_formula_sum` is properly constructed
CHEMS02	1	Check that the stated category is consistent with the formula of the compound
CHEMW01	1	Check consistency between `_chemical_formula_weight` and `_chemical_formula_sum`
CHEMW03	2	Check consistency between weight, *Z*, symmetry and atom list
CRYSC01	1	Check that colour of crystal is consistent with expected colour code combinations
CRYSR01	1	Check that the radius of the crystal is given for a spherical or cylindrical crystal
CRYSS01	1	Check consistency of crystal dimensions
CRYSS02	3	Check that the values of `_exptl_crystal_size_`* are not larger than expected
DENSD01	1	Check consistency of density, cell volume and weight
DENSX01	1	Check that `_exptl_crystal_density_meas` matches `_exptl_crystal_density_diffrn`
DIFMN01	1	Check that `_refine_diff_density_min` is less than `_refine_diff_density_max`
DIFMN02	2	Check that `_refine_diff_density_min` is within expected limits
DIFMN03	1	Check for adjacent site information if `_refine_diff_density_min` is outside expected limits
DIFMX01	2	Check that `_refine_diff_density_max` is within expected limits
DIFMX02	1	Check for adjacent site information if `_refine_diff_density_max` is outside expected limits
FCOEF01	1	Check that the value of `_refine_ls_structure_factor_coef` is recognized
FORMU01	1/2	Check consistency between formulae and atom site data
GOODF01	1/2	Check that `_refine_ls_goodness_of_fit_ref` is within expected limits
HYDTR01	1	Check that the value of `_refine_ls_hydrogen_treatment` is recognized
RADNT01	1	Check that the radiation type is recognized
RADNW01	1	Check that `_diffrn_radiation_wavelength` matches `_diffrn_radiation_type`
REFLE01	3	Check that `_reflns_threshold_expression` contains a multiplier which is below the limit
REFLG01	1	Check that `_reflns_number_gt` is less than or equal to `_diffrn_reflns_number`
REFLL01	1	Check that `_diffrn_reflns_limit_` values are in the correct order
REFLT01	1	Check that `_reflns_number_total` is less than or equal to `_diffrn_reflns_number`
REFLT02	1	Check that `_reflns_number_total` is greater than or equal to `_reflns_number_gt`
REFLT03	1/3/4	Check consistency of `_reflns_number_total` with cell volume, symmetry and θ_{max}
REFNR01	3	Check the ratio of `_refine_ls_number_reflns` and `_refine_ls_number_parameters`
RFACG01	3	Check that `_refine_ls_R_factor_gt` is within expected limits
RFACR01	3	Check that `_refine_ls_wR_factor_ref` is within expected limits
RINTA01	3	Check that `_diffrn_reflns_av_R_equivalents` is within expected limits
SHFSU01	2	Check that `_refine_ls_shift/su_max` is within expected limits
STRDE01	1	Check that `_refine_ls_abs_structure_details` is present if necessary
STRVA01	2/4	Check that `_refine_ls_abs_structure_Flack` is within expected limits
STRVA02	2/3/4	Check that `_refine_ls_abs_structure_Rogers` is within expected limits
SYMMG01	1	Check that the `_symmetry_space_group_name_H-M` value is recognized

Table A5.7.2.1 (*cont.*).

SYMMG02	1	Check consistency between space group name and symmetry positions
SYMMS01	1	Check that the **_symmetry_cell_setting** matches one of the keywords
SYMMS02	1	Check consistency between cell setting and cell parameters
THETM01	3	Check that **_diffrn_reflns_theta_max** is greater than expected limits
WEIGH01	1	Check that the value of **_refine_ls_weighting_scheme** is recognized

