

MODELING AND SIMULATION LAB REPORT

[Target Protein: Human 4 aminobutyrate]

SUBMITTED BY: ONEZA HASSAN ALVI

REGISTRATION NUMBER: 04281913032

SUMBITTED TO: SIR FAISAL AHMED

MODELING AND SIMULATION (BIF-213)

BSBIF NCB QAU



LAB REPORT:

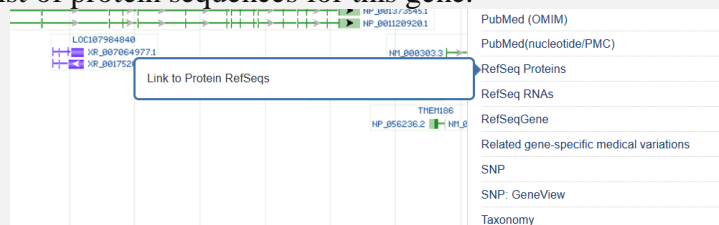
- Download sequence file for Human 4 aminobutyrate
- Generate a homology model using SWISS-model server <http://www.expasy.ch/swissmod/>
- Download the template structure from www.rcsb.org
- Compare the model and template structures
- Validate the Structure

Download the protein sequence in FASTA format:

- Go to the NCBI Gene website and enter the gene ID 18 in the search box.
- Click on the gene name “ABAT 4-aminobutyrate aminotransferase [Homo sapiens (human)]” to go to the gene summary page.



- Scroll down to the “Related information” section and click on the link “Protein (RefSeq)” under the “Gene” category. This will take you to the NCBI Protein website with a list of protein sequences for this gene.



- Click on the protein accession number “NP_001120920.1” to go to the protein summary page. This is the protein sequence that corresponds to the longest transcript variant of this gene.

An official website of the United States government [Here's how you know](#)

NIH National Library of Medicine
National Center for Biotechnology Information

Protein [Advanced](#) [Help](#)

GenPept

4-aminobutyrate aminotransferase, mitochondrial isoform 1 precursor [Homo sapiens]

NCBI Reference Sequence: NP_001120920.1
[Identical Proteins](#) [FASTA](#) [Graphics](#)

[Go to:](#)

LOCUS NP_001120920 500 aa linear PRI 29-MAY-2023
DEFINITION 4-aminobutyrate aminotransferase, mitochondrial isoform 1 precursor [Homo sapiens].
ACCESSION NP_001120920
VERSION NP_001120920.1
DBSOURCE REFSEQ: accession [NM_001127448.2](#)
KEYWORDS RefSeq.
SOURCE Homo sapiens (human)
ORGANISM Homo sapiens

Analyze this sequence
[Run BLAST](#)
[Identify Conserved Domains](#)
[Highlight Sequence Features](#)
[Find in this Sequence](#)
[Show in Genome Data Viewer](#)

Articles about the ABAT gene

- Click on the “FASTA” link under the “Display Settings” section to download the protein sequence in FASTA format.

FASTA

4-aminobutyrate aminotransferase, mitochondrial isoform 1 precursor [Homo sapiens]

NCBI Reference Sequence: NP_001120920.1
[GenPept](#) [Identical Proteins](#) [Graphics](#)

>NP_001120920.1 4-aminobutyrate aminotransferase, mitochondrial isoform 1 precursor [Homo sapiens]
MASMLLAQRLACSFQHSYRLLVPGSRHSQAQAKVDVEFDYDGLMKTEVPGPRSQELMKQLNIIQNAEA
VHFFCNYEESRGNLYVDVGNRMLDLYSQISSVPIGYSHPALKLIIQPPQNASMFVNRPALGILPPENFV
EKLRSLLSVAPKQMSQLITMACGSCSNENALKTFMWRYSKERGQRGSQEELTCMIQAPGCPDYSI
LSFMGAHFGRMTGCLATHTSKAIHKIDIPSFOWPIAPFPRLYPLEEFVKEHQEEARCLEEVEDLIVKY
RKKKKTAVAGIIVEPIQSEGGDNHASDDFRKLRLDIARKHGCAFLVDEVQTGGCTGKFWAHEHGLDDPA
DMVTFSKKMMTGFGFHFKEFRPINAPYRIFNTNLGDPKSNLLAEVINIIXREDLNNAAHAGKALLTGLL
DLQARYPQFISRVGRGTFCSDTPDDSIKRLLLIARNKGVVLGGCGDKSIRFRPTLVFRDHHAHLFLN
IFSDILADFK

Choose Destination
☒ File ☐ Clipboard
☐ Collections ☐ Analysis Tool

Download 1 item.
Format
Show GI ☐

Generate a homology model using SWISS-model server:

