

# Resource Summary Report

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## SHELX

RRID:SCR\_014220

Type: Tool

### Proper Citation

SHELX (RRID:SCR\_014220)

### Resource Information

**URL:** <http://shelx.uni-ac.gwdg.de/SHELX/>

**Proper Citation:** SHELX (RRID:SCR\_014220)

**Description:** A set of software programs that utilizes dual spaces algorithms for the determination of small and macromolecular crystal structures by single crystal X-ray and neutron diffraction. Libraries, extra files and environment variables are not required for the executables. SHELX is intended to be run on a command prompt but may be called from GUIs such as shelXle, Olex2, Oscail or WinGX, or hkl2map., THIS RESOURCE IS NO LONGER IN SERVICE. Documented on September 16,2025.

**Resource Type:** image analysis software, software resource, software application, image reconstruction software, data processing software, standalone software

**Defining Citation:** [DOI:10.1107/S2053273314026370](https://doi.org/10.1107/S2053273314026370)

**Keywords:** standalone software, image reconstruction software, image analysis software, crystal structure, crystal xray, neutron diffraction, bio.tools

**Availability:** THIS RESOURCE IS NO LONGER IN SERVICE

**Resource Name:** SHELX

**Resource ID:** SCR\_014220

**Alternate IDs:** biotools:shelx

**Alternate URLs:** <https://bio.tools/shelx>

**Record Creation Time:** 20220129T080319+0000

**Record Last Update:** 20260728T043436+0000

### Ratings and Alerts

No rating or validation information has been found for SHELX .

No alerts have been found for SHELX .

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## Data and Source Information

**Source:** [SciCrunch Registry](#)

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## Usage and Citation Metrics

We found 520 mentions in open access literature.

**Listed below are recent publications.** The full list is available at [nidm-terms](#) .

Majumdar D, et al. (2025) Synthesis, characterization, crystal engineering, DFT, and biological evaluation of a novel Cu(II)-perchlorate Schiff base complex. BMC chemistry, 19(1), 227.

Sourjah A, et al. (2025) Physicochemical Properties of New Ionic Liquids and Plastic Crystal Based on Huckel Anions. Chemistry (Weinheim an der Bergstrasse, Germany), 31(16), e202403681.

Arakcheeva A, et al. (2025) Cu<sub>2</sub>OSeO<sub>3</sub> turns trigonal with structural transformation and implications for skyrmions. Scientific reports, 15(1), 31945.

Stoian C, et al. (2025) Heavier Diferrocenylpnictogenium Ions. Chemistry (Weinheim an der Bergstrasse, Germany), 31(1), e202403555.

Ben Elhaj Y, et al. (2025) Novel lead-free bismuth-based perovskite-like (BrC<sub>5</sub>H<sub>13</sub>N)3Bi2Br9: synthesis, structural investigations and optoelectronic properties. RSC advances, 15(16), 12834.

Riesebeck T, et al. (2025) Synthesis and Characterization of Platinum(II) Complexes with Bis(3-(trifluoromethyl)-pyrazolyl)-borate Auxiliary Ligands. Inorganic chemistry, 64(31), 15881.

Gutmańska K, et al. (2025) From Donor-Acceptor Ligands to Smart Coordination Polymers: Cyanothiazole-Cu(I) Complexes for Multifunctional Electronic Devices. Chemistry (Weinheim an der Bergstrasse, Germany), 31(31), e202500215.

Takeyama T, et al. (2025) A Series of AnVIO<sub>22</sub><sup>+</sup> Complexes (An = U, Np, Pu) with N<sub>3</sub>O<sub>2</sub>-Donating Schiff-Base Ligands: Systematic Trends in the Molecular Structures and Redox Behavior. Inorganic chemistry, 64(3), 1313.

Ahmed A, et al. (2025) (Z)-N-(3-([1,1'-biphenyl]-2-yl)-4-heptyl-4-hydroxythiazolidin-2-ylidene)-4-bromobenzamide as carbonic anhydrase inhibitor: exploration of its in vitro and in silico studies. BMC chemistry, 19(1), 65.

Voigt J, et al. (2025) An aperiodic chiral tiling by topological molecular self-assembly. Nature communications, 16(1), 83.

di Lorenzo D, et al. (2025) Application of modular isoxazoline-2,2-amino acid-based peptidomimetics as chemical model systems for studying the tau misfolding. *iScience*, 28(4), 112272.

García-Valdivia AA, et al. (2025) In Situ Ligand Transformation for the Development of Luminescent 3D Metal-Organic Frameworks with Diamond-like Topology. *Crystal growth & design*, 25(3), 703.

Yamaguchi Y, et al. (2025) Ligand triplet energy escape in lanthanide complexes for developing luminescent molecular thermometers. *Communications chemistry*, 8(1), 269.

Vrabie R, et al. (2025) Unlocking the potential of trifluoromethyl pyrrole derivatives in chronic wounds management: rapid synthesis, structural insights, and potent antimicrobial activity. *Journal of enzyme inhibition and medicinal chemistry*, 40(1), 2513406.

Lister TM, et al. (2025) Engineered enzymes for enantioselective nucleophilic aromatic substitutions. *Nature*, 639(8054), 375.

López-Chamorro C, et al. (2025) Silver Binding Dichotomy for 7-Deazaadenine/Thymine: Preference for Watson-Crick Pairing over Homobase Interactions in DNA. *Inorganic chemistry*, 64(28), 14455.

Niazov-Elkan A, et al. (2025) Lattice bond chains administer kink anisotropy and inform strategies of theophylline crystal self-healing. *iScience*, 28(7), 112866.

Namoto K, et al. (2024) NIBR-LTSi is a selective LATS kinase inhibitor activating YAP signaling and expanding tissue stem cells in vitro and in vivo. *Cell stem cell*, 31(4), 554.

Mahana Y, et al. (2024) Structural evidence for protein-protein interaction between the non-canonical methyl-CpG-binding domain of SETDB proteins and C11orf46. *Structure (London, England : 1993)*, 32(3), 304.

Bai S, et al. (2024) Calix[2]azolum[2]benzimidazolone hosts for selective binding of neutral substrates in water. *Nature communications*, 15(1), 6616.