[CheckMyMetal(CMM)](#) report for PDB code: 7a94

PDB title: [Sars-cov-2 spike glycoprotein with 1 ace2 bound](#) (3.9Å)

ID	Res.	Metal	Occupancy	B factor (env.)[1]	Ligands	Valence[2]	nVECSUM[3]	Geometry[1,4]	gRMSD(°)[1]	Vacancy[1]	Bidentate	Alt. metal
D:901	ZN	Zn	1	N/A	O_1N_2	**0.5**	**0.46**	Tetrahedral	_20.4°_	25%	0	
			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 pdb7a94.ent in comparison with CSD
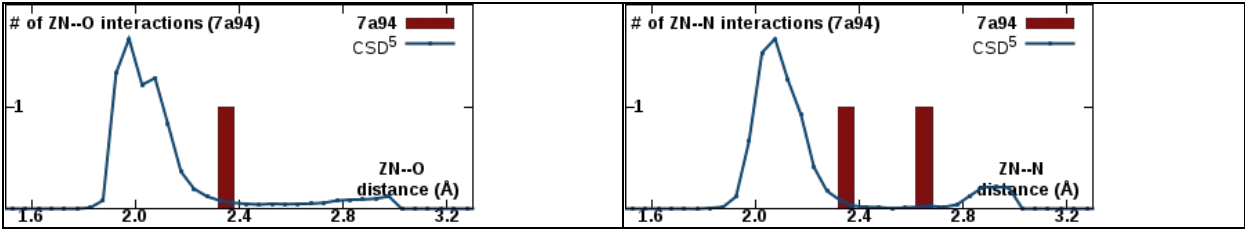
[(1) Zheng H, Chordia MD, Cooper DR, Chruszcz M, Müller P, Sheldrick GM, Minor W (2014) _Nature Protocols, 9(1),_ 156-70.](#)
[(2) Brown ID (2009) _Chem. Rev., 109,_ 6858-6919.](#)
[(3) Müller P, Köpke S, Sheldrick GM (2003) _Acta Crystallogr. D Biol. Crystallogr., 59,_ 32-37.](#)
[(4) Kuppuraj G, Dudev M, Lim C (2009) _J. Phys. Chem. B, 113,_ 2952-2960.](#)
[(5) _CSD: Cambridge Structural Database_](#)
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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.](#)