

PMCA

ATP-Mg

1°pose = -9,3 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	2.04	2.87	140.17	✓	×	3620 [Nam]	9235 [O3]
2	477A	THR	2.22	2.87	123.19	✓	✓	3632 [O3]	9238 [O3]
3	477A	THR	2.43	3.33	152.14	✓	×	3629 [Nam]	9235 [O3]
4	708A	THR	2.22	3.16	161.81	×	✓	9238 [O3]	5438 [O3]
5	708A	THR	2.64	3.55	156.07	✓	✓	5438 [O3]	9235 [O3]
6	709A	GLY	3.04	4.00	166.23	✓	×	5442 [Nam]	9238 [O3]
7	797A	ASP	2.26	3.21	166.25	×	✓	9251 [O3]	6136 [O2]
8	799A	THR	2.99	3.34	102.84	✓	✓	6147 [O3]	9250 [Npl]
9	799A	THR	3.30	4.04	133.53	✓	×	6144 [Nam]	9248 [Nar]
10	801A	ASP	2.85	3.42	118.63	×	✓	9240 [O3]	6164 [O2]
11	801A	ASP	2.43	3.26	142.78	×	✓	9228 [O3]	6164 [O2]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	476A	LYS	5.47	✓	Phosphate	9236, 9236, 9235, 9237, 9238, 9239
2	773A	LYS	4.71	✓	Phosphate	9227, 9227, 9226, 9228, 9229, 9230

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.planar (3)						
1	1Z	LIG	9234	9233	2.12	ligand
2	1Z	LIG	9234	9235	2.12	ligand
3	475A	ASP	9234	3616	2.23	protein.sidechain

2°pose = -9,0 kcal/mol

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	475A	ASP	2.98	3.64	127.03	✗	✓	9240 [O3]	3616 [O2]
2	476A	LYS	2.25	3.14	148.93	✓	✗	3620 [Nam]	9232 [O2]
3	477A	THR	2.32	2.94	121.24	✓	✓	3632 [O3]	9239 [O3]
4	477A	THR	2.79	3.66	148.12	✓	✗	3629 [Nam]	9232 [O2]
5	708A	THR	2.31	3.22	155.02	✓	✓	5438 [O3]	9232 [O2]
6	709A	GLY	2.92	3.89	167.40	✓	✗	5442 [Nam]	9239 [O3]
7	710A	ASP	2.78	3.72	162.00	✗	✓	9238 [O3]	5450 [O2]
8	773A	LYS	3.59	3.94	102.64	✓	✓	5960 [N3]	9240 [O3]
9	797A	ASP	2.11	2.97	146.53	✗	✓	9251 [O3]	6136 [O2]
10	798A	GLY	3.73	4.05	101.93	✓	✗	6140 [Nam]	9251 [O3]
11	799A	THR	2.84	3.73	150.32	✓	✗	6144 [Nam]	9244 [Nar]
12	800A	ASN	2.44	2.98	113.43	✗	✓	9250 [Npl]	6155 [O2]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	476A	LYS	4.12	✓	Phosphate	9236, 9236, 9235, 9237, 9238, 9239
2	582A	ARG	5.29	✓	Phosphate	9236, 9236, 9235, 9237, 9238, 9239

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9234	9226	2.49	ligand
2	1Z	LIG	9234	9233	2.12	ligand
3	1Z	LIG	9234	9235	2.12	ligand

