

1. naloga

DOI: [10.1074/mcp.O111.013706](https://doi.org/10.1074/mcp.O111.013706)

pot do rešitve:

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☐ Meta-Analysis
☐ Randomized Controlled Trial
☐ Review
☐ Systematic Review

3 results

1 **A human ubiquitin conjugating enzyme (E2)-HECT E3 ligase structure-function screen.**
Sheng Y, Hong JH, Doherty R, Srikumar T, Shloush J, Avvakumov GV, Walker JR, Xue S, Neculai D, Wan JW, Kim SK, Arrowsmith CH, Raught B, Dhe-Paganon S.
Mol Cell Proteomics. 2012 Aug;11(8):329-41. doi: 10.1074/mcp.O111.013706. Epub 2012 Apr 10.
PMID: 22496338 [Free PMC article](#).
Here we describe a systematic structure-function analysis of the human ubiquitin (Ub) E2 conjugating proteins, consisting of the determination of 15 new high-resolution three-dimensional structures of E2 catalytic domains, and autoubiquitylation assays for 26 ...

2 **Recognition mechanism of p63 by the E3 ligase Itch: novel strategy in the study and inhibition of this interaction.**
Bellomaria A, Barbato G, Melino G, Paci M, Melino S.
Cell Cycle. 2012 Oct 1;11(19):3638-48. doi: 10.4161/cc.21918. Epub 2012 Aug 30.
PMID: 22935697 [Free PMC article](#).
The HECT-containing E3 ubiquitin ligase Itch mediates the degradation of several proteins, including p63 and p73, involved in cell specification and fate. ...Several signaling complexes containing these domains have been associated with human diseases such as ...

3 **The E3 ligase HOIP specifies linear ubiquitin chain assembly through its RING-IBR-RING domain and the unique LDD extension.**
Smit JJ, Monteferrario D, Noordermeer SM, van Dijk WJ, van der Reijden BA, Sixma TK.
EMBO J. 2012 Oct 3;31(19):3833-44. doi: 10.1038/emboj.2012.217. Epub 2012 Aug 3.
PMID: 22863777 [Free PMC article](#).
Activation of the NF-kappaB pathway requires the formation of Met1-linked 'linear' ubiquitin chains on NEMO, which is catalysed by the Linear Ubiquitin Chain Assembly Complex (LUBAC) E3 consisting of HOIP, HOIL-1L and Sharpin. Here, we show that both LUBAC catalytic activi ...

2. naloga

pdb koda: 2OB4

ekspresijski sistem: [Escherichia coli BL21\(DE3\)](#)

ločljivost in metoda: X-RAY DIFFRACTION, 2.40 Å

pH in temperatura: 298K in 8,5

Structure Summary Structure Annotations Experiment Sequence Genome Versions

2OB4 | pdb_00002ob4

Human Ubiquitin-Conjugating Enzyme CDC34

X-RAY DIFFRACTION

Crystallization

Crystallization Experiments

ID	Method	pH	Temperature	Details
1	VAPOR DIFFUSION, HANGING DROP	8.5	298	The protein was dissolved at 42 mg/ml in 20 mM Tris-HCl, pH 8.0, 0.15 M NaCl, 5% glycerol and 2 mM DTT. Crystals were grown in hanging drops by mixing 2 microl. protein solution with 2 microl. well solution (28% PEG 4000, 0.1 M Tris-HCl, pH 8.5, 0.2 M MgCl2, 1 mM DTT and 7.5 mM glycyl-glycyl-glycine) at 21 deg C. For cryoprotection, the crystals were soaked in the well solution supplemented with 25% ethylene glycol, VAPOR DIFFUSION, HANGING DROP, temperature 298K

Crystal Properties

Matthews coefficient	Solvent content
2.13	42.21

Crystal Data

Unit Cell	Symmetry
Length (Å)	Space Group
a = 42.28	I 2 2 2
b = 66.31	
c = 124.61	
Angle (°)	
α = 90	
β = 90	
γ = 90	

3. naloga

vse piše na GenBank

delež CDS regije: 50,1 % (dolžina CDS regije: 710 bp, dolžina celotnega zaporedja: 1418 bp)

število eksonov: 5

fosforilirani ak ostanki: 5

vezavna regija SCF: YCVKTKAPAPDEGSDLFYDDYYEDGEVEEEEADSCFGDDEDDSGTEES

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FASTA ▾

ubiquitin-conjugating enzyme E2 R1 [Homo sapiens]

NCBI Reference Sequence: NP_004350.1
[GenPept](#) [Identical Proteins](#) [Graphics](#)

>NP_004350.1:190-236 ubiquitin-conjugating enzyme E2 R1 [Homo sapiens]
YCVKTKAPAPDEGSDLFYDDYYEDGEVEEEEADSCFGDDEDDSGTEES

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Change region shown ▴

☐ Whole sequence
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from: 190 to: end

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Protein 3D Structure ▴

(NEDD8)-CRL2VHL-MZ1-Brd4BD2-Ub(G76S, K48C)-UBE2R1(C93K, S138C)
PDB: 8RX0
Source: Homo sapiens
Method: Electron Microscopy
Resolution: 3.7 Å

