CheckMyMetal(CMM) report for PDB code: 6zoj

PDB title: Sars-cov-2-nsp1-40s complex, composite map (2.8Å)

Warning: *Valence* and *nVECSUM* parameters should be interpreted with great care due to the presence of multi-nuclear metal clusters around 2:2004 2:2012 2:2031 2:2043 2:2065 2:2071 2:2090 2:2106 2:2145 2:2148

ID	Res.	Metal	*Occupancy*	*B factor (env.)*[1]	*Ligands*	*Valence*[2]	*nVECSUM*[3]	*Geometry*[1,4]	*gRMSD*(°)[1]	*Vacancy*[1]	Bidentate	Alt. metal
2:2001	MG	Mg	1	N/A	O_2	**0.7**	**0.33**	**Trigonal Planar**	**23.8°**	*33%*	0	
2:2002	MG	Mg	1	N/A	O_1	**0.09**	**1**	**Poorly Coordinated**	N/A	N/A	0	
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	**0.11**	**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		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2007	MG	Mg	1	N/A	O_1	**0.2**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2008	MG	Mg	1	N/A	O_1	**0.3**	**0.98**	**Poorly Coordinated**	N/A	N/A	0	
2:2009	MG	Mg	1	N/A	O_1	**0.16**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2010	MG	Mg	1	N/A	O_2	**0.2**	**0.72**	**Square Planar**	2.3°	**50%**	0	
2:2011	MG	Mg	1	N/A	O_1	**0.2**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2012	MG	Mg	1	N/A	O_2	**0.3**	**0.71**	**Square Planar**	5.2°	**50%**	0	K
2:2013	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2014	MG	Mg	1	N/A	O_2	**0.3**	**0.65**	**Tetrahedral**	5.7°	**50%**	0	K
2:2015	MG	Mg	1	N/A	N_1	**0.5**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2016	MG	Mg	1	N/A	O_3	**0.5**	**0.67**	Octahedral	12.2°	**50%**	0	
2:2017	MG	Mg	1	N/A	O_2	**0.7**	0.078	**Linear**	5.5°	0	0	
2:2018	MG	Mg	1	N/A	O_1	**0.16**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2019	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2020	MG	Mg	1	N/A	O_1	**0.4**	**0.99**	**Poorly Coordinated**	N/A	N/A	0	
2:2021	MG	Mg	1	N/A	O_2	**0.6**	**0.47**	**Trigonal Planar**	*16.9°*	*33%*	0	
2:2022	MG	Mg	1	N/A	O_1	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2023	MG	Mg	1	N/A	O_1	**0.09**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2024	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2025	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2026	MG	Mg	1	N/A	O_1	**0.17**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2027	MG	Mg	1	N/A	O_1	**0.09**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2029	MG	Mg	1	N/A	O_1	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2030	MG	Mg	1	N/A	O_1	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2031	MG	Mg	1	N/A	O_2	**0.7**	**0.37**	**Trigonal Planar**	*18.5°*	*33%*	0	
2:2032	MG	Mg	1	N/A	O_1	**0.09**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2033	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2034	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2035	MG	Mg	1	N/A	O_1	**0.4**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2036	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2037	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	

2:2038	MG	Mg	1	N/A	**O_1**	**0.14**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2039	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2040	MG	Mg	1	N/A	**O_1**	**0.18**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2041	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2042	MG	Mg	1	N/A	**O_1**	**0.09**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2043	MG	Mg	1	N/A	*O_2*	**0.3**	**0.74**	**Square Planar**	1.1°	**50%**	0	K
2:2044	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2045	MG	Mg	1	N/A	**O_1**	**0.16**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2046	MG	Mg	1	N/A	**O_1**	**0.1**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2047	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2048	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2049	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2050	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2051	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2052	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2053	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2054	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2055	MG	Mg	1	N/A	**O_1**	**0.09**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2056	MG	Mg	1	N/A	O_2	**0.5**	**0.5**	**Trigonal Planar**	*18°*	*33%*	0	
2:2057	MG	Mg	1	N/A	**O_1**	**0.2**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2058	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2060	MG	Mg	1	N/A	**O_1**	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2061	MG	Mg	1	N/A	**O_1**	**0.13**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2062	MG	Mg	1	N/A	**O_1**	**0.11**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2063	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2065	MG	Mg	1	N/A	*O_2*	**0.5**	**0.84**	**Square Planar**	13.3°	**50%**	0	
2:2066	MG	Mg	1	N/A	*O_1*	**0.3**	**0.99**	**Poorly Coordinated**	N/A	N/A	0	
2:2067	MG	Mg	1	N/A	*O_2*	**0.2**	**0.82**	**Square Planar**	*16.9°*	**50%**	0	
2:2068	MG	Mg	1	N/A	**O_1**	**0.2**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2069	MG	Mg	1	N/A	**N_1**	**0.5**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2070	MG	Mg	1	N/A	**O_1**	**0.11**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2071	MG	Mg	1	N/A	*O_2*	**0.4**	**0.8**	**Square Planar**	*14.6°*	**50%**	0	K
2:2072	MG	Mg	1	N/A	**O_1**	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2073	MG	Mg	1	N/A	*O_2*	**0.4**	**0.78**	**Square Planar**	8.8°	**50%**	0	K
2:2074	MG	Mg	1	N/A	O_3	**0.7**	**0.37**	**Square Planar**	12.6°	*25%*	0	Na
2:2075	MG	Mg	1	N/A	*O_2*	**0.4**	**0.79**	**Square Planar**	13.4°	**50%**	0	
2:2076	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2077	MG	Mg	1	N/A	**O_1**	**0.12**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2078	MG	Mg	1	N/A	*O_2*	**0.5**	**0.78**	**Square Planar**	10°	**50%**	0	
2:2079	MG	Mg	1	N/A	**O_1**	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2081	MG	Mg	1	N/A	**O_1**	**0.1**	**1**	**Poorly Coordinated**	N/A	N/A	0	
								Poorly				

