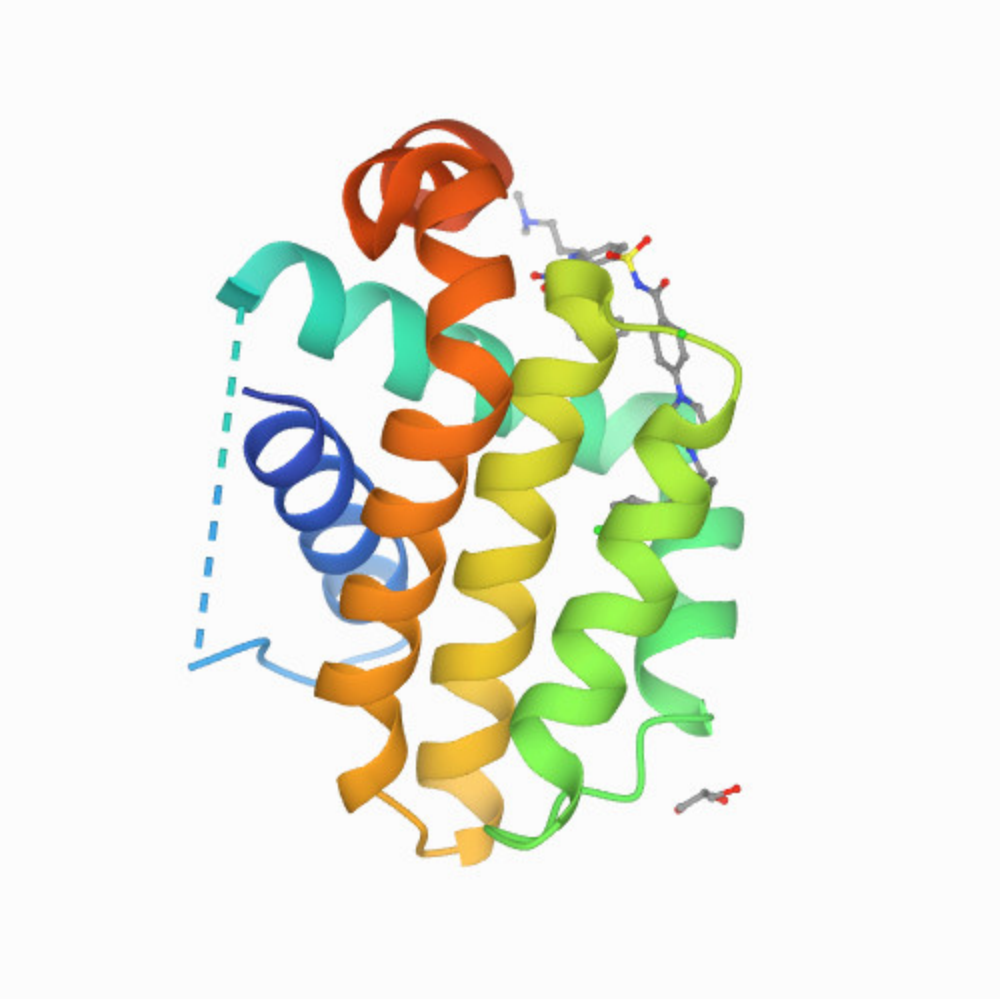
2YXJ

rcsb.org/structure/2YXJ

Biological Assembly 1



Macromolecule Content

- Total Structure Weight: 43.36 kDa
- Atom Count: 2608
- Modelled Residue Count: 279
- Deposited Residue Count: 362
- Unique protein chains: 1

Crystal structure of Bcl-xL in complex with ABT-737

PDB DOI: 10.2210/pdb2YXJ/pdb

Classification: APOPTOSIS
Organism(s): Homo sapiens
Expression System: Escherichia coli
Mutation(s): No

Deposited: 2007-04-26 **Released:** 2007-05-22
Deposition Author(s): Czabotar, P.E., Lee, E.F., Smith, B.J., Deshayes, K., Zobel, K., Fairlie, W.D., Colman, P.M.

