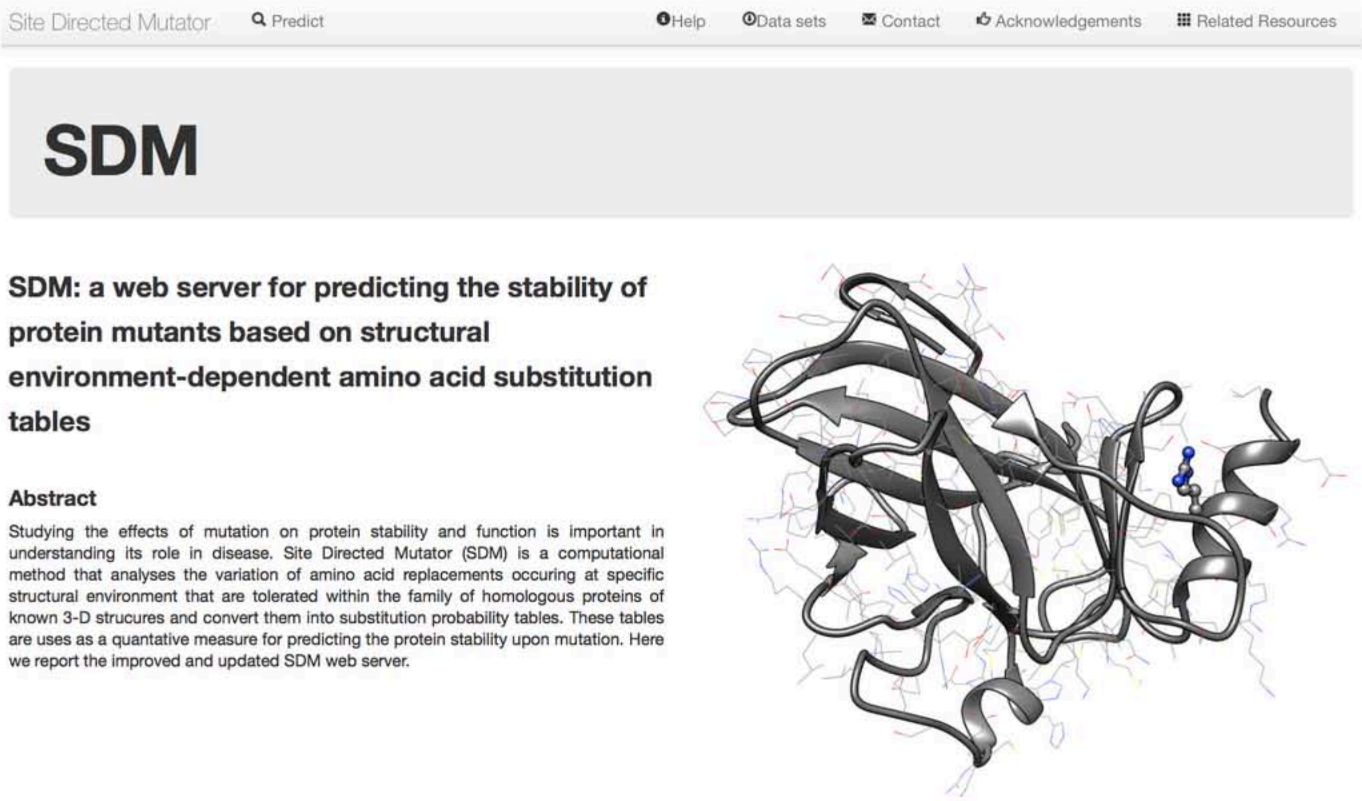
# Help - How to use SDM

## Main page



# SDM

**SDM: a web server for predicting the stability of protein mutants based on structural environment-dependent amino acid substitution tables**

**Abstract**

Studying the effects of mutation on protein stability and function is important in understanding its role in disease. Site Directed Mutator (SDM) is a computational method that analyses the variation of amino acid replacements occuring at specific structural environment that are tolerated within the family of homologous proteins of known 3-D strucures and convert them into substitution probability tables. These tables are uses as a quantative measure for predicting the protein stability upon mutation. Here we report the improved and updated SDM web server.

## About SDM

SDM is a computational method to predict the change in protein stability upon the introduction of a single mutation. It is a knowledge-based approach that uses conformationally constrained environment-dependent amino acid substitution tables to predict the change the protein stability between wildtype and mutant protein.

