

T417/1A418,419 KIT D4D5

X-ray source	NSLS X25
Number of crystals	1
Wavelength (Å)	1.1000
Unit Cell dimensions	C2
a (Å)	163.6
b (Å)	63.5
c (Å)	81.5
	$\beta=117.4$
Resolution (Å) ^a	50-2.4 (2.49-2.40)
No. of total reflections	178278
No. of unique reflections	29387
Completeness (%) ^a	99.9 (98.7)
Number of degrees collected (°)	330
Redundancy ^a	6.1 (5.3)
$I/\sigma I$ ^a	15.5 (2)
R_{sym} (%) ^a	10.8 (82.4)
Wilson B	56.8
Refinement	
Resolution (Å) ^a	42.4 – 2.4 (2.49 – 2.4)
R_{work} (%) ^a	23.2 (31.8)
R_{free} (%) ^a	26.2 (37.6)
No. of atoms	
Protein	4402
N-acetylglucosamine	42
Water	82
Cobalt	5
Residue range built	
Chain A	308-506
Chain B	309-423/426-505
Chain C	308-420/425-443/459-478/491-506
Model quality	
Rmsd bond length (Å)	0.0024
Rmsd bond angles (°)	0.71
B-factor (Å²)	
Average overall	79.6
Chain A	73.5
D4	66.2

D5	80.8
Chain B	88.5
D4	83.5
D5	93.8
Chain C	77.6
D4	63.9
D5	99.6
Water	60.1
Cobalt	92.6
NAG	126.6

MolProbity

Ramachandran plot (%) favored/outliers

96/0

MolProbity score

1.5 (99th percentile)

PDB Accession Code

4PGZ