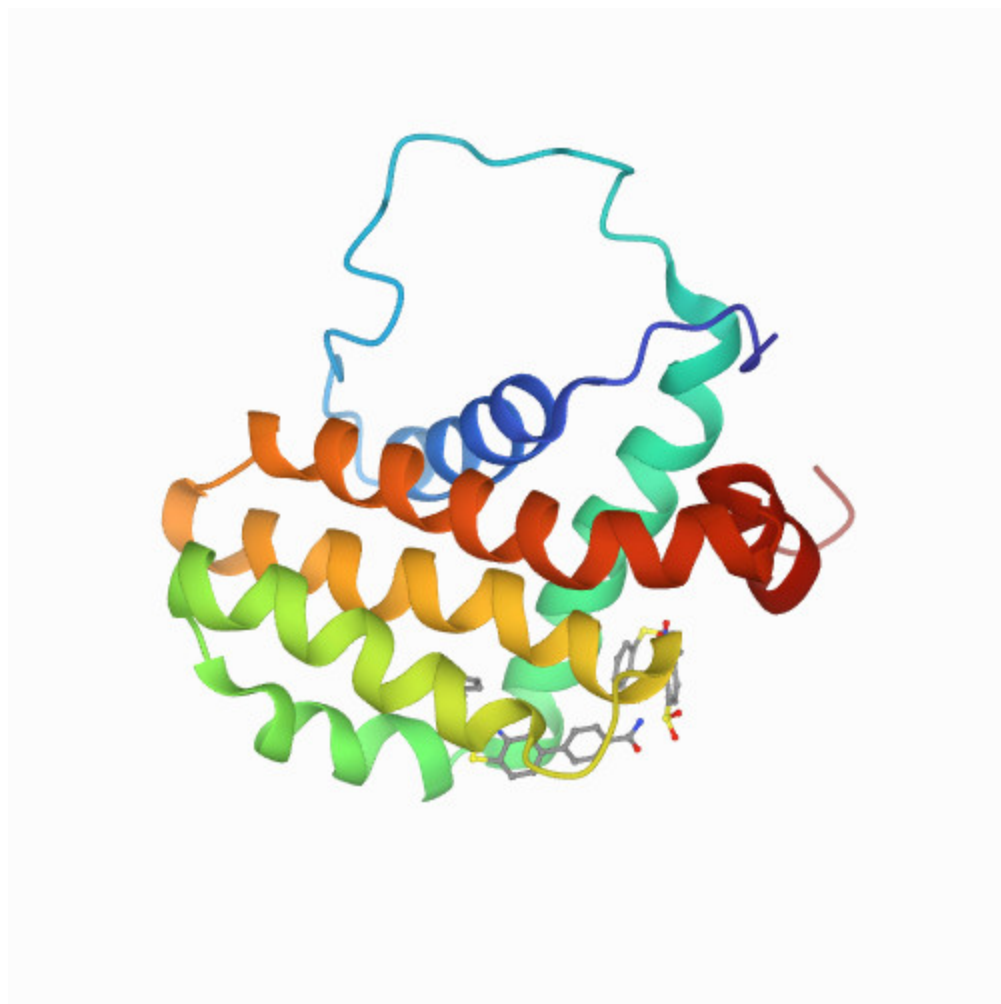


1YSW

 rcsb.org/structure/1ysw

NMR Ensemble



Macromolecule Content

- Total Structure Weight: 19.85 kDa
- Atom Count: 1398
- Modelled Residue Count: 164
- Deposited Residue Count: 164
- Unique protein chains: 1

Solution structure of the anti-apoptotic protein Bcl-2 complexed with an acyl-sulfonamide-based ligand

PDB DOI: [10.2210/pdb1YSW/pdb](https://doi.org/10.2210/pdb1YSW/pdb)

Classification: **APOPTOSIS**

Organism(s): [Homo sapiens](#)

