CheckMyMetal(CMM) report for PDB code: 2g9t

PDB title: Crystal structure of the sars coronavirus nsp10 at 2.1a (2.1Å)

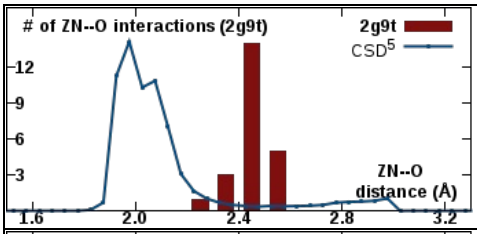
ID	Res.	Metal	*Occupancy*	*B factor (env.)*[1]	*Ligands*	*Valence*[2]	*nVECSUM*[3]	*Geometry*[1,4]	*gRMSD*(°)[1]	*Vacancy*[1]	Bidentate	Alt. metal
A:998	ZN	Zn	1	27.1 (29.7)	N_1S_3	2.3	0.081	Tetrahedral	8.1°	0	0	
A:999	ZN	Zn	1	36.6 (31.6)	O_1S_3	1.7	**0.26**	Tetrahedral	3.3°	0	0	Cu, Zn, Co
B:998	ZN	Zn	1	27.3 (27)	N_1S_3	2.3	0.096	Tetrahedral	6°	0	0	
B:999	ZN	Zn	1	41.2 (35.7)	O_1S_3	*1.3*	**0.27**	Tetrahedral	1.7°	0	0	Cu
C:998	ZN	Zn	1	27.4 (28.9)	N_1S_3	2.2	*0.12*	Tetrahedral	6°	0	0	
C:999	ZN	Zn	1	*36 (30.5)*	O_1S_3	*1.5*	*0.23*	Tetrahedral	3.6°	0	0	Cu, Co
D:998	ZN	Zn	1	27.5 (29.3)	N_1S_3	2.2	0.071	Tetrahedral	7.7°	0	0	
D:999	ZN	Zn	1	*37 (52.6)*	O_1S_3	**3.7**	**0.59**	Tetrahedral	**24.4°**	0	0	
E:998	ZN	Zn	1	27.6 (28.5)	N_1S_3	2.3	0.093	Tetrahedral	6.8°	0	0	
E:999	ZN	Zn	1	36 (34.7)	O_1S_3	*1.6*	*0.23*	Tetrahedral	4.5°	0	0	Cu, Zn, Co
F:998	ZN	Zn	1	27.2 (28.4)	N_1S_3	2.3	0.086	Tetrahedral	6°	0	0	
F:999	ZN	Zn	1	38.5 (34.7)	O_1S_3	*1.6*	**0.27**	Tetrahedral	4.2°	0	0	Cu, Zn, Co
G:998	ZN	Zn	1	27.2 (26.2)	N_1S_3	*2.4*	0.078	Tetrahedral	4.7°	0	0	
G:999	ZN	Zn	1	38.4 (33.7)	O_1S_3	*1.5*	**0.24**	Tetrahedral	2.8°	0	0	Cu, Co
H:998	ZN	Zn	1	29.7 (32.3)	N_1S_3	2.3	0.059	Tetrahedral	6.8°	0	0	
H:999	ZN	Zn	1	39.8 (41.5)	O_1S_3	1.7	**0.24**	Tetrahedral	4°	0	0	Cu, Zn, Co
I:998	ZN	Zn	1	25.5 (26.6)	N_1S_3	2.3	0.076	Tetrahedral	7.8°	0	0	
I:999	ZN	Zn	1	35.4 (32.8)	O_1S_3	1.8	*0.23*	Tetrahedral	3°	0	0	
J:998	ZN	Zn	1	27.9 (27)	N_1S_3	2.3	0.066	Tetrahedral	6°	0	0	
J:999	ZN	Zn	1	35.7 (36)	O_1S_3	*1.6*	**0.25**	Tetrahedral	4.4°	0	0	Cu, Zn, Co
K:998	ZN	Zn	1	29.3 (30.6)	N_1S_3	2.3	0.072	Tetrahedral	5.9°	0	0	
K:999	ZN	Zn	1	37.1 (34.6)	O_1S_3	1.7	**0.26**	Tetrahedral	6.2°	0	0	Cu, Zn, Co
L:998	ZN	Zn	1	27.3 (27.4)	N_1S_3	*2.4*	0.092	Tetrahedral	4.9°	0	0	
L:999	ZN	Zn	1	35.2 (33.2)	O_1S_3	2	**0.27**	Tetrahedral	3°	0	0	
M:998	ZN	Zn	1	27.4 (26.7)	N_1S_3	*2.4*	0.099	Tetrahedral	6.6°	0	0	
M:999	ZN	Zn	1	43.2 (38.3)	O_1S_3	*1.6*	**0.29**	Tetrahedral	3.7°	0	0	Cu, Zn, Co
N:998	ZN	Zn	1	29.4 (30.2)	N_1S_3	2.2	0.065	Tetrahedral	6.8°	0	0	
N:999	ZN	Zn	1	41.8 (39.7)	O_1S_3	*1.5*	**0.31**	Tetrahedral	4.3°	0	0	Cu, Co
O:998	ZN	Zn	1	34.4 (34.7)	N_1S_3	2.2	0.03	Tetrahedral	5.2°	0	0	
O:999	ZN	Zn	1	42.1 (39.8)	O_1S_3	*1.3*	*0.23*	Tetrahedral	4.9°	0	0	Cu