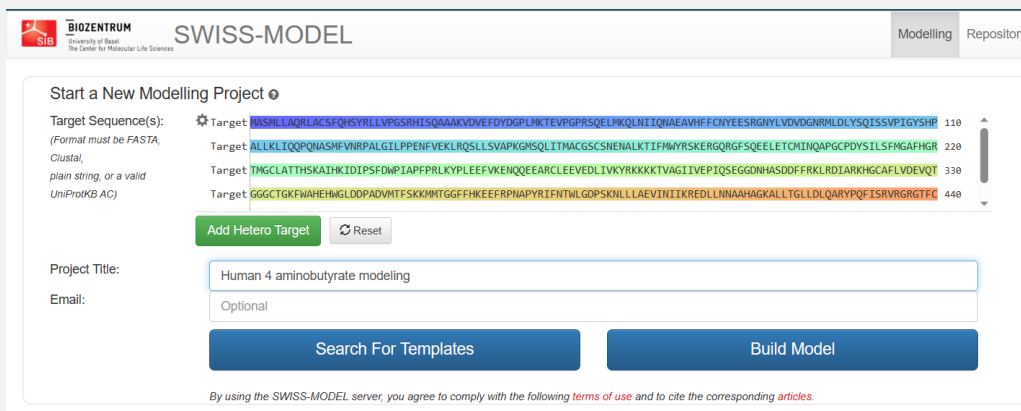
- Go to the SWISS-model website and click on the “Start Modelling” button or select the option “myWorkspace” from the navigation bar.

SWISS-MODEL [Modelling](#) [Repository](#) [Tools](#) [Documentation](#) [Log In](#) [Create Account](#)

SWISS-MODEL
is a fully automated protein structure homology-modelling server, accessible via the [ExPASy web server](#), or from the program [DeepView](#) (Swiss Pdb-Viewer).
The purpose of this server is to make protein modelling accessible to all life science researchers worldwide.

Repository
Every week we model all the sequences for thirteen core species based on the latest UniProtKB proteome. Is your protein already modelled and up to date in **SWISS-MODEL Repository**?

- Paste the protein sequence or provide the UniprotKB AC (P61851) of your target sequence in the input form. A project title is automatically suggested from the information retrieved from SWISS-MODEL’s own copy of the UniprotKB annotation, if a UniProtKB AC is used.



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SWISS-MODEL

Modelling Repository

Start a New Modelling Project

Target Sequence(s):
(Format must be FASTA, Clustal, plain string, or a valid UniProtKB AC)

Target:

Target:

Target:


Target:

Project Title:

Email:

By using the SWISS-MODEL server, you agree to comply with the following [terms of use](#) and to cite the corresponding [articles](#).

- Click on the “Search for Templates” button to find available template structures for your target sequence. The template search may take some time, depending on the complexity of your target sequence and the availability of templates.



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SWISS-MODEL

Modelling Repository Tools Documentation Log In Create Account

All Projects

Human 4 aminobutyrate modeling Created: today at 11:47

Template Results

The search for templates matching your target sequence is currently queuing. Please wait.

Queuing

If you want to come back later, bookmark this link:
<https://swissmodel.expasy.org/interactive/3ktcr/>

NASHLLAQLACSFQHSYRLLVPGSRHISQAAAKVDVEFDYDGLPHKTEVPGPRSQELHKLNIQNAEAVHFFCNYYEESRGNLYVDVGNRHLDLYSQISSVPIGYSHH
ALLKLTQQPNASMEFVNRPALGILPPENFEVKLRQSLLSVAPKMSQLITMACGSCSNENALKTFHMYRSKERGRGFSQEELETCHINQAPGCPDYSILSFMGAFHGR
TMGCLATTHSKATHKIDIPSFDMPIAPFPRLKYPLEEFVKENQEEARCLEEVEDLVKRYRKKKTVAGIIVEPIQSEGGDNHASDDFFRKLRLDIARKHGCAFLVDEVQT
GGGCTGKFWAHEHGLDDPADVMTFSKKMTGGFFHKEEFRPNAPYRIFNTWLGOPSKNLLAEVINIKREDLLNNAAHAGKALLTGLDLQARYPQFISRVGRGRTFCSDTDDSI
GGVLLGGCGDKSIRFRPTLVFRDHHALFLNIFSDILADFK

Antoine M. J. B. de Waele

- When the template search is finished, you will see a table showing the list of available templates ranked according to the expected quality of the resulting models. You can select a template based on the GMQE (Global Model Quality Estimation), QSQE (Quaternary Structure Quality Estimation), sequence identity, and the presence of ligands or metal-binding sites. You can also visualize the template in 3D by clicking on the checkbox next to the template ID.