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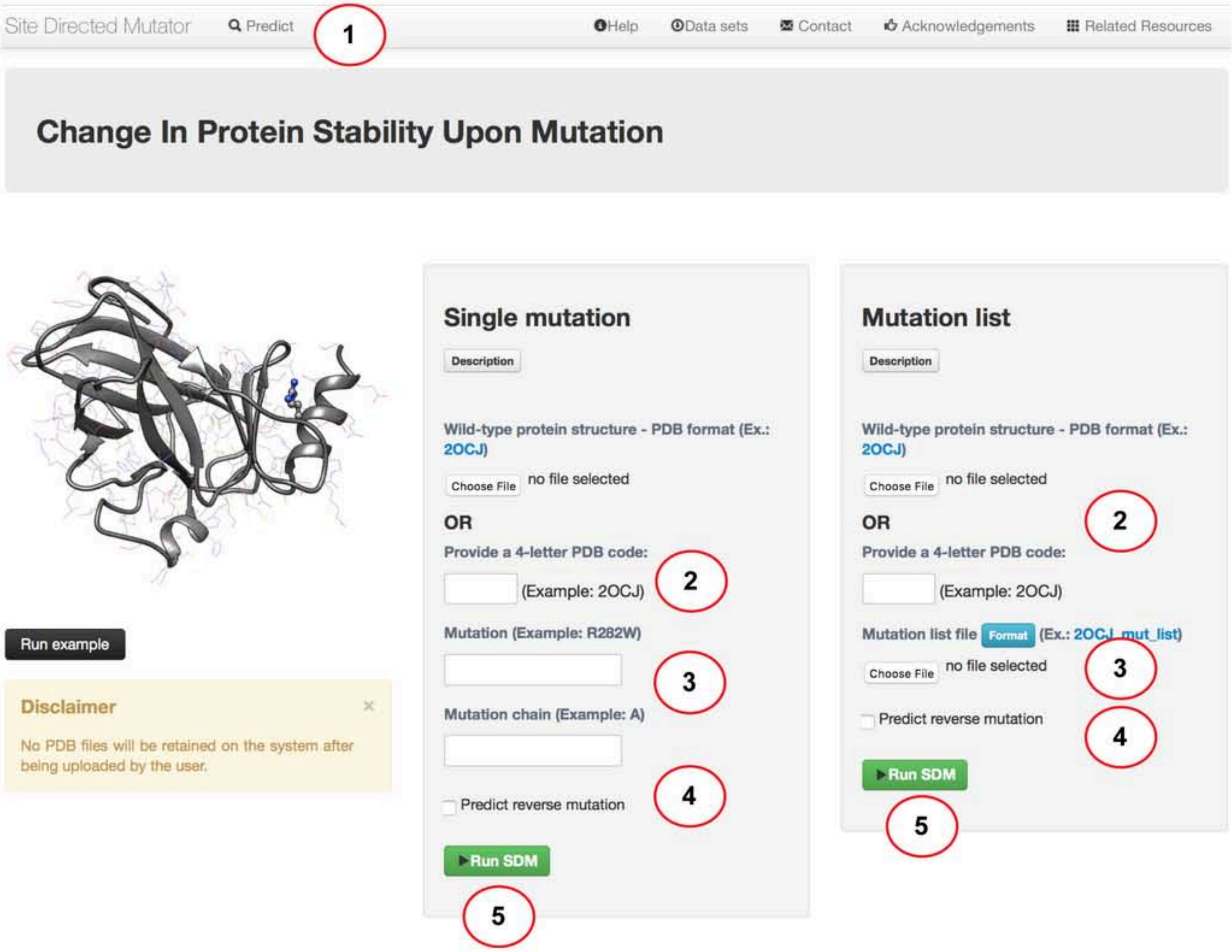
## Submission page



Site Directed Mutator   Predict   Help   Data sets   Contact   Acknowledgements   Related Resources

Change In Protein Stability Upon Mutation

Run example

**Disclaimer**

No PDB files will be retained on the system after being uploaded by the user.

