

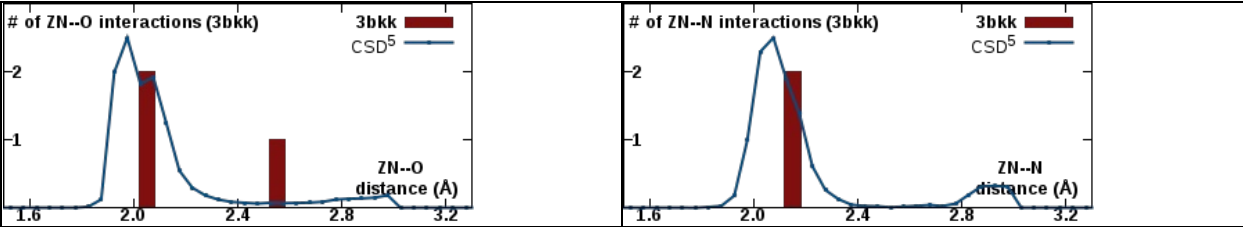
CheckMyMetal(CMM) report for PDB code: 3bkk

PDB title: Tesis ace co-crystal structure with ketone ace inhibitor kaf (2.2Å)

| Warning: Valence and nVECSUM parameters should be interpreted with great care due to potential cation-pi interactions observed around A:701 | | | | | | | | | | | | |
|---|------|-------|----------------|------------------------------|-------------------------------|----------------------|----------------------|-------------------------|-----------------------|----------------------|-----------|------------|
| ID | Res. | Metal | Occupancy | B factor (env.) ¹ | Ligands | Valence ² | nVECSUM ³ | Geometry ^{1,4} | gRMSD(°) ¹ | Vacancy ¹ | Bidentate | Alt. metal |
| A:701 | ZN | Zn | 1 | 15.8 (14.1) | O ₃ N ₂ | 1.5 | 0.084 | Trigonal Bipyramidal | 14.6° | 0 | 0 | Co |
| A:702 | CL | Cl | 1 | 12.2 (16.4) | | N/A | N/A | Free | N/A | N/A | N/A | |
| A:703 | CL | Cl | 1 | 14.5 (14.2) | | N/A | N/A | Free | N/A | N/A | N/A | |
| Legend: | | | Not applicable | Outlier | Borderline | Acceptable | | | | | | |

| Column | Description |
|------------------------------|---|
| Occupancy | Occupancy of ion under consideration |
| B factor (env.) ¹ | Metal ion B factor, with valence-weighted environmental average B factor in parenthesis |
| Ligands | Elemental composition of the coordination sphere |
| Valence ² | Summation of bond valence values for an ion binding site. Valence accounts for metal-ligand distances |
| nVECSUM ³ | Summation of ligand vectors, weighted by bond valence values and normalized by overall valence. Increase when the coordination sphere is not symmetrical due to incompleteness. |
| Geometry ^{1,4} | Arrangement of ligands around the ion, as defined by the NEIGHBORHOOD algorithm |
| gRMSD(°) ¹ | R.M.S. Deviation of observed geometry angles (L-M-L angles) compared to ideal geometry, in degrees |
| Vacancy ¹ | Percentage of unoccupied sites in the coordination sphere for the given geometry |
| Bidentate | Number of residues that form a bidentate interaction instead of being considered as multiple ligands |
| Alt. metal | A list of alternative metal(s) is proposed in descending order of confidency, assuming metal environment is accurately determined. This feature is still experimental. It requires user discrimination and cannot be blindly accepted |

Metal-ligand distance distributions for pdb3bkk.ent in comparison with CSD



(1) Zheng H, Chordia MD, Cooper DR, Chruszcz M, Müller P, Sheldrick GM, Minor W (2014) *Nature Protocols*, 9(1), 156-70.
(2) Brown ID (2009) *Chem. Rev.*, 109, 6858-6919.
(3) Müller P, Köpke S, Sheldrick GM (2003) *Acta Crystallogr. D Biol. Crystallogr.*, 59, 32-37.
(4) Kuppuraj G, Dudev M, Lim C (2009) *J. Phys. Chem. B*, 113, 2952-2960.
(5) CSD: Cambridge Structural Database
Maintained by: Heping Zheng <dust@iwonka.med.virginia.edu>

Citing CheckMyMetal (CMM):
Validation of metal-binding sites in macromolecular structures with the CheckMyMetal web server. Zheng,H., Chordia,M.D., Cooper,D.R., Chruszcz,M., Müller,P., Sheldrick,G.M., Minor,W. (2014) *Nature Protocols*, 9(1), 156-70.