Table A5.7.2.2. *List of data-validation tests applied by PLATON*

Test name	Type	Purpose
PLAT020	3	Check *R*(int)
PLAT021	1	Check expected number of reflections (max = 1 centro, 2 non-centro)
PLAT022	3	Check expected number of reflections
PLAT023	3	Check $\theta_{\max}$
PLAT024	4	Check for required Friedel pair averaging $Z \leq$ Si
PLAT025	1	Check for $h_{\min} \ldots l_{\max}$
PLAT026	3	Check for weak data
PLAT027	3	Check **_diffrn_reflns_theta_full**
PLAT028	3	Check **_diffrn_measured_fraction_theta_max**
PLAT029	3	Check **_diffrn_measured_fraction_theta_full**
PLAT030	1	Check **_diffrn_reflns_number** > **_reflns_number_total**
PLAT031	4	Check need for extinction correction parameter
PLAT032	4	Check s.u. Flack parameter
PLAT033	2	Check Flack parameter value
PLAT034	1	Check for Flack parameter value specified $Z >$ Si, non-centro
PLAT035	1	Check for **_chemical_absolute_configuration**
PLAT036	1	Check for missing Flack parameter s.u.
PLAT037	1	Check **_diffrn_reflns_theta_full**
PLAT038	1	Check **_diffrn_measured_fraction_theta_max**
PLAT039	1	Check **_diffrn_measured_fraction_theta_full**
PLAT040	1	Test for H atoms [0, 1]
PLAT041	1	Test sum formula
PLAT042	1	Test moiety formula
PLAT043	1	Test for molecular weight
PLAT044	1	Check reported with calculated density
PLAT045	1	Check reported and calculated *Z*
PLAT046	1	Check reported density with calculated density from $Z * MW$
PLAT047	1	Test sum formula given
PLAT048	1	Test moiety formula given
PLAT049	1	Check calculated density > 1.0
PLAT050	1	Test for μ given [0, 1]
PLAT051	1	Test for difference μ(cif) with μ(calc) [%]
PLAT052	1	Test for specification of absorption correction method [0, 1]
PLAT053	1	Test for specification crystal dimension min [0, 1]
PLAT054	1	Test for specification crystal dimension mid [0, 1]
PLAT055	1	Test for specification crystal dimension max [0, 1]
PLAT056	1	Test for specification crystal radius [0, 1]
PLAT057	3	Test for correction for absorption needed
PLAT058	1	Test for specification $T_{\max}$ [0, 1]
PLAT059	1	Test for specification $T_{\min}$ [0, 1]
PLAT060	3	*RR* test
PLAT061	3	RR' test
PLAT062	4	Rescale $T_{\min}$ and $T_{\max}$
PLAT063	3	Test for crystal size
PLAT064	1	Test for $T_{\max} \geq T_{\min}$
PLAT065	3	Test for applicability of (semi-)empirical absorption correction [0, 1]
PLAT066	1	Test whether predicted and reported transmission ranges are identical
PLAT067	1	Ensure that minimum dimension < max dimension
PLAT068	1	Test for $F(000)$ calc/reported difference
PLAT070	1	Test for duplicate labels
PLAT071	1	Test for uninterpretable labels
PLAT074	1	Test for occupancy = 0.0
PLAT075	1	Test for occupancy greater than 1.0
PLAT076	1	Test for occupancy less than 1.0 for atom on special position
PLAT077	4	Test for non-integral number of atoms in unit cell
PLAT080	2	Test maximum shift/error
PLAT081	1	Test for maximum shift/error given
PLAT082	2	Test for reasonable *R*1
PLAT083	2	Test for extreme second weighting parameter (*SHELXL*)
PLAT084	2	Test for reasonable *wR*2
PLAT085	2	Test for default *SHELXL* weighting scheme
PLAT086	2	Test for reasonable *S* (too low)
PLAT087	2	Test for reasonable *S* (too high)
PLAT088	3	Test for reasonable data/parameter ratio (centro)
PLAT089	3	Test for reasonable data/parameter ratio (non-centro) ($Z_{\max} < 18$)
PLAT090	3	Test for reasonable data/parameter ratio (non-centro) ($Z_{\max} > 18$)
PLAT091	1	Test for 'No wavelength given'
PLAT092	4	Test for wavelength type [Cu, Mo, Ag] [0, 1]
PLAT093	1	Test for inconsistency 'mixed' *versus* 'no refined H'
PLAT094	2	Test for maximum/minimum residual density ratio
PLAT095	1	Test for residual density maximum given [0, 1]
PLAT096	1	Test for residual density minimum given [0, 1]
PLAT097	2	Test maximum residual density
PLAT098	2	Test for minimum residual density

Table A5.7.2.2 (*cont.*).

