



# UNIVERSIDAD NACIONAL DE SAN AGUSTÍN

FACULTAD DE INGENIERÍA DE PRODUCCIÓN Y SERVICIOS  
CIENCIA DE LA COMPUTACIÓN

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## **Práctica 09: Estructura de Proteínas**

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**CURSO:**

BIOINFORMÁTICA

**ALUMNO**

KELVIN PAUL PUCHO ZEVALLOS

**DOCENTE:**

GUADALUPE DEL ROSARIO QUISPE SAJI

13 de Agosto del 2022

# Tarea

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RCSB PDB 194011 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

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PDB-101 PDB EMDatabank Protein Data Bank Worldwide Protein Data Bank Foundation

Structure Summary 3D View Annotations Experiment Sequence Genome Versions

Biological Assembly 1

2C8R

insuline(60sec) and UV laser excited fluorescence

PDB DOI: 10.2210/pdb2C8R/pdb

Classification: **HORMONE**

Organism(s): *Homo sapiens*

Mutation(s): No

Deposited: 2005-12-06 Released: 2006-03-08

Deposition Author(s): Vernede, X., Lavault, B., Ohana, J., Nurizzo, D., Joly, J., Jacquamet, L., Felisaz, F., Cipriani, F., Bourgeois, D.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.50 Å

R-Value Free: 0.224

R-Value Work: 0.206

R-Value Observed: 0.207

wwPDB Validation

3D Report Full Report

Metric	Percentile Ranks	Value
Rfree		0.220
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		4.1%

3D View: Structure | 1D-3D View | Electron Density | Validation Report

Global Symmetry: Cyclic - C2 (3D View)

1. A partir de la secuencia fasta indicada:  
> FVNQHLCGSHLVEALYLVCGERGFFYTPK
2. Identificar la proteína a la que corresponde : código de 4 letras y descripción de la proteína
  - Buscar la proteína en BLAST

Standard Protein BLAST

blastn **blastp** blastx tblastn tblastx

BLASTP programs search protein databases using a protein query. more...

Enter Query Sequence

Enter accession number(s), gi(s), or FASTA sequence(s) ? Clear

> test1  
FVNQHLCGSHLVEALYLVCGERGFFYTPK

Query subrange ?

From

To

Or, upload file

Elegir archivo No se ha seleccio...do ningún archivo ?

Job Title

test1

Enter a descriptive title for your BLAST search ?

☐ Align two or more sequences ?

Choose Search Set

Databases

☒ Standard databases (nr etc.): **New** ☐ Experimental databases

Compare

☐ Select to compare standard and experimental database ?

Standard

Database

Protein Data Bank proteins(pdb)

Organism

Optional

Enter organism name or id--completions will be suggested

☐ exclude **Add organism**

Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown. ?

Exclude

Optional

☐ Models (XM/XP) ☐ Non-redundant RefSeq proteins (WP) ☐ Uncultured/environmental sample sequences

**Try experimental clustered nr database**

For more info see [What is clustered nr?](#)

- Escogemos la secuencia con el alineamiento de la proteína de Homo Sapiens con una cobertura de 100% y con una identidad de 100%

**Your search parameters were adjusted to search for a short input sequence.**

Job Title	test1
RID	FG1NV6AH013 <small>Search expires on 08-15 04:16 am</small> <a href="#">Download All</a> ▼
Program	BLASTP <a href="#">Citation</a> ▼
Database	pdb <a href="#">See details</a> ▼
Query ID	Icl Query_65681
Description	test1
Molecule type	amino acid
Query Length	29
Other reports	<a href="#">Distance tree of results</a> <a href="#">Multiple alignment</a> <a href="#">MSA viewer</a> ?

### Filter Results

**Organism** only top 20 will appear ☐ exclude

  
[+ Add organism](#)

---

**Percent Identity**      **E value**      **Query Coverage**

to

to

to

Filter
Reset

**Descriptions**

Graphic Summary

Alignments

Taxonomy

**Sequences producing significant alignments**

[Download](#) ▼    [Select columns](#) ▼    Show 100 ▼    ?

