Table A6.1.2.2. *List of data-validation tests applied by PLATON*

Test name	Type	Purpose
PLAT001	1	Check for '**_shelx_res_file**' refinement instruction file
PLAT002	2	Report number of atom sites with distance/angle restraints
PLAT003	2	Report number of non-H atoms with U_{iso} or U_{ij} restraints
PLAT004	5	Report dimensionality of polymer
PLAT005	5	Check for refinement instruction file
PLAT006	5	Check for extinction parameter refinement
PLAT007	5	Report on unrefined *D*—H atoms
PLAT008	5	Check for refinement reflections details
PLAT009	1	Check for potential radiation type and standard wavelength conflict
PLAT010	1	Test for reflection data for validation and archival
PLAT011	1	Test for any ATOMS found in CIF
PLAT012	1	Check for valid **_shelx_res_checksum**
PLAT013	1	Check for **_shelx_hkl_checksum**
PLAT014	1	Check for **_shelxl_fab_checksum**
PLAT015	5	Check for refinement reflections details (*SHELXL*20*xy*)
PLAT016	5	Check for refinement FAB file (*SHELXL*20*xy*)
PLAT017	1	Check the consistency of Scattering type
PLAT018	1	Check **_diffrn_measured_fraction_theta_max** and *__full** equality
PLAT019	1	Check **_diffrn_measured_fraction_theta_max/full** consistency
PLAT020	3	Check for unusually high R_{int} value
PLAT021	4	Check expected number of reflections (max = 1 centro, 2 non-centro)
PLAT022	3	Check expected number of reflections (completeness)
PLAT023	3	Check θ_{max}
PLAT024	4	Check for required Friedel pair averaging Z≤Si (obsolete 1/1/2011)
PLAT025	1	Check for $h_{min} \ldots l_{max}$
PLAT026	3	Check for a weak data set
PLAT027	3	Check **_diffrn_reflns_theta_full**
PLAT028	3	Check the reported **_diffrn_measured_fraction_theta_max**
PLAT029	3	Check the reported **_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	4	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 against 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 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	4	*RR* test

Table A6.1.2.2. *(cont.)*

Test name	Type	Purpose
PLAT061	4	RR' test
PLAT062	4	Rescale T_{min} and T_{max}
PLAT063	4	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 < maximum dimension
PLAT068	1	Test for $F(000)$ calc/reported difference
PLAT069	1	Test for label without numerical part
PLAT070	1	Test for duplicate labels
PLAT071	1	Test for uninterpretable labels
PLAT072	2	Test for extreme first weighting parameter value (*SHELXL*)
PLAT073	1	Test for inconsistency 'constr' versus 'H atoms refined'
PLAT074	1	Test for occupancy = 0.0
PLAT075	1	Test for occupancy > 1.0
PLAT076	1	Test for occupancy < 1.0 for atom on special position
PLAT077	4	Test for non-integral number of atoms in unit cell
PLAT078	1	Test for inconsistency 'geom' versus 'no H atoms'
PLAT079	1	Test for inconsistency 'mixed' versus 'no H atoms'
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 value (*SHELXL*)
PLAT084	3	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, Ga, Mo, Ag, In Ka]
PLAT093	1	Test for inconsistency 'mixed' versus 'no refined H positions'
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 for maximum residual density (reported)
PLAT098	2	Test for minimum residual density (reported)
PLAT099	1	Test for minimum residual density greater zero [0, 1]
PLAT100	5	Report non-integer reported *Z* value in CIF
PLAT101	2	Test for insufficient digits for special position $\frac{1}{3}$ and $\frac{2}{3}$ in *x* coordinate
PLAT102	2	Test for insufficient digits for special position $\frac{1}{3}$ and $\frac{2}{3}$ in *y* coordinate
PLAT103	2	Test for insufficient digits for special position $\frac{1}{3}$ and $\frac{2}{3}$ in *z* coordinate
PLAT104	1	Test for additional translational symmetry [0, 1]
PLAT105	1	Test for inconsistent reported wavelengths in CIF and .res file
PLAT107	2	Test validity of inversion twinning operation
PLAT108	2	Test validity of the twinning operation
PLAT109	2	Test the twinning operation as alternate inversion twinning
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
PLAT115	5	Test for non-crystallographic centre of symmetry [0, 100]
PLAT116	2	Report implemented (pseudo) lattice translation
PLAT119	1	Report problem with symmetry operator syntax
PLAT120	1	Test for consistent **_symmetry_space_group_name_H-M** and symmetry operations