SWISS-MODEL

Human 4 aminobutyrate modeling Created: today at 11:47

Summary Templates 60 Models Project Data

Template Results

IF Sort	Coverage	GMQE	QMQE	Identity	Method	Oligo State	Ligands
<input checked="" type="checkbox"/> 4y0h.1.A 4-aminobutyrate aminotransferase, mitochondrial	0.93	0.94	95.67	X-ray, 1.6Å	homo-dimer ✓	1 x FES ¹² , 2 x PLP ¹²	
<input checked="" type="checkbox"/> 4y0d.1.A 4-aminobutyrate aminotransferase, mitochondrial	0.93	0.94	95.67	X-ray, 2.2Å	homo-dimer ✓	1 x FES ¹² , 2 x RW2 ¹²	
<input checked="" type="checkbox"/> 4y0i.1.B 4-aminobutyrate aminotransferase, mitochondrial	0.93	0.94	95.65	X-ray, 1.7Å	homo-dimer ✓	2 x PSZ ¹² , 1 x FES ¹²	
<input checked="" type="checkbox"/> 4y0i.1.B 4-aminobutyrate aminotransferase, mitochondrial	0.92	0.94	95.66	X-ray, 1.7Å	homo-dimer ✓	2 x PSZ ¹² , 1 x FES ¹²	

Build Models 1

Clear Selection

- After selecting a template, you can click on the “Build Model” button to start the modelling process. You can also adjust the target-template alignment if needed by clicking on the “Edit Alignment” button. The model building may take some time, depending on the size and complexity of your target sequence and template structure.

Human 4 aminobutyrate modeling Created: today at 11:47

Summary Templates 60 Models 1 Project Data

A model already exists for your chosen template.

Model Results

Order by: GMQE

1 500

Model 01

Structure Assessment

Oligo-State

Homo-dimer (matching prediction)

GMQE

0.91

QMEANDisCo Global: 0.91 ± 0.05

Ligands

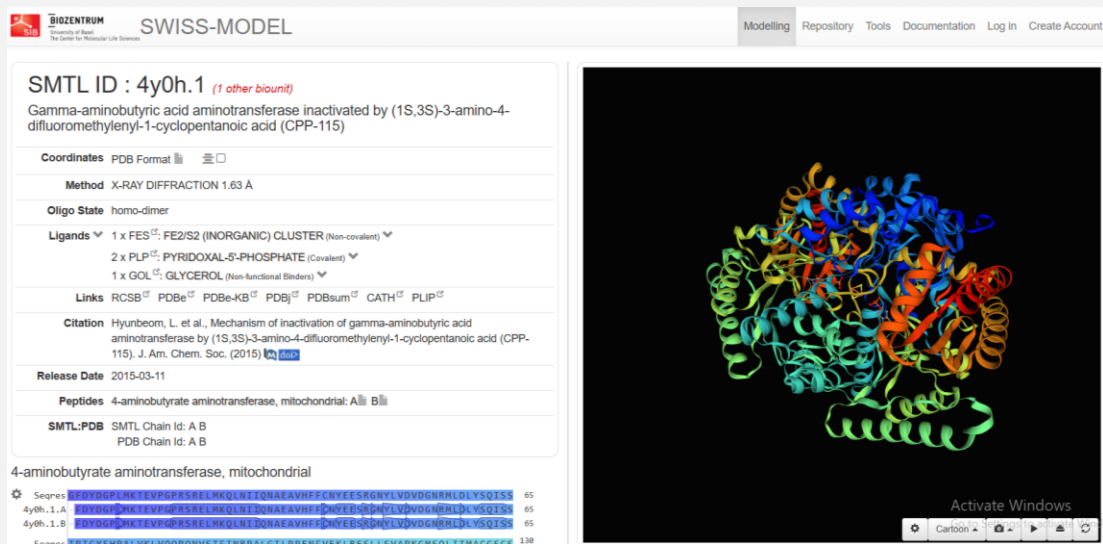
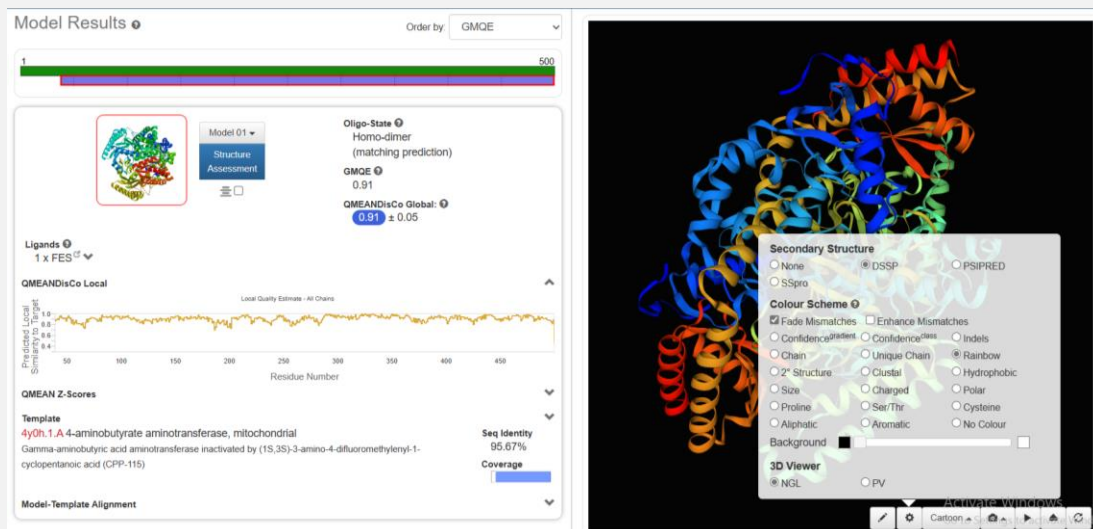
1 x FES¹²


QMEANDisCo Local

Local Quality Estimate - All Chains

Activate Windows

- When the model is built, you will see a summary of the modelling results, including a 3D visualization of your model, a quality assessment score (QMEAN), and a report of potential errors or issues in your model. You can download your model in PDB format by clicking on the “Download Model” button.




