CheckMyMetal(CMM) report for PDB code: 7l2c

PDB title: Crystallographic structure of neutralizing antibody 2-51 in complex with sars-cov-2 spike n-terminal domain (ntd) (3.6Å)

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

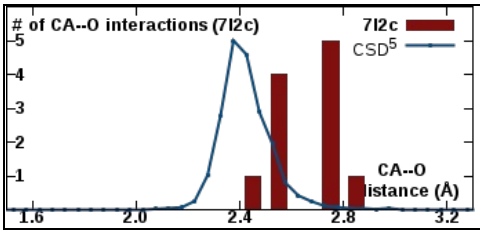
ID	Res.	Metal	*Occupancy*	*B factor (env.)*[1]	*Ligands*	*Valence*[2]	*nVECSUM*[3]	*Geometry*[1,4]	*gRMSD(°)*[1]	*Vacancy*[1]	Bidentate	Alt. metal
A:408	CA	Ca	1	*61.8 (52)*		N/A	N/A	**Free**	N/A	N/A	N/A	
A:409	CA	Ca	1	60.4 (56.5)		N/A	N/A	**Free**	N/A	N/A	N/A	
A:411	CA	Ca	1	*74.9 (120.6)*		N/A	N/A	**Free**	N/A	N/A	N/A	
A:412	CA	Ca	1	95.4 (108.4)		N/A	N/A	**Free**	N/A	N/A	N/A	
A:413	CA	Ca	1	80.4 (79.6)		N/A	N/A	**Free**	N/A	N/A	N/A	
A:417	CAC	As	1	**172.4 (88.8)**	O_2	2.3	**0.57**	Tetrahedral	0.5°	**50%**	0	Cu, Co
B:407	CA	Ca	1	92 (85.1)	O_2	**0.4**	**0.64**	**Tetrahedral**	2.1°	**50%**	0	
B:408	CA	Ca	1	71.8 (80.3)	O_1	**0.11**	**1**	**Poorly Coordinated**	N/A	N/A	0	
B:409	CA	Ca	1	88.1 (88)		N/A	N/A	**Free**	N/A	N/A	N/A	
B:410	CA	Ca	1	72.9 (84)	O_1	**0.2**	**1**	**Poorly Coordinated**	N/A	N/A	0	
B:412	CA	Ca	1	*100.4 (84.8)*	O_1	**0.19**	**1**	**Poorly Coordinated**	N/A	N/A	0	
H:301	CA	Ca	1	64.9 (59.2)		N/A	N/A	**Free**	N/A	N/A	N/A	
H:302	CA	Ca	1	*71.1 (57.7)*		N/A	N/A	**Free**	N/A	N/A	N/A	
H:303	CA	Ca	1	*74 (60.1)*		N/A	N/A	**Free**	N/A	N/A	N/A	
H:304	CA	Ca	1	89.7 (101.6)		N/A	N/A	**Free**	N/A	N/A	N/A	
H:305	CA	Ca	1	87.8 (92.8)	O_1	**0.11**	**1**	**Poorly Coordinated**	N/A	N/A	0	
H:306	CA	Ca	1	*103.1 (76)*	O_1	**0.1**	**1**	**Poorly Coordinated**	N/A	N/A	0	
H:307	CA	Ca	1	72.7 (77.7)	O_1	**0.1**	**1**	**Poorly Coordinated**	N/A	N/A	0	
L:301	CA	Ca	1	81.5 (82.5)		N/A	N/A	**Free**	N/A	N/A	N/A	
L:302	CA	Ca	1	75.8 (75.1)		N/A	N/A	**Free**	N/A	N/A	N/A	
C:302	CA	Ca	1	*77.9 (50.4)*		N/A	N/A	**Free**	N/A	N/A	N/A	
C:304	CA	Ca	1	**78.6 (0)**		N/A	N/A	**Free**	N/A	N/A	N/A	
C:305	CA	Ca	1	*72.3 (112.8)*		N/A	N/A	**Free**	N/A	N/A	N/A	
C:306	CA	Ca	1	73.8 (73.6)		N/A	N/A	**Free**	N/A	N/A	N/A	
C:307	CA	Ca	1	*90.3 (66)*	O_2	**0.4**	*0.28*	**Linear**	**31.4°**	0	0	
C:309	CA	Ca	1	*82.6 (67.5)*		N/A	N/A	**Free**	N/A	N/A	N/A	
C:310	CA	Ca	1	**68.9 (0)**		N/A	N/A	**Free**	N/A	N/A	N/A	
C:311	CA	Ca	1	*82.9 (62.6)*		N/A	N/A	**Free**	N/A	N/A	N/A	
D:301	CA	Ca	1	*65.6 (43.4)*		N/A	N/A	**Free**	N/A	N/A	N/A	
D:302	CA	Ca	1	*80.5 (62.4)*		N/A	N/A	**Free**	N/A	N/A	N/A	
D:303	CA	Ca	1	84 (73)		N/A	N/A	**Free**	N/A	N/A	N/A	
D:304	CA	Ca	1	*66.1 (52.6)*	O_1	**0.09**	**1**	**Poorly Coordinated**	N/A	N/A	0	
D:305	CA	Ca	1	98.3 (89.9)		N/A	N/A	**Free**	N/A	N/A	N/A	
D:306	CA	Ca	1	79.4 (79.4)		N/A	N/A	**Free**	N/A	N/A	N/A	

Not

Legend:	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 distribution for pdb7l2c.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.