Table A6.1.2.2. *(cont.)*

Test name	Type	Purpose
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 space_**group** settings
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 one 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
PLAT148	3	S.u.on a, b or c – axis too large
PLAT149	3	S.u.on α, β or γ too large
PLAT150	1	Check reported unit-cell volume value
PLAT151	1	Check for s.u. on volume
PLAT152	1	Check for consistency of s.u. on volume and cell parameters
PLAT153	1	Test for equal axial s.u.'s
PLAT154	1	Test for equal cell angle s.u.'s
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
PLAT158	4	Check for standard reduced cell
PLAT159	1	Check β angle value for monoclinic c
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
PLAT167	3	Test DANG restraint value in CIF-embedded .res file
PLAT168	4	Check for EXYZ record(s) in CIF-embedded shelxl.res file
PLAT169	4	Check for AFIX 1 record(s) in CIF-embedded shelxl.res file
PLAT170	4	Check for sufficient data in in atom data loop
PLAT171	4	Check for Ea.d.p. record(s) in CIF-embedded shelxl.res file
PLAT172	4	Check for DFIX record(s) in CIF-embedded shelxl.res file
PLAT173	4	Check for DANG record(s) in CIF-embedded shelxl.res file
PLAT174	4	Check for FLAT record(s) in CIF-embedded shelxl.res file
PLAT175	4	Check for SAME record(s) in CIF-embedded shelxl.res file
PLAT176	4	Check for SADI record(s) in CIF-embedded shelxl.res file
PLAT177	4	Check for DELU record(s) in CIF-embedded shelxl.res file
PLAT178	4	Check for SIMU record(s) in CIF-embedded shelxl.res file
PLAT179	4	Check for CHIV record(s) in CIF-embedded shelxl.res file
PLAT180	4	Check rounding of cell axes and angles
PLAT181	1	Check for all angles exactly 90 degrees in monoclinic
PLAT182	1	Check for at least one s.u. greater than zero in monoclinic

