Structural Parameters Analyzed by SAnDReS

Structural Parameter	Unit
Crystallographic high-resolution limit	Å
Crystallographic low-resolution limit	Å
Crystallographic R-factor[1]	Unitless
Crystallographic R-free[2]	Unitless
Error for crystallographic R-free	Å
Minimum fobs/sigma	Unitless
Number of reflections	Unitless
Completeness	Unitless
B-value from Wilson plot	$Å^2$
ESD[3] from Luzzati plot	Å
ESD from sigmaa plot	Å
Cross-validated ESD from Luzzati plot	Å
Cross-validated ESD from sigmaa plot	Å
ESU[4] based on R-value	Å
ESU based on R-free	Å
ESU based on maximum likelihood	Å
ESU for B-values based on maximum likelihood	$Å^2$
Correlation coefficient for Fo-Fc	Unitless
Correlation coefficient for Fo-Fc free	Unitless
RMSD[5] from ideal values (bond length)	Å
RMSD from ideal values (bond length others)	Å
RMSD from ideal values (bond angle)	Degree
RMSD from ideal values (bond angle others)	Degree
Angle distances (SHELXL[6])	Å
Distances from restraint planes (SHELXL)	Å
Zero chiral volumes (SHELXL)	$Å^3$

Non-zero chiral volumes (SHELXL)	$Å^3$
Anti-bumping distance restraints (SHELXL)	Å
RMSD from ideal (torsion angle period 1)	Degree
RMSD from ideal (torsion angle period 2)	Degree
RMSD from ideal (torsion angle period 3)	Degree
RMSD from ideal (torsion angle period 4)	Degree
Torsion angles from Buster-TNT[7] program	Degree
Trigonal carbon planes (Buster-TNT)	Å
General planes (Buster-TNT)	Å
Isotropic thermal factors (Buster-TNT)	$Å^2$
Non-bonded contacts (Buster-TNT)	Å
RMSD for omega pep. torsion angle (Buster-TNT)	Degree
Coordinate error (max-like. method) (PHENIX[8])	Å
Phase error (max-like. method) (PHENIX)	Degree
RMSD for chirality (PHENIX)	$Å^3$
RMSD for planarity (PHENIX)	Å
RMSD for dihedral (PHENIX)	Degree
RMSD for chiral center restraints	$Å^3$
RMSD for general planes refined atoms	Å
RMSD for general planes other atoms	Å
RMSD for non-bonded contacts refined atoms	Å
RMSD for non-bonded contacts other atoms	Å
RMSD for non-bonded torsions	Å
RMSD for non-bonded torsion others	Å
RMSD for H-bonds (X...Y) refined atoms	Å
RMSD for H-bonds (X...Y) refined other atoms	Å
RMSD for potential metal-ion refined atoms	Å
RMSD for symmetry VDW refined atoms	Å

RMSD for symmetry VDW refined other atoms	Å
RMSD for symmetry H-bond refined atoms	Å
RMSD for symmetry metal-ion refined atoms	Å
Crystal temperature	Kelvin
X-ray wavelength	Å
Number of unique reflections	Unitless
Resolution range low	Å
Completeness for range (data)	Unitless
I/sigma(I) for data set	Unitless
Highest resolution shell for data set	Å
Highest resolution shell low for data set	Å
Completeness for shell for data set	Unitless
I/sigma(I) for shell for data set	Unitless
Solvent content	Unitless
Matthews coefficient	$Å^3$/Da
Information about missing residues	Unitless
Number of rotatable bonds in the ligand	Unitless
Number of protein atoms	Unitless
Number of ligand atoms	Unitless
Number of solvent atoms	Unitless
Number of all atoms	Unitless
Number of active-ligand atoms	Unitless
Protein molecular weight	Da
Mean B-value (ligand and co-factors)	$Å^2$
Mean occupancy (ligand and co-factors)	Unitless
Mean B-value (water molecules)	$Å^2$
Mean occupancy (water molecules)	Unitless
Mean B-value (whole structure)	$Å^2$