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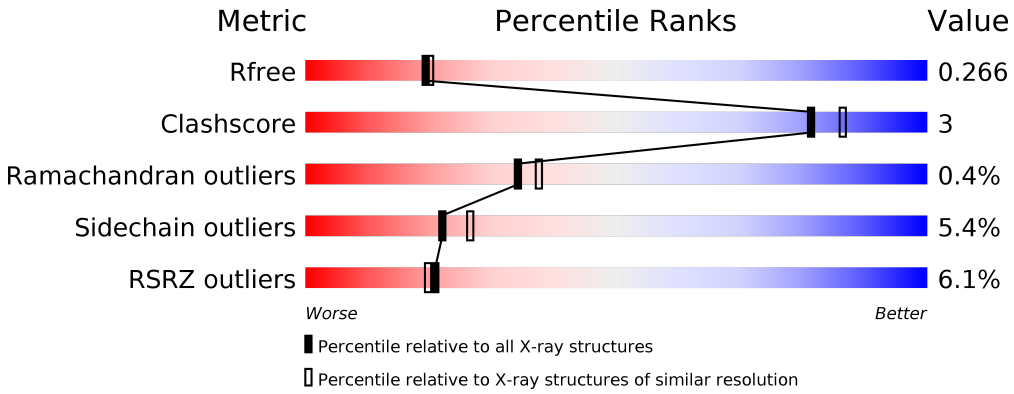
wwPDB Validation

3D Report Full Report

Ligand Structure Quality Assessment



This is version 1.3 of the entry. See complete history.

Crystal structure of ABT-737 complexed with Bcl-xL: implications for selectivity of antagonists of the Bcl-2 family

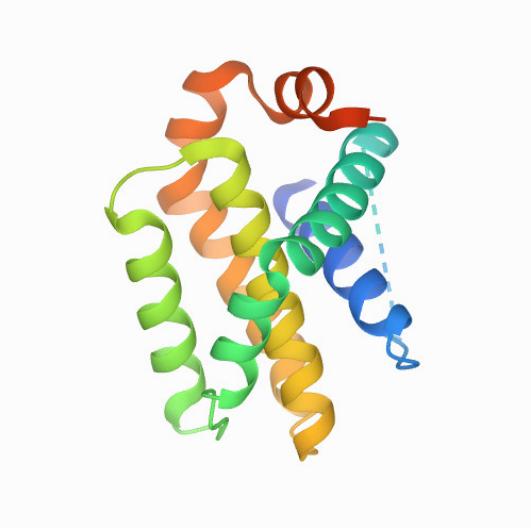
Lee, E.F., Czabotar, P.E., Smith, B.J., Deshayes, K., Zobel, K., Colman, P.M., Fairlie, W.D. (2007) Cell Death Differ **14**: 1711-1713

PubMed: 17572662
DOI: 10.1038/sj.cdd.4402178
Primary Citation of Related Structures:
2YXJ

Macromolecules

Find similar proteins by:

(by identity cutoff) | 3D Structure

Entity ID: 1					
Molecule					
Chains					
Sequence Length					
Organism					
Details					
Image					
Apoptosis regulator Bcl-X	A, B	181	Homo sapiens	**Mutation(s)**: 0 **Gene Names:** Bcl-xL	

