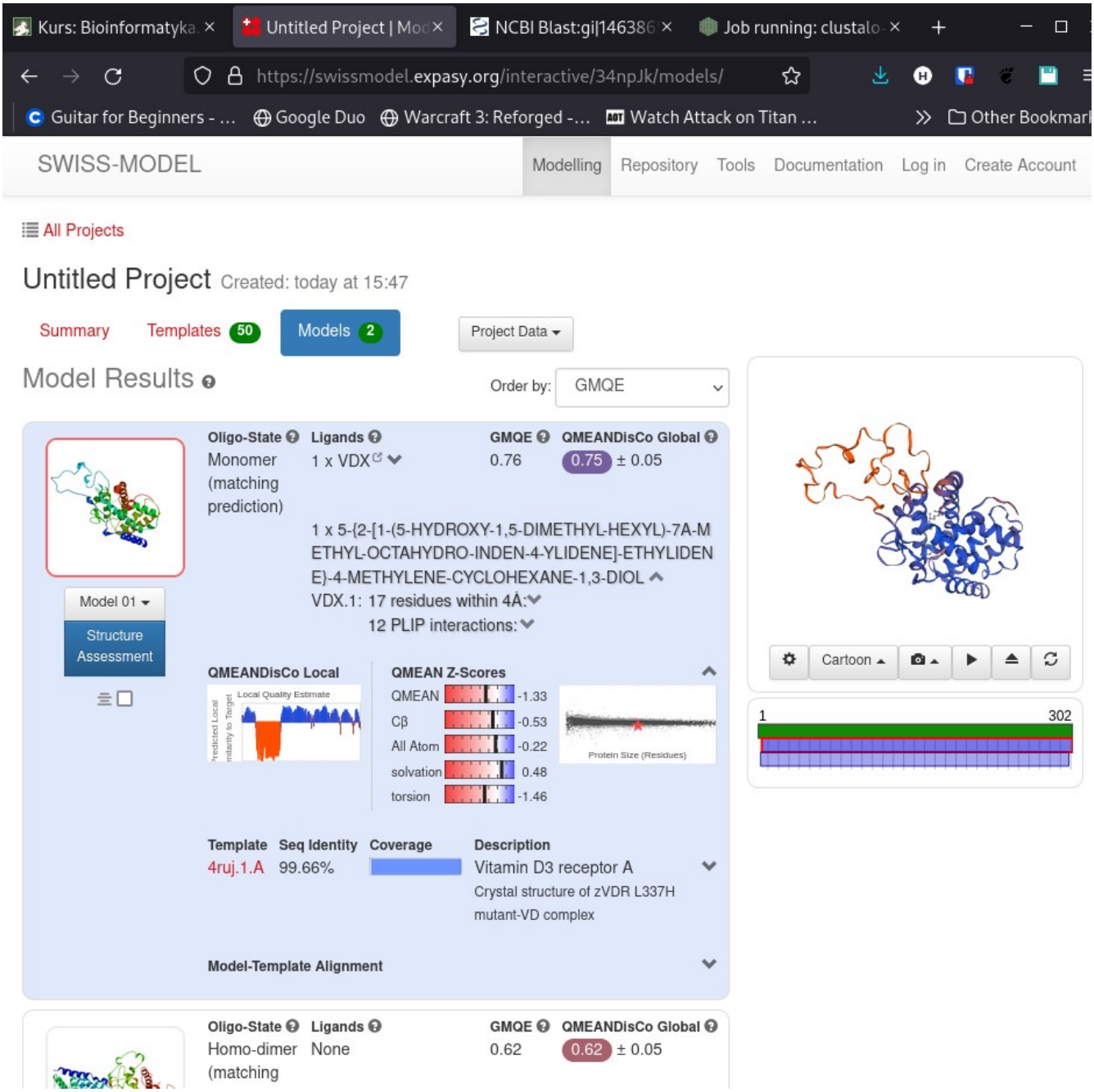
Łatwy cel


Kurs: Bioinformatyka
Untitled Project | Mod
NCBI Blast:gi|146386
Job running: clustalo
https://swissmodel.expasy.org/interactive/34npJk/models/
Guitar for Beginners - ...
Google Duo
Warcraft 3: Reforged -...
Watch Attack on Titan ...
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All Projects
Untitled Project Created: today at 15:47
Summary
Templates 50
Models 2
Project Data
Model Results
Order by: GMQE
Oligo-State
Ligands
GMQE
QMEANDisCo Global
Monomer (matching prediction)
1 x VDX
0.76
0.75 ± 0.05
1 x 5-{2-[1-(5-HYDROXY-1,5-DIMETHYL-HEXYL)-7A-METHYL-OCTAHYDRO-INDEN-4-YLIDENE]-ETHYLIDENE}-4-METHYLENE-CYCLOHEXANE-1,3-DIOL
VDX.1: 17 residues within 4Å:
12 PLIP interactions:
Model 01
Structure Assessment
QMEANDisCo Local
Local Quality Estimate
QMEAN Z-Scores
QMEAN -1.33
Cβ -0.53
All Atom -0.22
solvation 0.48
torsion -1.46
Protein Size (Residues)
Template
Seq Identity
Coverage
Description
4ruj.1.A
99.66%
Vitamin D3 receptor A
Crystal structure of zVDR L337H mutant-VD complex
Model-Template Alignment
Oligo-State
Ligands
GMQE
QMEANDisCo Global
Homo-dimer (matching
None
0.62
0.62 ± 0.05
Cartoon
1
302

302

Other reports

Distance tree of results Multiple alignment MSA viewer

Descriptions | Graphic Summary | Alignments | Taxonomy

Sequences producing significant alignments

Download | New Select columns | Show 100

select all *100 sequences selected*

GenPept Graphics Distance tree of results Multiple alignment New MSA Viewer

	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accessio