Mean occupancy (whole structure)	Unitless
Mean B-value (main-chain protein atoms)	$Å^2$
Mean occupancy (main-chain protein atoms)	Unitless
Mean B-value (side-chain protein atoms)	$Å^2$
Mean occupancy (side-chain protein atoms)	Unitless
Mean B-value (active ligand)	$Å^2$
Mean occupancy (active ligand)	Unitless
Unit cell volume	$Å^3$
Reciprocal unit cell volume	$Å^{-3}$
Total number of possible reflections	Unitless
Radius of gyration for non-H atoms in protein	Å
Mean B-value (radius ≤ 15.0 Å)	$Å^2$
Mean occupancy (radius ≤ 15.0 Å)	Unitless
Mean B-value (radius ≤ 15.0 Å MC[9] atoms)	$Å^2$
Mean occupancy (radius ≤ 15.0 Å MC atoms)	Unitless
Mean B-value (radius ≤ 15.0 Å SC[10] atoms)	$Å^2$
Mean occupancy (radius ≤ 15.0 Å SC atom)	Unitless
Matthews coefficient (radius ≤ 15.0 Å)	$Å^3$/Da
Mean B-value (radius ≤ 20.0 Å)	$Å^2$
Mean occupancy (radius ≤ 20.0 Å)	Unitless
Mean B-value (radius ≤ 20.0 Å MC atoms)	$Å^2$
Mean occupancy (radius ≤ 20.0 Å MC atoms)	Unitless
Mean B-value (radius ≤ 20.0 Å SC atoms)	$Å^2$
Mean occupancy (radius≤ 20.0 Å SC atoms)	Unitless
Matthews coefficient (radius ≤ 20.0 Å)	$Å^3$/Da
Mean B-value (radius ≤ 25.0 Å)	$Å^2$
Mean occupancy (radius ≤ 25.0 Å)	Unitless
Mean B-value (radius ≤ 25.0 Å MC atoms)	$Å^2$

Mean occupancy (radius ≤ 25.0 Å MC atoms)	Unitless
Mean B-value (radius ≤ 25.0 Å SC atoms)	$Å^2$
Mean occupancy (radius ≤ 25.0 Å SC atom)	Unitless
Matthews coefficient (radius ≤ 25.0 Å)	$Å^3$/Da

[1] R-factor is given by the following equation: $R\text{-}\,factor = 100.\frac{\sum|F_{obs} - F_{calc}|}{\sum F_{obs}}$, where F_{obs} and F_{calc} are observed and calculated structure factors, respectively. The sums being taken over all reflections with $F/\sigma(F) > 2\sigma(F)$, σ is the standard deviation for F.

[2] R-free = R-factor for 10% of the data that were not included during crystallographic refinement.

[3] ESD: Estimated standard deviation

[4] ESU: Estimated overall coordinate error

[5] RMSD: Root-mean square deviation

[6] SHELXS: Program for crystallographic refinement (Sheldrick GM, Schneider TR. SHELXL: high-resolution refinement. Methods Enzymol. 1997; 277: 319-343)

[7] Buster-TNT: Program for crystallographic refinement (Blanc E, Roversi P, Vonrhein C, Flensburg C, Lea SM, Bricogne G. Refinement of severely incomplete structures with maximum likelihood in BUSTER-TNT. Acta Crystallogr D Biol Crystallogr. 2004; 60(Pt 12 Pt 1):2210-21.).

[8] PHENIX: Program for crystallographic refinement (Adams PD, Afonine PV, Bunkóczi G, Chen VB, Davis IW, Echols N, Headd JJ, Hung LW, Kapral GJ, Grosse-Kunstleve RW, McCoy AJ, Moriarty NW, Oeffner R, Read RJ, Richardson DC, Richardson JS, Terwilliger TC, Zwart PH. PHENIX: a comprehensive Python-based system for macromolecular structure solution. Acta Crystallogr D Biol Crystallogr. 2010; 66(Pt 2):213-21).

[9] MC: main-chain

[10] SC: Side-chain