205,701 Structures from the PDB
1,068,577 Computed Structure Models (CSM)

Enter search term(s), Entry ID(s), or sequence
 Include CSM ☐

Advanced Search | Browse Annotations

PDB-101 | PDB | EMDatResource | UNIPROT | wwPDB | PDB-Dev

Structure Summary | 3D View | Annotations | Experiment | Sequence | Genome | Ligands | Versions

Biological Assembly 1

4Y0H
 Gamma-aminobutyric acid aminotransferase inactivated by (1S,3S)-3-amino-4-difluoromethylethyl-1-cyclopentanoic acid (CPP-115)
 PDB DOI: <https://doi.org/10.2210/pdb4Y0H/pdb>

Classification: TRANSFERASE
Organism(s): *Sus scrofa*
Expression System: *Sus scrofa*
Mutation(s): No

Deposited: 2015-02-06 Released: 2015-03-11
 Deposition Author(s): Rui, W., Ruslan, S., Hyunbeom, L., Emma, H.D., Jose, I.J., Neil, K., Richard, B.S., Dali, L.

Experimental Data Snapshot
 Method: X-RAY DIFFRACTION
 Resolution: 1.63 Å
 R-Value Free: 0.203
 R-Value Work: 0.176
 R-Value Observed: 0.178

wwPDB Validation
 3D Report | Full Report

Metric	Percentile Ranks	Value
Rfree		0.210
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		2.8%
RSRZ outliers		1.2%

Global Symmetry: Cyclic - C2 (3D View)
 Global Statistics: Monomer 2 mar. 67

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

Display Files | Download Files

- To download the template structure in PDB format, click on the “Download Files” button on the top right corner of the page. A drop-down menu will appear with different

Structure Summary | 3D View | Annotations | Experiment | Sequence | Genome | Ligands | Versions

4Y0H
 Gamma-aminobutyric acid aminotransferase inactivated by (1S,3S)-3-amino-4-difluoromethylethyl-1-cyclopentanoic acid (CPP-115)

Sequence of 4Y0H | Gamm... Chain 1: 4-aminobut... A

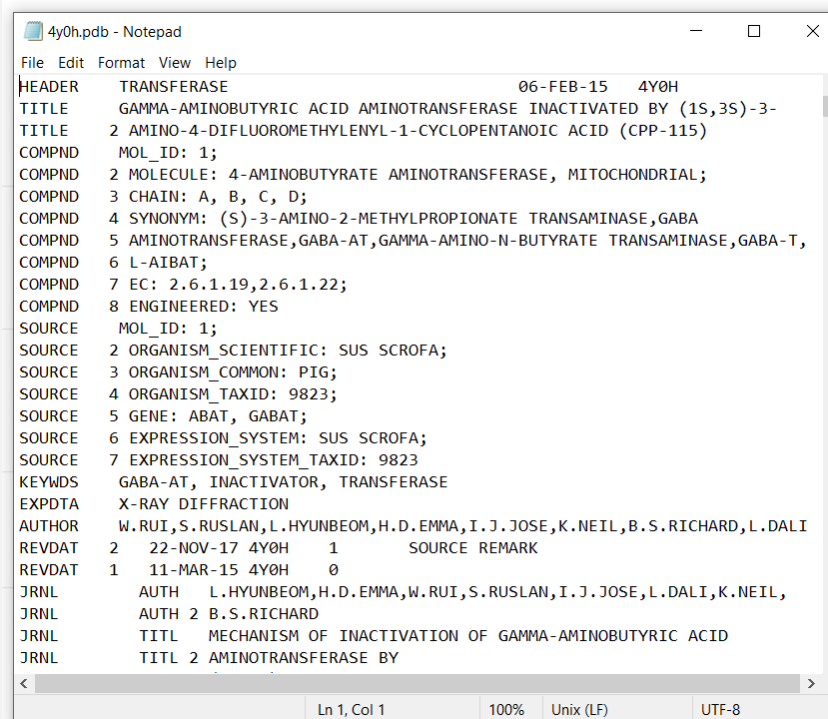
@FDYDGLMKEVTPGPRSLMKQLNIIQNAEAVHFFCHYEESRGNVIVVDGSRMLDLYSQISSIPIGYSHFALVKLVQPPQNVSTFINRFPALGILFPENFVEKLRSLISV
 APKMGSLITNACGSCSNENAFKTIIMWYRSKERGESAFSKEELETCHINQAPGCPQVSIILSFMGAHGRTHGCLATHSKAIHKIDIPSTFDFLAPFFFLKYLEEFVKENQ
 QEARCLLEEVEDLIVKYRKKKTKVAGIIVEPIQSEGGDNHADDFFRKLKRDISRKHGCAFLVDVQCTGGGSGTKFWAHEHWGLDOPADVMTFSKQDGTGGFFHKEEFPHAPY

Display Files | Download Files

- FASTA Sequence
- PDBx/mmCIF Format
- PDBx/mmCIF Format (gz)
- PDB Format
- PDB Format (gz)
- PDBML/XML Format (gz)
- Structure Factors (CIF)
- Structure Factors (CIF - gz)

file formats and options. Select “PDB Format” to download the structure in PDB format. You can also choose other formats or options depending on your needs.