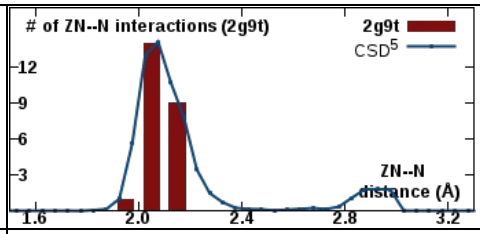
P:998	ZN	Zn	1	28.7 (29)	N_1S_3	2.2	*0.13*	Tetrahedral	5.2°	0	0	
P:999	ZN	Zn	1	*38.1 (32.4)*	O_1S_3	*1.6*	*0.23*	Tetrahedral	3.5°	0	0	Cu, Zn, Co
Q:998	ZN	Zn	1	25.6 (26.8)	N_1S_3	2.3	*0.13*	Tetrahedral	5.4°	0	0	
Q:999	ZN	Zn	1	37.1 (33.2)	O_1S_3	2	**0.26**	Tetrahedral	3°	0	0	
R:998	ZN	Zn	1	28 (28.3)	N_1S_3	*2.4*	0.099	Tetrahedral	7.3°	0	0	
R:999	ZN	Zn	1	34.8 (33.4)	O_1S_3	*1.6*	**0.29**	Tetrahedral	4.9°	0	0	Cu, Zn, Co
S:998	ZN	Zn	1	27.6 (29.1)	N_1S_3	2.2	0.083	Tetrahedral	5.1°	0	0	
S:999	ZN	Zn	1	32.8 (30.4)	O_1S_3	1.8	*0.21*	Tetrahedral	2.7°	0	0	
T:998	ZN	Zn	1	27 (27.7)	N_1S_3	2.3	0.096	Tetrahedral	6.1°	0	0	
T:999	ZN	Zn	1	43.1 (47.8)	O_1S_3	*1.4*	**0.58**	Tetrahedral	**27.6°**	0	0	Cu, Co
U:998	ZN	Zn	1	26.5 (28.4)	N_1S_3	2.3	*0.12*	Tetrahedral	6°	0	0	
U:999	ZN	Zn	1	33.6 (31)	O_1S_3	1.7	**0.25**	Tetrahedral	3.8°	0	0	Cu, Zn, Co
V:998	ZN	Zn	1	29.9 (31.8)	N_1S_3	2.3	0.1	Tetrahedral	7°	0	0	
V:999	ZN	Zn	1	**73 (24.5)**	**S_1**	**0.4**	**1**	**Poorly Coordinated**	N/A	N/A	0	
W:998	ZN	Zn	1	28.7 (29.6)	N_1S_3	2.2	0.066	Tetrahedral	6.7°	0	0	
W:999	ZN	Zn	1	35 (33.1)	O_1S_3	1.9	**0.24**	Tetrahedral	3.5°	0	0	
X:998	ZN	Zn	1	24.7 (26.3)	N_1S_3	*2.4*	0.093	Tetrahedral	6.5°	0	0	
X:999	ZN	Zn	1	*37 (48.2)*	O_1S_3	**5.2**	**0.74**	*Square Planar*	**30.6°**	0	0	

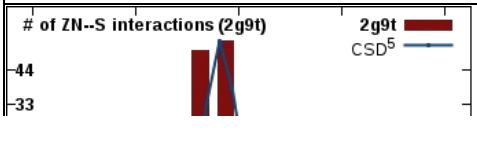
Legend: Not applicable | **Outlier** | *Borderline* | Acceptable

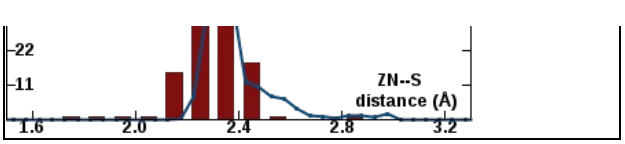
Column	Description
Occupancy	Occupancy of ion under consideration
B factor (env.)[1]	Metal ion B factor, with valence-weighted environmental average B factor in parenthesis
Ligands	Elemental composition of the coordination sphere
Valence[2]	Summation of bond valence values for an ion binding site. *Valence* 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 pdb2g9t.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.