Table A6.1.2.2. *(cont.)*

Test name	Type	Purpose
PLAT183	1	Check for **_cell_measured_reflns_used** value reported
PLAT184	1	Check for **_cell_measured_theta_min** value reported
PLAT185	1	Check for **_cell_measured_theta_max** value reported
PLAT186	4	Check for ISOR record(s) in CIF-embedded shelxl.res file
PLAT187	4	Check for RIGU record(s) in CIF-embedded shelxl.res file
PLAT188	3	Test SIMU restraint value in CIF-embedded .res file
PLAT189	3	Test SAME restraint value in CIF-embedded .res file
PLAT190	3	Test RIGU restraint value in CIF-embedded .res file
PLAT191	3	Test SADI restraint value in CIF-embedded .res file
PLAT192	3	Test DELU restraint value in CIF-embedded .res file
PLAT193	1	Test for consistency of cell and diffraction temperatures
PLAT194	3	Report on non-default DEFS restraint values in CIF-embedded .res file
PLAT195	3	Test DFIX restraint value in CIF-embedded .res file
PLAT196	1	Test for measurement temperature $\neq 293$ K and no TEMP record
PLAT197	1	Test for specification of unit-cell measurement temperature
PLAT198	1	Test for specification of data collection temperature
PLAT199	1	Test for *SHELXL* room-temperature default (cell)
PLAT200	1	Test for *SHELXL* room-temperature default (datacollection)
PLAT201	2	Test for isotropic non-H atoms in main residue(s)
PLAT202	3	Test for isotropic non-H atoms in anion ? or solvent ?
PLAT203	2	Test for negative non-hydrogen U(iso)
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? and 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
PLAT218	3	Test for constrained U_{ij}'s
PLAT220	2	Test $U_{\rm eq}$(max)/$U_{\rm eq}$(min) range for non-H atoms in non-solvent
PLAT221	2	Test $U_{\rm eq}$(max)/$U_{\rm eq}$(min) range for non-H atoms in solvent
PLAT222	3	Test $U_{\rm iso}$(max)/$U_{\rm iso}$(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
PLAT224	1	Test for difference in implicit and explicit $U_{\rm eq}$
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]
PLAT234	4	Hirshfeld rigid-bond test [*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
PLAT245	2	Test for unusually low H $U_{\rm eq}$ as compared with bonded atom
PLAT250	2	Test for unusual anisotropic average U_{ij}
PLAT260	2	Test for high average $U_{\rm eq}$ for residue
PLAT300	4	Test for fixed partial occupancy
PLAT301	3	Test for main residue(s) disorder %
PLAT302	4	Test for (anion/solvent) disorder %
PLAT303	2	Test for more than one connection to hydrogen atoms
PLAT304	4	Test for non-integer number of atoms in residue
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

Table A6.1.2.2. *(cont.)*

Test name	Type	Purpose
PLAT312	2	Test for C=O—H
PLAT313	2	Test for O with three covalent bonds
PLAT314	2	Test for metal-O—H angle of H_2O
PLAT315	2	Test for single bonded carbon atom
PLAT316	2	Check for too many H's on C in C=N bond in main residue(s)
PLAT317	2	Check for too many H's on C in C=N bond in solvent/ion (s)
PLAT318	2	Hybridization problem on N in main residue(s)
PLAT319	2	Hybridization problem on N in solvent/ion
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 H on potentially sp^3 carbon
PLAT327	2	Check for possibly missing H on potentially sp^3 carbon
PLAT328	4	Check for a possibly missing H on potentially sp^3 phosphorus
PLAT329	4	Check for unclear carbon atom hybridization
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 multiple substituted benzene type C—C
PLAT334	2	Check average in multiple substituted benzene type C—C
PLAT335	2	Check multiple substituted benzene type C—C range
PLAT336	2	Check unusual bond distance
PLAT338	4	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 ($Z_{max} > 39$)
PLAT343	2	Hybridization problem on C in main residue(s)
PLAT344	2	Hybridization problem on C in solvent/ion
PLAT350	3	Test for short C—H (ångström difference) X-ray: 0.96 neutron: 1.08
PLAT351	3	Test for long C—H (ångström difference) X-ray: 0.96 neutron: 1.08
PLAT352	3	Test for short N—H (ångström difference) X-ray: 0.87 neutron: 1.009
PLAT353	3	Test for long N—H (ångström difference) X-ray: 0.87 neutron: 1.009
PLAT354	3	Test for short O—H (ångström difference) X-ray: 0.82 neutron: 0.983
PLAT355	3	Test for long O—H (ångström difference) X-ray: 0.82 neutron: 0.983
PLAT356	3	Test for short B—H distance in *X*—BH_3 moiety
PLAT357	3	Test for long B—H distance in *X*—BH_3 moiety
PLAT358	3	Test for short B—H distance in (X,Y,Z)-B—H moiety
PLAT359	3	Test for long B—H distance in (X,Y,Z)-B—H moiety
PLAT360	2	Test for short C4 —C4 (ångström difference) X-ray: 1.54
PLAT361	2	Test for long C4 —C4 (ångström difference) X-ray: 1.54
PLAT362	2	Test for short C4 —C3 (ångström difference) X-ray: 1.52
PLAT363	2	Test for long C4 —C3 (ångström difference) X-ray: 1.52
PLAT364	2	Test for short C4 —C2 (ångström difference) X-ray: 1.46
PLAT365	2	Test for long C4 —C2 (ångström difference) X-ray: 1.46
PLAT366	2	Test for short C? —C? (ångström difference) X-ray: 1.50
PLAT367	2	Test for long C? —C? (ångström difference) X-ray: 1.50
PLAT368	2	Test for short C3 —C3 (ångström difference) X-ray: 1.34
PLAT369	2	Test for long C3 —C3 (ångström difference) X-ray: 1.34
PLAT370	2	Test for short C3 —C2 (ångström difference) X-ray: 1.31
PLAT371	2	Test for long C3 —C2 (ångström difference) X-ray: 1.31
PLAT372	2	Test for short C2 —C2 (ångström difference) X-ray: 1.25
PLAT373	2	Test for long C2 —C2 (ångström difference) X-ray: 1.25
PLAT374	2	Test for long N—N bond (> 1.45 Å)
PLAT375	2	Test for C—O—H with large C—O distance
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