3°pose = -8,9 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	2.06	2.88	139.49	✓	×	3620 [Nam]	9235 [O3]
2	477A	THR	2.32	2.96	122.54	✓	✓	3632 [O3]	9238 [O3]
3	477A	THR	2.39	3.29	150.85	✓	×	3629 [Nam]	9235 [O3]
4	582A	ARG	2.86	3.27	105.95	✓	✓	4467 [Ng+]	9244 [Nar]
5	708A	THR	2.19	3.12	160.77	×	✓	9238 [O3]	5438 [O3]
6	708A	THR	2.58	3.50	157.03	✓	✓	5438 [O3]	9235 [O3]
7	709A	GLY	2.93	3.89	166.49	✓	×	5442 [Nam]	9238 [O3]
8	799A	THR	2.64	3.24	120.15	✓	×	6144 [Nam]	9240 [O3]
9	800A	ASN	2.25	3.10	144.24	✓	×	6151 [Nam]	9240 [O3]
10	801A	ASP	2.25	3.08	143.10	×	✓	9228 [O3]	6164 [O2]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	476A	LYS	5.45	✓	Phosphate	9236, 9236, 9235, 9237, 9238, 9239
2	773A	LYS	4.71	✓	Phosphate	9227, 9227, 9226, 9228, 9229, 9230

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9234	9233	2.12	ligand
2	1Z	LIG	9234	9235	2.12	ligand
3	475A	ASP	9234	3616	2.24	protein.sidechain

4°pose = -8,9 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	1.98	2.80	138.78	✓	✗	3620 [Nam]	9235 [O3]
2	477A	THR	2.17	2.85	125.95	✓	✓	3632 [O3]	9238 [O3]
3	477A	THR	2.36	3.25	151.14	✓	✗	3629 [Nam]	9235 [O3]
4	708A	THR	2.13	3.07	163.25	✗	✓	9238 [O3]	5438 [O3]
5	708A	THR	2.64	3.55	155.74	✓	✓	5438 [O3]	9235 [O3]
6	709A	GLY	3.03	4.00	167.85	✓	✗	5442 [Nam]	9238 [O3]
7	797A	ASP	2.67	3.60	161.20	✗	✓	9251 [O3]	6136 [O2]
8	799A	THR	2.57	3.47	151.68	✓	✗	6144 [Nam]	9245 [Nar]
9	800A	ASN	2.67	3.06	103.58	✗	✓	9250 [Npl]	6155 [O2]
10	801A	ASP	3.02	3.51	112.32	✗	✓	9240 [O3]	6164 [O2]
11	801A	ASP	2.48	3.31	144.44	✗	✓	9228 [O3]	6164 [O2]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	476A	LYS	5.38	✓	Phosphate	9236, 9236, 9235, 9237, 9238, 9239
2	773A	LYS	4.81	✓	Phosphate	9227, 9227, 9226, 9228, 9229, 9230

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9234	9233	2.12	ligand
2	1Z	LIG	9234	9235	2.12	ligand
3	475A	ASP	9234	3616	2.23	protein.sidechain

5°pose = -8,7 kcal/mol

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	475A	ASP	3.40	3.83	109.40	✗	✓	9240 [O3]	3616 [O2]
2	475A	ASP	3.17	3.91	134.51	✗	✓	9238 [O3]	3616 [O2]
3	476A	LYS	2.41	2.99	117.58	✓	✗	3620 [Nam]	9235 [O3]
4	477A	THR	3.25	3.85	121.25	✓	✓	3632 [O3]	9233 [O3]
5	477A	THR	1.83	2.81	172.64	✓	✗	3629 [Nam]	9235 [O3]
6	582A	ARG	3.65	4.02	105.44	✓	✓	4467 [Ng+]	9226 [O3]
7	708A	THR	2.22	2.90	125.98	✓	✓	5438 [O3]	9233 [O3]
8	709A	GLY	2.07	3.01	160.41	✓	✗	5442 [Nam]	9233 [O3]
9	768A	SER	3.01	3.83	142.69	✗	✗	9229 [O3]	5925 [O2]
10	797A	ASP	2.47	3.18	128.98	✗	✓	9251 [O3]	6136 [O2]
11	798A	GLY	3.50	3.87	104.37	✓	✗	6140 [Nam]	9251 [O3]
12	799A	THR	2.83	3.74	153.44	✓	✗	6144 [Nam]	9244 [Nar]
13	800A	ASN	2.63	3.27	123.01	✗	✓	9250 [Npl]	6155 [O2]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	5.33	✓	Phosphate	9231, 9231, 9230, 9233, 9239, 9232