- A pop-up window will appear asking you to save the file to your computer. Choose a location and a name for your file and click save. You have now downloaded the template structure in PDB format.



```
4y0h.pdb - Notepad
File Edit Format View Help
HEADER          TRANSFERASE                                06-FEB-15  4Y0H
TITLE           GAMMA-AMINOBUTYRIC ACID AMINOTRANSFERASE INACTIVATED BY (1S,3S)-3-
TITLE           2 AMINO-4-DIFLUOROMETHYLENYL-1-CYCLOPENTANOIC ACID (CPP-115)
COMPND          MOL_ID: 1;
COMPND          2 MOLECULE: 4-AMINOBUTYRATE AMINOTRANSFERASE, MITOCHONDRIAL;
COMPND          3 CHAIN: A, B, C, D;
COMPND          4 SYNONYM: (S)-3-AMINO-2-METHYLPROPIONATE TRANSAMINASE,GABA
COMPND          5 AMINOTRANSFERASE,GABA-AT,GAMMA-AMINO-N-BUTYRATE TRANSAMINASE,GABA-T,
COMPND          6 L-AIBAT;
COMPND          7 EC: 2.6.1.19,2.6.1.22;
COMPND          8 ENGINEERED: YES
SOURCE          MOL_ID: 1;
SOURCE          2 ORGANISM_SCIENTIFIC: SUS SCROFA;
SOURCE          3 ORGANISM_COMMON: PIG;
SOURCE          4 ORGANISM_TAXID: 9823;
SOURCE          5 GENE: ABAT, GABAT;
SOURCE          6 EXPRESSION_SYSTEM: SUS SCROFA;
SOURCE          7 EXPRESSION_SYSTEM_TAXID: 9823
KEYWDS          GABA-AT, INACTIVATOR, TRANSFERASE
EXPDTA          X-RAY DIFFRACTION
AUTHOR          W.RUI,S.RUSLAN,L.HYUNBEOM,H.D.EMMA,I.J.JOSE,K.NEIL,B.S.RICHARD,L.DALI
REVSTAT        2  22-NOV-17  4Y0H   1      SOURCE REMARK
REVSTAT        1  11-MAR-15  4Y0H   0
JRNL            AUTH  L.HYUNBEOM,H.D.EMMA,W.RUI,S.RUSLAN,I.J.JOSE,L.DALI,K.NEIL,
JRNL            AUTH 2 B.S.RICHARD
JRNL            TITL  MECHANISM OF INACTIVATION OF GAMMA-AMINOBUTYRIC ACID
JRNL            TITL 2 AMINOTRANSFERASE BY
```

Compare the model and template structures using TM-align or DALI:

- Go to the TM-align website or the DALI website (I chose TM-align).
- Click on the “Choose file” button and select your model file in PDB format from your computer. Repeat the same for your template file in PDB format.
- Click on the “RUN TM-align” button to start the alignment. The alignment may take a few seconds or minutes, depending on the size and complexity of your structures.

- DeepFold
- DeepFoldRNA
- FoldDesign
- COFACTOR
- COACH
- MetaGO
- TripletGO
- IonCom
- FG-MD
- ModRefiner
- REMO
- DEMO
- DEMO-EM
- SPRING
- COTH
- Threpp
- PEPPI
- BSPred
- ANGLOR
- EDock
- BSP-SLIM
- SAXSTER
- FUPred
- ThreaDom
- ThreaDomEx
- EvoDesign
- BindProf
- BindProfX

Note: This server is only for pair-wise structure comparison. If you want to match one protein structure with all proteins in the PDB library, you can do it in [COFACTOR Server](#)

- Input Structure 1 in [PDB format](#) or [PDBx/mmCIF format](#) (mandatory):
Please copy and paste your structure file here. [Sample input](#)

Or upload the structure file:
 model_01.pdb

- Input Structure 2 in [PDB format](#) or [PDBx/mmCIF format](#) (mandatory):
Please copy and paste your structure file here. [Sample input](#)

Or upload the structure file:
 4y0h.pdb

- Input Email: (optional, where results will be sent to)
-

- When the alignment is finished, you will see a summary of the results, including a score and a visualization of the structural similarity between your model and template. The score is a measure of how well your structures match each other, based on their shape and orientation. A higher score means a better alignment and a more similar structure. The visualization shows your structures in different colors, superimposed on each other. You can rotate, zoom, or change the display options of the visualization using the buttons or mouse controls.