UniProt & NIH Common Fund Data Resources

Find proteins for Q07817 *(Homo sapiens)*

Explore Q07817

Go to UniProtKB: Q07817

PHAROS: Q07817

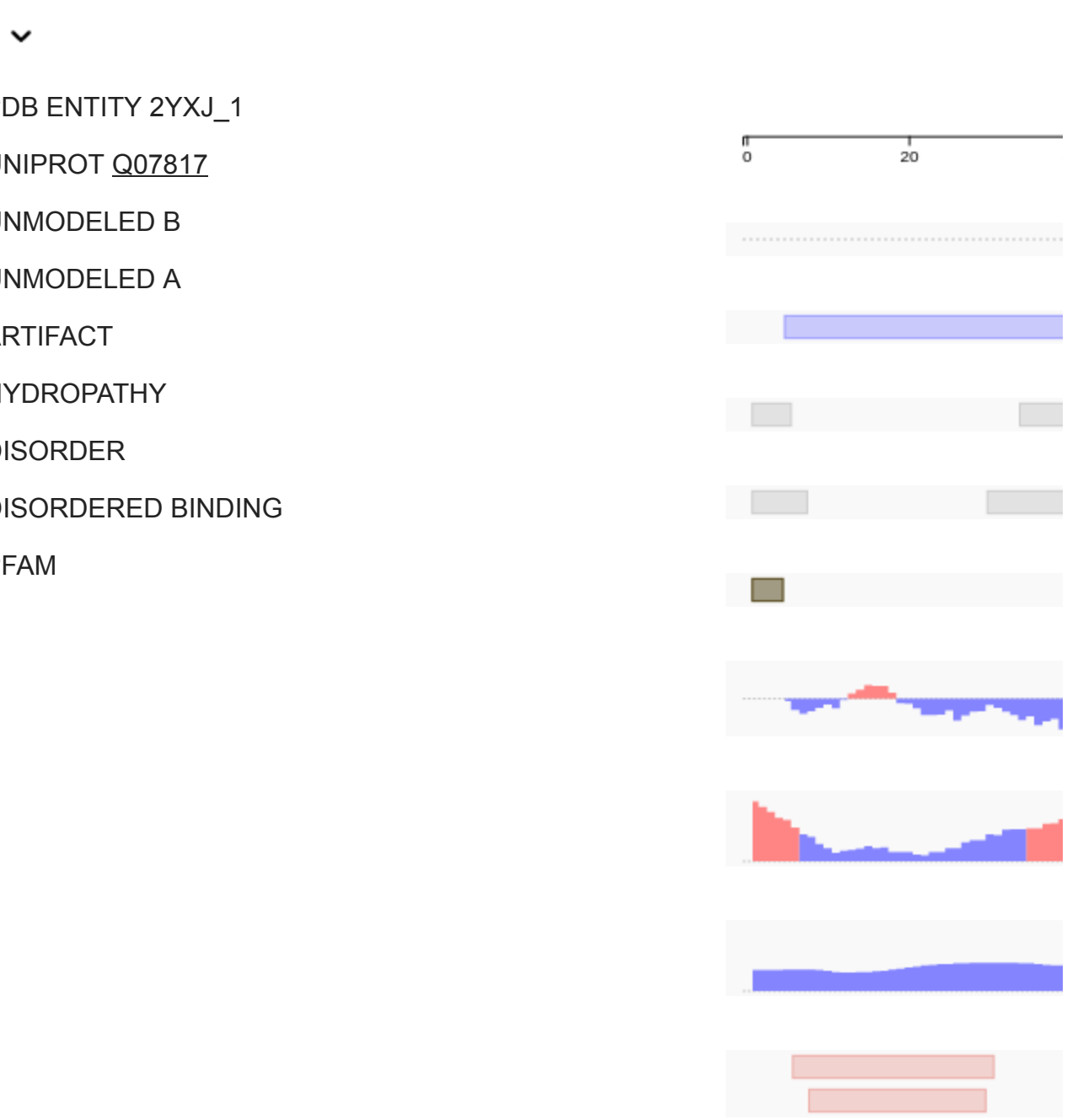
GTEx: ENSG00000171552

Protein Feature View

Expand

Reference Sequence

2YXJ_1



Small Molecules

Ligands 3 Unique

ID	Chains	Name / Formula / InChI Key	2D Diagram	3D Interactions
N3C (Subject of Investigation/LOI)	D [auth A], F [auth B]	**4-{4-[(4'-CHLOROBIPHENYL-2-YL)METHYL]PIPERAZIN-1-YL}-N-{[4-({(1R)-3-(DIMETHYLAMINO)-1-[(PHENYLTHIO)METHYL]PROPYL}AMINO)-3-NITROPHENYL]SULFONYL}BENZAMIDE** C_{42} H_{45} Cl N_6 O_5 S_2 HPLNQCPCUACXLM-PGUFJCEWSA-N		Ligand Interacti
GOL	E [auth A]	**GLYCEROL** C_3 H_8 O_3 PEDCQBHIVMGVHV-UHFFFAOYSA-N		Ligand Interacti
CL	C [auth A]	**CHLORIDE ION** Cl VEXZGXHMUGYJMC-UHFFFAOYSA-M		Ligand Interacti

Binding Affinity Annotations		
ID		
Source		
Binding Affinity		
N3C	PDBBind: 2YXJ	**Ki:** 0.5 (nM) from 1 assay(s)
	Binding MOAD: 2YXJ	**IC50:** 9 (nM) from 1 assay(s)

Experimental Data & Validation

Experimental Data