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9234	9233	2.12	ligand
2	1Z	LIG	9234	9235	2.12	ligand
3	708A	THR	9234	5438	2.41	protein.sidechain

6°pose = -8,7 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	2.37	3.06	126.30	✓	×	3620 [Nam]	9238 [O3]
2	477A	THR	2.29	2.86	116.19	×	×	9250 [Npl]	3635 [O2]
3	477A	THR	3.11	3.77	126.98	✓	✓	3632 [O3]	9235 [O3]
4	477A	THR	2.00	2.93	155.77	✓	×	3629 [Nam]	9238 [O3]
5	707A	VAL	3.16	4.00	144.97	×	×	9238 [O3]	5434 [O2]
6	708A	THR	2.87	3.82	166.19	✓	✓	5438 [O3]	9238 [O3]
7	709A	GLY	2.14	3.09	161.57	✓	×	5442 [Nam]	9235 [O3]
8	799A	THR	2.32	3.04	128.87	✓	×	6144 [Nam]	9251 [O3]
9	800A	ASN	2.49	3.13	121.99	✓	×	6151 [Nam]	9251 [O3]

▼ π-Cation Interactions

Index	Residue	AA	Distance	Offset	Protein charged?	Ligand Group	Ligand Atoms
1	582A	ARG	5.78	1.45	✓	Aromatic	9241, 9242, 9243, 9245, 9247

▼ Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	5.40	✓	Phosphate	9227, 9227, 9226, 9228, 9229, 9230
2	582A	ARG	4.33	✓	Phosphate	9231, 9231, 9230, 9233, 9239, 9232

▼ Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, linear (2)						
1	1Z	LIG	9234	9233	2.12	ligand
2	1Z	LIG	9234	9235	2.12	ligand

7°pose = -8,7 kcal/mol

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	475A	ASP	2.27	3.18	155.14	✗	✓	9251 [O3]	3616 [O2]
2	477A	THR	3.03	3.99	167.17	✓	✗	3629 [Nam]	9244 [Nar]
3	477A	THR	2.78	3.46	127.35	✓	✓	3632 [O3]	9248 [Nar]
4	582A	ARG	3.12	3.74	122.98	✓	✓	4467 [Ng+]	9245 [Nar]
5	708A	THR	2.03	2.92	151.59	✓	✓	5438 [O3]	9248 [Nar]
6	709A	GLY	2.63	3.55	156.72	✓	✗	5442 [Nam]	9248 [Nar]
7	797A	ASP	2.70	3.31	123.33	✓	✓	6137 [O3]	9235 [O3]
8	797A	ASP	3.26	4.05	139.05	✓	✗	6132 [Nam]	9240 [O3]
9	798A	GLY	2.56	3.00	106.46	✓	✗	6140 [Nam]	9240 [O3]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	4.69	✓	Phosphate	9227, 9227, 9226, 9228, 9229, 9230
2	582A	ARG	4.73	✓	Phosphate	9231, 9231, 9230, 9233, 9239, 9232

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9234	9233	2.12	ligand
2	1Z	LIG	9234	9235	2.12	ligand
3	797A	ASP	9234	6137	2.62	protein.sidechain