TM-align Results

```

*****
*                               TM-align (Version 20190822)                               *
* An algorithm for protein structure alignment and comparison                             *
* Based on statistics:                                                         *
*   0.0 < TM-score < 0.30, random structural similarity                         *
*   0.5 < TM-score < 1.00, in about the same fold                             *
* Reference: Y Zhang and J Skolnick, Nucl Acids Res 33, 2302-9 (2005)         *
* Please email your comments and suggestions to: zhng@umich.edu               *
*****

```

```

Name of Chain_1: A918153
Name of Chain_2: B918153
Length of Chain_1: 461 residues
Length of Chain_2: 461 residues

```

```

Aligned length= 461, RMSD= 0.07, Seq_ID=n_identical/n_aligned= 0.957
TM-score= 0.99992 (if normalized by length of Chain_1)
TM-score= 0.99992 (if normalized by length of Chain_2)
(You should use TM-score normalized by length of the reference protein)

```

```

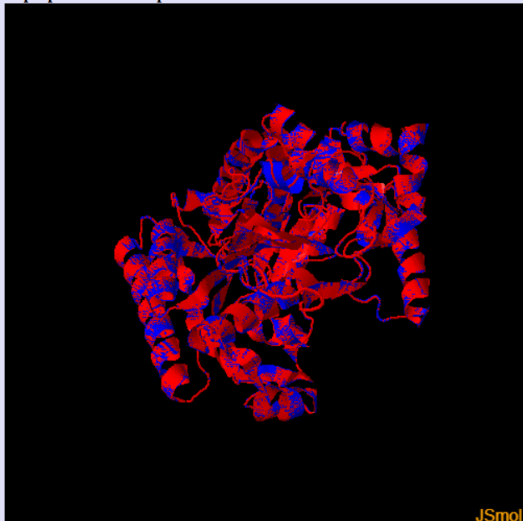
(":" denotes aligned residue pairs of d < 5.0 A, "." denotes other aligned residues)
FDYDGPLMKTEVPGRSQELMKQLNIIQNAEAVHFFCNYYEESRGNYLVDVDGNRMLDLYSQISSVPIGYSHPALKLIIQQPNASMEVNRPALG
::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
FDYDGPLMKTEVPGRSRELKQLNIIQNAEAVHFFCNYYEESRGNYLVDVDGNRMLDLYSQISSIPIGYSHPALVKLVQQPNVSTFINRPALG

```

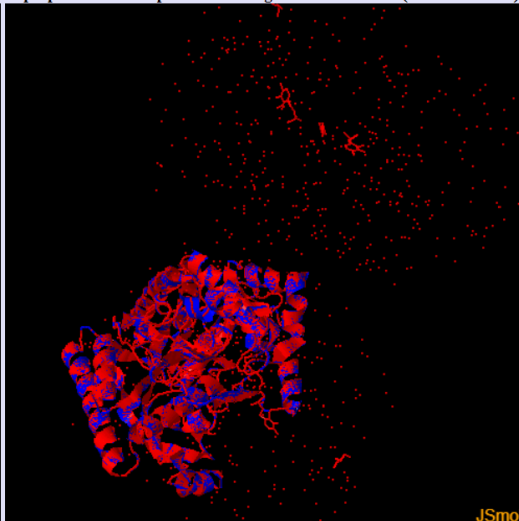
- You can also download the aligned structures or the alignment file for further analysis.

Visualization (Protein-1 in blue and Protein-2 in red)

Superposition of two proteins



Superposition of two proteins with ligands and solvents (when available)



Document downloads

- Click [A918153.pdb](#) to download the first structure (model_01.pdb) that you submitted.
- Click [B918153.pdb](#) to download the second structure (4y0h.pdb) that you submitted.

Validate the structure of your model:

- Go to the QMEAN website or the MolProbity website.
- Click on the “Browse” button and select your model file in PDB format from your computer.
- Click on the “Submit” button to start the analysis. The analysis may take a few seconds or minutes, depending on the size and complexity of your model.

SWISS-MODEL

Modelling Repository Tools Documentation Log in Create Account

QMEAN Qualitative Model Energy Analysis CAMEO evaluation Help Examples

[+Select Coordinate File...](#)

model_01.pdb 4 atoms were removed!

removing atoms with zero occupancy
 -> removed 0 atoms with zero occupancy
 removing hydrogen atoms
 -> removed 0 hydrogen atoms
 _FES1 is not a standard amino acid -> removed

For optimum performance, please add the SEQRES of your model here

Segres
 Method

☒ QMEANDisCo
 The default method used by SWISS-MODEL homology modelling pipeline and Structure Assessment - a single model method combining statistical potentials and agreement terms with a distance constraints (DisCo) score. DisCo evaluates consistencies of pairwise CA-CA distances from a model with constraints extracted from homologous structures. All scores are combined using a neural network trained to predict per-residue ICDT scores.

☐ QMEAN
 A single model method combining statistical potentials and agreement terms in a linear manner.