4. naloga

iskanje po UniProtu

aktivno mesto: C-93

mesto nahajanja: jedro, citoplazma

Formula: $C_{1199}H_{1817}N_{301}O_{381}S_6$ (protparam)

web.expasy.org/cgi-bin/protparam/protparam

His (H)	4	0.8%
Ile (I)	9	3.8%
Leu (L)	19	8.1%
Lys (K)	14	5.9%
Met (M)	3	1.3%
Phe (F)	9	3.8%
Pro (P)	20	8.5%
Ser (S)	15	6.4%
Thr (T)	13	5.5%
Trp (W)	4	1.7%
Tyr (Y)	13	5.5%
Val (V)	17	7.2%
Pyl (O)	0	0.0%
Sec (U)	0	0.0%
(B)	0	0.0%
(Z)	0	0.0%
(X)	0	0.0%

Total number of negatively charged residues (Asp + Glu): 45
Total number of positively charged residues (Arg + Lys): 24

Atomic composition:

Carbon	C	1199
Hydrogen	H	1817
Nitrogen	N	301
Oxygen	O	381
Sulfur	S	6

Formula: C₁₁₉₉H₁₈₁₇N₃₀₁O₃₈₁S₆
Total number of atoms: 3704

Extinction coefficients:
Extinction coefficients are in units of M⁻¹ cm⁻¹, at 280 nm measured in water.
Ext. coefficient 41495
Abs 0.1% (=1 g/l) 1.552, assuming all pairs of Cys residues form cystines

Ext. coefficient 41370
Abs 0.1% (=1 g/l) 1.547, assuming all Cys residues are reduced

Estimated half-life:
The N-terminal of the sequence considered is M (Met).
The estimated half-life is: 30 hours (mammalian reticulocytes, in vitro).
>20 hours (yeast, in vivo).
>10 hours (Escherichia coli, in vivo).

Instability index:
The instability index (II) is computed to be 51.59
This classifies the protein as unstable.

Aliphatic index: 72.25
Grand average of hydropathicity (GRAVY): -0.612

5. naloga

Na pdb od 3RZ3 poiščeš kodo za ligand (U94)

rcsb.org/structure/3RZ3

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Sequence Clusters 30% Identity 50% Identity 70% Identity 80% Identity 90% Identity 100% Identity

UniProt Group P49427

Sequence Annotations Expand

Reference Sequence 3RZ3_1

3RZ3_1
UNIPROT P49427
UNMODELED
ARTIFACT
HYDROPATHY
DISORDER
DISORDERED BINDING
PFAM

Small Molecules

Ligands

ID	Chains	Name / Formula / InChI Key	2D Diagram	3D Interactions
U94 Query on U94	E [auth A], F [auth B], G [auth C], H [auth D]	4,5-dideoxy-5-(3',5'-dichlorobiphenyl-4-yl)-4- [(methoxyacetyl)amino]-L-arabinonic acid C ₂₀ H ₂₁ Cl ₂ N O ₆ NTCBTNCWNRCBGX-YTQUADARSA-N		Interactions Interactions & Density

Download Ideal Coordinates CCD File
Download Instance Coordinates

Experimental Data & Validation

Experimental Data Structure Validation

poiščeš SMILES kodo liganda.

✓ Prepare target **Reset target**


swissdock.ch

✓ Prepare target Reset target

3 - Define search space

Search box center 32 19 14 Å

Search box size 24 24 25 Å



Hydrogen bonds Ionic interactions Cation- π interactions Hydrophobic contacts π -stacking interactions Show protein surface Reset

rezultat:

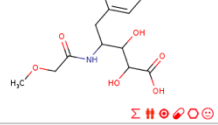
swissdock.ch/results.php?job=87923935

Box size: 24 - 24 - 25



If you publish these results, please, cite the following papers:

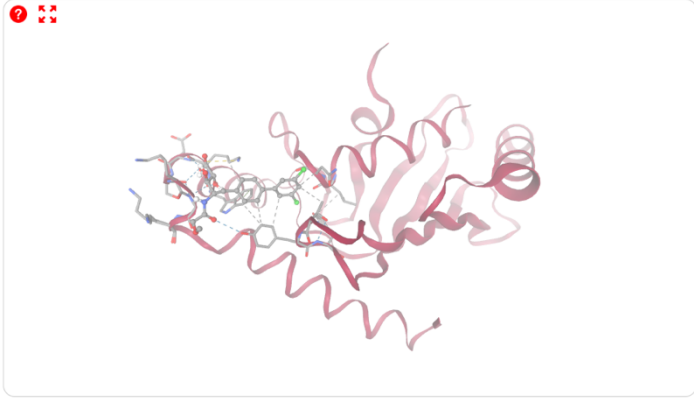
Bugnon M, Röhrig UF, Gouilleux M, Perez MAS, Dains A, Michielin O, Zoete V. *SwissDock 2024: major enhancements for small-molecule docking with Attracting Cavities and AutoDock Vina*. *Nucleic Acids Res.* **2024**

Eberhardt J, Santos-Martins D, Tillack AF, Forli S. *AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings*. *J. Chem. Inf. Model.* **2021**



Results

Export your results:  



Hydrogen bonds Ionic interactions Cation- π interactions Hydrophobic contacts π -stacking interactions Show protein surface Reset

Model	Calculated affinity (kcal/mol)
1	-6.140
2	-5.925

interakcije: vodikove vezi, ionske, hidrofobne, pi-pi interakcije