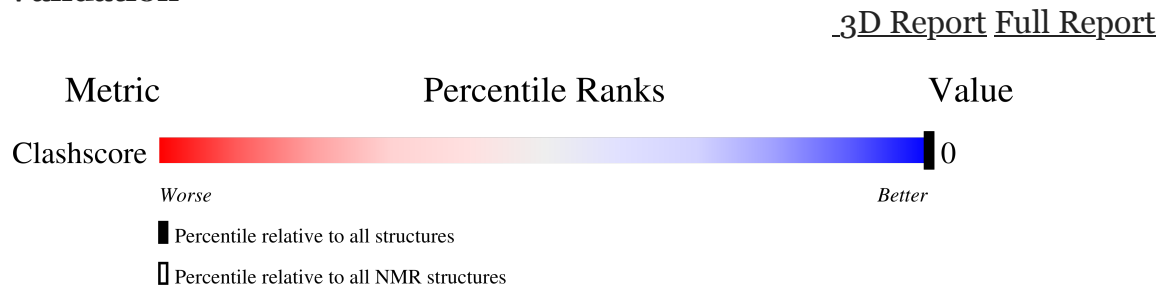
Expression System: [Escherichia coli BL21\(DE3\)](#)

Mutation(s): No

Deposited: 2005-02-09 **Released:** 2005-06-07

Deposition Author(s): [Oltersdorf, T.](#), [Elmore, S.W.](#), [Shoemaker, A.R.](#), [Armstrong, R.C.](#), [Augeri, D.J.](#), [Belli, B.A.](#), [Bruncko, M.](#), [Deckwerth, T.L.](#), [Dinges, J.](#), [Hajduk, P.J.](#), [Joseph, M.K.](#), [Kitada, S.](#), [Korsmeyer, S.J.](#), [Kunzer, A.R.](#), [Letai, A.](#), [Li, C.](#), [Mitten, M.J.](#), [Nettesheim, D.G.](#), [Ng, S.](#), [Nimmer, P.M.](#), [O'Connor, J.M.](#), [Oleksijew, A.](#), [Petros, A.M.](#), [Reed, J.C.](#), [Shen, W.](#), [Tahir, S.K.](#), [Thompson, C.B.](#), [Tomaselli, K.J.](#), [Wang, B.](#), [Wendt, M.D.](#), [Zhang, H.](#), [Fesik, S.W.](#), [Rosenberg, S.H.](#)

wwPDB Validation



This is version 1.3 of the entry. See complete [history](#).

An inhibitor of Bcl-2 family proteins induces regression of solid tumours

[Oltersdorf, T.](#), [Elmore, S.W.](#), [Shoemaker, A.R.](#), [Armstrong, R.C.](#), [Augeri, D.J.](#), [Belli, B.A.](#), [Bruncko, M.](#), [Deckwerth, T.L.](#), [Dinges, J.](#), [Hajduk, P.J.](#), [Joseph, M.K.](#), [Kitada, S.](#), [Korsmeyer, S.J.](#), [Kunzer, A.R.](#), [Letai, A.](#), [Li, C.](#), [Mitten, M.J.](#), [Nettesheim, D.G.](#), [Ng, S.](#), [Nimmer, P.M.](#), [O'Connor, J.M.](#), [Oleksijew, A.](#), [Petros, A.M.](#), [Reed, J.C.](#), [Shen, W.](#), [Tahir, S.K.](#), [Thompson, C.B.](#), [Tomaselli, K.J.](#), [Wang, B.](#), [Wendt, M.D.](#), [Zhang, H.](#), [Fesik, S.W.](#), [Rosenberg, S.H.](#)

(2005) *Nature* **435**: 677-681

PubMed: [15902208](#)

DOI: [10.1038/nature03579](https://doi.org/10.1038/nature03579)

Primary Citation of Related Structures:

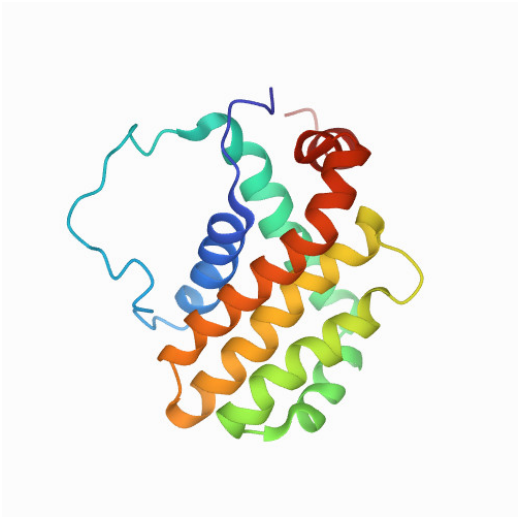
[1YSG](#), [1YSL](#), [1YSN](#), [1YSW](#), [1YSX](#)