Method: X-RAY DIFFRACTION
Resolution: 2.20 Å
R-Value Free: 0.249
R-Value Work: 0.199
R-Value Observed: 0.201
Space Group: P 2_1 2_1 2_1

Unit Cell:

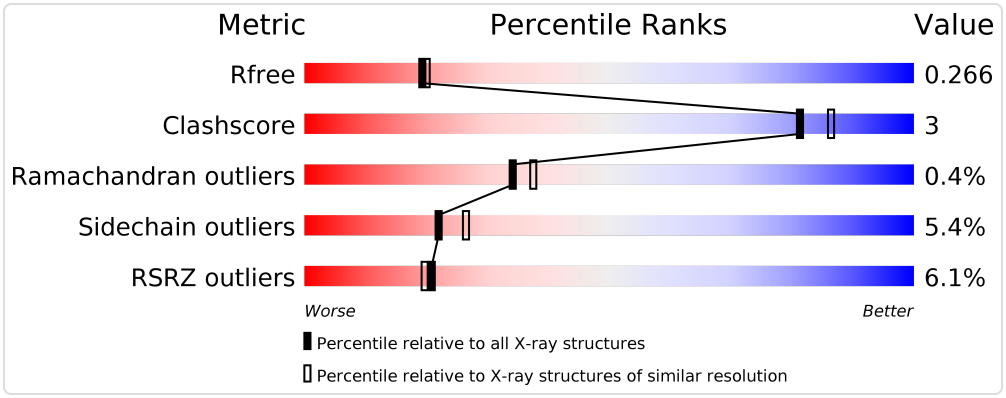
Length (Å)	Angle (˚)
a = 66.321	α = 90
b = 75.37	β = 90
c = 87.778	γ = 90

Software Package:

Software Name	Purpose
REFMAC	refinement
CrystalClear	data collection
HKL-2000	data reduction
HKL-2000	data scaling
PHASER	phasing

Structure Validation

View Full Validation Report



Ligand Structure Quality Assessment

Entry History

Deposition Data

Deposited Date: 2007-04-26
Released Date: 2007-05-22
Deposition Author(s): Czabotar, P.E., Lee, E.F., Smith, B.J., Deshayes, K., Zobel, K., Fairlie, W.D., Colman, P.M.

Revision History (Full details and data files)

- **Version 1.0: 2007-05-22**
  Type: Initial release
- **Version 1.1: 2008-04-30**
  Changes: Version format compliance
- **Version 1.2: 2011-07-13**
  Changes: Non-polymer description, Version format compliance
- **Version 1.3: 2017-08-16**
  Changes: Source and taxonomy