☑	Chain A, Vitamin D receptor [Danio rerio]	Danio rerio	619	619	100%	0.0	100.00%	302	2HBH_A
☑	Structure-activity relationship study of vitamin D analogs with oxol…	Danio rerio	618	618	100%	0.0	100.00%	317	5NMB_2
☑	Crystal structure of zVDR L337H mutant-VD complex [Danio rerio]	Danio rerio	616	616	100%	0.0	99.67%	302	4RUJ_A
☑	Development of synthetically accessible non-secosteroidal hybrid …	Danio rerio	615	615	99%	0.0	100.00%	300	4FHH_A
☑	Crystal structure of the VDR LBD complexed to seocalcitol [Homo…	Homo sa…	377	377	100%	2e-132	63.87%	263	1S0Z_A
☑	Synthesis, Structure, and Biological Activity of des-Side Chain An…	Homo sa…	377	377	100%	3e-132	63.87%	280	3P8X_A
☑	Crystal Structure Of The Nuclear Receptor For Vitamin D Comple…	Homo sa…	375	375	98%	9e-132	64.67%	259	1DB1_A
☑	Crystal structure of the human vitamin D receptor (H305F) ligand …	Homo sa…	374	374	100%	3e-131	63.55%	263	3A2I_A
☑	Crystal structure of the human vitamin D receptor (H305F/H397F)…	Homo sa…	371	371	100%	4e-130	63.23%	263	3A2J_A
☑	Human VDR ligand binding domain in complex with maxacalcitol […	Homo sa…	370	370	97%	7e-130	64.86%	254	3B0T_A
☑	Crystal Structure Analysis of Vitamin D receptor [Homo sapiens]	Homo sa…	370	370	97%	9e-130	64.86%	253	3AZ1_A

Clustal Omega

Input form | Web services | Help & Documentation | Bioinformatics Tools FAQ

Tools > Multiple Sequence Alignment > Clustal Omega

Results for job clustalo-I20220201-150345-0977-5895192-p2m

Alignments | Result Summary | Phylogenetic Tree | Results Viewers | Submission Details

