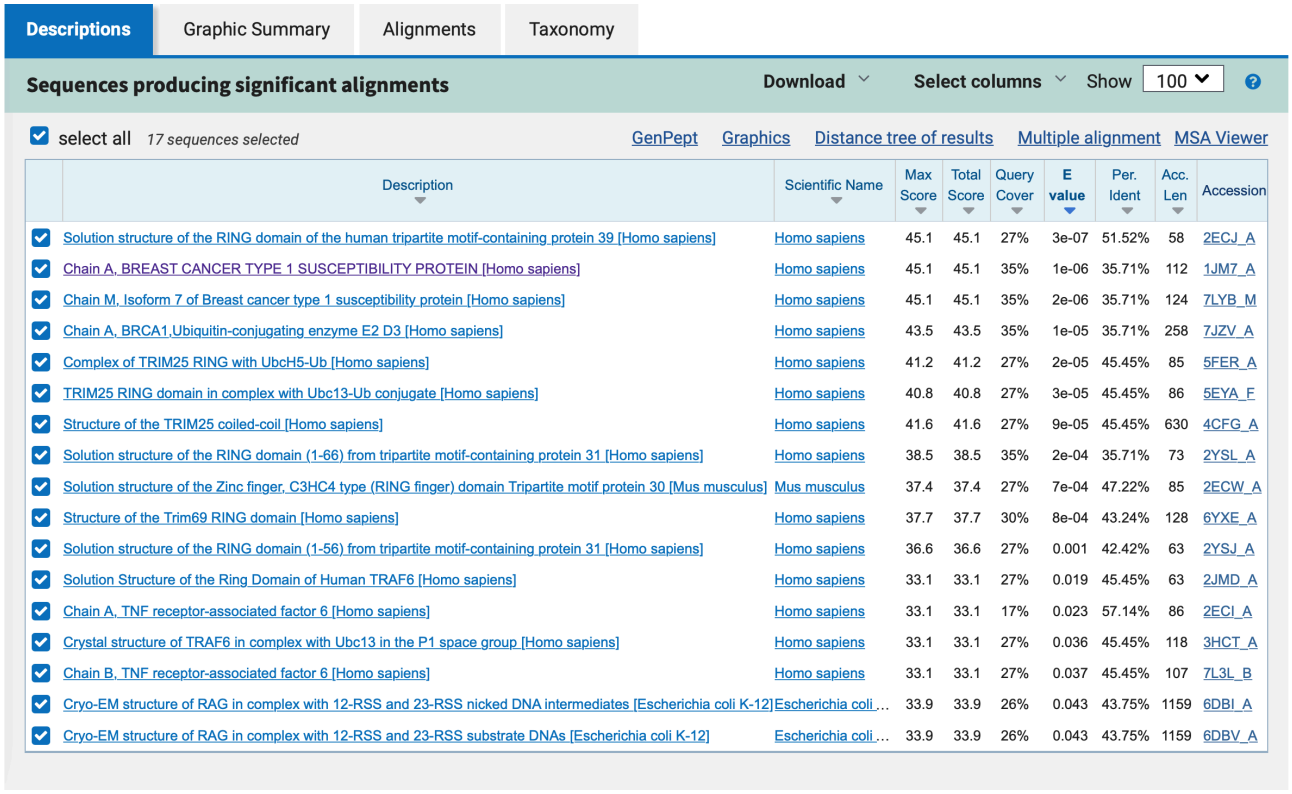
IQB Assignment 3

Name : Aayush Gakhar
Roll no : 2020006

```
>protein
MALPAGPAEAACALCQRAPREPVRADCGHRFCRACVVRFWAEEDGPFPCPECADDCWQRA
VEPGRPPLSRRLLALEEAAAAPARDGPASEAALQLLCRADAGPLCAACRMAAGPEPPEWE
```

1.