**Single mutation**

Description

Wild-type protein structure - PDB format (Ex.: 2OCJ)

Choose File no file selected

OR

Provide a 4-letter PDB code:

(Example: 2OCJ)

Mutation (Example: R282W)

Mutation chain (Example: A)

☐ Predict reverse mutation

Run SDM

**Mutation list**

Description

Wild-type protein structure - PDB format (Ex.: 2OCJ)

Choose File no file selected

OR

Provide a 4-letter PDB code:

(Example: 2OCJ)

Mutation list file Format (Ex.: 2OCJ_mut_list)

Choose File no file selected

☐ Predict reverse mutation

Run SDM

## How to run a prediction

To run a prediction:

**(1)** Click on "Predict" to open the submission page.

**(2)** Provide the structure of the wild-type protein, which must comply with the PDB format.

**(3)** A **single mutation** or a **file** with a list of mutations to be analysed should be provided. For single mutation mode, a mutation code consists of *wild-type* code, residue *position* and *mutant* code (using the one letter amino acid code as shown in example). Similar format is used to list mutations in a file (An an example mutant list file could be downloaded by clicking the like "2OCJ_mut_list". A maximumm of 20 mutations are allowed in the mutant list file. Residue position must be consistent with the PDB file. The *chain ID* must also be provided for both single muation and mutation list option.

**(4)** Check this option to predict reverse mutation.

**(5)** You are then ready to submit your query for analysis.

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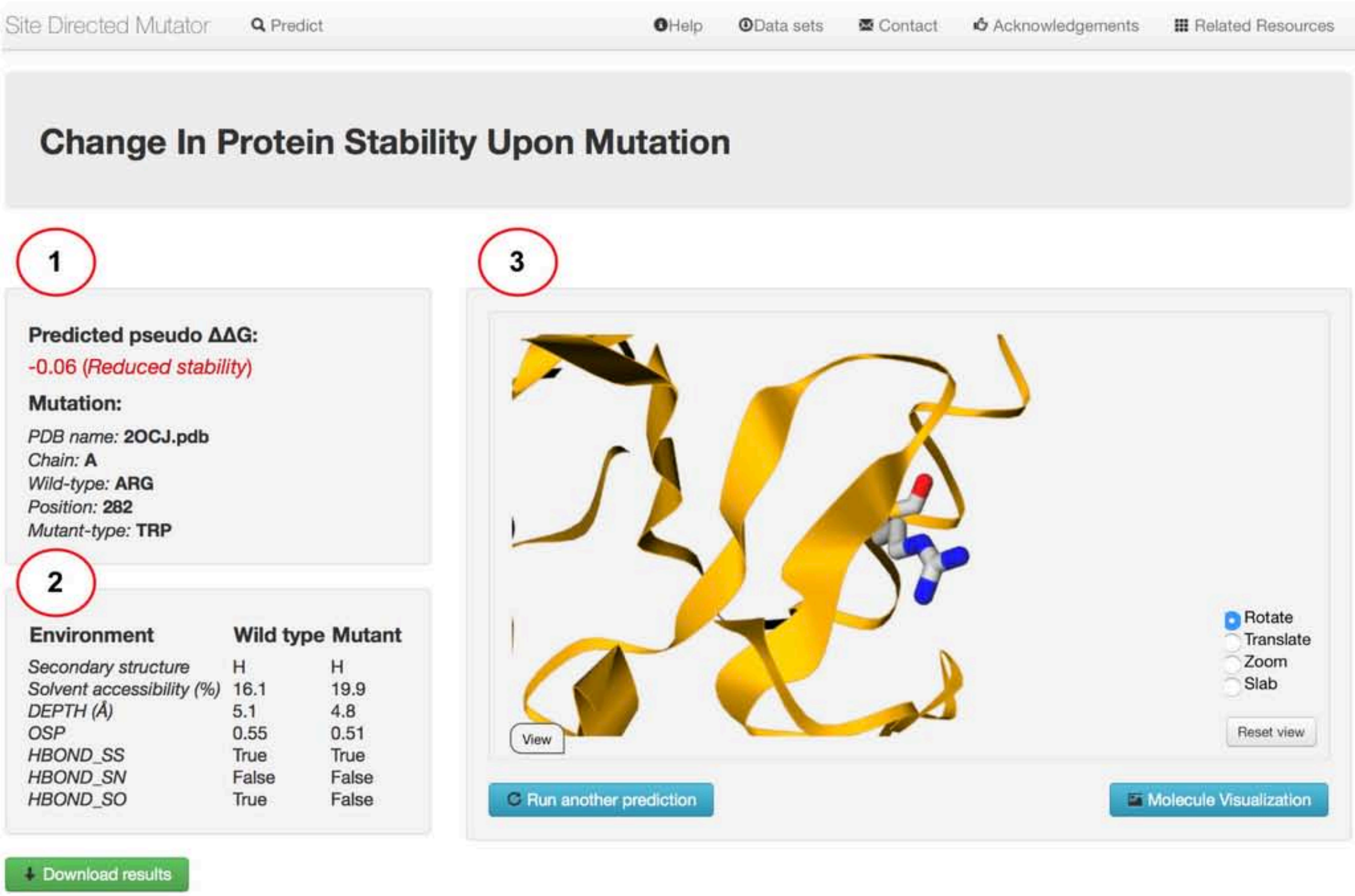
## Results page