Download Alignment File | Show Colors

```
CLUSTAL O(1.2.4) multiple sequence alignment


gi|146386501|The      GSHMLSDEQMQIINSLVEAHHKTYDDSYSDFVRFRPPVREGPVTRSASRAASLHSLSDAS      60
2HBH_A                GSHMLSDEQMQIINSLVEAHHKTYDDSYSDFVRFRPPVREGPVTRSASRAASLHSLSDAS      60
                      ************************************************************

gi|146386501|The      SDSFNHSPESVDTKLNFSNLLMMYQDSGSPDSSEEDQQSRLSMLPHLADLVSYSIQKVIG      120
2HBH_A                SDSFNHSPESVDTKLNFSNLLMMYQDSGSPDSSEEDQQSRLSMLPHLADLVSYSIQKVIG      120
                      ************************************************************

gi|146386501|The      FAKMIPGFRDLTAEDQIALLKSSAIEIIMLRSNQSFSLEDMSWSCGGPDFKYCINDVTKA      180
2HBH_A                FAKMIPGFRDLTAEDQIALLKSSAIEIIMLRSNQSFSLEDMSWSCGGPDFKYCINDVTKA      180
                      ************************************************************

gi|146386501|The      GHTLELLEPLVKFQVGLKKLKLHEEEHVLLMAICLLSPDRPGVQDHVRIEALQDRLCDVL      240
2HBH_A                GHTLELLEPLVKFQVGLKKLKLHEEEHVLLMAICLLSPDRPGVQDHVRIEALQDRLCDVL      240
                      ************************************************************

gi|146386501|The      QAYIRIQHPGGRLLYAKMIQKLADLRSLNEEHSKQYRSLSFQPEHSMQLTPLVLEVFGSE      300
2HBH_A                QAYIRIQHPGGRLLYAKMIQKLADLRSLNEEHSKQYRSLSFQPEHSMQLTPLVLEVFGSE      300
                      ************************************************************

gi|146386501|The      VS        302
2HBH_A                VS        302
                      **
```

PLEASE NOTE: Showing colors on large alignments is slow.

lab14_protein2.pdb

All Projects

Untitled Project Created: today at 16:47

Summary | Templates 50 | Models 1 | Project Data

Model Results

Order by: GMQE

Oligo-State	Ligands	GMQE	QMEANDisCo Global
Homo-dimer (matching prediction)	None	0.98	0.93 ± 0.05

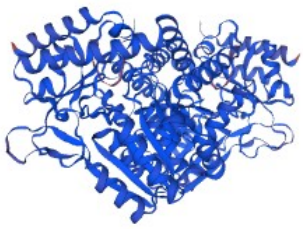
QMEANDisCo Local | QMEAN Z-Scores

Model 01

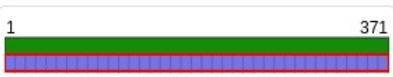
Structure Assessment

Template	Seq Identity	Coverage	Description
3ke3.1.A	100.00%		Putative serine-pyruvate aminotransferase Crystal structure of Putative serine-pyruvate aminotransferase (YP_263484.1) from PSYCHROBACTER ARCTICUM 273-4 at 2.20 A resolution

Model-Template Alignment



Cartoon



Email: Optional

amino acid

Query Length

371

Other reports

Distance tree of results | Multiple alignment | MSA viewer

Descriptions | Graphic Summary | Alignments | Taxonomy

Sequences producing significant alignments

Download | New Select columns | Show 100

select all *3 sequences selected*

GenPept | Graphics | Distance tree of results | Multiple alignment | New MSA Viewer

	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accessio
☑	Chain A, Putative serine-pyruvate aminotransferase [Psychrobacter …	Psychrob…	739	739	100%	0.0	97.57%	379	3KE3_A
☑	Crystal structure and substrate specificity of a thermophilic archaeal …	Saccharol…	95.1	95.1	87%	3e-21	28.96%	384	3ZRP_A
☑	Crystal structure of alanine-pyruvate aminotransferase with 2-methyl…	Thermus t…	69.7	69.7	96%	1e-12	27.22%	353	2YRI_A

Results for job clustalo-I20220201-155049-0014-92730217-p1m

Alignments | Result Summary | Phylogenetic Tree | Results Viewers | Submission Details

