

Target Thresholds      >= 25      <= 20      <= 5      <= 8.5      Ignore      Ignore      >= 75

| Design                       | Stable-Stable | Unstable-Unstable | RLSASA_paratop | RLSASA_epitop | Unstable_With_Stal | Stablized_Percentage |       |
|------------------------------|---------------|-------------------|----------------|---------------|--------------------|----------------------|-------|
| insulin_epitope1_design440_0 | 20.83         | 33.33             | 11.6           | 2.79          | 8                  | 6                    | 75    |
| insulin_epitope1_design444_1 | 3.7           | 44.44             | 8.62           | 3.55          | 8                  | 8                    | 100   |
| insulin_epitope1_design490_1 | 18.75         | 25                | 11.51          | 4.8           | 5                  | 4                    | 80    |
| insulin_epitope1_design632_0 | 0             | 38.1              | 12.51          | 3.87          | 6                  | 5                    | 83.33 |
| insulin_epitope1_design642_0 | 3.33          | 50                | 13.17          | 2.64          | 6                  | 5                    | 83.33 |
| insulin_epitope1_design821_0 | 14.29         | 50                | 14.98          | 3.21          | 11                 | 10                   | 90.91 |
| insulin_epitope2_design12_0  | 29.41         | 41.18             | 3.77           | 2.14          | 2                  | 2                    | 100   |
| insulin_epitope2_design16_0  | 36.11         | 16.67             | 2.34           | 6.6           | 1                  | 1                    | 100   |
| insulin_epitope2_design16_1  | 21.62         | 18.92             | 4.15           | 4.85          | 9                  | 7                    | 77.78 |
| insulin_epitope2_design180_1 | 20.83         | 33.33             | 11.76          | 3.8           | 6                  | 4                    | 66.67 |
| insulin_epitope2_design207_0 | 20            | 35                | 3.45           | 2.93          | 5                  | 5                    | 100   |
| insulin_epitope2_design207_1 | 13.04         | 26.09             | 7.1            | 6.08          | 5                  | 5                    | 100   |
| insulin_epitope2_design223_0 | 18.52         | 37.04             | 6.92           | 4.96          | 5                  | 4                    | 80    |
| insulin_epitope2_design230_0 | 15.79         | 36.84             | 7.82           | 4.15          | 10                 | 9                    | 90    |
| insulin_epitope2_design230_1 | 20            | 23.33             | 8.06           | 7.23          | 8                  | 7                    | 87.5  |
| insulin_epitope2_design277_0 | 44.74         | 18.42             | 7.58           | 5.94          | 6                  | 6                    | 100   |
| insulin_epitope2_design289_0 | 31.03         | 20.69             | 7.21           | 1.87          | 4                  | 3                    | 75    |
| insulin_epitope2_design345_1 | 28            | 24                | 9.74           | 4.19          | 7                  | 6                    | 85.71 |
| insulin_epitope2_design350_1 | 25            | 25                | 11.1           | 4.54          | 8                  | 6                    | 75    |
| insulin_epitope2_design36_1  | 30            | 40                | 7.12           | 4.01          | 9                  | 7                    | 77.78 |
| insulin_epitope2_design376_0 | 28.12         | 28.12             | 5.61           | 6.34          | 8                  | 5                    | 62.5  |
| insulin_epitope2_design376_1 | 21.21         | 39.39             | 3.88           | 2.94          | 6                  | 6                    | 100   |
| insulin_epitope2_design422_0 | 29.03         | 29.03             | 5.22           | 3.82          | 4                  | 2                    | 50    |
| insulin_epitope2_design432_0 | 8.7           | 43.48             | 11.05          | 4.23          | 8                  | 6                    | 75    |
| insulin_epitope2_design480_0 | 25.64         | 28.21             | 5.61           | 6.5           | 7                  | 4                    | 57.14 |
| insulin_epitope2_design480_1 | 32.26         | 22.58             | 2.77           | 4.36          | 8                  | 7                    | 87.5  |
| insulin_epitope2_design481_0 | 20            | 20                | 4.33           | 5.96          | 9                  | 6                    | 66.67 |
| insulin_epitope2_design494_1 | 23.08         | 30.77             | 5.77           | 5.56          | 6                  | 3                    | 50    |
| insulin_epitope2_design49_1  | 18.52         | 29.63             | 7.13           | 6.59          | 8                  | 8                    | 100   |
| insulin_epitope2_design538_1 | 34.38         | 15.62             | 4.11           | 5.22          | 1                  | 0                    | 0     |

