Predicted versus actual oxygen for datapoint 717

2	2
2 0 -0	0
2 - 0	2 0
	$\begin{bmatrix} 1 & -2 & 1 \\ -2 & 1 & 1 \end{bmatrix}$
	2
-2 2	$\begin{bmatrix} 0 \\ -2 \end{bmatrix}$
- 0 2 -2	- 0 -2
- 0 -2 -2	- 0 -2
0 -2	0 _2
2 0 -0	0
- 0	- 0
	2 - 0
2 - 0	$\begin{bmatrix} -2 \\ 0 \end{bmatrix}$
	2 0
	$\begin{bmatrix} & & & \\ & -2 & & \\ & 2 & & \\ & 0 & & \end{bmatrix}$
	2
-2 2	0 _2
- 0 2 -2	0 -2
- 0 2 -2	- 0 -2
- 0 2 -2	- 0 -2 -2
- 0 -2 -2	0 -2
- 0 2	0 _2
2 - 0 -2	0
- 0	- 0
2 - 0	2 - 0
	2 2 0
	2 2 0
2	2
-0	-2