

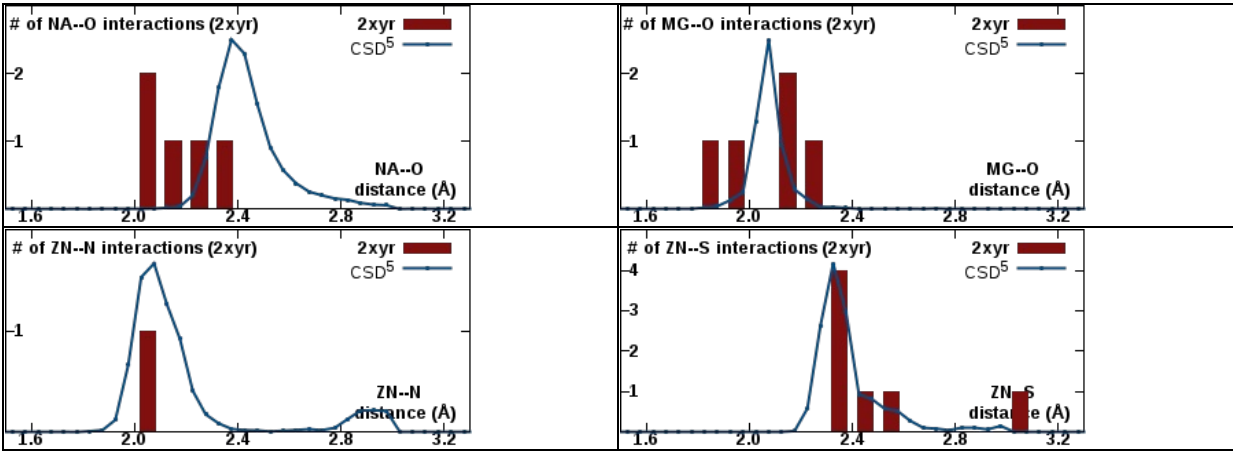
CheckMyMetal(CMM) report for PDB code: 2xyr

PDB title: Crystal structure of the nsp16 nsp10 sars coronavirus complex (2.5Å)

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:1293	NA	Na	1	42.9 (59.5)	O <sub>5</sub>	1.9	0.056	Trigonal Bipyramidal	14.3°	0	0	
A:1294	CL	Cl	1	55.3 (48.6)		N/A	N/A	Free	N/A	N/A	N/A	
A:1295	CL	Cl	1	58 (53.6)		N/A	N/A	Free	N/A	N/A	N/A	
A:1296	CL	Cl	1	61.2 (42.5)		N/A	N/A	Free	N/A	N/A	N/A	
A:1297	CL	Cl	1	55.7 (46.6)		N/A	N/A	Free	N/A	N/A	N/A	
A:1299	MG	Mg	0.5	39.2 (39.5)	O <sub>5</sub>	1.7	0.14	Trigonal Bipyramidal	13.2°	0	0	Co
B:1132	ZN	Zn	1	51.3 (52.5)	N <sub>1</sub> S <sub>3</sub>	1.8	0.061	Tetrahedral	4.9°	0	0	
B:1133	ZN	Zn	1	75.4 (76.3)	S <sub>4</sub>	1.3	0.17	Tetrahedral	19.8°	0	0	Cu
B:1134	CL	Cl	1	56.6 (63)		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. <i>Valence</i> 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 <i>NEIGHBORHOOD</i> 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

Metal-ligand distance distributions for pdb2xyr.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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