8°pose = -8,4 kcal/mol

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	475A	ASP	2.33	3.00	125.82	✗	✓	9251 [O3]	3616 [O2]
2	476A	LYS	3.20	3.55	101.60	✓	✓	3626 [N3]	9250 [Npl]
3	476A	LYS	2.57	3.55	173.92	✗	✓	9250 [Npl]	3626 [N3]
4	477A	THR	2.86	3.50	124.09	✓	✗	3629 [Nam]	9248 [Nar]
5	477A	THR	2.35	3.11	134.32	✓	✓	3632 [O3]	9248 [Nar]
6	582A	ARG	3.43	4.06	123.30	✓	✓	4466 [Ng+]	9245 [Nar]
7	708A	THR	1.99	2.91	158.61	✓	✓	5438 [O3]	9248 [Nar]
8	709A	GLY	3.06	3.99	158.46	✓	✗	5442 [Nam]	9248 [Nar]
9	797A	ASP	2.95	3.47	116.27	✓	✓	6137 [O3]	9235 [O3]
10	799A	THR	2.94	3.85	155.09	✓	✗	6144 [Nam]	9230 [O3]
11	800A	ASN	3.12	3.51	105.80	✗	✓	9228 [O3]	6155 [O2]
12	800A	ASN	2.09	3.03	159.72	✓	✗	6151 [Nam]	9229 [O2]

Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	4.78	✓	Phosphate	9231, 9231, 9230, 9233, 9239, 9232

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9234	9233	2.12	ligand
2	1Z	LIG	9234	9235	2.12	ligand
3	797A	ASP	9234	6137	2.46	protein.sidechain

9°pose = -8,4 kcal/mol

▼ Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	475A	ASP	2.64	3.25	120.78	✗	✓	9251 [O3]	3616 [O2]
2	476A	LYS	3.33	4.04	128.64	✓	✓	3626 [N3]	9250 [Npl]
3	477A	THR	2.11	3.00	148.62	✗	✓	9250 [Npl]	3632 [O3]
4	477A	THR	3.23	3.92	128.01	✓	✗	3629 [Nam]	9245 [Nar]
5	477A	THR	2.53	3.05	114.19	✓	✓	3632 [O3]	9245 [Nar]
6	582A	ARG	2.16	3.04	148.80	✓	✓	4466 [Ng+]	9248 [Nar]
7	582A	ARG	3.16	3.87	130.00	✓	✓	4467 [Ng+]	9248 [Nar]
8	708A	THR	2.69	3.58	152.46	✓	✓	5438 [O3]	9245 [Nar]
9	709A	GLY	3.18	4.09	155.07	✓	✗	5442 [Nam]	9245 [Nar]
10	768A	SER	3.36	3.90	117.01	✓	✓	5923 [O3]	9251 [O3]
11	799A	THR	2.47	3.36	149.43	✓	✗	6144 [Nam]	9238 [O2]
12	800A	ASN	2.34	3.20	145.22	✓	✗	6151 [Nam]	9232 [O2]
13	801A	ASP	2.85	3.32	110.33	✓	✗	6159 [Nam]	9232 [O2]
14	801A	ASP	2.46	3.05	119.46	✗	✓	9240 [O3]	6164 [O2]

▼ Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	4.50	✓	Phosphate	9227, 9227, 9226, 9228, 9229, 9230

▼ Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9234	9229	2.69	ligand
2	1Z	LIG	9234	9233	2.12	ligand
3	1Z	LIG	9234	9235	2.12	ligand

10°pose = -8,3 kcal/mol

▼ Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	477A	THR	3.52	3.94	108.05	✓	×	3629 [Nam]	9251 [O3]
2	477A	THR	2.33	2.72	103.49	×	×	9251 [O3]	3635 [O2]
3	768A	SER	2.38	3.14	133.79	×	×	9250 [Npl]	5925 [O2]
4	799A	THR	2.40	3.32	156.18	✓	×	6144 [Nam]	9229 [O3]
5	800A	ASN	2.20	3.08	148.37	✓	×	6151 [Nam]	9228 [O2]

▼ Salt Bridges

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	582A	ARG	4.38	✓	Phosphate	9231, 9231, 9230, 9233, 9239, 9232
2	582A	ARG	5.12	✓	Phosphate	9236, 9236, 9235, 9237, 9238, 9239

▼ Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Mg, trigonal.pyramidal (3)						
1	1Z	LIG	9234	9228	2.71	ligand
2	1Z	LIG	9234	9233	2.12	ligand
3	1Z	LIG	9234	9235	2.12	ligand