☒ select all    100 sequences selected

[GenPept](#)    [Graphics](#)    [Distance tree of results](#)    [Multiple alignment](#)    [MSA Viewer](#)

	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
<input checked="" type="checkbox"/>	Crystallographic and solution studies of N-lithocholyli insulin: a new generation of prolonged-acting insulins [Homo sapiens]	Homo sapiens	99.0	99.0	100%	4e-28	100.00%	29	1UZ9_B
<input checked="" type="checkbox"/>	CONFORMATIONAL CHANGES IN CUBIC INSULIN CRYSTALS IN THE pH RANGE 7-11 [Bos taurus]	Bos taurus	99.0	99.0	100%	5e-28	100.00%	30	1AFH_B
<input checked="" type="checkbox"/>	Chain B_R6 INSULIN HEXAMER [Homo sapiens]	Homo sapiens	99.0	99.0	100%	5e-28	100.00%	30	1AI0_B
<input checked="" type="checkbox"/>	Modified A22Gly-B31Arg Human Insulin [Homo sapiens]	Homo sapiens	99.0	99.0	100%	5e-28	100.00%	31	2LGB_B
<input checked="" type="checkbox"/>	Structure of Glargine insulin in 20% acetic acid d4 (pH 1.0) [synthetic construct]	synthetic construct	99.0	99.0	100%	6e-28	100.00%	32	6K5D_B

- Vemos que las secuencias son idénticas

[Download](#)
[GenPept](#)
[Graphics](#)

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[Previous](#)
[Descriptions](#)

### Crystallographic and solution studies of N-lithocholyl insulin: a new generation of prolonged-acting insulins. [Homo sapiens]

Sequence ID: [1UZ9\\_B](#) Length: 29 Number of Matches: 1

[See 31 more title\(s\)](#)
[See all Identical Proteins\(IPG\)](#)

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Range 1: 1 to 29 [GenPept](#) [Graphics](#)

[Next Match](#)
[Previous Match](#)

Score	Expect	Identities	Positives	Gaps
99.0 bits(226)	4e-28	29/29(100%)	29/29(100%)	0/29(0%)
Query 1	FVNQHLCGSHLVEALYLVCGERGFFYTPK 29			
	FVNQHLCGSHLVEALYLVCGERGFFYTPK			
Sbjct 1	FVNQHLCGSHLVEALYLVCGERGFFYTPK 29			

#### Related Information

[Structure](#) - 3D structure displays  
[Identical Proteins](#) - Identical proteins to 1UZ9\_B

- Copiamos el código PDB 1UZ9

## Chain B, Insulin

PDB: [1UZ9\\_B](#)

[Identical Proteins](#) [FASTA](#) [Graphics](#)

Go to: ☐

LOCUS 1UZ9\_B 29 aa linear PRI 01-DEC-2020  
 DEFINITION Chain B, Insulin.  
 ACCESSION 1UZ9\_B  
 VERSION 1UZ9\_B  
 DBSOURCE pdb: molecule 1UZ9, chain B, release Dec 7, 2012;  
 deposition: Mar 8, 2004;  
 class: Insulin;  
 source: Mmdb\_id: [51748](#), Pdb\_id 1: 1UZ9;  
 Exp. method: X-Ray Diffraction.  
 KEYWORDS .  
 SOURCE Homo sapiens (human)  
 ORGANISM [Homo sapiens](#)  
 Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;  
 Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini;  
 Catarrhini; Hominidae; Homo.  
 REFERENCE 1 (residues 1 to 29)  
 AUTHORS Whittingham, J.L., Jonassen, I., Havelund, S., Roberts, S.M.,  
 Dodson, E.J., Verma, C.S., Wilkinson, A.J. and Dodson, G.G.  
 TITLE Crystallographic and solution studies of N-lithocholyl insulin: a  
 new generation of prolonged-acting human insulins  
 JOURNAL Biochemistry 43 (20), 5987-5995 (2004)  
 PUBMED [15147182](#)

- Buscamos en el Protein Data Bank (PDB)
- <https://www.rcsb.org/structure/1UZ9>

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PDB Archive 1UZ9

in PDB ID(s) 1UZ9

Help

PDB-101 PDDB WORLDWIDE PDB EMDDataResource Nucleic Acid Database Worldwide Protein Data Bank

Structure Summary 3D View Annotations Experiment Sequence Genome Versions

Biological Assembly 1

1UZ9

Crystallographic and solution studies of N-lithocholyl insulin: a new generation of prolonged-acting insulins.

PDB DOI: 10.2210/pdb1UZ9/pdb

Classification: **INSULIN**

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

Mutation(s): No

Deposited: 2004-03-08 Released: 2005-03-03

Deposition Author(s): Whittingham, J.L., Jonassen, I., Havelund, S., Roberts, S.M., Dodson, E.J., Verma, C.S., Wilkinson, A.J., Dodson, G.G.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.60 Å

