

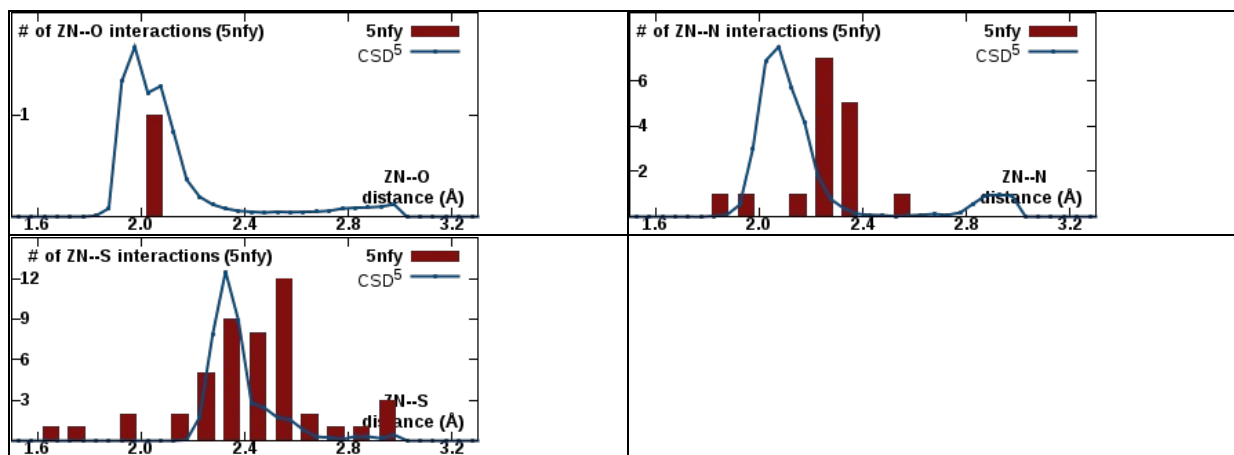
CheckMyMetal(CMM) report for PDB code: 5nfy

PDB title: Sars-cov nsp10/nsp14 dynamic complex (3.4Å)

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:601	ZN	Zn	1	161.4 (75.9)	N <sub>1</sub> S <sub>2</sub>	2.8	0.47	Tetrahedral	14.1°	25%	0	Cu, Fe
A:602	ZN	Zn	1	102.2 (93.5)	N <sub>2</sub> S <sub>2</sub>	1.2	0.26	Tetrahedral	13°	0	0	
A:603	ZN	Zn	1	92.3 (159.8)	N <sub>1</sub> S <sub>3</sub>	15.2	0.93	Trigonal Bipyramidal	13.3°	20%	0	
B:601	ZN	Zn	1	123.8 (109.2)	O <sub>1</sub> N <sub>1</sub> S <sub>2</sub>	1.3	0.2	Tetrahedral	19.4°	0	0	
B:602	ZN	Zn	1	111.2 (86.1)	N <sub>2</sub> S <sub>2</sub>	1.5	0.26	Tetrahedral	14.8°	0	0	Cu, Co
B:603	ZN	Zn	1	119.2 (140.4)	S <sub>3</sub>	1.8	0.6	Square Planar	17.2°	25%	0	Cu, Co, Zn, Ni
C:601	ZN	Zn	1	155.8 (69.8)	N <sub>1</sub> S <sub>3</sub>	10.6	0.74	Tetrahedral	18.1°	0	0	
C:602	ZN	Zn	1	107.5 (86.4)	N <sub>2</sub> S <sub>2</sub>	1.2	0.27	Tetrahedral	18.4°	0	0	
C:603	ZN	Zn	1	168.7 (128.2)	S <sub>2</sub>	1.1	0.72	Square Planar	1.8°	50%	0	
D:601	ZN	Zn	1	144.4 (143.1)	N <sub>1</sub> S <sub>3</sub>	7	0.87	Square Planar	24.6°	0	0	
D:602	ZN	Zn	1	107.8 (81.5)	N <sub>2</sub> S <sub>2</sub>	1.6	0.27	Tetrahedral	15.1°	0	0	Cu, Zn, Co
D:603	ZN	Zn	1	115.9 (120)	S <sub>3</sub>	0.9	0.57	Trigonal Bipyramidal	9.5°	40%	0	
M:201	ZN	Zn	1	112.8 (83.8)	N <sub>1</sub> S <sub>3</sub>	1.9	0.14	Tetrahedral	8.9°	0	0	
M:202	ZN	Zn	1	155.9 (137.3)	S <sub>3</sub>	0.6	0.44	Tetrahedral	13.4°	25%	0	
N:201	ZN	Zn	1	88 (77.5)	N <sub>1</sub> S <sub>3</sub>	1.5	0.075	Tetrahedral	12.5°	0	0	
N:202	ZN	Zn	1	148.9 (129.8)	S <sub>2</sub>	0.5	0.78	Square Planar	7.5°	50%	0	
O:201	ZN	Zn	1	196.1 (93.3)	N <sub>1</sub> S <sub>3</sub>	1.3	0.45	Trigonal Bipyramidal	14.3°	20%	0	
O:202	ZN	Zn	1	175.6 (147.4)	S <sub>2</sub>	0.6	0.63	Tetrahedral	8°	50%	0	
P:201	ZN	Zn	1	161.8 (79.8)	S <sub>3</sub>	7.8	0.17	Trigonal Planar	14.1°	0	0	
P:202	ZN	Zn	1	142.3 (123.7)	S <sub>2</sub>	0.4	0.73	Square Planar	3.7°	50%	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. <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 pdb5nfy.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.