Submitting the given sequence for blastp, we get the following result:



Descriptions | Graphic Summary | Alignments | Taxonomy

Sequences producing significant alignments Download Select columns Show 100

select all *17 sequences selected* GenPept Graphics Distance tree of results Multiple alignment MSA Viewer

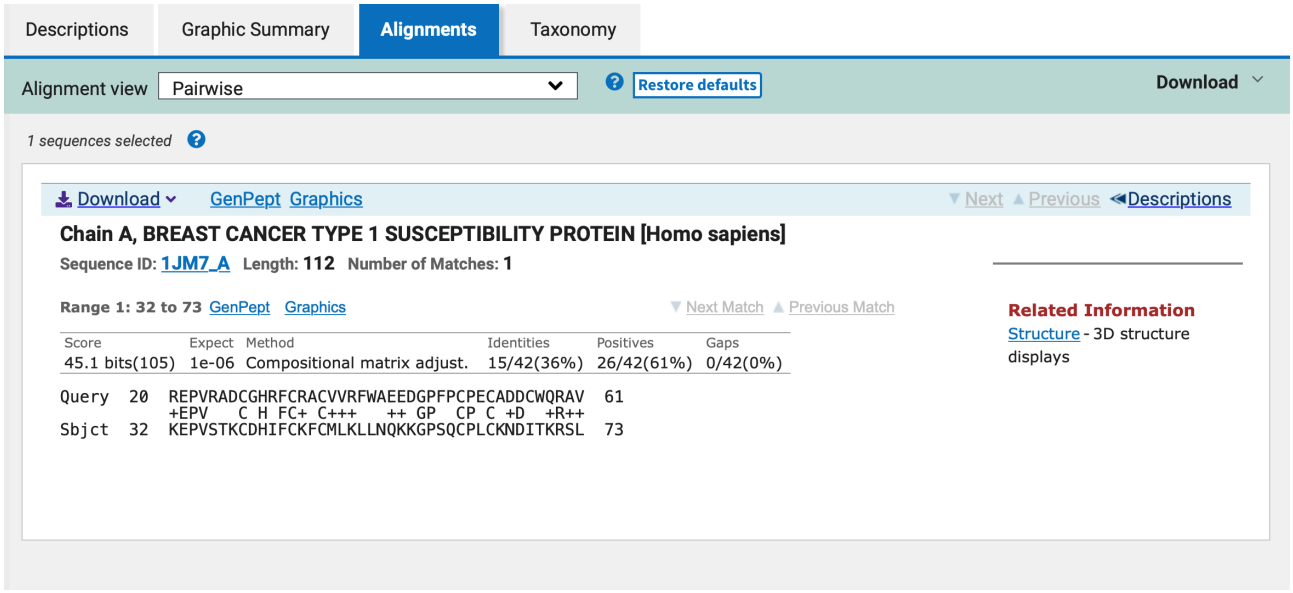
Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
Solution structure of the RING domain of the human tripartite motif-containing protein 39 [Homo sapiens]	Homo sapiens	45.1	45.1	27%	3e-07	51.52%	58	2ECJ_A
Chain A, BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN [Homo sapiens]	Homo sapiens	45.1	45.1	35%	1e-06	35.71%	112	1JM7_A
Chain M, Isoform 7 of Breast cancer type 1 susceptibility protein [Homo sapiens]	Homo sapiens	45.1	45.1	35%	2e-06	35.71%	124	7LYB_M
Chain A, BRCA1,Ubiquitin-conjugating enzyme E2 D3 [Homo sapiens]	Homo sapiens	43.5	43.5	35%	1e-05	35.71%	258	7JZV_A
Complex of TRIM25 RING with UbcH5-Ub [Homo sapiens]	Homo sapiens	41.2	41.2	27%	2e-05	45.45%	85	5FER_A
TRIM25 RING domain in complex with Ubc13-Ub conjugate [Homo sapiens]	Homo sapiens	40.8	40.8	27%	3e-05	45.45%	86	5EYA_F
Structure of the TRIM25 coiled-coil [Homo sapiens]	Homo sapiens	41.6	41.6	27%	9e-05	45.45%	630	4CFG_A
Solution structure of the RING domain (1-66) from tripartite motif-containing protein 31 [Homo sapiens]	Homo sapiens	38.5	38.5	35%	2e-04	35.71%	73	2YSL_A
Solution structure of the Zinc finger, C3HC4 type (RING finger) domain Tripartite motif protein 30 [Mus musculus]	Mus musculus	37.4	37.4	27%	7e-04	47.22%	85	2ECW_A
Structure of the Trim69 RING domain [Homo sapiens]	Homo sapiens	37.7	37.7	30%	8e-04	43.24%	128	6YXE_A
Solution structure of the RING domain (1-56) from tripartite motif-containing protein 31 [Homo sapiens]	Homo sapiens	36.6	36.6	27%	0.001	42.42%	63	2YSJ_A
Solution Structure of the Ring Domain of Human TRAF6 [Homo sapiens]	Homo sapiens	33.1	33.1	27%	0.019	45.45%	63	2JMD_A
Chain A, TNF receptor-associated factor 6 [Homo sapiens]	Homo sapiens	33.1	33.1	17%	0.023	57.14%	86	2ECI_A
Crystal structure of TRAF6 in complex with Ubc13 in the P1 space group [Homo sapiens]	Homo sapiens	33.1	33.1	27%	0.036	45.45%	118	3HCT_A
Chain B, TNF receptor-associated factor 6 [Homo sapiens]	Homo sapiens	33.1	33.1	27%	0.037	45.45%	107	7L3L_B
Cryo-EM structure of RAG in complex with 12-RSS and 23-RSS nicked DNA intermediates [Escherichia coli K-12]	Escherichia coli …	33.9	33.9	26%	0.043	43.75%	1159	6DBI_A
Cryo-EM structure of RAG in complex with 12-RSS and 23-RSS substrate DNAs [Escherichia coli K-12]	Escherichia coli …	33.9	33.9	26%	0.043	43.75%	1159	6DBV_A

