

PMCA

ATA-Mg

1°pose = -9,6 kcal/mol

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	770A	PRO	3.82	9226	5936

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	477A	THR	3.30	4.07	136.20	✓	✗	3629 [Nam]	9242 [O2]
2	477A	THR	2.92	3.45	114.99	✓	✓	3632 [O3]	9242 [O2]
3	708A	THR	2.73	3.64	156.67	✓	✓	5438 [O3]	9242 [O2]
4	709A	GLY	3.10	3.96	146.89	✓	✗	5442 [Nam]	9242 [O2]
5	768A	SER	3.51	3.98	112.36	✓	✓	5923 [O3]	9238 [O3]

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, linear (2)						
1	1Z	LIG	9220	9221	2.00	ligand
2	1Z	LIG	9220	9222	1.66	ligand
Complex 2: Mg, tetrahedral (4)						
5	1Z	LIG	9240	9241	1.65	ligand
6	1Z	LIG	9240	9238	2.11	ligand
7	475A	ASP	9240	3616	2.35	protein.sidechain
8	707A	VAL	9240	5434	2.53	protein.mainchain
Complex 3: Mg, linear (2)						
3	1Z	LIG	9251	9252	1.65	ligand
4	1Z	LIG	9251	9249	2.15	ligand

2°pose = -9,5 kcal/mol

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	800A	ASN	3.66	9248	6153

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	477A	THR	2.79	3.59	139.14	✓	✗	3629 [Nam]	9242 [O2]
2	477A	THR	2.75	3.17	107.45	✓	✓	3632 [O3]	9242 [O2]
3	582A	ARG	3.20	3.96	135.23	✓	✓	4466 [Ng+]	9221 [O3]
4	768A	SER	3.64	4.05	108.40	✓	✓	5923 [O3]	9238 [O3]
5	799A	THR	1.97	2.85	148.38	✓	✗	6144 [Nam]	9249 [O3]
6	800A	ASN	2.99	3.86	148.51	✓	✗	6151 [Nam]	9249 [O3]

π-Cation Interactions

Index	Residue	AA	Distance	Offset	Protein charged?	Ligand Group	Ligand Atoms
1	582A	ARG	4.23	1.54	✓	Aromatic	9225, 9226, 9227, 9228, 9229, 9230

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	4.36	✓	Carboxylate	9252, 9253

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, linear (2)						
3	1Z	LIG	9220	9221	2.00	ligand
4	1Z	LIG	9220	9222	1.66	ligand
Complex 2: Mg, tetrahedral (4)						
5	1Z	LIG	9240	9241	1.65	ligand
6	1Z	LIG	9240	9238	2.11	ligand
7	475A	ASP	9240	3616	2.43	protein.sidechain
8	707A	VAL	9240	5434	2.42	protein.mainchain
Complex 3: Mg, linear (2)						
1	1Z	LIG	9251	9252	1.65	ligand
2	1Z	LIG	9251	9249	2.15	ligand

3°pose = -9,3 kcal/mol

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	581A	VAL	3.56	9229	4456
2	581A	VAL	3.41	9230	4455
3	800A	ASN	3.65	9248	6153

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	799A	THR	1.97	2.79	141.23	✓	✓	6147 [O3]	9221 [O3]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	4.68	✓	Carboxylate	9241, 9242
2	582A	ARG	4.91	✓	Carboxylate	9252, 9253

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9220	9221	2.00	ligand
2	1Z	LIG	9220	9222	1.66	ligand
7	220A	TYR	9220	1680	2.39	protein.mainchain
Complex 2: Mg, linear (2)						
3	1Z	LIG	9240	9241	1.65	ligand
4	1Z	LIG	9240	9238	2.11	ligand
Complex 3: Mg, linear (2)						
5	1Z	LIG	9251	9252	1.65	ligand
6	1Z	LIG	9251	9249	2.14	ligand

4°pose = -9,2 kcal/mol

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	800A	ASN	3.53	9237	6153

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	477A	THR	2.88	3.69	139.54	✓	✗	3629 [Nam]	9253 [O2]
2	477A	THR	2.90	3.22	100.49	✓	✓	3632 [O3]	9253 [O2]
3	768A	SER	3.68	4.08	107.48	✓	✓	5923 [O3]	9249 [O3]
4	799A	THR	2.01	2.85	141.51	✓	✗	6144 [Nam]	9238 [O3]
5	800A	ASN	2.86	3.76	152.21	✓	✗	6151 [Nam]	9238 [O3]