Table A6.1.2.2. *(cont.)*

Test name	Type	Purpose
PLAT395	2	Test general *X*—O—*Y* angle value
PLAT396	2	Test Si—O—Si angle value
PLAT397	2	Test B—O—B angle value
PLAT398	2	Test C—O—C angle value
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 XH_3)
PLAT413	2	Test for short non-bonding inter H···H contacts (involving XH_3)
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 bonds without acceptor
PLAT430	2	Test for short non-bonding inter D···*A* contacts
PLAT431	2	Test for short non-bonding inter HL···*A* contacts (HL = halogen)
PLAT432	2	Test for short non-bonding inter X···*Y* contacts
PLAT433	4	Test for short non-bonding minor..minor inter X···*Y* contacts
PLAT434	2	Test for short non-bonding inter HL···HL contacts (HL = halogen)
PLAT480	4	Test for too large H···*A*
PLAT481	4	Test for too large D···*A*
PLAT482	4	Test for too small *D*—H···*A* angle
PLAT484	4	Test for not rounded *D*—H···*A* angle
PLAT601	2	Test for (unreported) solvent accessible voids
PLAT602	2	Test for too large (unreported) solvent accessible voids
PLAT603	4	Test for too large unit cell for VOID search
PLAT605	4	Test for (reported) solvent accessible voids
PLAT606	4	Test for too large (reported) solvent accessible voids
PLAT607	4	Test for skipped VOID Test
PLAT608	4	Test for too many atoms for *ADDSYM* test as part of *checkcif*
PLAT609	4	Check for missing SQUEEZE or MASK Info
PLAT650	4	Report the use of the *SHELXL*/SWAT instruction
PLAT660	1	Test for radiation type specification
PLAT697	1	Check for BLANK records in embedded *hkl* file
PLAT698	1	Check for **`_shelx_include_file_checksum`**
PLAT699	1	Test for **`_exptl_crystal_description`** value
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···*A* distances and coordinates in CIF
PLAT707	1	Test for consistency of H-bond D···*A* distances and coordinates in CIF
PLAT708	1	Test for consistency of H-bond *D*—H···*A* angles and coordinates in CIF
PLAT710	4	Test for linear torsions in CIF
PLAT711	1	Test for label problems 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···*A* distances in CIF
PLAT717	1	Test for label problem for H-bond D···*A* distances in CIF
PLAT718	1	Test for label problem for H-bond *D*—H···*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	2	Test for consistency of contact distances and coordinates in CIF
PLAT725	2	Test for consistency of H-bond *D*—H distances and coordinates in CIF
PLAT726	2	Test for consistency of H-bond H···*A* distances and coordinates in CIF
PLAT727	1	Test for consistency of H-bond D···*A* distances and coordinates in CIF

