Summary - Int 6, Group A, 𝚫𝚫G Version

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# *Intermediate 6*

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_34 + dip\_x\_1 + L\_3\_9 | 0.644 | 0.488 | 0.590 |
| ddg ~ diff\_NBO\_31\_32 + Aniso.Polar + loc.B5\_9\_3 | 0.600 | 0.432 | 0.691 |

***3-Fold cross-validation***

| Q2 | MAE |
| --- | --- |
| 0.324 | 0.767 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_34 | 7.488 |
| dip\_x\_1 | 3.403 |
| L\_3\_9 | 5.216 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.122 | 0.162 | 6.912 | 0.0000072 |
| NPA\_34 | 2.237 | 0.457 | 4.893 | 0.0002373 |
| dip\_x\_1 | 1.073 | 0.308 | 3.483 | 0.0036534 |
| L\_3\_9 | 1.632 | 0.381 | 4.278 | 0.0007657 |