

Data Collection

Overall

Outer Shell

Low resolution limit	none	2.74
High resolution limit	2.60	2.60
R_{merge}	0.044	0.467
R_{meas} (all I+ & I-)	0.056	0.615
Total number of observations (all I+ & I-)	77375	11410
Total number unique (all I+ & I-)	19071	2767
$\langle I / \sigma(I) \rangle$	20.2	2.5
Completeness	99.5	99.9
Multiplicity	4.1	4.1

Refinement

Total Number of Bins Used	20	1
Resolution Range High	2.6 Å	2.6 Å
Resolution Range Low	31.34 Å	2.667 Å
Data Cutoff (Fs)	0	0
Completeness for Range	99.42 %	99.86 %
Number of Reflections	17100	1261

Goodness of Fit of Model to Data

Cross-Validation Method	Throughout	Throughout
Free R Value (Test Set Selection)	Random	Random
R Value (Working Set)	0.20222	0.412
Free R Value	0.23876	0.42
Free R Value Test Set Size	10.2 %	12.9 %
Free R Value Test Set Count	1949	163
Number of Non-Hydrogen Atoms	3089	
Mean B Value	78.591 Å ²	

Estimated Overall Coordinate Error

ESU Based on R Value	0.441 Å
ESU Based on Free R Value	0.274 Å
ESU Based on (max. likelihood)	0.252 Å
ESU for b Values (max. likelihood)	26.738 Å ²

RMS Deviations from Ideal Values

Bond Lengths Refined Atoms	0.01 Å
Bond Angles Refined Atoms	1.955°
General Planes Refined Atoms	0.006 Å
Non-Bonded Contacts Refined Atoms	0.204 Å
Non-Bonded Torsion Refined Atoms	0.284 Å

Isotropic Thermal Factor Restraints

Side-Chain Bond Refined Atoms	1.101 Å ²
Side-Chain Angle Refined Atoms	1.857 Å ²