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2QD9

P38 Alpha Map Kinase inhibitor based on heterobicyclic scaffolds

PDB DOI: <https://doi.org/10.2210/pdb2QD9/pdb>

Classification: TRANSFERASE

Organism(s): Homo sapiens

Expression System: Escherichia coli

Mutation(s): No

Deposited: 2007-06-20 Released: 2007-08-21

Deposition Author(s): Sack, J.S.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.70 Å

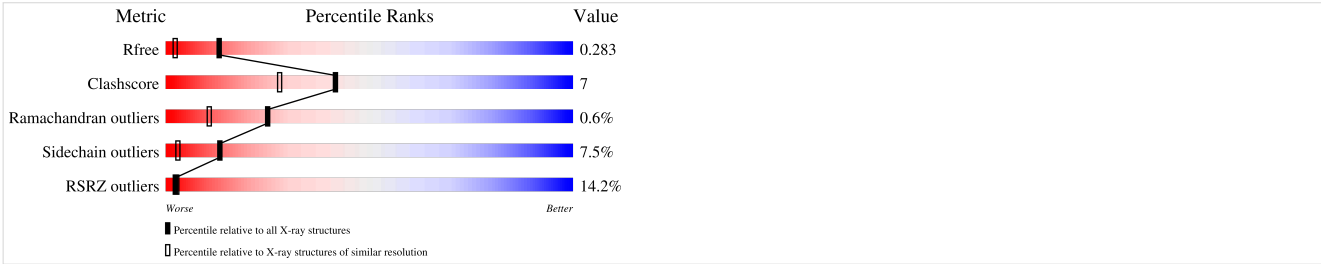
R-Value Free: 0.282

R-Value Work: 0.251

R-Value Observed: 0.252

wwPDB Validation

3D Report Full Report



Ligand Structure Quality Assessment



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

Literature

Synthesis and SAR of p38alpha MAP kinase inhibitors based on heterobicyclic scaffolds.

[Murali Dhar, T.G.](#), [Wroblewski, S.T.](#), [Lin, S.](#), [Furch, J.A.](#), [Nirschl, D.S.](#), [Fan, Y.](#), [Todderud, G.](#), [Pitt, S.](#), [Doweyko, A.M.](#), [Sack, J.S.](#), [Mathur, A.](#), [McKinnon, M.](#), [Barrish, J.C.](#), [Dodd, J.H.](#), [Schieven, G.L.](#), [Leftheris, K.](#)
(2007) Bioorg Med Chem Lett 17: 5019-5024

PubMed: [17664068](#)
DOI: <https://doi.org/10.1016/j.bmcl.2007.07.029>

Primary Citation of Related Structures:
2QD9

PubMed Abstract:
The synthesis and structure-activity relationships (SAR) of p38alpha MAP kinase inhibitors based on heterobicyclic scaffolds are described. This effort led to the identification of compound (21) as a potent inhibitor of p38alpha MAP kinase with good cellular potency toward the inhibition of TNF-alpha production. X-ray co-crystallography of an oxalamide analog (24) bound to unphosphorylated p38alpha is also disclosed.

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[Explore in 3D](#): [Structure](#) | [Sequence Annotations](#) | [Electron Density](#) | [Validation Report](#) | [Ligand Interaction \(LGF\)](#)

Global Symmetry: Asymmetric - C1
Global Stoichiometry: Monomer - A1

[Find Similar Assemblies](#)

Biological assembly 1 assigned by authors.

Macromolecules

Find similar proteins by:

Sequence ▼

 (by identity cutoff) | 3D Structure

Entity ID: 1					
Molecule	Chains	Sequence Length	Organism	Details	Image
Mitogen-activated protein kinase 14	A	366	Homo sapiens	Mutation(s): 0 Gene Names: MAPK14 , CSBP , CSBP1 , CSBP2 , CSPB1 , MXI2 EC: 2.7.11.24	

UniProt & NIH Common Fund Data Resources

Find proteins for [Q16539](#) (*Homo sapiens*)
Explore [Q16539](#)

Go to UniProtKB: [Q1653](#)