Test name	Type	Purpose
PLAT099	1	Test for minimum residual density less than zero [0, 1]
PLAT110	2	Test for additional translational symmetry [0, 1]
PLAT111	2	Test for additional centre of symmetry [0, 100]
PLAT112	2	Test for additional symmetry [0, 1]
PLAT113	2	Report new space group suggested by *ADDSYM*
PLAT114	2	Report on *ADDSYM* problem
PLAT120	1	Test for consistent **_symmetry_space_group_name_H-M** and symmetry operations
PLAT121	1	Test for valid **_symmetry_space_group_name_H-M**
PLAT122	1	Test for ? **_symmetry_space_group_name_H-M**
PLAT123	1	Test for interpretable space-group symmetry
PLAT124	1	Test for **_symmetry_equiv_pos_as_xyz** present
PLAT125	4	Test for ? **_symmetry_space_group_name_Hall**
PLAT126	1	Test for **_symmetry_space_group_name_Hall** error
PLAT127	1	Test for **_symmetry_space_group_name_Hall** consistency
PLAT128	4	Test for non-standard monoclinic space-group setting
PLAT129	4	Test for unusual non-standard space-group name
PLAT130	1	Test for cubic: $a = b = c$
PLAT131	1	Test for cubic: $\alpha = \beta = \gamma = 90$
PLAT132	1	Test for trigonal/hexagonal: $a = b$
PLAT133	1	Test for trigonal/hexagonal: $\alpha = \beta = 90$
PLAT134	1	Test for trigonal/hexagonal: $\gamma = 120$
PLAT135	1	Test for tetragonal: $a = b$
PLAT136	1	Test for tetragonal: $\alpha = \beta = \gamma = 90$
PLAT137	1	Test for orthorhombic: $\alpha = \beta = \gamma = 90$
PLAT138	1	Test for monoclinic more than 1 angle off 90 degrees
PLAT139	1	Test for rhombohedral $a = b = c$
PLAT140	1	Test for rhombohedral $\alpha = \beta = \gamma$
PLAT141	4	S.u. on *a* axis small or missing
PLAT142	4	S.u. on *b* axis small or missing
PLAT143	4	S.u. on *c* axis small or missing
PLAT144	4	S.u. on α small or missing
PLAT145	4	S.u. on β small or missing
PLAT146	4	S.u. on γ small or missing
PLAT147	1	S.u. on symmetry restricted cell angle
PLAT150	1	Check volume
PLAT151	1	Check for s.u. on volume
PLAT152	1	Check for consistency of s.u. on volume and cell parameters
PLAT155	4	Check for reduced cell *aP*
PLAT156	4	Check for non-standard axial order
PLAT157	4	Check for non-standard monoclinic β angle < 90 degrees
PLAT161	4	Missing *x*-coordinate s.u.
PLAT162	4	Missing *y*-coordinate s.u.
PLAT163	4	Missing *z*-coordinate s.u.
PLAT164	4	Check for refined C—H H atoms
PLAT165	3	Check for *R*-flagged non-H atoms
PLAT166	4	Check for calc flagged atoms with s.u.'s on coordinates
PLAT170	4	Check for sufficient data in atom data loop
PLAT199	1	Test for *SHELXL* room-temperature default (cell)
PLAT200	1	Test for *SHELXL* room-temperature default (data collection)
PLAT201	2	Test for isotropic non-H atoms in main residue(s)
PLAT202	3	Test for isotropic non-H atoms in anion? or solvent?
PLAT210	3	Test for all-isotropic a.d.p.(s)
PLAT211	2	Test for NPD a.d.p.'s (1.0) in main residue(s)
PLAT212	2	Test for NPD a.d.p.'s in anion? & solvent? [0, 1]
PLAT213	2	Test ratio a.d.p. max/min in main residue(s)
PLAT214	2	Test ratio a.d.p. max/min in anion? or solvent?
PLAT215	3	Test for unusual disordered atom a.d.p. in main residue
PLAT216	3	Test for unusual disordered atom a.d.p. in minor residue
PLAT217	1	Test for incomplete U_{ij} data
PLAT220	2	Test $U_{\rm eq}$(max)/$U_{\rm eq}$(min) range for non-H atoms in non-solvent
PLAT221	4	Test $U_{\rm eq}$(max)/$U_{\rm eq}$(min) range for non-H atoms in solvent
PLAT222	3	Test $U_{\rm eq}$(max)/$U_{\rm eq}$(min) range for H atoms in non-solvent
PLAT223	4	Test $U_{\rm eq}$(max)/$U_{\rm eq}$(min) range for H atoms in solvent
PLAT230	2	Hirshfeld rigid-bond test [*Acta Cryst.* (1976), A**32**, 239–244]
PLAT231	4	Hirshfeld rigid-bond test [*Acta Cryst.* (1976), A**32**, 239–244]
PLAT232	2	Hirshfeld rigid-bond test (metal-*X*) [*Acta Cryst.* (1976), A**32**, 239–244]
PLAT233	4	Hirshfeld rigid-bond test (metal-*X*) [*Acta Cryst.* (1976), A**32**, 239–244]
PLAT241	2	Test for unusually high $U_{\rm eq}$ as compared with bonded neighbours
PLAT242	2	Test for unusually low $U_{\rm eq}$ as compared with bonded neighbours
PLAT243	4	Test for unusually high solvent $U_{\rm eq}$ as compared with bonded neighbours
PLAT244	4	Test for unusually low solvent $U_{\rm eq}$ as compared with bonded neighbours
PLAT250	2	Test for unusual anisotropic average U_{ij}
PLAT301	3	Test for main residue(s) disorder
PLAT302	4	Test for (anion/solvent) disorder
PLAT305	2	Test for isolated hydrogen atoms
PLAT306	2	Test for isolated oxygen atoms
PLAT307	2	Test for isolated metal atoms
PLAT308	2	Test for single-bonded metal atoms
PLAT309	2	Test for single-bonded oxygen atoms
PLAT310	2	Test for 'too close' (symmetry-related) full-weight atoms
PLAT311	2	Test for isolated disordered oxygen atoms
PLAT312	2	Test for C=O—H
PLAT313	2	Test for O with three covalent bonds
PLAT318	2	Hybridization problem on N in main residue(s)
PLAT319	2	Hybridization problem on N in solvent/ion

