CheckMyMetal(CMM) report for PDB code: 7koj

PDB title: The crystal structure of papain-like protease of sars cov-2, c111s mutant, in complex with plp_snyder494 inhibitor (2.0Å)

Warning: Due to a lack of high-resolution structural data the validity of *Valence* and *nVECSUM* parameters has not been established for rarely observed metals

Warning: *Valence* and *nVECSUM* parameters should be interpreted with great care due to potential cation-pi interactions observed around A:513 A:523; and the presence of multi-nuclear metal clusters around A:504 A:512 A:513 A:515 A:516 A:518 A:519 A:520 A:521 A:523

Warning: Coordinating ligands by symmetry operation are labeled with prefix 'sym-'

Warning: Partial occupancy of the metal is not adjusted upon symmetry operation

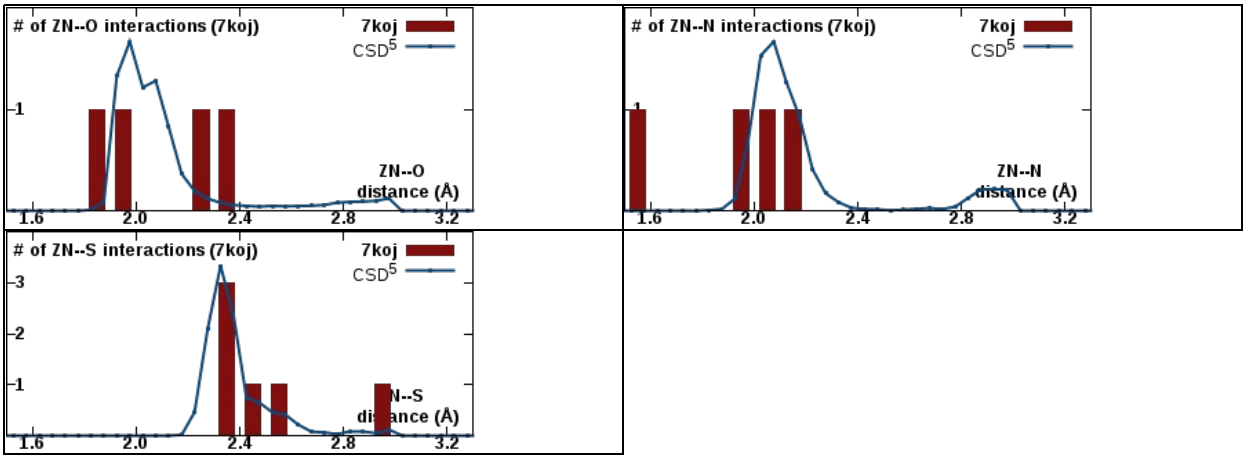
ID	Res.	Metal	*Occupancy*	*B factor (env.)*[1]	*Ligands*	*Valence*[2]	*nVECSUM*[3]	*Geometry*[1,4]	*gRMSD*(°)[1]	*Vacancy*[1]	Bidentate	Alt. metal
A:502	ZN	Zn	1	128 (126.1)	S_4	*1.5*	**0.28**	*Trigonal Bipyramidal*	11.6°	*20%*	0	Co
A:503	ZN	Zn	*0.7*	98 (87.8)	O_1N_1	2	**0.78**	**Linear**	*18.5°*	0	0	
A:504	ZN	Zn	0.5	*41 (56.9)*	$O_1N_1S_1$	2	*0.18*	Tetrahedral	*14.1°*	*25%*	0	
A:504	ZN	Zn	0.5	63.8 (59.7)	$O_1N_1S_1$	*1.5*	**0.29**	Tetrahedral	*13.9°*	*25%*	0	Cu, Co
A:505	ZN	Zn	1	57.7 (60)	O_1N_1	2.2	0.098	**Trigonal Planar**	0.9°	**33%**	0	Cu
A:506	CL	Cl	1	58.5 (68)		N/A	N/A	**Free**	N/A	N/A	N/A	
A:507	CL	Cl	1	57.6 (66.3)		N/A	N/A	**Free**	N/A	N/A	N/A	
A:508	CL	Cl	1	65.1 (64.7)		N/A	N/A	**Free**	N/A	N/A	N/A	
A:512	UNX	Unk	1	69.9 (60.7)	O_1N_1	**0.2**	**0.29**	**Linear**	**32.4°**	0	0	
A:513	UNX	Unk	1	67.4 (63.5)	N_1	**0.4**	**1**	**Poorly Coordinated**	N/A	N/A	0	
A:514	UNX	Unk	1	73.2 (63.5)		N/A	N/A	**Free**	N/A	N/A	N/A	
A:515	UNX	Unk	1	65.8 (60.5)	O_1N_1	**0.2**	**0.54**	**Trigonal Planar**	2.3°	**33%**	0	
A:516	UNX	Unk	1	*78.5 (61.7)*	N_1	**0.09**	**1**	**Poorly Coordinated**	N/A	N/A	0	
A:517	UNX	Unk	1	*70.2 (59.8)*		N/A	N/A	**Free**	N/A	N/A	N/A	
A:518	UNX	Unk	1	*70.1 (81.7)*	N_1	**0.4**	**1**	**Poorly Coordinated**	N/A	N/A	0	
A:519	UNX	Unk	1	73.3 (82)	N_1	**0.14**	**1**	**Poorly Coordinated**	N/A	N/A	0	
A:520	UNX	Unk	1	58.9 (62.1)	O_1	**0.16**	**1**	**Poorly Coordinated**	N/A	N/A	0	
A:521	UNX	Unk	1	79.9 (82)	N_1	**0.17**	**1**	**Poorly Coordinated**	N/A	N/A	0	
A:522	UNX	Unk	1	*70.1 (82)*		N/A	N/A	**Free**	N/A	N/A	N/A	
A:523	UNX	Unk	1	64.9 (61.1)	O_1	**0.15**	**1**	**Poorly Coordinated**	N/A	N/A	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 pdb7koj.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.