CheckMyMetal(CMM) report for PDB code: 6zok

PDB title: Sars-cov-2-nsp1-40s complex, focused on body (2.8Å)

Warning: *Valence* and *nVECSUM* parameters should be interpreted with great care due to the presence of multi-nuclear metal clusters around 2:1911 2:1936 2:1952 2:1990 2:1993

ID	Res.	Metal	*Occupancy*	*B factor (env.)*[1]	*Ligands*	*Valence*[2]	*nVECSUM*[3]	*Geometry*[1,4]	*gRMSD*(°)[1]	*Vacancy*[1]	Bidentate	Alt. metal
2:1901	MG	Mg	1	N/A	O_1	0.09	1	Poorly Coordinated	N/A	N/A	0	
2:1902	MG	Mg	1	N/A	*O_2*	0.3	0.34	Trigonal Planar	*20.7°*	*33%*	0	
2:1903	MG	Mg	1	N/A	O_1	0.3	1	Poorly Coordinated	N/A	N/A	0	
2:1904	MG	Mg	1	N/A		N/A	N/A	Free	N/A	N/A	N/A	
2:1906	MG	Mg	1	N/A	O_1	0.3	1	Poorly Coordinated	N/A	N/A	0	
2:1907	MG	Mg	1	N/A	O_1	0.15	1	Poorly Coordinated	N/A	N/A	0	
2:1908	MG	Mg	1	N/A	O_1	0.09	1	Poorly Coordinated	N/A	N/A	0	
2:1909	MG	Mg	1	N/A		N/A	N/A	Free	N/A	N/A	N/A	
2:1911	MG	Mg	1	N/A	*O_2*	0.5	0.77	Square Planar	7.4°	50%	0	
2:1912	MG	Mg	1	N/A	*O_1*	0.3	0.99	Poorly Coordinated	N/A	N/A	0	
2:1913	MG	Mg	1	N/A	*O_2*	0.2	0.81	Square Planar	*17.4°*	50%	0	
2:1914	MG	Mg	1	N/A	O_1	0.2	1	Poorly Coordinated	N/A	N/A	0	
2:1915	MG	Mg	1	N/A	N_1	0.6	1	Poorly Coordinated	N/A	N/A	0	
2:1916	MG	Mg	1	N/A	O_1	0.12	1	Poorly Coordinated	N/A	N/A	0	
2:1917	MG	Mg	1	N/A	*O_2*	0.4	0.77	Square Planar	10.7°	50%	0	
2:1918	MG	Mg	1	N/A	O_1	0.2	1	Poorly Coordinated	N/A	N/A	0	
2:1919	MG	Mg	1	N/A	*O_2*	0.3	0.75	Square Planar	6.7°	50%	0	K
2:1920	MG	Mg	1	N/A	O_3	0.8	0.35	Square Planar	8°	*25%*	0	Na
2:1921	MG	Mg	1	N/A	*O_2*	0.5	0.78	Square Planar	11.8°	50%	0	
2:1922	MG	Mg	1	N/A		N/A	N/A	Free	N/A	N/A	N/A	
2:1923	MG	Mg	1	N/A	O_1	0.13	1	Poorly Coordinated	N/A	N/A	0	
2:1924	MG	Mg	1	N/A	*O_2*	0.5	0.8	Square Planar	13.1°	50%	0	
2:1925	MG	Mg	1	N/A	O_1	0.3	1	Poorly Coordinated	N/A	N/A	0	
2:1926	MG	Mg	1	N/A		N/A	N/A	Free	N/A	N/A	N/A	
2:1927	MG	Mg	1	N/A	O_1	0.14	1	Poorly Coordinated	N/A	N/A	0	
2:1928	MG	Mg	1	N/A	O_1	0.13	1	Poorly Coordinated	N/A	N/A	0	
2:1930	MG	Mg	1	N/A	O_1	0.11	1	Poorly Coordinated	N/A	N/A	0	
2:1932	MG	Mg	1	N/A	O_1	0.3	1	Poorly Coordinated	N/A	N/A	0	
2:1933	MG	Mg	1	N/A		N/A	N/A	Free	N/A	N/A	N/A	
2:1934	MG	Mg	1	N/A	O_1	0.3	1	Poorly Coordinated	N/A	N/A	0	
2:1935	MG	Mg	1	N/A		N/A	N/A	Free	N/A	N/A	N/A	
2:1936	MG	Mg	1	N/A	O_3	0.8	*0.27*	Square Planar	8.4°	*25%*	0	Na
2:1937	MG	Mg	1	N/A		N/A	N/A	Free	N/A	N/A	N/A	
2:1938	MG	Mg	1	N/A	O_1	0.11	1	Poorly Coordinated	N/A	N/A	0	