Table A5.7.2.2 (*cont.*).

Test name	Type	Purpose
PLAT320	2	Hybridization problem on C in main residue(s)
PLAT321	2	Hybridization problem on C in solvent/ion
PLAT322	2	Hybridization problem on non-C in main residue(s)
PLAT323	2	Hybridization problem on non-C in solvent/ion
PLAT324	2	Check for possibly missing H on coordinating *X*—N—*X* in main residue
PLAT325	2	Check for possibly missing H on coordinating *X*—N—*X* in solvent/anion
PLAT326	2	Check for possibly missing hydrogen atom on carbon with sp^3-like geometry in the main residue
PLAT327	2	Check for possibly missing hydrogen atom on carbon with sp^3-like geometry in the solvent/anion
PLAT328	2	Check for possibly missing H on potentially sp^3 P
PLAT330	2	Check average phenyl C—C
PLAT331	2	Check average phenyl C—C
PLAT332	2	Check phenyl C—C range
PLAT333	2	Check average in multiply substituted benzene C—C
PLAT334	2	Check average in multiply substituted benzene C—C
PLAT335	2	Check multiply substituted benzene C—C range
PLAT338	2	Check average torsion angle in cyclohexane ring
PLAT340	3	Check bond precision for C—C in light-atom structures [$Z(\max) < 20$]
PLAT341	3	Check bond precision for C—C in structures [$19 < Z(\max) < 40$]
PLAT342	3	Check bond precision for C—C in structures [$Z(\max) > 39$]
PLAT350	3	Test for short C—H (ångstrom difference) XRAY: 0.96
PLAT351	3	Test for long C—H (ångstrom difference) XRAY: 0.96
PLAT352	3	Test for short N—H (ångstrom difference) XRAY: 0.87
PLAT353	3	Test for long N—H (ångstrom difference) XRAY: 0.87
PLAT354	3	Test for short O—H (ångstrom difference) XRAY: 0.82
PLAT355	3	Test for long O—H (ångstrom difference) XRAY: 0.82
PLAT360	2	Test for short C4—C4 (ångstrom difference) XRAY: 1.54
PLAT361	2	Test for long C4—C4 (ångstrom difference) XRAY: 1.54
PLAT362	2	Test for short C4—C3 (ångstrom difference) XRAY: 1.52
PLAT363	2	Test for long C4—C3 (ångstrom difference) XRAY: 1.52
PLAT364	2	Test for short C4—C2 (ångstrom difference) XRAY: 1.46
PLAT365	2	Test for long C4—C2 (ångstrom difference) XRAY: 1.46
PLAT366	2	Test for short C?—C? (ångstrom difference) XRAY: 1.50
PLAT367	2	Test for long C?—C? (ångstrom difference) XRAY: 1.50
PLAT368	2	Test for short C3—C3 (ångstrom difference) XRAY: 1.34
PLAT369	2	Test for long C3—C3 (ångstrom difference) XRAY: 1.34
PLAT370	2	Test for short C3—C2 (ångstrom difference) XRAY: 1.31
PLAT371	2	Test for long C3—C2 (ångstrom difference) XRAY: 1.31
PLAT372	2	Test for short C2—C2 (ångstrom difference) XRAY: 1.25
PLAT373	2	Test for long C2—C2 (ångstrom difference) XRAY: 1.25
