CheckMyMetal(CMM) report for PDB code: 7d30

PDB title: Structure of sybody mr17-sr31 fusion in complex with the sars-cov-2 s receptor binding domain (rbd) (2.1Å)

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 the presence of multi-nuclear metal clusters around A:1317 A:1323 A:1325

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:1314	CD	Cd	0.5	*69.2 (87.2)*	O_7	**3**	0.079	Octahedral	**24.3°**	0	1	Co, Cu
A:1315	CD	Cd	0.48	*129.7 (73.1)*	O_3	**1.2**	*0.19*	Tetrahedral	*18°*	*25%*	0	Na
A:1316	CD	Cd	*0.56*	*107.3 (69.9)*		N/A	N/A	**Free**	N/A	N/A	N/A	
A:1317	CD	Cd	*0.6*	**150.9 (48.5)**	O_3	**0.9**	**0.35**	Tetrahedral	10°	*25%*	0	
A:1318	CD	Cd	0.32	*129.1 (95.4)*	O_4	1.7	**0.5**	Tetrahedral	**32.5°**	0	0	
A:1319	CD	Cd	0.39	*103 (88.4)*	O_4	1.7	**0.39**	*Square Planar*	**31.5°**	0	0	
A:1320	CD	Cd	*0.61*	*143.3 (104)*	O_1	**0.5**	**1**	**Poorly Coordinated**	N/A	N/A	0	
A:1321	CD	Cd	0.5	**135.2 (69.1)**		N/A	N/A	**Free**	N/A	N/A	N/A	
A:1322	CD	Cd	0.49	**107 (52)**	O_1	**0.4**	**1**	**Poorly Coordinated**	N/A	N/A	0	
A:1323	CD	Cd	0.27	**123.5 (49.8)**	O_3	**1.2**	**0.29**	*Square Planar*	*18.5°*	*25%*	0	
A:1324	CD	Cd	*0.71*	*39.8 (52.4)*	O_4	*1.6*	*0.22*	**Trigonal Planar**	12.5°	0	1	
A:1325	CD	Cd	0.31	*65.1 (51.4)*	O_2	**0.4**	**0.33**	**Trigonal Planar**	*21.4°*	**33%**	0	
B:2114	CD	Cd	0.5	*112.5 (84)*	O_5	2	*0.14*	Octahedral	*17.9°*	*16%*	0	Ca
B:2115	CD	Cd	*0.66*	67.5 (62.3)	O_6	*2.5*	0.081	*Trigonal Bipyramidal*	9°	0	1	
B:2116	CD	Cd	0.38	*141.1 (93.4)*	O_4	1.7	**0.37**	*Trigonal Bipyramidal*	11.2°	**40%**	1	
B:2117	CD	Cd	*0.52*	**127.1 (48.2)**	O_1	**0.4**	**1**	**Poorly Coordinated**	N/A	N/A	0	
B:2118	CD	Cd	0.31	94.3 (85.6)	O_1	**0.4**	**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

(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.