CheckMyMetal(CMM) report for PDB code: 6xez

PDB title: Structure of sars-cov-2 replication-transcription complex bound to nsp13 helicase - nsp13(2)-rtc (3.5Å)

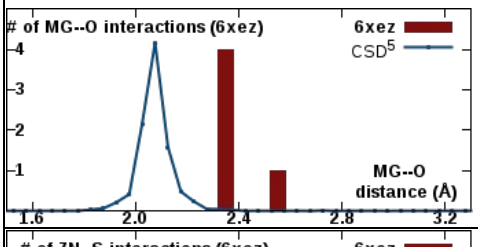
Warning: *Valence* and *nVECSUM* parameters should be interpreted with great care due to potential cation-pi interactions observed around A:1002; the presence of multi-nuclear metal clusters around E:705 F:1004; and the presence of small molecules in the coordinate sphere of the metal ion E:705 F:1004

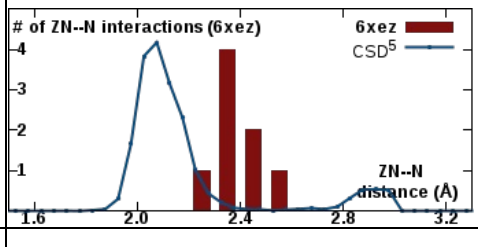
ID	Res.	Metal	*Occupancy*	*B factor (env.)*[1]	*Ligands*	*Valence*[2]	*nVECSUM*[3]	*Geometry*[1,4]	*gRMSD*(°)[1]	*Vacancy*[1]	Bidentate	Alt. metal
A:1001	ZN	Zn	1	N/A	N_1S_3	2	0.21	Tetrahedral	10.1°	0	0	
A:1002	ZN	Zn	1	N/A	N_1S_3	1.7	**0.34**	Tetrahedral	*13.6°*	0	0	Cu, Zn, Co
A:1003	MG	Mg	1	N/A	O_5	*1*	**0.43**	**Trigonal Bipyramidal**	*18.8°*	0	0	
E:701	ZN	Zn	1	N/A	S_4	2.3	0.13	Tetrahedral	12.4°	0	0	
E:702	ZN	Zn	1	N/A	N_1S_3	1.7	**0.34**	*Trigonal Bipyramidal*	8.1°	20%	0	Co, Zn
E:703	ZN	Zn	1	N/A	N_2S_2	1.6	**0.54**	*Trigonal Bipyramidal*	12.6°	20%	0	Co, Zn
E:705	AF3	Al	1	N/A	O_2	2.4	**0.36**	*Square Planar*	**29.8°**	**50%**	0	Cu, Fe, Ni
E:706	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
F:1000	ZN	Zn	1	N/A	S_4	1.3	0.21	*Square Planar*	**24.3°**	0	0	Cu
F:1001	ZN	Zn	1	N/A	N_1S_3	1.6	**0.44**	*Octahedral*	13°	*33%*	0	Co, Cu, Zn
F:1002	ZN	Zn	1	N/A	N_2S_2	*1*	*0.31*	Tetrahedral	*18.6°*	0	0	
F:1004	AF3	Al	1	N/A	O_2	2.4	**0.36**	*Square Planar*	**29.8°**	**50%**	0	Cu, Fe, Ni
F:1005	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	

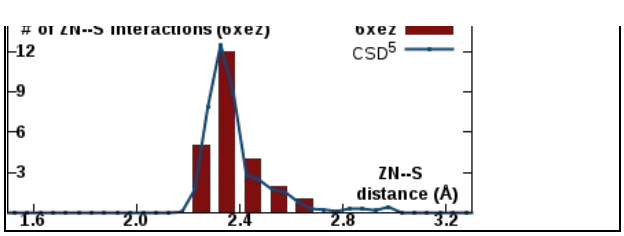
Legend: Not applicable | **Outlier** | *Borderline* | Acceptable

Column	Description
Occupancy	Occupancy of ion under consideration
B factor (env.)[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 pdb6xez.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.