CheckMyMetal(CMM) report for PDB code: 7kgt

PDB title: Crystal structure of hla-a*0201 in complex with sars-cov-2 n226-234 (1.9Å)

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.)_[1]**	**_Ligands_**	**_Valence_[2]**	**_nVECSUM_[3]**	**_Geometry_[1,4]**	**_gRMSD(°)_[1]**	**_Vacancy_[1]**	**Bidentate**	**Alt. metal**
A:301	CD	Cd	1	18.5 (17.4)	O_4N_2	_1.6_	0.078	_Trigonal Bipyramidal_	5.4°	0	1	
A:302	CD	Cd	1	_55.2 (39.2)_	_N_2_	**0.4**	**0.71**	_Square Planar_	0.4°	**50%**	0	
A:303	NA	Na	1	_47.6 (32.8)_	**N_1**	**0.13**	**1**	**Poorly Coordinated**	N/A	N/A	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

(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.