CheckMyMetal(CMM) report for PDB code: 1zv8

PDB title: A structure-based mechanism of sars virus membrane fusion (1.9Å)

Warning: *Valence* and *nVECSUM* parameters should be interpreted with great care due to the presence of multi-nuclear metal clusters around G:201; and the presence of small molecules in the coordinate sphere of the metal ion G:201

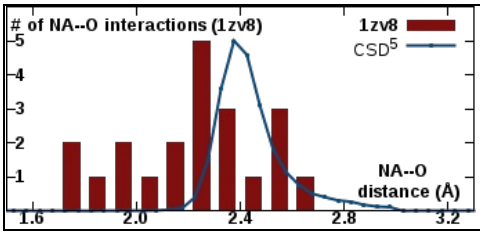
Warning: Coordinating ligands by symmetry operation are labeled with prefix 'sym-'

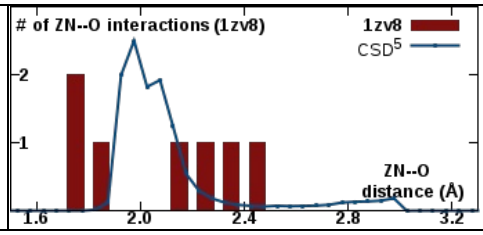
ID	Res.	Metal	*Occupancy*	*B factor (env.)*[1]	*Ligands*	*Valence*[2]	*nVECSUM*[3]	*Geometry*[1,4]	*gRMSD*(°)[1]	*Vacancy*[1]	Bidentate	Alt. metal
A:209	NA	Na	1	*41.5 (32.3)*	O_3	*0.6*	**0.51**	*Square Planar*	*18.8°*	*25%*	0	
B:206	NA	Na	1	*56.6 (40)*	O_4	*1.4*	*0.15*	*Square Planar*	*17.4°*	*25%*	1	
G:201	CAC	As	1	*40.1 (34.4)*	*O_2*	1.7	**0.57**	Tetrahedral	1.6°	**50%**	0	
G:204	ZN	Zn	1	*44.4 (30.9)*	*O_3*	*1.4*	**0.51**	Tetrahedral	11.9°	*25%*	0	
G:208	NA	Na	1	*50.7 (40.7)*	O_3	0.7	**0.74**	Octahedral	*19.3°*	**50%**	0	
H:203	ZN	Zn	1	38.5 (36.7)	*O_4*	1.7	*0.22*	*Square Planar*	**29.1°**	0	0	Cu, Co
H:210	NA	Na	1	*45.9 (55.1)*	O_3	1	**0.35**	*Tetrahedral*	**24.2°**	*25%*	0	
J:207	NA	Na	1	35.5 (33.6)	O_4	**2.3**	**0.47**	*Tetrahedral*	*13.8°*	0	0	Cu, Co
K:205	NA	Na	1	36.6 (39.5)	O_4	**2**	**0.63**	Octahedral	10.8°	**33%**	0	Cu

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 pdb1zv8.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

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