

**Table 8. Hologram (HQSAR) output for UPPS**

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Hologram lengths	97, 151, 199, 257, 307, 353
Minimum atoms in fragment	4
Maximum atoms in fragment	5
Include bond information	1
Include connection information	1
Include hydrogens	1
Use chiral fragments	0
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<b>Cross-validated model</b>	
$R^2$	0.737
StdErr	0.472
<b>Full model</b>	
$R^2$	0.859
StdErr	0.346
<b>Ensemble model</b>	
$R^2$	0.707
StdErr	0.499
Best length	97
Components	3

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Sybyl 7.3 HQSAR module (Tripos Inc., St. Louis, MO)