

Variable	Value	
Resolution limits	0.000	3.200
Number of used reflections	8466	
Percentage observed	100.0000	
Percentage of free reflections	0.0000	
Overall R factor	0.3441	
Average Fourier shell correlation	0.8318	
Overall weighted R factor	0.3441	
Overall weighted R2 factor	0.3658	
Average correlation coefficient	0.6964	
Overall correlation coefficient	0.7825	
Cruickshanks DPI for coordinate error	0.5793	
Overall figure of merit	0.9890	
ML based su of positional parameters	0.3171	
ML based su of thermal parameters	18.8472	