π-Cation Interactions

Index	Residue	AA	Distance	Offset	Protein charged?	Ligand Group	Ligand Atoms
1	582A	ARG	4.25	0.23	✓	Aromatic	9225, 9226, 9227, 9228, 9229, 9230

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	5.41	✓	Carboxylate	9222, 9223
2	582A	ARG	4.24	✓	Carboxylate	9241, 9242

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, linear (2)						
3	1Z	LIG	9220	9221	2.01	ligand
4	1Z	LIG	9220	9222	1.66	ligand
Complex 2: Mg, linear (2)						
1	1Z	LIG	9240	9241	1.65	ligand
2	1Z	LIG	9240	9238	2.11	ligand
Complex 3: Mg, tetrahedral (4)						
5	1Z	LIG	9251	9252	1.65	ligand
6	1Z	LIG	9251	9249	2.14	ligand
7	475A	ASP	9251	3616	2.46	protein.sidechain
8	707A	VAL	9251	5434	2.43	protein.mainchain

5°pose = -9,1 kcal/mol

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	476A	LYS	3.34	4.05	130.39	✓	×	3620 [Nam]	9238 [O3]
2	582A	ARG	2.98	3.64	124.92	✓	✓	4466 [Ng+]	9253 [O2]
3	799A	THR	3.36	3.97	121.89	✓	×	6144 [Nam]	9223 [O2]

π-Cation Interactions

Index	Residue	AA	Distance	Offset	Protein charged?	Ligand Group	Ligand Atoms
1	582A	ARG	4.43	1.85	✓	Aromatic	9225, 9226, 9227, 9228, 9229, 9230

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	773A	LYS	5.26	✓	Carboxylate	9241, 9242

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, linear (2)						
1	1Z	LIG	9220	9221	2.00	ligand
2	1Z	LIG	9220	9222	1.66	ligand
Complex 2: Mg, trigonal.planar (3)						
5	1Z	LIG	9240	9241	1.65	ligand
6	1Z	LIG	9240	9238	2.11	ligand
7	707A	VAL	9240	5434	2.21	protein.mainchain
Complex 3: Mg, trigonal.pyramidal (3)						
3	1Z	LIG	9251	9252	1.65	ligand
4	1Z	LIG	9251	9249	2.15	ligand
8	709A	GLY	9251	5445	2.61	protein.mainchain

6°pose = -9,1 kcal/mol

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	770A	PRO	3.67	9228	5936
2	800A	ASN	3.81	9230	6153

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	477A	THR	2.82	3.66	144.07	✓	✗	3629 [Nam]	9253 [O2]
2	477A	THR	3.01	3.38	104.25	✓	✓	3632 [O3]	9253 [O2]
3	768A	SER	3.52	3.98	111.60	✓	✓	5923 [O3]	9249 [O3]
4	799A	THR	2.33	3.01	125.37	✓	✗	6144 [Nam]	9221 [O3]
5	800A	ASN	2.64	3.59	163.72	✓	✗	6151 [Nam]	9221 [O3]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	5.12	✓	Carboxylate	9241 , 9242

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, linear (2)						
1	1Z	LIG	9220	9221	2.00	ligand
2	1Z	LIG	9220	9222	1.66	ligand
Complex 2: Mg, linear (2)						
3	1Z	LIG	9240	9241	1.65	ligand
4	1Z	LIG	9240	9238	2.11	ligand
Complex 3: Mg, tetrahedral (4)						
5	1Z	LIG	9251	9252	1.65	ligand
6	1Z	LIG	9251	9249	2.14	ligand
7	475A	ASP	9251	3616	2.54	protein.sidechain
8	707A	VAL	9251	5434	2.20	protein.mainchain

7°pose = -9,0 kcal/mol

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	581A	VAL	3.22	9245	4455
2	581A	VAL	3.98	9248	4456
3	770A	PRO	3.95	9233	5936

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	773A	LYS	3.58	3.92	102.16	✓	✓	5960 [N3]	9221 [O3]
2	799A	THR	2.48	2.93	107.78	✓	✓	6147 [O3]	9249 [O3]