We can see the that Chain A, BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN [Homo sapiens] can serve as the best template for modelling the E3 ubiquitin-protein ligase structure.

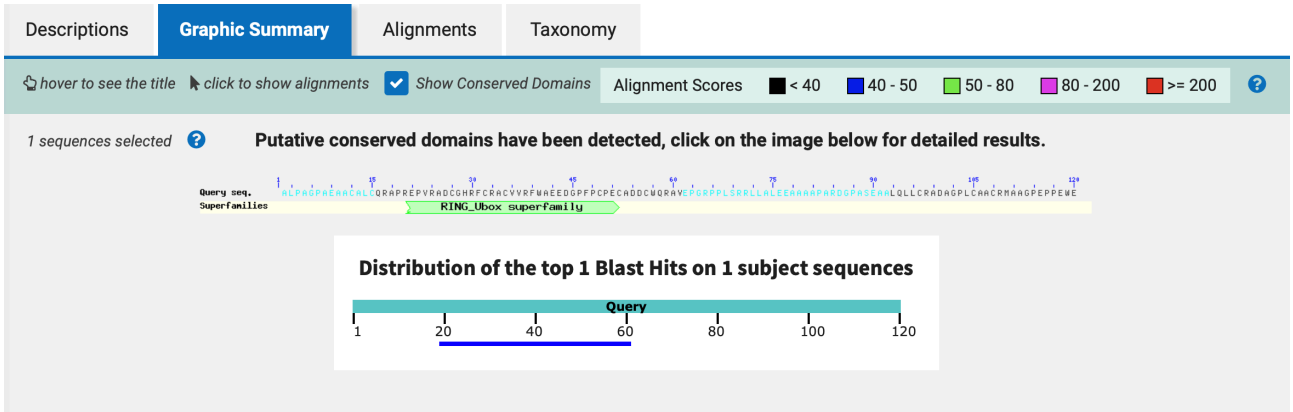
1. Query cover: It has the highest query cover of all the results of 35%. this indicates it is more aligned to out query protein.
2. E value: E value is also second highest. e value shows whar percentage of local alignment is there. The high E value makes it agood choice.
3. Score: The score is also very good of 45.1%.

2.

Below is the alignmrnt of the template we chose.



We donot get coverage after protein number 60 in any of the .
The coverage is highest among all other options.



So we can only use this as our template.

3.

SOLUTION NMR method was used to solve this structure. Their are 2 chains in this structure a and b. We need the chain a.

