

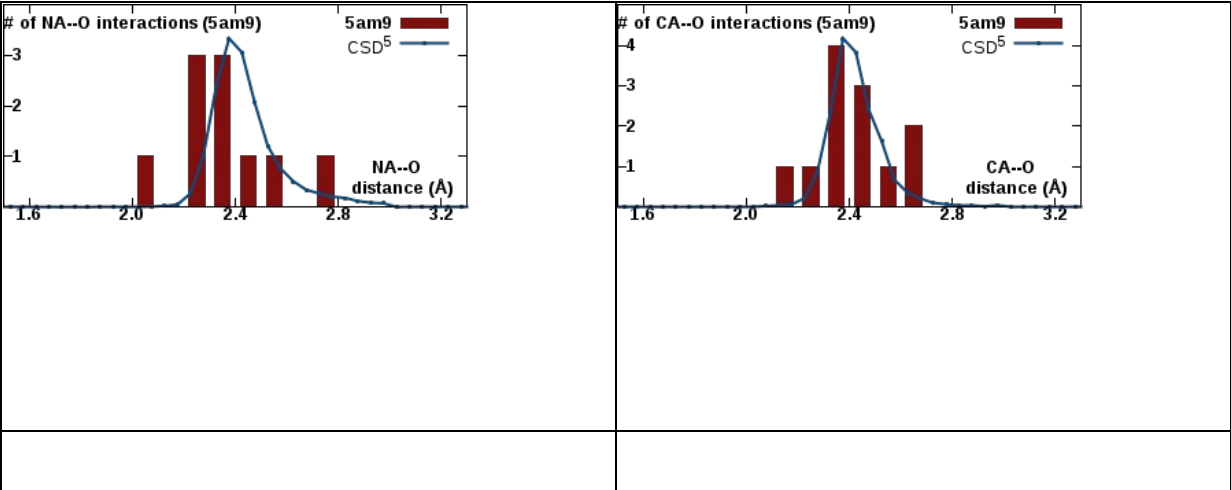
CheckMyMetal(CMM) report for PDB code: 5am9

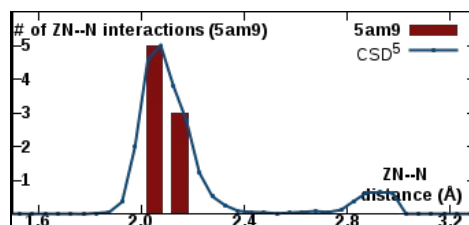
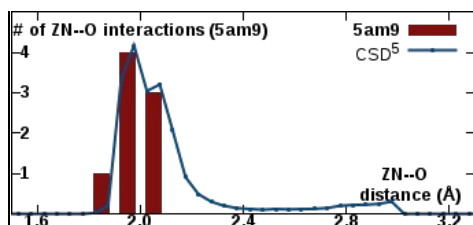
PDB title: Crystal structure of the angiotensin-1 converting enzyme n- domain in complex with amyloid-beta 10-16 (1.8Å)

Warning: Valence and nVECSUM parameters should be interpreted with great care due to potential cation-pi interactions observed around A:1001 C:1001												
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:1001	ZN	Zn	1	20.9 (19.5)	O <sub>2</sub> N <sub>2</sub>	1.8	0.16	Tetrahedral	10.5°	0	0	
A:1002	CL	Cl	1	21.7 (20.6)		N/A	N/A	Free	N/A	N/A	N/A	
A:1003	NA	Na	1	30.2 (33.1)	O <sub>6</sub>	1.2	0.2	Octahedral	7.5°	0	0	
B:1001	ZN	Zn	1	18.5 (17.2)	O <sub>2</sub> N <sub>2</sub>	1.7	0.2	Tetrahedral	11.7°	0	0	
B:1002	CL	Cl	1	19 (19.5)		N/A	N/A	Free	N/A	N/A	N/A	
B:1003	CA	Ca	1	41.5 (29.6)	O <sub>6</sub>	1.7	0.29	Octahedral	7.9°	0	0	
C:1001	ZN	Zn	1	17.9 (15.8)	O <sub>2</sub> N <sub>2</sub>	1.7	0.21	Tetrahedral	10.5°	0	0	
C:1002	CL	Cl	1	17.7 (18.2)		N/A	N/A	Free	N/A	N/A	N/A	
C:1003	CA	Ca	1	25.6 (21.6)	O <sub>6</sub>	1.9	0.12	Octahedral	7.6°	0	0	
D:1001	ZN	Zn	1	19.5 (18.1)	O <sub>2</sub> N <sub>2</sub>	1.8	0.16	Tetrahedral	11.3°	0	0	
D:1002	CL	Cl	1	20.3 (19.4)		N/A	N/A	Free	N/A	N/A	N/A	
D:1003	NA	Na	1	40.3 (32.7)	O <sub>4</sub>	1.2	0.32	Square Planar	6.7°	0	0	
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. Valence 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 NEIGHBORHOOD 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 pdb5am9.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.