π-Cation Interactions

Index	Residue	AA	Distance	Offset	Protein charged?	Ligand Group	Ligand Atoms
1	582A	ARG	5.51	1.57	✓	Aromatic	9225, 9226, 9227, 9228, 9229, 9230

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, tetrahedral (4)						
5	1Z	LIG	9220	9221	2.00	ligand
6	1Z	LIG	9220	9222	1.66	ligand
7	475A	ASP	9220	3616	2.70	protein.sidechain
9	801A	ASP	9220	6164	2.73	protein.sidechain
Complex 2: Mg, linear (2)						
3	1Z	LIG	9240	9241	1.65	ligand
4	1Z	LIG	9240	9238	2.11	ligand
Complex 3: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9251	9252	1.65	ligand
2	1Z	LIG	9251	9249	2.15	ligand
8	799A	THR	9251	6147	2.46	protein.sidechain

8°pose = -9,0 kcal/mol

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	581A	VAL	3.44	9228	4456
2	581A	VAL	3.66	9245	4456
3	581A	VAL	3.72	9248	4456
4	819A	THR	3.77	9245	6282

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	799A	THR	2.78	3.61	144.42	✓	✓	6147 [O3]	9253 [O2]
2	799A	THR	2.99	3.81	141.38	✓	✗	6144 [Nam]	9249 [O3]

π-Stacking

Index	Residue	AA	Distance	Angle	Offset	Stacking Type	Ligand Atoms
1	220A	TYR	5.00	75.10	1.09	T	9225, 9226, 9227, 9228, 9229, 9230

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	219A	LYS	4.01	✓	Carboxylate	9241, 9242

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9220	9221	2.00	ligand
2	1Z	LIG	9220	9222	1.66	ligand
7	220A	TYR	9220	1676	2.36	protein.sidechain
Complex 2: Mg, linear (2)						
3	1Z	LIG	9240	9241	1.65	ligand
4	1Z	LIG	9240	9238	2.11	ligand
Complex 3: Mg, linear (2)						
5	1Z	LIG	9251	9252	1.65	ligand
6	1Z	LIG	9251	9249	2.15	ligand

9°pose = -8,9 kcal/mol

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	220A	TYR	3.88	9244	1673
2	581A	VAL	3.28	9228	4456
3	581A	VAL	3.71	9245	4454
4	581A	VAL	3.49	9248	4456
5	819A	THR	3.55	9232	6282
6	819A	THR	3.49	9243	6282

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	799A	THR	2.99	3.83	145.87	✓	✓	6147 [O3]	9253 [O2]
2	799A	THR	2.62	3.59	166.65	✓	✗	6144 [Nam]	9249 [O3]

π-Stacking

Index	Residue	AA	Distance	Angle	Offset	Stacking Type	Ligand Atoms
1	220A	TYR	4.81	68.05	1.09	T	9225, 9226, 9227, 9228, 9229, 9230

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9220	9221	2.00	ligand
2	1Z	LIG	9220	9222	1.66	ligand
7	220A	TYR	9220	1676	2.44	protein.sidechain
Complex 2: Mg, linear (2)						
3	1Z	LIG	9240	9241	1.65	ligand
4	1Z	LIG	9240	9238	2.11	ligand
Complex 3: Mg, linear (2)						
5	1Z	LIG	9251	9252	1.65	ligand
6	1Z	LIG	9251	9249	2.14	ligand

10°pose = -8,9 kcal/mol

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	581A	VAL	3.48	9230	4455
2	581A	VAL	3.54	9226	4456
3	819A	THR	3.62	9226	6282

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	797A	ASP	2.55	3.35	143.34	✓	✓	6137 [O3]	9242 [O2]
2	799A	THR	1.98	2.80	140.59	✓	✓	6147 [O3]	9221 [O3]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	219A	LYS	5.48	✓	Carboxylate	9222, 9223
2	582A	ARG	3.50	✓	Carboxylate	9252, 9253

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9220	9221	2.00	ligand
2	1Z	LIG	9220	9222	1.66	ligand
7	220A	TYR	9220	1680	2.34	protein.mainchain
Complex 2: Mg, linear (2)						
3	1Z	LIG	9240	9241	1.65	ligand
4	1Z	LIG	9240	9238	2.11	ligand
Complex 3: Mg, linear (2)						
5	1Z	LIG	9251	9252	1.65	ligand
6	1Z	LIG	9251	9249	2.14	ligand