Download Alignment File | Show Colors

```
CLUSTAL O(1.2.4) multiple sequence alignment


original      ------DIDPNGLLEYSVV-YTDRALNHMSKAFQEVMNDLLSNLKTVY---NAEAAVIIP      50
template      MDKLLLHVGPTTIKEDVLVAGLENNVGFTSKEFVEALAYSLKGLRYVMGASKNYQPLIIP      60
                    .:.*. : *  :*   :. :.. ** * *.:   *..*: *    :    :***

original      GSGTYGMEAVARQLTIDEDCLIIRNGWFSYRWTQILEKGKFAKSSTVLTAERTEDTEAPK      110
template      GGGTSAMESVTSLLKPNDKILVVSNGVFGDRWEQIFKRYPVNVK--VLRPSPG-D-----      112
              *.** .**:*:  *. ::. *:: ** *. ** **:::  .  .  **  .   *

original      PFAPVDIETAVAKIKEDKSAIVYAPHVETSSGIILSEEYIKALSEAVHSVGGLLVIDC-I      169
template      YVKPGEVEE---EVRKSEYKLVALTHVETSTGVREPV---KDVINKIRKYVELIVVDGVS      166
               . * ::*    ::::.:  :*   *****:*:       * : : ::.   *:*:*

original      ASGCVWLDMKELGIDVLISAPQKGWSSTPCAGLVMLSAAAIKKVESTE-SNCFSLDLKQW      228
template      SVGAEEVKAEEWNVDVYLTASQKALGSAAGLGLLLLSPKALSILDSQNSIAGYYLDLRNW      226
              : *.  :. :* .:** ::* **. .*:   **::**  *:. ::* :    : ***::*

original      LTIMRAYENGGHAYHATMPTDSLRQFRDAILEAKEIGFDILRDAQWELGNRVRKVLTDKG      288
template      LPVMRGAEEGKAAYFATPPVHVILQLAEAFRLIEKEGIENRIKRHTMVASAIRAGLEALG      286
              * :**. *:*  **.** *.. : *: :*:   :: *::   . :  :.. :*  *   *

original      IESVAAEG--F--EAPGVVVSYTERDDMHKGSAFAEAGLQIAAGVPLKVGEPDNFKTFRL      344
template      LEIVARRPESYSNTVTGVILKVADPQKVL--------AGTVNEGVEFAPGVHPAFKYFRI      338
              :* ** .   :   . **::. :: :.:         .  :  ** :  *    ** **:

original      GLFGLDKLTDIDGTVERFEKALDEV----------------LA---    371
template      GHMGWVTPNDAIIAISVIERTLRKLGEPIRFGEGVKAVEEVLFSAR    384
              * :*  . .*   ::. :*::* ::                *
```

PLEASE NOTE: Showing colors on large alignments is slow.

Start a New Modelling Project

For the uploaded target-template alignment, 10 biounits and / or chains were found to match your template. Please select which biounit you wish to use as the template.
You can avoid this step by using the SMTL ID as the template name in your input alignment, (SMTL ID is <PDB ID>.<biological assembly>.<Chain ID>)

Supported Inputs

- Sequence(s)
- Target-Template Alignmen
- User Template
- DeepView Project

```
Target  ------DIDPNGLLEYSVV-YTDRALNHMSKAFQEVMNDLLSNLKTVY---NAEAAVIIPGSGTY
3zrp.1.A MDKLLLHVGPTTIKEDVLVAGLENNVGFTSKEFVEALAYSLKGLRYVMGASKNYQPLIIPGGGTS

Target  GMEAVARQLTIDEDCLIIRNGWFSYRWTQILEKGKFAKSSTVLTAERTEDTEAPKPFAPVDIETA
3zrp.1.A AMESVTSLLKPNDKILVVSNGVFGDRWEQIFKRYPVNVK--VLRPSPG-D-----YVKPGEVEE-

Target  VAKIKEDKSAIVYAPHVETSSGIILSEEYIKALSEAVHSVGGLLVIDC-IASGCVWLDMKELGID
```

Sequence Identity: 27.51

Build Model | Reset

```
Target  ------DIDPNGLLEYSVV-YTDRALNHMSKAFQEVMNDLLSNLKTVY---NAEAAVIIPGSGTY
3zrp.1.B MDKLLLHVGPTTIKEDVLVAGLENNVGFTSKEFVEALAYSLKGLRYVMGASKNYQPLIIPGGGTS

Target  GMEAVARQLTIDEDCLIIRNGWFSYRWTQILEKGKFAKSSTVLTAERTEDTEAPKPFAPVDIETA
3zrp.1.B AMESVTSLLKPNDKILVVSNGVFGDRWEQIFKRYPVNVK--VLRPSPG-D-----YVKPGEVEE-

Target  VAKIKEDKSAIVYAPHVETSSGIILSEEYIKALSEAVHSVGGLLVIDC-IASGCVWLDMKELGID
```