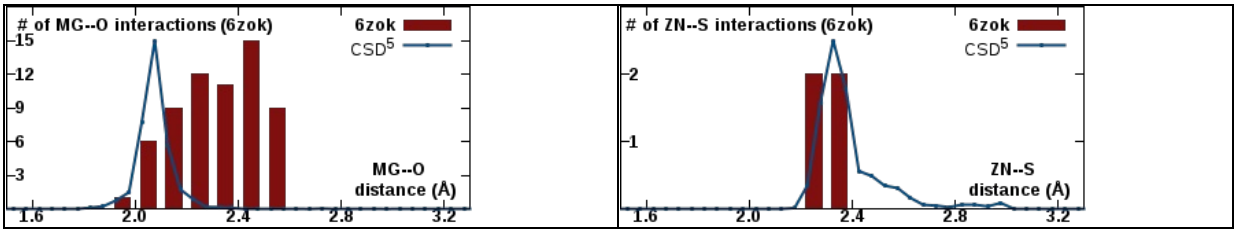
2:1939	MG	Mg	1	N/A	**O_1**	**0.11**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1940	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1942	MG	Mg	1	N/A	**O_1**	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1943	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1944	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1945	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1946	MG	Mg	1	N/A	**O_1**	**0.15**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1947	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1948	MG	Mg	1	N/A	**O_1**	**0.12**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1949	MG	Mg	1	N/A	**O_1**	**0.09**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1951	MG	Mg	1	N/A	**O_1**	**0.13**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1952	MG	Mg	1	N/A	**O_1**	**0.08**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1953	MG	Mg	1	N/A	**O_1**	**0.15**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1954	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1955	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1956	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1957	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1958	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1959	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1960	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1961	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1962	MG	Mg	1	N/A	**O_1**	**0.4**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1964	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1965	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1966	MG	Mg	1	N/A	**O_1**	**0.1**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1967	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1968	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1970	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1971	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1972	MG	Mg	1	N/A	**O_1**	**0.12**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1973	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1974	MG	Mg	1	N/A	**O_1**	**0.19**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1975	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1976	MG	Mg	1	N/A	*O_2*	**0.2**	**0.8**	**Square Planar**	*14.5°*	**50%**	0	
2:1977	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1979	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1980	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1981	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1982	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1983	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1984	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1985	MG	Mg	1	N/A	**O_1**	**0.13**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1986	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1987	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1988	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1989	MG	Mg	1	N/A	**O_1**	**0.11**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1990	MG	Mg	1	N/A	*O_2*	**0.2**	**0.84**	**Square Planar**	*19.9°*	**50%**	0	
2:1991	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1992	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	

2:1993	MG	Mg	1	N/A	**O_1**	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1994	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1995	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1996	MG	Mg	1	N/A	**O_1**	**0.11**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1997	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:1998	MG	Mg	1	N/A	**O_1**	**0.12**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:1999	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2000	MG	Mg	1	N/A	*O_2*	**0.2**	**0.62**	**Tetrahedral**	4.3°	**50%**	0	
2:2001	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2002	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2003	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2004	MG	Mg	1	N/A	**O_1**	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2005	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2006	MG	Mg	1	N/A	*O_2*	**0.4**	**0.87**	**Square Planar**	**31.9°**	**50%**	0	
L:201	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
X:201	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
X:202	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
a:201	ZN	Zn	1	N/A	S_4	2.3	0.061	Tetrahedral	2.3°	0	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 pdb6zok.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.