☐ QMEANBran
 QMEANBran is a combination of statistical potentials targeted at local quality estimation of membrane protein models in their naturally occurring oligomeric state: after identifying the transmembrane region using an implicit solvation model, specifically trained statistical potentials get applied on the different regions of a protein model.

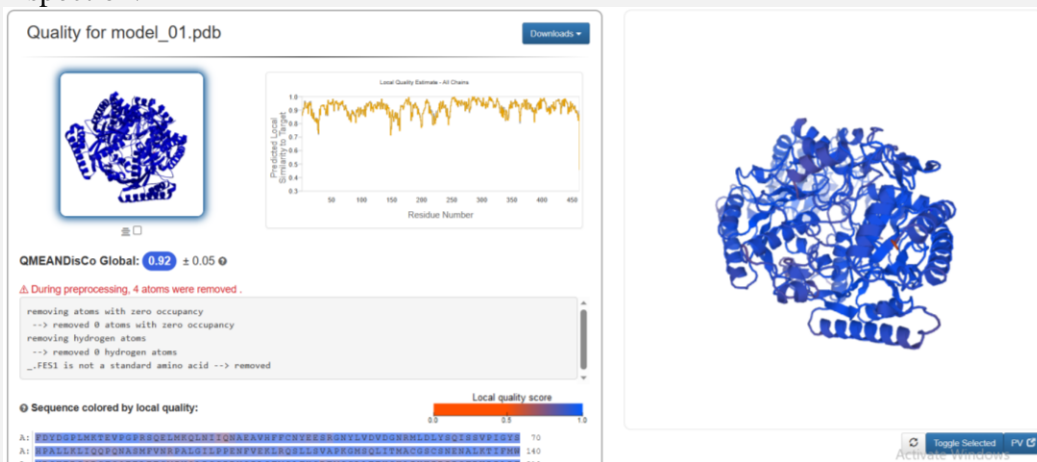
Project Name (Optional)

Email (Optional)

[Submit](#)

Activate Windows
Go to Settings to activate Windows

- When the analysis is finished, you will see a summary of the results, including a score and a report of potential errors or issues in your model. The score is a measure of how well your model conforms to the expected stereochemistry and geometry of a protein structure, based on various criteria such as bond lengths, bond angles, torsion angles, clashes, and packing. A higher score means a better quality and a more reliable model. The report lists the specific errors or issues that were detected in your model, such as missing atoms, outliers, bad contacts, or Ramachandran violations. You can also download the annotated model or the report file for further inspection.



model_001_processed.pdb - Notepad

FileEditFormatViewHelp

ATOM	1	N	PHE	A	1	42.840	27.292	48.646	1.00	0.87	N
ATOM	2	CA	PHE	A	1	41.590	26.524	48.963	1.00	0.87	C
ATOM	3	C	PHE	A	1	41.160	25.503	47.921	1.00	0.87	C
ATOM	4	O	PHE	A	1	40.693	24.439	48.322	1.00	0.87	O
ATOM	5	CB	PHE	A	1	40.447	27.519	49.318	1.00	0.87	C
ATOM	6	CG	PHE	A	1	40.683	28.176	50.662	1.00	0.87	C
ATOM	7	CD1	PHE	A	1	41.348	29.410	50.772	1.00	0.87	C
ATOM	8	CD2	PHE	A	1	40.216	27.559	51.835	1.00	0.87	C
ATOM	9	CE1	PHE	A	1	41.557	30.002	52.025	1.00	0.87	C
ATOM	10	CE2	PHE	A	1	40.413	28.155	53.087	1.00	0.87	C
ATOM	11	CZ	PHE	A	1	41.094	29.372	53.183	1.00	0.87	C
ATOM	12	N	ASP	A	2	41.321	25.759	46.604	1.00	0.89	N
ATOM	13	CA	ASP	A	2	40.847	24.873	45.575	1.00	0.89	C
ATOM	14	C	ASP	A	2	41.587	25.292	44.302	1.00	0.89	C
ATOM	15	O	ASP	A	2	42.143	26.396	44.300	1.00	0.89	O
ATOM	16	CB	ASP	A	2	39.321	25.095	45.447	1.00	0.89	C
ATOM	17	CG	ASP	A	2	38.621	23.834	44.984	1.00	0.89	C
ATOM	18	OD1	ASP	A	2	39.227	22.733	45.084	1.00	0.89	O
ATOM	19	OD2	ASP	A	2	37.463	23.958	44.528	1.00	0.89	O
ATOM	20	N	TYR	A	3	41.634	24.445	43.246	1.00	0.92	N
ATOM	21	CA	TYR	A	3	42.048	24.792	41.879	1.00	0.92	C
ATOM	22	C	TYR	A	3	40.809	25.238	41.083	1.00	0.92	C
ATOM	23	O	TYR	A	3	39.694	25.119	41.585	1.00	0.92	O
ATOM	24	CB	TYR	A	3	42.712	23.596	41.133	1.00	0.92	C
ATOM	25	CG	TYR	A	3	44.027	23.190	41.739	1.00	0.92	C
ATOM	26	CD1	TYR	A	3	45.233	23.722	41.258	1.00	0.92	C
ATOM	27	CD2	TYR	A	3	44.082	22.192	42.723	1.00	0.92	C
ATOM	28	CE1	TYR	A	3	46.462	23.289	41.774	1.00	0.92	C
ATOM	29	CE2	TYR	A	3	45.314	21.688	43.168	1.00	0.92	C
ATOM	30	CZ	TYR	A	3	46.504	22.281	42.739	1.00	0.92	C

