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Table 1. Refinement statistics for **1c**-NADPH-hDHFR complex

Lattice constants, Å	86.259,77.637	
Space group	R3	
Resolution range	8.0-2.1 Å	
Reflections collected	9706	
Reflections used (8-2.1 Å ; 2 σ)	8970	
R factor, %	15.9	
Protein atoms	1568	
Water molecules	72	
B factor (protein average) Å ²	19.34	
	Target σ	Root mean square σ
Distances, Å		
Bonds	0.020	0.018
Angles	0.040	0.050
Planar 1-4	0.050	0.051
Planar groups	0.020	0.014
Chiral volume	0.150	0.191
Non-bonded distances		
Single torsion	0.500	0.197
Multiple torsion	0.500	0.262
Possible hydrogen bonds	0.500	0.259
Torsion angles, degrees		
Planar	3.0	2.4
Staggered	15.0	19.4
Orthonormal	15.0	22.5