Sequence Identity: 27.51

Build Model | Reset

```
Target  ------DIDPNGLLEYSVV-YTDRALNHMSKAFQEVMNDLLSNLKTVY---NAEAAVIIPGSGTY
3zrr.1.C MDKLLLHVGPTTIKEDVLVAGLENNVGFTSKEFVEALAYSLKGLRYVMGASKNYQPLIIPGGGTS

Target  GMEAVARQLTIDEDCLIIRNGWFSYRWTQILEKGKFAKSSTVLTAERTEDTEAPKPFAPVDIETA
3zrr.1.C AMESVTSLLKPNDKILVVSNGVFGDRWEQIFKRYPVNVK--VLRPSPG-D-----YVKPGEVEE-

Target  VAKIKEDKSAIVYAPHVETSSGIILSEEYIKALSEAVHSVGGLLVIDC-IASGCVWLDMKELGID
```

Sequence Identity: 27.51

Build Model | Reset

```
Target  ------DIDPNGLLEYSVV-YTDRALNHMSKAFQEVMNDLLSNLKTVY---NAEAAVIIPGSGTY
3zrr.1.A MDKLLLHVGPTTIKEDVLVAGLENNVGFTSKEFVEALAYSLKGLRYVMGASKNYQPLIIPGGGTS

Target  GMEAVARQLTIDEDCLIIRNGWFSYRWTQILEKGKFAKSSTVLTAERTEDTEAPKPFAPVDIETA
3zrr.1.A AMESVTSLLKPNDKILVVSNGVFGDRWEQIFKRYPVNVK--VLRPSPG-D-----YVKPGEVEE-

Target  VAKIKEDKSAIVYAPHVETSSGIILSEEYIKALSEAVHSVGGLLVIDC-IASGCVWLDMKELGID
```

FATCAT comparison of structures original and model

(Structure pairs with P-value < 0.05 are significantly similar. For explanation see help)

These two structures are significantly similar with P-value of 0.00e+00 (raw FATCAT score is 654.27)
They have 335 equivalent positions with an RMSD of 2.75Å without twists.

Detailed results:

- FATCAT alignment file
- Graph of FATCAT chaining result (postscript version)
- Superimposed structures (a pdb file with structure original and modified structure model stored as chains A and B)
- Transformation matrices for alignment blocks
- Differential Distance Matrix Decomposition
- Get the 'complete' structure of model superimposed onto original; or the 'complete' structure of original superimposed onto model (help)
- Interactive viewer (structures, alignment, contact map)

The results are stored for one month(s)

lab14_protein3.pdb

Model Results

Order by: GMQE

Model 03

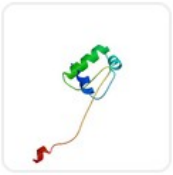
Structure Assessment

Oligo-State	Ligands	GMQE	QMEANDisCo Global
Monomer	None	0.18	0.42 ± 0.11

QMEANDisCo Local | QMEAN Z-Scores

Template	Seq Identity	Coverage	Description
4fe4.2.A	5.71%		Xylose operon regulatory protein Crystal structure of apo E. coli XylR

Model-Template Alignment



Model 02

Structure Assessment

Oligo-State	Ligands	GMQE	QMEANDisCo Global
Monomer	None	0.21	0.55 ± 0.11

QMEANDisCo Local | QMEAN Z-Scores

Template	Seq Identity	Coverage	Description
6w2s.1.b	12.16%		Eukaryotic translation initiation factor 3 subunit E Structure of the Cricket Paralysis Virus 5-UTR IRES (CrPV 5-UTR-IRES) bound to the small ribosomal subunit in the open state (Class 1)

Model-Template Alignment

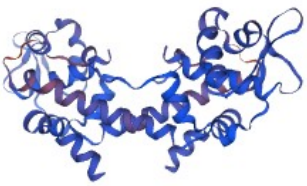
Model 01

Structure Assessment

Oligo-State	Ligands	GMQE	QMEANDisCo Global
Homo-dimer (matching prediction)	None	0.93	0.86 ± 0.05

