CheckMyMetal(CMM) report for PDB code: 7kgq

PDB title: Crystal structure of hla-a*0201in complex with sars-cov-2 n222-230 (1.3Å)

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: *Valence* and *nVECSUM* parameters should be interpreted with great care due to the presence of multi-nuclear metal clusters around A:302

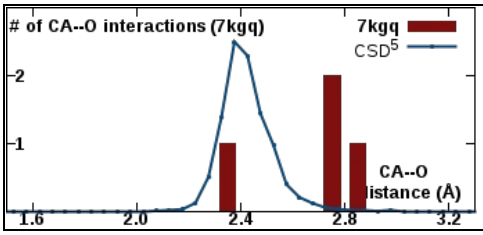
Warning: Coordinating ligands by symmetry operation are labeled with prefix 'sym-'

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	14.1 (14.6)	O_4N_2	2.1	0.022	*Trigonal Bipyramidal*	6.7°	0	1	
A:302	CD	Cd	1	*29.4 (24.3)*	O_2N_2	*1.4*	**0.39**	*Trigonal Bipyramidal*	10.6°	*20%*	0	
A:303	CA	Ca	1	**58.8 (26.7)**		N/A	N/A	**Free**	N/A	N/A	N/A	
B:101	CA	Ca	1	35.5 (32.7)	O_4	**0.6**	**0.58**	Octahedral	7.6°	**33%**	0	K

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 distribution for pdb7kgq.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.