Table A6.1.2.2. *(cont.)*

Test name	Type	Purpose
PLAT728	1	Test for consistency of H-bond *D*—H···*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 angles and coordinates in CIF s.u.'s
PLAT733	1	Test for consistency of torsions and coordinates in CIF s.u's
PLAT734	1	Test for consistency of contact distance s.u. and coordinate s.u. in CIF
PLAT735	1	Test for consistency of H-bond *D*—H distance s.u. and coordinate s.u in CIF
PLAT736	1	Test for consistency of H-bond H···*A* distance s.u. and coordinates in CIF
PLAT737	1	Test for consistency of H-bond D···*A* distance s.u. and coordinates in CIF
PLAT738	1	Test for consistency of H-bond *D*—H···*A* angle and coordinates in CIF s.u.
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···*A* distance s.u. in CIF
PLAT747	1	Test for missing H-bond D···*A* distance s.u. in CIF
PLAT748	1	Test for missing H-bond *D*—H···*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···*A* distance s.u. in CIF
PLAT757	4	Test for senseless H-bond D···*A* distance s.u. in CIF
PLAT758	4	Test for Senseless H-bond *D*—H···*A* angle s.u. in CIF
PLAT760	1	Test for the presence of at least one torsion angle in the 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
PLAT766	4	Test for erroneous LIST 8 instruction in embedded .ins file
PLAT767	4	Test for erroneous LIST 6 instruction in embedded .ins file
PLAT768	4	Test for CIF/RES embedded explicit scattering factor values
PLAT769	4	Test for CIF embedded explicit scattering factor values
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)
PLAT774	1	Test for too large / erroneous bond distance
PLAT775	1	Test for too large / erroneous contact distance
PLAT776	1	Test for too large / erroneous H-bond *D*—H distance
PLAT777	2	Check for N···H···*X*+ bonds in CIF
PLAT778	2	Check for O···H···*X*+ bonds in CIF
PLAT779	4	Test for suspect angle in CIF (not caught otherwise)
PLAT780	1	Test whether coordinates form a connected set
PLAT781	1	Test for Flack *x* value for centrosymmetric space-group
PLAT782	2	Test for unusual C—NO_2 and C—CO_2 moiety bond geometry
PLAT787	4	Test for El1 in sum formula
PLAT788	4	Test for El1 in moiety formula
PLAT789	4	Report the number of atoms with negative **`_atom_site_disorder_group`**
PLAT790	4	Test whether c.g. residue in unit-cell box
PLAT791	4	Check the absolute configuration of chiral atom in Sohnke space group
PLAT792	1	Check the absolute configuration of chiral atom in a polar non-Sohnke space group
PLAT793	4	Check the absolute configuration of chiral atom in a centrosymmetric space group
PLAT794	5	Report the calculated 'valence bond' valency for metals
PLAT795	4	Test for C-atom labels ordered