QMEANDisCo Local | QMEAN Z-Scores

Template	Seq Identity	Coverage	Description
3k69.1.A	98.65%		Putative transcription regulator CRYSTAL STRUCTURE OF A PUTATIVE TRANSCRIPTIONAL REGULATOR (LP_0360) FROM



Cartoon

Descriptions | Graphic Summary | Alignments | Taxonomy

Sequences producing significant alignments

Download | New Select columns | Show 500

3 sequences selected | GenPept | Graphics | Distance tree of results | Multiple alignment | New MSA Viewer

Sequences with E-value BETTER than threshold

select all 3 sequences selected — **PSI-BLAST iteration 1**

	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession	Select for PSI blast	Used to build PSSM	New adde
☑	CRYSTAL STRUCTURE OF A PUTATIVE TR…	Lactipla…	287	287	99%	5e-101	94.12%	162	3K69_A	☑		
☑	Crystal structure of a putative DNA binding pro…	Bacillus …	44.3	44.3	89%	7e-06	28.57%	145	1XD7_A	☑		
☑	X-ray crystal structure of BC1842 protein from …	Bacillus …	42.7	42.7	85%	3e-05	28.91%	149	1YLF_A	☑		

Run PSI-BLAST Iteration 2 with max number of sequences 500 **Run**

Results for job clustalo-I20220202-021129-0020-88826466-p1m

Alignments | Result Summary | Phylogenetic Tree | Results Viewers | Submission Details

Download Alignment File | Show Colors

```
CLUSTAL O(1.2.4) multiple sequence alignment


original        ---MKLDFSVAVHSILYLDAHRDSKVASRELAQSLHLNPVMIRNILSVLHKHGYLTGTVG      57
template        MSLINSRLAVAIHILSL--ISMDEKTSSEIIADSVNTNPVVVRRMISLLKKADILTSRAG      58
                   ::  ::**:* :       *.*.:*. :*:*:: ***::*.::*:*:* . **. .*


original        KNGGYQLDLALADMNLGDLYDLTIPPTISYARFITGPSKQSPIAANISETLTDLFTVADR      117
template        VPGAS-LKKDPADISLLEVYRAVQKQEEL-FAVHENPNPKCPVGKKIQNALDETFESVQR      116
                  *.  *.   **:.* ::*  .         .  .*. :.*:. :*.::* : *  .:*


original        QYRAYYHQFTMADLQADLNHHGTFLQHEQDS   148
template        AMENELASKSLKDVMNHLFEGGSHHHHHH--   145
                  .    . :: *:  .* . *:. :*.:
```

SWISS-MODEL | Modelling | Repository | Tools | Documentation | Log in | Create Account

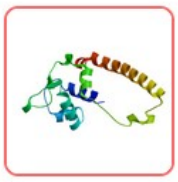
All Projects

Template Alignment: 1xd7.1 Created: today at 03:12

Summary | Templates 1 | Models 1 | Project Data

Model Results

Order by: GMQE



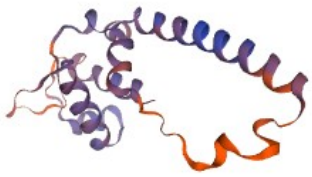
Oligo-State	Ligands	GMQE	QMEANDisCo Global
Monomer (requested by user)	None	0.57	0.65 ± 0.07

QMEANDisCo Local | QMEAN Z-Scores

Template	Seq Identity	Coverage	Description
1xd7.1.B	24.24%		ywnA

Model-Template Alignment

Model 01 | Structure Assessment



Cartoon

FATCAT comparison of structures original and model

(Structure pairs with P-value < 0.05 are significantly similar. For explanation see help)

These two structures are significantly similar with P-value of 1.22e-10 (raw FATCAT score is 260.91)
They have 128 equivalent positions with an RMSD of 3.04Å without twists.

Detailed results:

- FATCAT alignment file
- Graph of FATCAT chaining result (postscript version)
- Superimposed structures (a pdb file with structure original and modified structure model stored as chains A and B)
- Transformation matrices for alignment blocks
- Differential Distance Matrix Decomposition
- Get the 'complete' structure of model superimposed onto original; or the 'complete' structure of original superimposed onto model (help)
- Interactive viewer (structures, alignment, contact map)

The results are stored for one month(s)