### Change In Protein Stability Upon Mutation

**Predicted pseudo ΔΔG:**
-0.06 *(Reduced stability)*

**Mutation:**
*PDB name:* **2OCJ.pdb**
*Chain:* **A**
*Wild-type:* **ARG**
*Position:* **282**
*Mutant-type:* **TRP**

| **Environment** | **Wild type** | **Mutant** |
|---|---|---|
| *Secondary structure* | H | H |
| *Solvent accessibility (%)* | 16.1 | 19.9 |
| *DEPTH (Å)* | 5.1 | 4.8 |
| *OSP* | 0.55 | 0.51 |
| *HBOND_SS* | True | True |
| *HBOND_SN* | False | False |
| *HBOND_SO* | True | False |

## Results - Single mutation

**(1)** Your results for a single mutation will be displayed once calculations are completed. The results will display the predicted change in protein stability upon mutation (pseudo ΔΔG). A negative (in red) and positive (in blue) value corresponds to mutation predicted to be destabilising and stabilising respectively. Complementary information displayed include:

**(2)** A summary of the mutation is presented highlighting the wild-type residue, position number, chain and the mutant residue. A separate panel list the structural features including the main chain conformation class of the secondary structure, solvent accessibility, residue depth, residue occuluded surface packing (OSP), sidechain-sidechain hydrogen bond (HBOND_SS), sidechain-main chain amide hydrogen bond (HBOND_SN), sidechain-main chain carbonyl hydrogen bond (HBOND_SO) for the wildtype and mutant residue.

**(3)** The protein structure with its wildtype residue environment can be visualised directly from the server.

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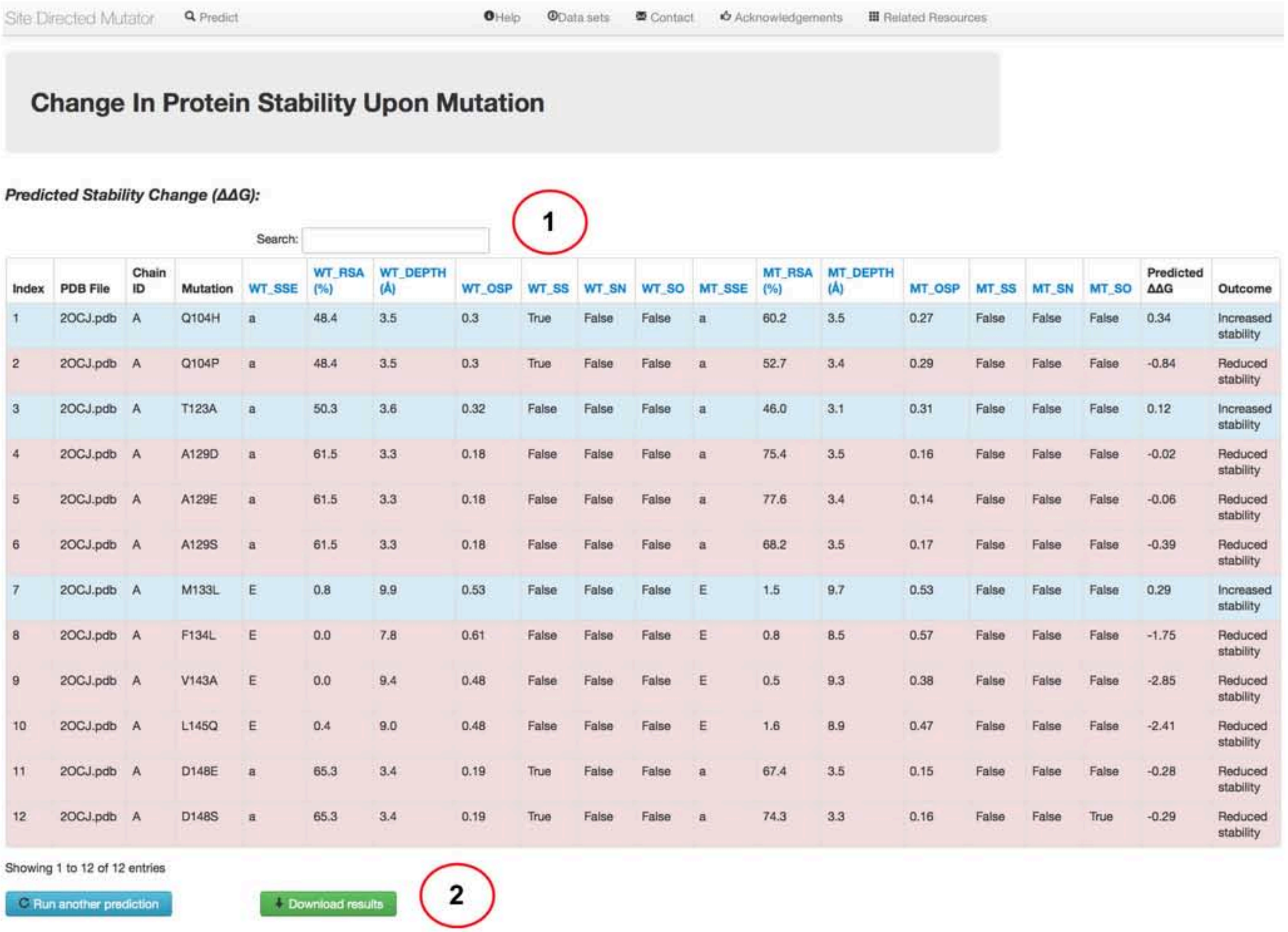
## Results page