R-Value Free: 0.206

R-Value Work: 0.179

R-Value Observed: 0.180

wwPDB Validation

3D Report Full Report

Metric Percentile Ranks Value

Clashscore 9

Ramachandran outliers 0

Sidechain outliers 2.3%

Worse Better

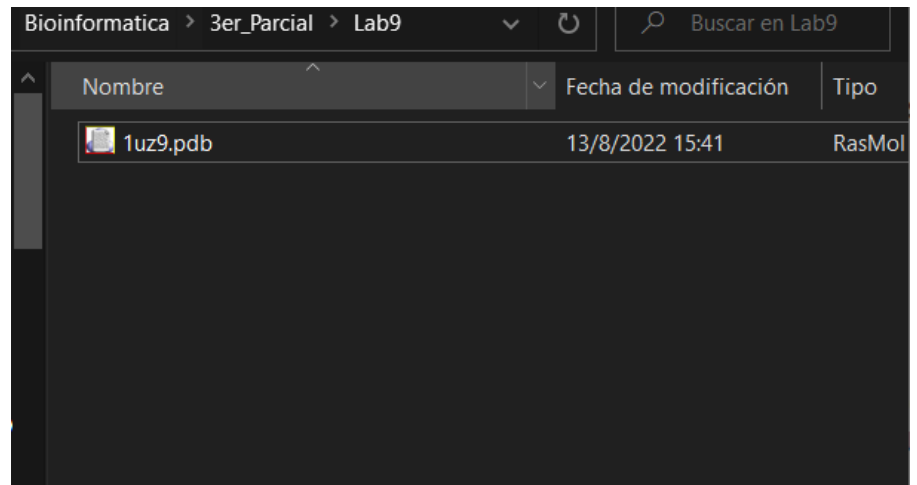
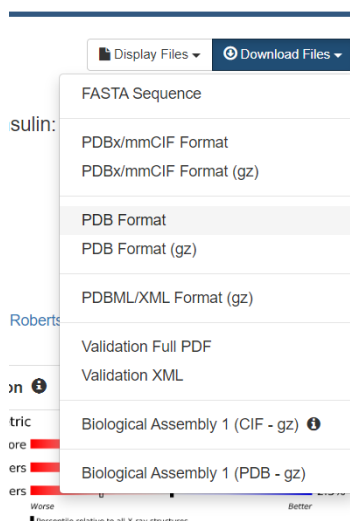
Percentile relative to all X-ray structures

Percentile relative to X-ray structures of similar resolution

3D View: Structure | 1D-3D View | Validation Report | Ligand Interaction

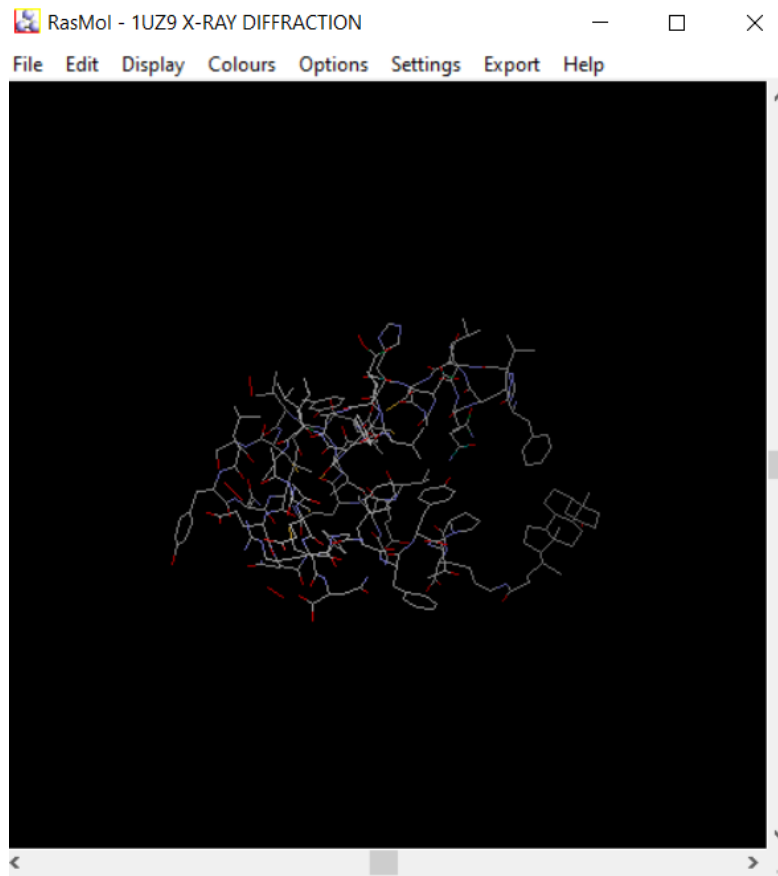
Global Symmetry: Dihedral - D3 (3D View)

- Y finalmente descargamos el .pdb de la proteína 1UZ9



### 3. Bajar el archivo .pdb correspondiente y mostrar la estructura en listones (ribbons) usando el programa RasMol

- Instalamos el programa RasMol y abrimos el archivo 1uz9.pdb



- Nos dirigimos a Display/Ribbons y mostramos la estructura en listones (ribbons)