Ln 1, Col 1100%Unix (LF)UTF-8

- QMEANDisCo Global is a score that measures the quality of a protein model based on various criteria, such as bond lengths, bond angles, torsion angles, clashes, and packing. It also takes into account the distance constraints derived from homologous structures in the Protein Data Bank. The score ranges from 0 to 1, where a higher score means a better quality and a more reliable model. The score is also normalized by the length of the model, to account for the different sizes of proteins. The value $0.92 \pm$

0.05 means that your model has a high quality and is very similar to the experimental structures of proteins of the same size. The value ± 0.05 means that there is a small uncertainty or variation in the score, which is normal for any prediction method. You can also look at the QMEANDisCo Local Quality Estimate and QMEAN Z-Scores to see how the quality of your model varies along the sequence and how it compares to other models.

Another method to validate the model: UCLA-DOE LAB --- SAVES v6.0

To validate your homology model structure using UCLA, you can use the SAVESv6.0 - Structure Validation Server¹. This server allows you to run various programs to check the quality of your model, such as ERRAT, VERIFY 3D, PROVE, PROCHECK and WHATCHECK. To use this server, you need to upload your structure in PDB format and select the programs you want to run.

UCLA-DOE LAB — SAVES v6.0



**To run any or all programs:
upload your structure, in PDB format only**

model_01.pdb

Customize job name:

model_01.pdb

Run programs

References

ERRAT

- Reference: Verification of protein structures: patterns of nonbonded atomic interactions, Colovos C and Yeates TO, 1993.
- C++ software

VERIFY 3D

- Profile Search Software [Bowie et al., 1991, Luethy et al., 1992].
- DSSP original and Wikipedia

UCLA-DOE LAB — SAVES v6.0

UCLA

Job 1369169 has been created

[New Job](#)

job #1369169: model_01.pdb [[job link](#)] [[3D Viewer](#)]

ERRAT Complete <u>Overall Quality Factor</u> 92.0354 Results	VERIFY Complete 77.46% of the residues have averaged 3D-1D score ≥ 0.1 Fail Fewer than 80% of the amino acids have scored ≥ 0.1 in the 3D/1D profile. Results	PROVE Temporarily down at the moment																																																																	
WHATCHECK Complete <table border="1"><tr><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td><td>6</td><td>7</td><td>8</td><td>9</td><td>10</td><td>11</td><td>12</td><td>13</td></tr><tr><td>14</td><td>15</td><td>16</td><td>17</td><td>18</td><td>19</td><td>20</td><td>21</td><td>22</td><td>23</td><td></td><td></td><td></td></tr><tr><td>24</td><td>25</td><td>26</td><td>27</td><td>28</td><td>29</td><td>30</td><td>31</td><td>32</td><td>33</td><td></td><td></td><td></td></tr><tr><td>34</td><td>35</td><td>36</td><td>37</td><td>38</td><td>39</td><td>40</td><td>41</td><td>42</td><td>43</td><td></td><td></td><td></td></tr><tr><td>44</td><td>45</td><td>46</td><td>47</td><td>48</td><td>49</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr></table> Results	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23				24	25	26	27	28	29	30	31	32	33				34	35	36	37	38	39	40	41	42	43				44	45	46	47	48	49								PROCHECK Complete Out of 9 evaluations • Errors: 4 • Warning: 3 • Pass: 2 Results	OPEN We are open to suggestions for a 6th program to operate in this window. If you know of a program that we could run locally on our server that would be most useful, please let us know: email holton at mbi dot ucla dot edu with your suggestion
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- **ERRAT:** The Overall Quality Factor is the percentage of the protein that falls below the 95% rejection limit for the error values. A higher value indicates a better quality model. This model has an Overall Quality Factor of 92.0354, which is quite good.
- **PROCHECK:** The program gives a summary of the results with Errors, Warnings, and Pass for each evaluation. Errors indicate serious problems, Warnings indicate potential problems, and Pass indicate acceptable results. This model has 4 Errors, 3 Warnings, and 2 Pass out of 9 evaluations, which suggests that your model has some issues that need to be fixed.
- **WHATCHECK:** The program gives a list of headings for each test result and highlights the problematic regions in red. You can select a test result box to see more details about the issues and how to fix them.
- **VERIFY3D:** The program also gives a percentage of residues that have a 3D-1D score above 0.1, which is considered a threshold for acceptable models. This model has 77.46% of residues above this threshold, which is slightly below the recommended value of 80%. This means that your model has some regions that are not well matched with their sequence.