

CheckMyMetal(CMM) report for PDB code: 7kgo

PDB title: Crystal structure of hla-a\*0201in complex with sars-cov-2 n351-359 (2.1Å)

Warning: Due to a lack of high-resolution structural data the validity of Valence and nVECSUM parameters has not been established for rarely observed metals												
Warning: Coordinating ligands by symmetry operation are labeled with prefix 'sym-'												
ID	Res.	Metal	Occupancy	B factor (env.) <sup>1</sup>	Ligands	Valence <sup>2</sup>	nVECSUM <sup>3</sup>	Geometry <sup>1,4</sup>	gRMSD(°) <sup>1</sup>	Vacancy <sup>1</sup>	Bidentate	Alt. metal
A:301	3NI	Ni	1	55.4 (34.7)		N/A	N/A	Free	N/A	N/A	N/A	
A:302	3NI	Ni	1	70.1 (35.7)		N/A	N/A	Free	N/A	N/A	N/A	
A:303	CL	Cl	1	49.9 (43.5)		N/A	N/A	Free	N/A	N/A	N/A	
A:304	CL	Cl	1	66.7 (39.8)		N/A	N/A	Free	N/A	N/A	N/A	
A:305	CD	Cd	1	40.1 (46)	O <sub>2</sub> N <sub>2</sub>	0.9	0.23	Square Planar	16.8°	0	0	
B:101	3NI	Ni	1	49.3 (44.9)		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.) <sup>1</sup>	Metal ion B factor, with valence-weighted environmental average B factor in parenthesis
Ligands	Elemental composition of the coordination sphere
Valence <sup>2</sup>	Summation of bond valence values for an ion binding site. Valence accounts for metal-ligand distances
nVECSUM <sup>3</sup>	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 <sup>1,4</sup>	Arrangement of ligands around the ion, as defined by the NEIGHBORHOOD algorithm
gRMSD(°) <sup>1</sup>	R.M.S. Deviation of observed geometry angles (L-M-L angles) compared to ideal geometry, in degrees
Vacancy <sup>1</sup>	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

(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.