

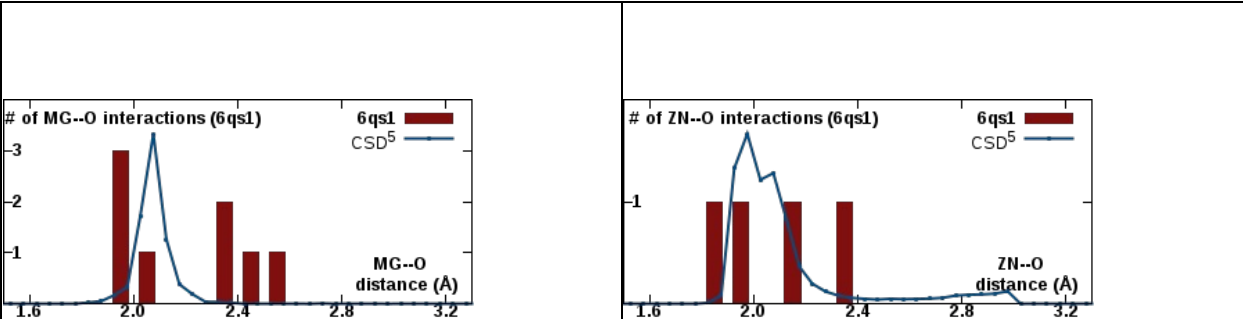
CheckMyMetal(CMM) report for PDB code: 6qs1

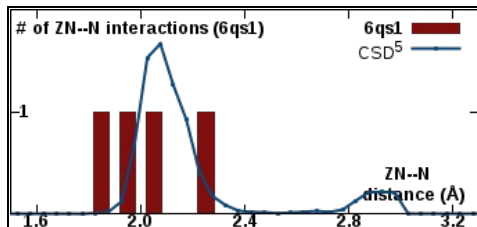
PDB title: Crystal structure of human angiotensin-1 converting enzyme n-domain in complex with bppb (1.8Å)

ID	Res.	Metal	Occupancy	B factor (env.) ¹	Ligands	Valence ²	nVECSUM ³	Geometry ^{1,4}	gRMSD(°) ¹	Vacancy ¹	Bidentate	Alt. metal
A:714	BO3	B	0.79	37.9 (42.9)	O ₃	3.3	0.15	Trigonal Planar	2.5°	0	0	
A:715	BO3	B	0.71	33.4 (32.3)	O ₃	3.2	0.11	Trigonal Planar	2.3°	0	0	
A:716	BO3	B	0.81	42 (42.2)	O ₃	3	0.084	Trigonal Planar	1.8°	0	0	
A:721	BO3	B	1	53.5 (53.8)	O ₃	3.1	0.027	Trigonal Planar	1.2°	0	0	
A:722	ZN	Zn	0.7	30.3 (28.9)	O ₂ N ₂	1.7	0.36	Tetrahedral	20.5°	0	0	Cu, Zn, Co
A:723	CL	Cl	1	25.2 (25)		N/A	N/A	Free	N/A	N/A	N/A	
A:724	CL	Cl	1	36.1 (32.4)		N/A	N/A	Free	N/A	N/A	N/A	
A:725	MG	Mg	0.68	39 (38.8)	O ₅	1.2	0.49	Square Planar	24.3°	0	1	
B:710	BO3	B	0.78	42.3 (40.6)	O ₃	3.1	0.037	Trigonal Planar	1.7°	0	0	
B:711	BO3	B	0.89	51.8 (52.2)	O ₃	3.1	0.051	Trigonal Planar	0.6°	0	0	
B:712	BO3	B	0.92	50.1 (54.5)	O ₃	3.2	0.054	Trigonal Planar	0.9°	0	0	
B:714	ZN	Zn	0.64	29.5 (31.5)	O ₂ N ₂	1.9	0.35	Tetrahedral	20.7°	0	0	Cu, Zn, Co
B:715	CL	Cl	1	32.8 (34.3)		N/A	N/A	Free	N/A	N/A	N/A	
B:716	CL	Cl	1	44.3 (45.3)		N/A	N/A	Free	N/A	N/A	N/A	
B:717	MG	Mg	1	47.9 (44)	O ₃	1.1	0.61	Octahedral	4.8°	50%	0	Ca
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. <i>Valence</i> 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 <i>NEIGHBORHOOD</i> 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 pdb6qs1.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*

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.