PLAT374	2	Test for long N—N bond (> 1.45 Å)
PLAT380	4	Test for incorrectly oriented methyl moiety
PLAT390	3	Test methyl moiety *X*—C—H bond angle
PLAT391	3	Test methyl moiety H—C—H bond angle
PLAT395	2	Test *X*—O—*Y* angle
PLAT396	2	Test Si—O—Si angle
PLAT410	2	Test for short non-bonding intra H···H contacts
PLAT411	2	Test for short non-bonding inter H···H contacts
PLAT412	2	Test for short non-bonding intra H···H contacts (involving *X*H3)
PLAT413	2	Test for short non-bonding inter H···H contacts (involving *X*H3)
PLAT414	2	Test for short non-bonding intra *D*—H···H—*X* contacts
PLAT415	2	Test for short non-bonding inter *D*—H···H—*X* contacts
PLAT416	2	Test for short non-bonding intra *D*—H···H—*D* contacts
PLAT417	2	Test for short non-bonding inter *D*—H···H—*D* contacts
PLAT420	2	Test for *D*—H without acceptor
PLAT430	2	Test for short non-bonding inter $D \cdots A$ contacts
PLAT431	2	Test for short non-bonding inter HL$\cdots A$ contacts (HL = halogen)
PLAT432	2	Test for short non-bonding inter $X \cdots Y$ contacts
PLAT433	4	Test for short non-bonding minor···minor inter $X \cdots Y$ contacts
PLAT480	4	Test for too large H$\cdots A$
PLAT481	4	Test for too large $D \cdots A$
PLAT482	4	Test for too small *D*—H$\cdots A$ angle
PLAT601	2	Test for solvent accessible voids
PLAT602	4	Test for too large solvent accessible voids
PLAT603	4	Test for too large unit cell for void search
PLAT604	4	Test for too many voids
PLAT701	1	Test for consistency of bonds and coordinates in CIF
PLAT702	1	Test for consistency of angles and coordinates in CIF
PLAT703	1	Test for consistency of torsions and coordinates in CIF
PLAT704	1	Test for consistency of contact distances and coordinates in CIF
PLAT705	1	Test for consistency of H-bond *D*—H distances and coordinates in CIF
PLAT706	1	Test for consistency of H-bond H$\cdots A$ distances and coordinates in CIF
PLAT707	1	Test for consistency of H-bond $D \cdots A$ distances and coordinates in CIF
PLAT708	1	Test for consistency of H-bond *D*—H$\cdots A$ angles and coordinates in CIF
PLAT710	4	Test for linear torsions in CIF
PLAT711	1	Test for label problem for bonds in CIF
PLAT712	1	Test for label problem for angles in CIF
PLAT713	1	Test for label problem for torsions in CIF
PLAT714	1	Test for label problem for contact distances in CIF
PLAT715	1	Test for label problem for H-bond *D*—H distances in CIF
PLAT716	1	Test for label problem for H-bond H$\cdots A$ distances in CIF
PLAT717	1	Test for label problem for H-bond $D \cdots A$ distances in CIF

Table A5.7.2.2 (*cont.*).