|                              |       |       |       |      |    |    |       |
|------------------------------|-------|-------|-------|------|----|----|-------|
| insulin_epitope2_design567_1 | 7.5   | 47.5  | 9.58  | 3.89 | 13 | 11 | 84.62 |
| insulin_epitope2_design56_1  | 21.88 | 34.38 | 10.31 | 4.83 | 9  | 7  | 77.78 |
| insulin_epitope2_design580_1 | 15.15 | 39.39 | 12.86 | 6    | 10 | 8  | 80    |
| insulin_epitope2_design586_0 | 42.86 | 14.29 | 12.38 | 3.3  | 3  | 3  | 100   |
| insulin_epitope2_design586_1 | 33.33 | 18.52 | 11.78 | 4.42 | 6  | 5  | 83.33 |
| insulin_epitope2_design590_1 | 20    | 32    | 2.49  | 2.98 | 6  | 6  | 100   |
| insulin_epitope2_design592_1 | 19.35 | 32.26 | 5.65  | 4.38 | 5  | 5  | 100   |
| insulin_epitope2_design642_1 | 29.63 | 14.81 | 9.65  | 3.3  | 7  | 7  | 100   |
| insulin_epitope2_design651_0 | 13.33 | 40    | 2.91  | 3.83 | 9  | 6  | 66.67 |
| insulin_epitope2_design661_0 | 26.09 | 17.39 | 3.75  | 2.89 | 3  | 3  | 100   |
| insulin_epitope2_design6_0   | 13.04 | 34.78 | 9.61  | 5.05 | 9  | 8  | 88.89 |
| insulin_epitope2_design700_1 | 12.12 | 30.3  | 5.97  | 6.98 | 11 | 9  | 81.82 |
| insulin_epitope2_design724_1 | 40.54 | 24.32 | 3.74  | 4.03 | 6  | 6  | 100   |
| insulin_epitope2_design727_1 | 31.25 | 28.12 | 9.58  | 6.54 | 7  | 5  | 71.43 |
| insulin_epitope2_design751_1 | 7.69  | 53.85 | 9.76  | 2.47 | 9  | 7  | 77.78 |
| insulin_epitope2_design766_0 | 8.82  | 44.12 | 5.35  | 7.46 | 10 | 9  | 90    |
| insulin_epitope2_design783_1 | 16.67 | 36.67 | 10.39 | 2.4  | 9  | 9  | 100   |
| insulin_epitope2_design790_1 | 37.5  | 29.17 | 3.06  | 2.79 | 4  | 2  | 50    |
| insulin_epitope2_design791_1 | 21.88 | 31.25 | 14.79 | 3.93 | 4  | 3  | 75    |
| insulin_epitope2_design819_0 | 35.48 | 16.13 | 7.17  | 3.29 | 5  | 5  | 100   |
| insulin_epitope2_design861_0 | 9.38  | 37.5  | 4.4   | 5.17 | 10 | 9  | 90    |
| insulin_epitope2_design861_1 | 15.62 | 31.25 | 5.14  | 5.47 | 7  | 6  | 85.71 |
| insulin_epitope2_design89_1  | 25.81 | 32.26 | 4.17  | 2.34 | 6  | 2  | 33.33 |
| insulin_epitope2_design952_0 | 26.67 | 30    | 5.63  | 2.1  | 7  | 5  | 71.43 |
| insulin_epitope3_design229_0 | 3.45  | 51.72 | 10.66 | 4.46 | 7  | 6  | 85.71 |
| insulin_epitope3_design626_1 | 29.03 | 25.81 | 6.68  | 4.87 | 4  | 4  | 100   |
| insulin_epitope3_design805_1 | 0     | 29.17 | 12.2  | 5.34 | 4  | 2  | 50    |
| insulin_epitope3_design843_0 | 7.69  | 42.31 | 9.66  | 5.68 | 5  | 4  | 80    |

<= 10 <= -2.5 >= 0.65

Primary Reason

PAE dG/BSA SC

8 -3.323 0.744

Need an epitope 1 design and these two appear equivalent so I've listed both

7 -3.665 0.727

8 -3.271 0.748

Need an epitope 1 design and these two appear equivalent so I've listed both

5 -3.265 0.736

8 -3.658 0.72

5 -3.718 0.708

6 -3.368 0.717

5 -3.592 0.719

Meets all stability criteria

5 -3.576 0.71

Good SC and generally good stability criteria

5 -3.347 0.738

7 -3.409 0.738

8 -3.272 0.735

6 -3.487 0.734

6 -3.367 0.707

7 -3.388 0.715

8 -3.596 0.751

Generally strong stability criteria

8 -3.635 0.726

Generally strong stability criteria

6 -3.643 0.761

7 -3.639 0.763

6 -3.682 0.728

5 -3.722 0.717

6 -3.852 0.735

7 -3.225 0.712

5 -3.369 0.702

7 -3.34 0.702

8 -3.895 0.774

Meets almost all criteria

4 -3.34 0.704

8 -3.488 0.743

6 -3.14 0.804

6 -3.572 0.709

Good stability criteria - the 0% is unimportant because it was 0 / 1

|   |        |       |   |
|---|--------|-------|---|
| 6 | -3.367 | 0.727 |   |
| 8 | -3.55  | 0.732 |   |
| 6 | -3.542 | 0.748 |   |
| 5 | -3.83  | 0.782 | Very good at everything but paratope RLSASA             |
| 5 | -3.27  | 0.735 | Very good at everything but paratope RLSASA             |
| 8 | -3.647 | 0.722 |   |
| 7 | -3.658 | 0.722 |   |
| 6 | -3.301 | 0.707 | Very good at everything but paratope RLSASA             |
| 6 | -3.641 | 0.721 |   |
| 5 | -3.414 | 0.713 | Meets every stability criteria                          |
| 6 | -3.381 | 0.741 |   |
| 6 | -3.62  | 0.731 |   |
| 6 | -3.772 | 0.74  | Meets almost all criteria                               |
| 5 | -3.597 | 0.727 |   |
| 7 | -3.304 | 0.74  |   |
| 6 | -3.293 | 0.728 |   |
| 5 | -3.474 | 0.725 |   |
| 6 | -3.587 | 0.732 |   |
| 6 | -3.777 | 0.759 |   |
| 7 | -3.491 | 0.718 | Very good at everything but paratope RLSASA             |
| 6 | -3.061 | 0.732 |   |
| 7 | -3.349 | 0.727 |   |
| 6 | -3.859 | 0.732 |   |
| 5 | -3.145 | 0.715 |   |
| 7 | -3.19  | 0.718 |   |
| 7 | -4.022 | 0.776 | Clearly the best epitope 3 design by stability criteria |
| 7 | -3.913 | 0.764 |   |
| 8 | -3.375 | 0.7   |   |