

# 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:** data processing software, image analysis software, image reconstruction software, software application, software resource, 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:** 20260821T194017+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 523 mentions in open access literature.

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

Sinyavskiy S, et al. (2026) Benzo[e][1,2,4]triazolo[1,5-c][1,2,3]triazines: Design, Synthesis, and Cytotoxic Effects. *Chemistry & biodiversity*, 23(6), e71416.

Chen CY, et al. (2026) Transcriptome-guided development of a fibrosis-reversal compound reduces skin scarring and allows regeneration via mitochondrial uncoupling. *Cell reports. Medicine*, 7(5), 102821.

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.

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.

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)<sub>3</sub>Bi<sub>2</sub>Br<sub>9</sub>: synthesis, structural investigations and optoelectronic properties. *RSC advances*, 15(16), 12834.

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.

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.

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.

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.

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.

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.

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

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.