Test name	Type	Purpose
PLAT718	1	Test for label problem for H-bond *D*—H$\cdots A$ angles in CIF
PLAT720	4	Test for unusual labels
PLAT721	1	Test for consistency of bonds and coordinates in CIF
PLAT722	1	Test for consistency of angles and coordinates in CIF
PLAT723	1	Test for consistency of torsions and coordinates in CIF
PLAT724	1	Test for consistency of contact distances and coordinates in CIF
PLAT725	1	Test for consistency of H-bond *D*—H distances and coordinates in CIF
PLAT726	1	Test for consistency of H-bond H$\cdots A$ distances and coordinates in CIF
PLAT727	1	Test for consistency of H-bond $D \cdots A$ distances and coordinates in CIF
PLAT728	1	Test for consistency of H-bond *D*—H$\cdots A$ angles and coordinates in CIF
PLAT731	1	Test for consistency of bond s.u.'s and coordinate s.u.'s in CIF
PLAT732	1	Test for consistency of angle s.u.'s and coordinate s.u.'s in CIF
PLAT733	1	Test for consistency of torsion s.u.'s and coordinate s.u.'s in CIF
PLAT734	1	Test for consistency of contact distance s.u.'s and coordinate s.u.'s in CIF
PLAT735	1	Test for consistency of H-bond *D*—H distance s.u.'s and coordinate s.u.'s in CIF
PLAT736	1	Test for consistency of H-bond H$\cdots A$ distance s.u.'s and coordinate s.u.'s in CIF
PLAT737	1	Test for consistency of H-bond $D \cdots A$ distance s.u.'s and coordinate s.u.'s in CIF
PLAT738	1	Test for consistency of H-bond *D*—H$\cdots A$ angle s.u.'s and coordinate s.u.'s in CIF
PLAT741	1	Test for missing bond s.u. in CIF
PLAT742	1	Test for missing angle s.u. in CIF
PLAT743	1	Test for missing torsion s.u. in CIF
PLAT744	1	Test for missing contact distance s.u. in CIF
PLAT745	1	Test for missing H-bond *D*—H distance s.u. in CIF
PLAT746	1	Test for missing H-bond H$\cdots A$ distance s.u. in CIF
PLAT747	1	Test for missing H-bond $D \cdots A$ distance s.u. in CIF
PLAT748	1	Test for missing H-bond *D*—H$\cdots A$ angle s.u. in CIF
PLAT751	4	Test for senseless bond s.u. in CIF
PLAT752	4	Test for senseless angle s.u. in CIF
PLAT753	4	Test for senseless torsion s.u. in CIF
PLAT754	4	Test for senseless contact distance s.u. in CIF
PLAT755	4	Test for senseless H-bond *D*—H distance s.u. in CIF
PLAT756	4	Test for senseless H-bond H$\cdots A$ distance s.u. in CIF
PLAT757	4	Test for senseless H-bond $D \cdots A$ distance s.u. in CIF
PLAT758	4	Test for senseless H-bond *D*—H$\cdots A$ angle s.u. in CIF
PLAT761	1	Test for the presence of at least one *X*—H in the CIF
PLAT762	1	Test for at least one *X*—*Y*—H or H—*Y*—H entry in the CIF
PLAT763	1	Test for missing bonds in CIF
PLAT764	4	Test for overcomplete bonds in CIF
PLAT770	2	Test for suspect C—H bonds in CIF (not caught otherwise)
PLAT771	2	Test for suspect N—H bonds in CIF (not caught otherwise)
PLAT772	2	Test for suspect O—H bonds in CIF (not caught otherwise)
PLAT773	2	Test for suspect C—C bonds in CIF (not caught otherwise)
PLAT779	2	Test for suspect angle in CIF (not caught otherwise)
PLAT780	2	Test whether coordinates form a connected set
PLAT790	4	Test whether c.g. residue in unit-cell box
PLAT798	4	Test for alphanumeric label on coordinate record
PLAT799	4	Test for alphanumeric label on displacement-parameter record
PLAT801	4	Test for missing, incomplete or out-of-order cell data
PLAT802	1	Test for input lines longer than 80 characters
PLAT803	1	Test for loop problem in CIF-read
PLAT804	4	Test for ARU-pack problem in *PLATON*
PLAT805	4	Test for insufficient coordinate data
PLAT806	4	Test for insufficient U_{ij} data
PLAT810	4	Test for out-of-memory problem
PLAT850	4	Test for BASF/TWIN problem in *SHELXL*

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