### Change In Protein Stability Upon Mutation

***Predicted Stability Change (ΔΔG):***

| Index | PDB File | Chain ID | Mutation | WT_SSE | WT_RSA (%) | WT_DEPTH (Å) | WT_OSP | WT_SS | WT_SN | WT_SO | MT_SSE | MT_RSA (%) | MT_DEPTH (Å) | MT_OSP | MT_SS | MT_SN | MT_SO | Predicted ΔΔG | Outcome |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2OCJ.pdb | A | Q104H | a | 48.4 | 3.5 | 0.3 | True | False | False | a | 60.2 | 3.5 | 0.27 | False | False | False | 0.34 | Increased stability |
| 2 | 2OCJ.pdb | A | Q104P | a | 48.4 | 3.5 | 0.3 | True | False | False | a | 52.7 | 3.4 | 0.29 | False | False | False | -0.84 | Reduced stability |
| 3 | 2OCJ.pdb | A | T123A | a | 50.3 | 3.6 | 0.32 | False | False | False | a | 46.0 | 3.1 | 0.31 | False | False | False | 0.12 | Increased stability |
| 4 | 2OCJ.pdb | A | A129D | a | 61.5 | 3.3 | 0.18 | False | False | False | a | 75.4 | 3.5 | 0.16 | False | False | False | -0.02 | Reduced stability |
| 5 | 2OCJ.pdb | A | A129E | a | 61.5 | 3.3 | 0.18 | False | False | False | a | 77.6 | 3.4 | 0.14 | False | False | False | -0.06 | Reduced stability |
| 6 | 2OCJ.pdb | A | A129S | a | 61.5 | 3.3 | 0.18 | False | False | False | a | 68.2 | 3.5 | 0.17 | False | False | False | -0.39 | Reduced stability |
| 7 | 2OCJ.pdb | A | M133L | E | 0.8 | 9.9 | 0.53 | False | False | False | E | 1.5 | 9.7 | 0.53 | False | False | False | 0.29 | Increased stability |
| 8 | 2OCJ.pdb | A | F134L | E | 0.0 | 7.8 | 0.61 | False | False | False | E | 0.8 | 8.5 | 0.57 | False | False | False | -1.75 | Reduced stability |
| 9 | 2OCJ.pdb | A | V143A | E | 0.0 | 9.4 | 0.48 | False | False | False | E | 0.5 | 9.3 | 0.38 | False | False | False | -2.85 | Reduced stability |
| 10 | 2OCJ.pdb | A | L145Q | E | 0.4 | 9.0 | 0.48 | False | False | False | E | 1.6 | 8.9 | 0.47 | False | False | False | -2.41 | Reduced stability |
| 11 | 2OCJ.pdb | A | D148E | a | 65.3 | 3.4 | 0.19 | True | False | False | a | 67.4 | 3.5 | 0.15 | False | False | False | -0.28 | Reduced stability |
| 12 | 2OCJ.pdb | A | D148S | a | 65.3 | 3.4 | 0.19 | True | False | False | a | 74.3 | 3.3 | 0.16 | False | False | True | -0.29 | Reduced stability |

Showing 1 to 12 of 12 entries

## Results - List of Mutations

**(1)** Your results for a list of mutations will be displayed in a table format with the following information:

Mutation field contain the information about the mutation including the wildtype single letter amino acid code followed by the mutation residue position and the mutant amino acid code.