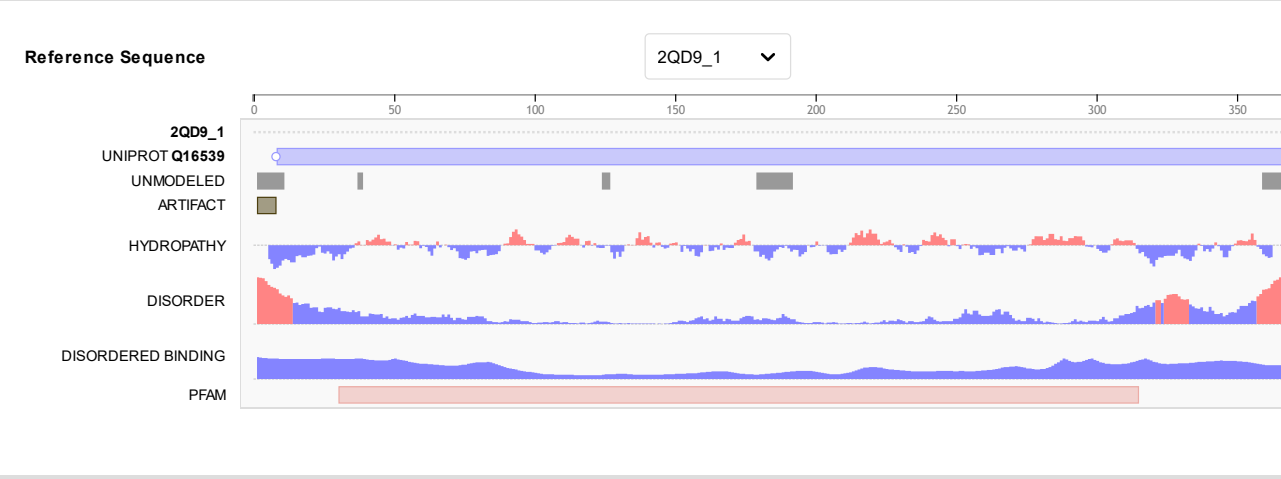
PHAROS: Q16539
GTE: ENSG00000112062

Entity Groups

Sequence Clusters 30% Identity 50% Identity 70% Identity 90% Identity 95% Identity 100% Identity

UniProt Group Q16539

Sequence Annotations Expa



Small Molecules

Ligands 1 Unique				
ID	Chains	Name / Formula / InChI Key	2D Diagram	3D Interactions
LG	B [auth F A]	1-[5-[[3-[2,4-bis(fluoranyl)phenyl]-6,8-dihydro-5~{H}-imidazo[1,5-a]pyrazin-7-yl]carbonyl]-6-methoxy-1~{H}-pyrrolo[2,3-b]pyridin-3-yl]-2-[(3~{R})-3-oxidanylpyrrolidin-1-yl]ethane-1,2-dione C ₂₇ H ₂₄ F ₂ N ₆ O ₅ GRRHHDRNCLEFSY-MRXNPFEDSA-N		Interactions Interactions & Densit
Download Instance Coordinates				

Binding Affinity Annotations		
ID	Source	Binding Affinity
LGF	BindingDB: 2QD9	IC ₅₀ : 13 (nM) from 1 assay(s)
	PDBBind: 2QD9	IC ₅₀ : 13 (nM) from 1 assay(s)

Experimental Data & Validation

Experimental Data

Method: X-RAY DIFFRACTION
Resolution: 1.70 Å
R-Value Free: 0.282
R-Value Work: 0.251
R-Value Observed: 0.252
Space Group: P2₁2₁

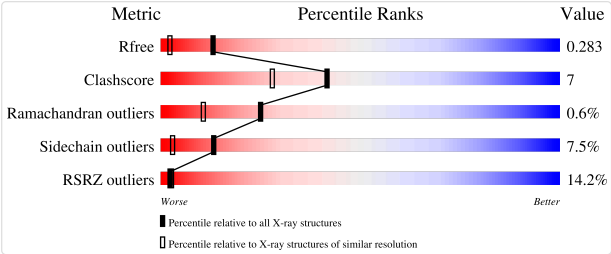
Unit Cell:	
Length (Å)	Angle (°)
a = 65.65	α = 90

Length (Å)	Angle (°)
b = 74.36	β = 90
c = 78.98	γ = 90

Software Package:	
Software Name	Purpose
REFMAC	refinement
DENZO	data reduction
SCALEPACK	data scaling

Structure Validation

View Full Validation Report



Ligand Structure Quality Assessment ⓘ



Entry History

Deposition Data

Released Date: 2007-08-21
Deposition Author(s): Sack, J.S.

Revision History (Full details and data files)

- Version 1.0: 2007-08-21**
Type: Initial release
- Version 1.1: 2011-07-13**
Changes: Version format compliance
- Version 1.2: 2018-12-12**
Changes: Advisory, Data collection, Derived calculations, Refinement description, Structure summary
- Version 1.3: 2024-02-21**
Changes: Data collection, Database references, Derived calculations, Refinement description

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