Table A6.1.2.2. *(cont.)*

Test name	Type	Purpose
PLAT796	4	Test for O-atom labels ordered
PLAT797	4	Test for N-atom labels ordered
PLAT798	4	Test for alphanumeric label on coordinate record
PLAT799	4	Test for alphanumeric label on displacement parameter record
PLAT800	4	Test for out-of-order symmetry data
PLAT801	4	Test for missing, incomplete or out-of-order cell data
PLAT802	4	Test for input lines longer than 80 characters
PLAT803	1	Test for loop problem in CIF-read
PLAT804	5	Test for ARU-pack problem(s) in *PLATON*
PLAT805	1	Test for insufficient 'coordinate data'
PLAT806	4	Test for insufficient 'U_{ij} data'
PLAT807	5	Test for maximum number of ATOMS exceeded problem
PLAT808	5	Test for parseable *SHELXL* style weighting scheme
PLAT809	1	Test the *SHELXL* style weighting scheme
PLAT810	5	Test for out-of-memory problem
PLAT811	5	Test for no *ADDSYM* analysis
PLAT812	5	Test for ALIAS OVERFLOW
PLAT813	1	Test for insufficient data on HKLF record in CIF
PLAT814	5	Test for (in)commensurate structure CIF
PLAT815	5	Test for number of population parameter overflow
PLAT816	5	Test for final refinement with detwinned HKLF 4 data
PLAT820	5	Report read problem in *PLATON*/PLA230
PLAT822	4	Check for negative PART record(s) in CIF-embedded shelxl.res file
PLAT850	4	Test for BASF/TWIN problem in *SHELXL*
PLAT860	3	Test for restraints used in refinement
PLAT868	4	Report the suppression of *Olex2*/**`_smtbx_masks`** use related ALERTS
PLAT869	4	Report the suppression of SQUEEZE use related ALERTS
PLAT870	4	Report the suppression of some twinning related ALERTS
PLAT871	4	Report the suppression of some Laue technique related ALERTS
PLAT872	4	Report the suppression of anharmonic refinement related ALERTS
PLAT880	1	Report missing datum for **`_diffrn_reflns_number`**
PLAT881	1	Report missing datum for **`_diffrn_reflns_av_R_equivalents`**
PLAT882	1	Report missing datum for **`__diffrn_reflns_av_unetI/netI`**
PLAT883	1	Report missing datum for **`_atom_sites_solution_primary`**
PLAT898	4	Check for duplicate H-M space-group symbol
PLAT899	4	Report the use of an older *SHELXL* version
PLAT900	1	Test for 'no-matching reflection file'
PLAT901	1	Test for CIF and FCF CELL not matching
PLAT902	1	Test for non-zero number of recognised reflections in FCF
PLAT903	1	Test for Fobs=Fcalc in FCF
PLAT904	1	Test for NREF > NPAR in the CIF
PLAT905	3	Report negative *K* values in the analysis of variance
PLAT906	3	Report large *K* values in the analysis of variance
PLAT907	2	Check whether the structure needs to be inverted
PLAT908	2	Report on max observed data in any resolution shell
PLAT909	3	Report of observed data at θ cutoff
PLAT910	3	Test for number of missing reflections below $\theta_{\min}$
PLAT911	3	Test for missing reflections between $\theta_{\min}$and $(\sin\theta)/\lambda = 0.6$
PLAT912	4	Test for missing reflections above $(\sin\theta)/\lambda = 0.6$
PLAT913	3	Test for missing strong reflections
PLAT914	3	Test for absence of Bijvoet pairs in non-centro structure
PLAT915	3	Test for low Friedel pair coverage in non-centro structure
PLAT916	2	Test for differing Flack *x* and Hooft *y* parameter values
PLAT917	2	Test/report whether FCF is basedon *a* BASF/TWIN refinement
PLAT918	3	Test for reflections with I(obs) $\ll$ I(calc)
PLAT919	3	Test for reflections affected by the beamstop
PLAT920	1	Test for $\theta_{\max}$ consistency between CIF and FCF
PLAT921	1	Test for *R*1 consistency between CIF and FCF (reported)
PLAT922	1	Test for *wR*2 consistency between CIF and FCF (reported)