2:2082	MG	Mg	1	N/A	**O_1**	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2084	MG	Mg	1	N/A	**O_1**	**0.17**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2085	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2086	MG	Mg	1	N/A	**O_1**	**0.2**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2087	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2088	MG	Mg	1	N/A	**O_1**	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2089	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2090	MG	Mg	1	N/A	O_3	**0.8**	**0.42**	**Square Planar**	11.7°	*25%*	0	Na
2:2091	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2092	MG	Mg	1	N/A	**O_1**	**0.18**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2093	MG	Mg	1	N/A	**O_1**	**0.08**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2094	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2095	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2096	MG	Mg	1	N/A	**O_1**	**0.2**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2097	MG	Mg	1	N/A	**O_1**	**0.11**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2098	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2099	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2100	MG	Mg	1	N/A	**O_1**	**0.12**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2101	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2102	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2103	MG	Mg	1	N/A	**O_1**	**0.08**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2105	MG	Mg	1	N/A	**O_1**	**0.1**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2106	MG	Mg	1	N/A	*O_1*	**0.2**	**0.98**	**Poorly Coordinated**	N/A	N/A	0	
2:2107	MG	Mg	1	N/A	**O_1**	**0.19**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2108	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2109	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2110	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2111	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2112	MG	Mg	1	N/A	**O_1**	**0.11**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2113	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2114	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2115	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2116	MG	Mg	1	N/A	**O_1**	**0.4**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2118	MG	Mg	1	N/A	**N_1**	**0.17**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2119	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2120	MG	Mg	1	N/A	**O_1**	**0.2**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2121	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2122	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2123	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2124	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2125	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2126	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2127	MG	Mg	1	N/A	*O_2*	**0.18**	**0.75**	**Square Planar**	7°	**50%**	0	
2:2128	MG	Mg	1	N/A	**O_1**	**0.17**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2129	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2130	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	

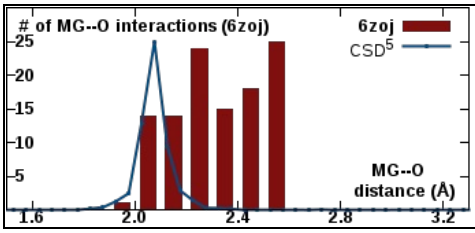
2:2131	MG	Mg	1	N/A	O_2	**0.3**	**0.82**	**Square Planar**	*15.4°*	**50%**	0	K
2:2132	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2134	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2135	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2136	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2137	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2138	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2139	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2140	MG	Mg	1	N/A	**O_1**	**0.1**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2141	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2142	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2143	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2144	MG	Mg	1	N/A	**O_1**	**0.18**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2145	MG	Mg	1	N/A	O_2	**0.4**	**0.87**	**Square Planar**	*17.1°*	**50%**	0	
2:2146	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2147	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2148	MG	Mg	1	N/A	**O_1**	**0.4**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2149	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2150	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2151	MG	Mg	1	N/A	**O_1**	**0.08**	**1**	**Poorly Coordinated**	N/A	N/A	0	
2:2152	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2153	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2154	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2155	MG	Mg	1	N/A	O_2	**0.2**	**0.65**	**Tetrahedral**	8.6°	**50%**	0	
2:2156	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2157	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2158	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
2:2159	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
G:301	MG	Mg	1	N/A	**O_1**	**0.3**	**1**	**Poorly Coordinated**	N/A	N/A	0	
O:201	MG	Mg	1	N/A	**O_1**	**0.08**	**1**	**Poorly Coordinated**	N/A	N/A	0	
O:202	MG	Mg	1	N/A	O_3	**0.7**	**0.7**	**Tetrahedral**	**27.7°**	*25%*	0	Na
S:201	MG	Mg	1	N/A		N/A	N/A	**Free**	N/A	N/A	N/A	
S:202	MG	Mg	1	N/A	O_3	**0.4**	**0.37**	**Square Planar**	*13.9°*	*25%*	0	K
T:201	MG	Mg	1	N/A	O_2	**0.3**	**0.74**	**Square Planar**	5.2°	**50%**	0	K
X:2301	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	0.033	Tetrahedral	1.7°	0	0	
d:201	ZN	Zn	1	N/A	S_4	2.3	0.081	Tetrahedral	3°	0	0	
f:500	ZN	Zn	1	N/A	S_4	2.1	0.08	Tetrahedral	1.7°	0	0	

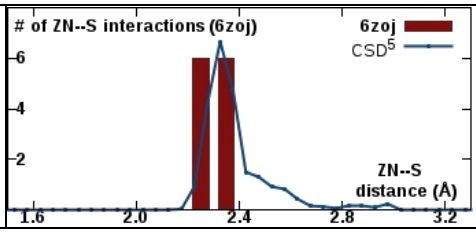
Legend: Not applicable | **Outlier** | *Borderline* | Acceptable

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
	A list of alternative metal(s) is proposed in descending order of confidency, assuming metal

Alt. metal	environment is accurately determined. This feature is still experimental. It requires user discrimination and cannot be blindly accepted

Metal-ligand distance distributions for pdb6zoj.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>

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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.