NMR Ensemble

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

Display Files | Download Files

1JM7

Solution structure of the BRCA1/BARD1 RING-domain heterodimer

PDB DOI: 10.2210/pdb1JM7/pdb

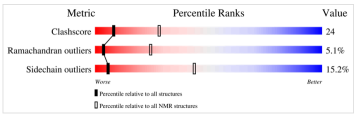
Classification: ANTITUMOR
Organism(s): Homo sapiens
Expression System: Escherichia coli BL21(DE3)
Mutation(s): No

Deposited: 2001-07-17 **Released:** 2001-10-03
Deposition Author(s): Brzovic, P.S., Rajagopal, P., Hoyt, D.W., King, M.-C., Klevit, R.E.

Experimental Data Snapshot

Method: SOLUTION NMR
Conformers Calculated: 25
Conformers Submitted: 14
Selection Criteria: structures with the least restraint violations, structures with the lowest energy

wwPDB Validation 3D Report | Full Report



Macromolecule Content

- Total Structure Weight: 26.25 kDa
- Atom Count: 1573
- Modelled Residue Count: 200
- Deposited Residue Count: 229
- Unique protein chains: 2

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

Literature — Download Primary Citation

Macromolecules

Find similar proteins by: Sequence (by identity cutoff) | 3D Structure

Entity ID: 1

Molecule	Chains	Sequence Length	Organism	Details	Image
BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN	A	112	Homo sapiens	Mutation(s): 0 Gene Names: BRCA1, RNF53 EC: 2.3.2.27	

UniProt & NIH Common Fund Data Resources

Find proteins for P38398 *(Homo sapiens)* — Go to UniProtKB: P38398

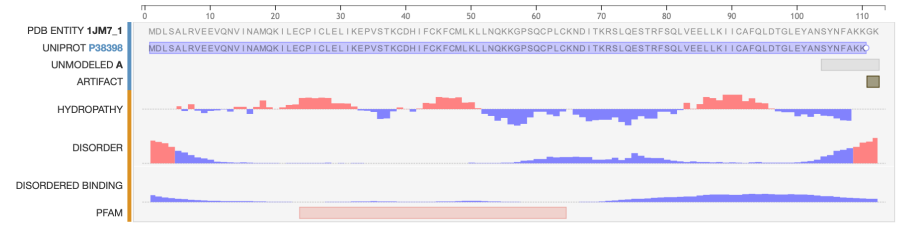
PHAROS: P38398 GTEx: ENSG00000012048

Entity Groups

Sequence Clusters	30% Identity	50% Identity	70% Identity	90% Identity	95% Identity	100% Identity
UniProt Group	P38398

Protein Feature View Expand

Reference Sequence: 1JM7_1



Entity ID: 2

Molecule	Chains	Sequence Length	Organism	Details	Image
BRCA1-ASSOCIATED RING DOMAIN PROTEIN 1	B	117	Homo sapiens	Mutation(s): 0 Gene Names: BARD1 EC: 2.3.2.27	

UniProt & NIH Common Fund Data Resources

Find proteins for Q99728 *(Homo sapiens)* — Go to UniProtKB: Q99728

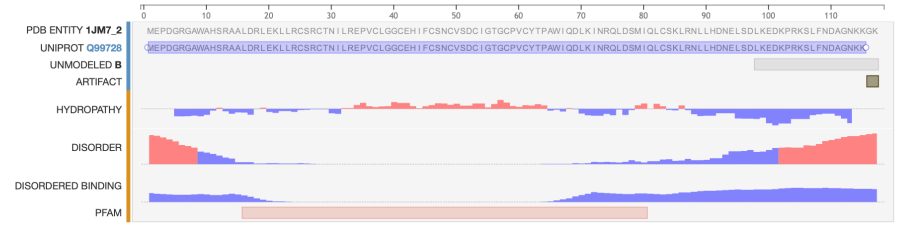
PHAROS: Q99728 GTEx: ENSG00000138376

Entity Groups

Sequence Clusters	30% Identity	50% Identity	70% Identity	90% Identity	95% Identity	100% Identity
UniProt Group	Q99728

Protein Feature View Expand

Reference Sequence: 1JM7_2



The chain B is different from our chain of interest.