Table A6.1.2.2. *(cont.)*

Test name	Type	Purpose
PLAT923	1	Test for *S* consistency between CIF and FCF (reported)
PLAT924	1	Test for consistency of the reported and calculated $\rho_{\min}$
PLAT925	1	Test for consistency of the reported and calculated $\rho_{\max}$
PLAT926	1	Test for *R*1 consistency between CIF and FCF (calculated)
PLAT927	1	Test for *wR*2 consistency between CIF and FCF (calculated)
PLAT928	1	Test for *S* consistency between CIF and FCF (calculated)
PLAT929	5	Test for interpretable weight parameters for *R*1, *wR*2 and *S* comparison
PLAT930	2	Test for missed twinning from FCF data
PLAT931	5	Test for missed twinning from FCF/CIF data
PLAT933	2	Report number of OMIT records in embedded .res file
PLAT934	3	Report number of outliers in the FCF file
PLAT935	2	Pseudo extinction parameter test
PLAT936	2	Test for DAMP instruction in embedded .res file
PLAT937	4	Report exponential term in *SHELXL* weight expression
PLAT939	3	Test for high not-weight-optimized S value
PLAT940	3	Test for *wR*2 refinement with all data
PLAT941	3	Test fit low measured *hkl* multiplicity
PLAT949	5	Test for Poisson type intensity Sigma distribution
PLAT950	5	Test for reported and calculated $H_{\max}$ difference (from CIF data)
PLAT951	5	Test for reported and calculated $K_{\max}$ difference (from CIF data)
PLAT952	5	Test for reported and calculated $L_{\max}$ difference (from CIF data)
PLAT953	1	Test for reported (in CIF) and actual $H_{\max}$ difference in the FCF file
PLAT954	1	Test for reported (in CIF) and actual $K_{\max}$ difference in the FCF file
PLAT955	1	Test for reported (in CIF) and actual $L_{\max}$ difference in the FCF file
PLAT956	1	Test for calculated ($\theta_{\max}$) and actual $H_{\max}$ difference in the FCF file
PLAT957	1	Test for calculated ($\theta_{\max}$) and actual $K_{\max}$ difference in the FCF file
PLAT958	1	Test for calculated ($\theta_{\max}$) and actual $L_{\max}$ difference in the FCF file
PLAT960	3	Test for reflections with $I < -2\sigma$
PLAT961	5	Test for absence of negative observed intensities
PLAT962	5	Test for input reflections with $\sigma(I) = 0.0$
PLAT963	2	Test for both weighting parameter values zero (*SHELXL*)
PLAT964	2	Test for consistency of *SHELXL* weight parameters in CIF and embedded .res file
PLAT965	2	Test whether the *SHELXL* weight optimization has converged
PLAT966	5	Test/report omit threshold criterion value
PLAT967	5	Report θ cutoff (OMIT) record in embedded .res file
PLAT969	5	Report 'Henn *et al.*' predicted and *R*-factor-gap values
PLAT970	5	Test/report electron diffraction
PLAT971	2	Test for large positive calculated residual density
PLAT972	2	Test for large negative calculated residual density
PLAT973	2	Test for large positive density on metal atom
PLAT974	2	Test for large negative density close to metal atom
PLAT975	2	Test for positive density near N or O
PLAT976	2	Test for negative density near N or O
PLAT977	2	Test for negative density on H atom positions
PLAT978	2	Report number of cases with positive density on C—C bonds
PLAT979	1	Report the use of *NoSpherA2* scattering factors
PLAT980	1	Test for non-zero number of anomalous scattering factors
PLAT981	1	Test for non-zero f'' anomalous scattering factor values
PLAT982	1	Test the anomalous scattering factor f' values against IT
PLAT983	1	Test the anomalous scattering factor f'' values against IT
PLAT984	1	Test the anomalous scattering factor f' values against B and C
PLAT985	1	Test the anomalous scattering factor f'' values against B and C
PLAT986	1	Test for non-zero f' anomalous scattering factor values
PLAT987	1	Test for the need of a TWIN/BASF refinement
PLAT988	1	Report the use of supplied f' for missing internally calculated value
PLAT989	1	Report the use of supplied f'' for missing internally calculated value
PLAT990	1	Report deprecated .res file based SQUEEZE job

Table A6.1.2.2. *(cont.)*

Test name	Type	Purpose
PLAT991	5	Report on generated *hkl* data
PLAT992	5	Report difference between reported and actual **`_reflns_number_gt`** values
PLAT993	1	Report missing .bodd include file
PLAT994	1	Report missing *SHELXL*/MERG instruction
PLAT995	1	Report problem with recreating FCF with *SHELXL*
PLAT996	1	Test validity of *SHELXL* style LIST 4 F_o/F_c FCF file
PLAT997	1	Test for acceptable CIF/FCF file combination for *SHELXL*
PLAT998	1	Test for LIST3
PLAT999	1	Test for LIST6