CheckMyMetal(CMM) report for PDB code: 6f06

PDB title: Cathepsin l in complex with (3s,14e)-8-(azetidin-3-yl)-19-chloro-n-(1- cyanocyclopropyl)-5-oxo-12,17-dioxa-4-azatricyclo[16.2.2.06, 11]docosa-1(21),6,8,10,14,18(22),19-heptaene-3-carboxamide (2.0Å)

Warning: *Valence* and *nVECSUM* parameters should be interpreted with great care due to potential cation-pi interactions observed around B:306 B:307; and the presence of multi-nuclear metal clusters around B:308 B:309

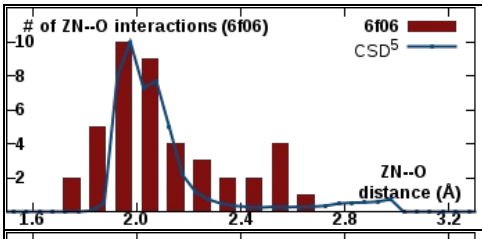
Warning: Coordinating ligands by symmetry operation are labeled with prefix 'sym-'

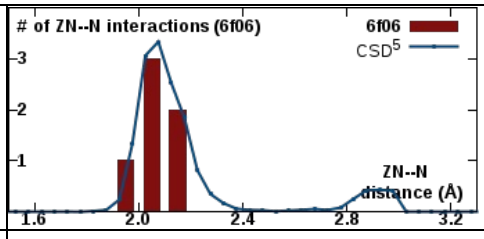
ID	Res.	Metal	*Occupancy*	*B factor (env.)*[1]	*Ligands*	*Valence*[2]	*nVECSUM*[3]	*Geometry*[1,4]	*gRMSD*(°)[1]	*Vacancy*[1]	Bidentate	Alt. metal
A:302	ZN	Zn	1	29.5 (29.4)	$O_1N_1S_1$	2.1	*0.16*	Tetrahedral	1.7°	*25%*	0	Cu, Zn, Fe, Mn, Co
A:303	ZN	Zn	1	38.2 (34)	*O_1N_1*	**0.9**	**0.67**	*Square Planar*	9.4°	**50%**	0	
A:304	ZN	Zn	1	*28.3 (23.7)*	*O_4*	1.9	*0.12*	Tetrahedral	6°	0	0	Cu, Zn, Co
A:305	ZN	Zn	1	*42.7 (32)*	*O_7*	2.1	**0.28**	Tetrahedral	7.8°	0	3	Cu, Zn, Co
A:306	ZN	Zn	1	31.5 (27.9)	*O_4*	2.1	0.1	Tetrahedral	11.5°	0	0	
A:307	ZN	Zn	1	*67.9 (38.9)*	*O_1N_1*	**0.5**	**0.86**	*Square Planar*	5.3°	**50%**	0	
A:308	CL	Cl	1	*37.1 (25)*		N/A	N/A	**Free**	N/A	N/A	N/A	
B:302	ZN	Zn	1	28.9 (30.1)	$O_1N_1S_1$	2.1	0.085	Tetrahedral	6.4°	*25%*	0	
B:303	ZN	Zn	1	42.6 (36.8)	O_2N_1	*1.4*	**0.26**	Tetrahedral	*14.1°*	*25%*	0	Cu
B:304	ZN	Zn	1	*35.7 (28.1)*	*O_3*	*1.4*	**0.4**	Tetrahedral	10.2°	*25%*	0	
B:305	ZN	Zn	1	33.6 (29)	*O_4*	1.8	*0.21*	Tetrahedral	7.3°	0	0	Cu, Co
B:306	ZN	Zn	1	38 (37.5)	*O_5*	1.9	*0.16*	Tetrahedral	8.7°	0	1	Cu, Zn, Co
B:307	ZN	Zn	1	39.3 (34.8)	O_3N_1	*1.4*	**0.27**	Tetrahedral	10°	0	0	
B:308	ZN	Zn	1	*62.9 (51.5)*	*O_3*	**0.8**	**0.63**	Tetrahedral	**23.8°**	*25%*	0	Na
B:309	ZN	Zn	1	*80.2 (54.3)*	*O_3*	**0.6**	**0.49**	Tetrahedral	**26.8°**	*25%*	0	
B:310	CL	Cl	1	33.4 (33.7)		N/A	N/A	**Free**	N/A	N/A	N/A	

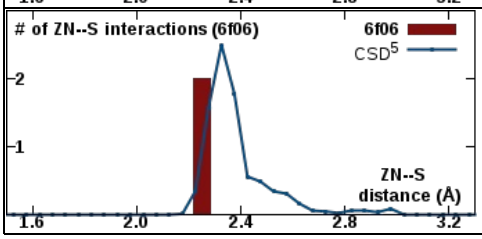
Legend: Not applicable | **Outlier** | *Borderline* | Acceptable

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 pdb6f06.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.