PubMed Abstract:

Macromolecules

Find similar proteins by:

(by identity cutoff) | [3D Structure](#)

Entity ID: 1					
Molecule					
Chains					
Sequence Length					
Organism					
Details					
Image					
Apoptosis regulator Bcl-2	A	164	Homo sapiens	Mutation(s): 0 Gene Names: BCL2	
UniProt & NIH Common Fund Data Resources					

Find proteins for [P10415](#) (*Homo sapiens*)

Explore [P10415](#)

Go to UniProtKB: [P10415](#)

PHAROS: [P10415](#)

GTEX: [ENSG00000171791](#)

Protein Feature View

[Expand](#)

Reference Sequence

1YSW_1



PDB ENTITY 1YSW_1

UNIPROT [P10415](#)

HYDROPATHY

DISORDER

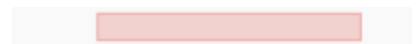
DISORDERED BINDING

PFAM



HAGRTGYDNREIMKYIHKLSQRGYB/DAGDDE

HAGRTGYDNREIMKYIHKLSQRGYB/DAG



Small Molecules

Ligands 1 Unique		
ID		
Chains		
Name / Formula / InChI Key		
2D Diagram		
3D Interactions		
43B (Subject of Investigation/LOI)	B [auth A]	3-NITRO-N-{4-[2-(2-PHENYLETHYL)-1,3-BENZOTHAZOL-5-YL]BENZOYL}-4-{[2-(PHENYLSULFANYL)ETHYL]AMINO}BENZENESULFONAMIDE C ₃₆ H ₃₀ N ₄ O ₅ S ₃ KYLSTDPZEIQYFX-UHFFFAOYSA-N

Experimental Data & Validation

Experimental Data

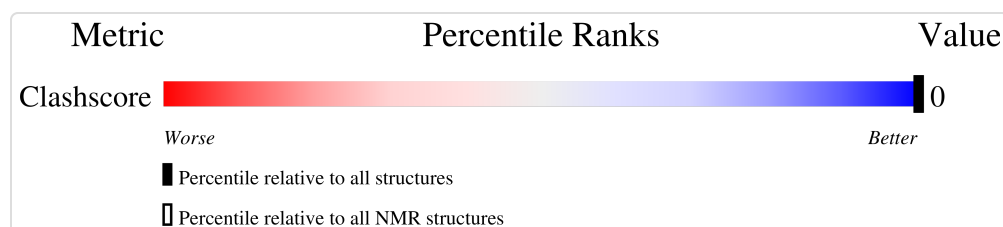
Method: SOLUTION NMR

Conformers Submitted: 1

OLDERADO: [1YSW](#) [Olderado](#)

Structure Validation

View [Full Validation Report](#)



Deposition Data

Deposited Date: 2005-02-09

Released Date: 2005-06-07

Deposition Author(s): Oltersdorf, T., Elmore, S.W., Shoemaker, A.R., Armstrong, R.C., Augeri, D.J., Belli, B.A., Bruncko, M., Deckwerth, T.L., Dinges, J., Hajduk, P.J., Joseph, M.K., Kitada, S., Korsmeyer, S.J., Kunzer, A.R., Letai, A., Li, C., Mitten, M.J., Nettesheim, D.G., Ng, S., Nimmer, P.M., O'Connor, J.M., Oleksijew, A., Petros, A.M., Reed, J.C., Shen, W., Tahir, S.K., Thompson, C.B., Tomaselli, K.J., Wang, B., Wendt, M.D., Zhang, H., Fesik, S.W., Rosenberg, S.H.

Revision History (Full details and data files)

- **Version 1.0: 2005-06-07**
Type: Initial release
- **Version 1.1: 2008-04-30**
Changes: Version format compliance
- **Version 1.2: 2011-07-13**
Changes: Version format compliance
- **Version 1.3: 2022-03-02**
Changes: Database references, Derived calculations