The main chain conformation class of the secondary structure for the wildtype (WT_SSE) and mutant (MT_SSE) residue.
Residue percentage relative solvent side chain accessibility (RSA) for wildtype (WT_RSA %) and mutant (MT_RSA %).

Residue depth for wildtype (WT_DEPTH) and mutant (MT_DEPTH) in angstrom units.

Residue occluded surface packing for wildtype (WT_OSP) and mutant (MT_OSP).

Sidechain-sidechain hydrogen bond (HBOND_SS), sidechain-main chain amide hydrogen bond (HBOND_SN) and sidechain-main chain carbonyl hydrogen bond (HBOND_SO) for the wildtype and mutant residue.

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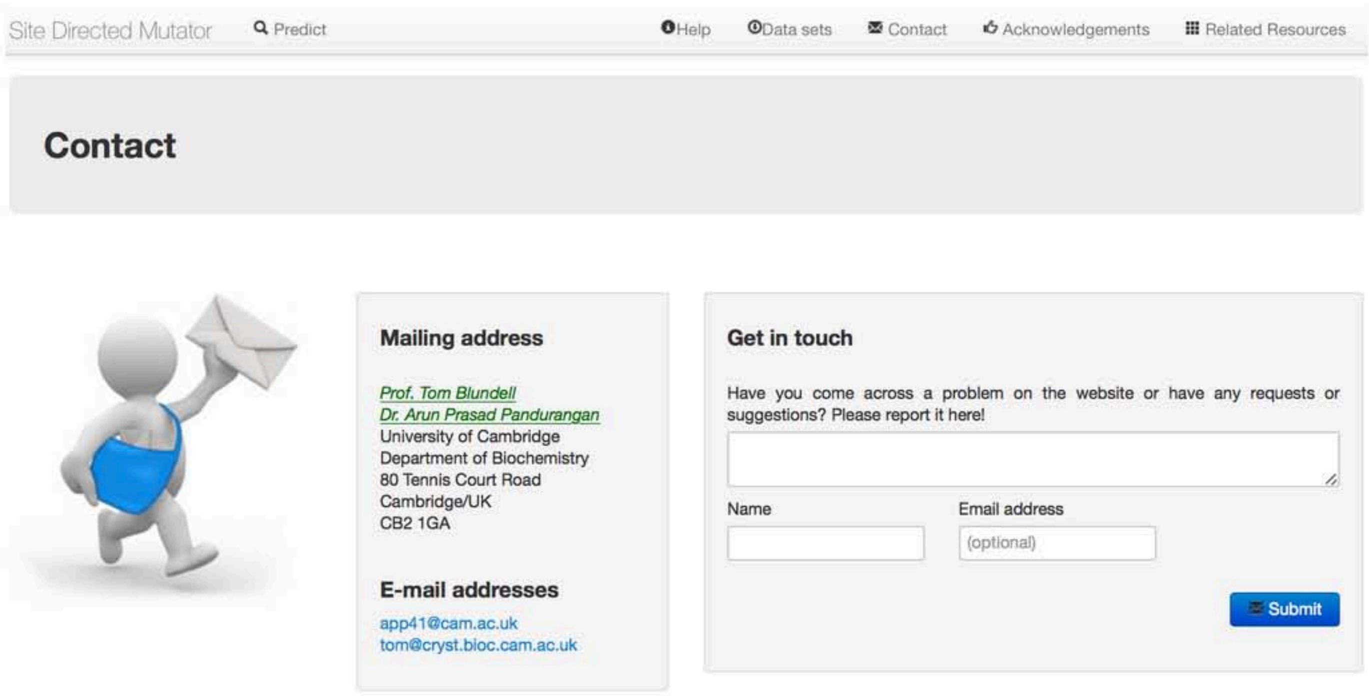

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**Get in touch**

Have you come across a problem on the website or have any requests or suggestions? Please report it here!

Name

Email address (optional)

## Getting in touch

In case you experience any trouble using SDM or have any suggestions or comments, please do not hesitate in contacting us either via e-mail or through the online form.

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