

Supplementary Materials

D- Mannoside FimH inhibitors as non-antibiotic alternatives for Uropathogenic *Escherichia coli*

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Table S1. Molecular coupling results obtained from the 4X5P code protein with the ligand b made in the AutoDock Vina software package.

Protein 4X5P			
Position s Ligand b	Afinity (kcal/ mol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.7	0.000	0.000
2	-6.7	0.462	1.215
3	-6.6	1.334	2.107
4	-6.6	1.346	1.847
5	-6.4	1.958	2.657
6	-6.4	0.882	1.394
7	-6.2	2.064	3.256
8	-6.1	1.208	1.863
9	-6.1	1.590	2.026

Table S2. Molecular coupling results obtained from the 4X5P code protein with the ligand c made in the AutoDock Vina software package.

Protein 4X5P			
Positions Ligand c	Afinity (kcal/ mol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.8	0.000	0.000
2	-6.8	1.102	1.900
3	-6.7	0.371	1.605
4	-6.6	1.629	2.341
5	-6.4	1.818	3.325
6	-6.4	1.171	1.971
7	-6.2	2.384	3.326
8	-6.1	1.749	3.517
9	-6.1	1.767	2.451

Table S3. Molecular coupling results obtained from the 4X5P code protein with the ligand d made in the AutoDock Vina software package.

Protein 4X5P			
Positio ns Ligand d	Afinity (kcal/ mol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-7.0	0.000	0.000
2	-6.9	0.096	1.111
3	-6.7	1.395	2.131
4	-6.7	1.418	1.921
5	-6.4	0.893	1.013
6	-6.4	2.048	2.772
7	-6.3	2.019	2.727
8	-6.2	2.136	3.183
9	-6.2	1.783	2.456

Table S4. Molecular coupling results obtained from the 4X5P code protein with the ligand e made in the AutoDock Vina software package.

Protein 4X5P			
Positio ns Ligand e	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.8	0.000	0.000
2	-6.8	0.080	1.117
3	-6.6	1.470	2.079
4	-6.6	1.500	1.858
5	-6.4	1.193	1.213
6	-6.3	2.301	2.776
7	-6.2	2.096	3.151
8	-6.1	2.577	3.014
9	-6.1	1.526	1.761

Table S5. Molecular coupling results obtained from the 4X5P code protein with the ligand f made in the AutoDock Vina software package.

Protein 4X5P			
Position s Ligand f	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.5	0.000	0.000
2	-6.3	1.437	1.750
3	-6.2	2.041	2.268
4	-6.2	1.374	2.007
5	-5.9	1.897	3.476
6	-5.9	2.080	3.134
7	-5.8	3.481	2.808
8	-5.7	2.204	3.054
9	-5.5	2.704	3.481

Table S7. Molecular coupling results obtained from the 4X5P code protein with the ligand h made in the AutoDock Vina software package.

Protein 4X5P			
Positions Ligand h	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.7	0.000	0.000
2	-6.5	2.166	3.111
3	-6.4	1.595	1.978
4	-6.3	1.189	1.325
5	-6.3	2.863	4.398
6	-6.3	1.419	1.938
7	-6.2	2.636	3.280
8	-6.1	27.602	29.642
9	-6.1	2.019	3.138

Table S6. Molecular coupling results obtained from the 4X5P code protein with the ligand g made in the AutoDock Vina software package.

Protein 4X5P			
Positions Ligand g	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.5	0.000	0.000
2	-6.5	2.411	2.812
3	-6.5	1.194	1.625
4	-6.4	1.782	3.080
5	-6.4	2.435	4.035
6	-6.4	2.023	3.354
7	-6.3	3.392	5.425
8	-6.2	2.061	2.570
9	-6.2	3.317	4.444

Table S8. Molecular coupling results obtained from the 4X5P code protein with the ligand i made in the AutoDock Vina software package.

Protein 4X5P			
Positions Ligand i	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.6	0.000	0.000
2	-6.6	0.525	1.343
3	-6.5	1.984	2.702
4	-6.5	1.954	2.467
5	-6.1	2.705	3.685
6	-6.1	2.902	3.669
7	-6.0	1.672	2.607
8	-5.9	1.555	3.073
9	-5.9	1.554	1.765

Table S9. Molecular coupling results obtained from the 4X5P code protein with the ligand j made in the AutoDock Vina software package.

Protein 4X5P			
Position s Ligand j	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.5	0.000	0.000
2	-6.5	0.366	3.804
3	-6.5	1.670	2.217
4	-6.4	0.945	3.572
5	-6.4	0.971	1.121
6	-6.4	1.479	4.061
7	-6.3	2.081	4.455
8	-6.3	1.623	2.591
9	-6.2	1.288	1.538

Table S10. Molecular coupling results obtained from the 4X5P code protein with the ligand k made in the AutoDock Vina software package.

Protein 4X5P			
Positions Ligand k	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.7	0.000	0.000
2	-6.4	2.370	3.483
3	-6.4	1.218	1.629
4	-6.4	1.910	2.484
5	-6.3	1.599	2.240
6	-6.3	1.411	2.324
7	-6.3	2.113	2.483
8	-6.2	2.207	2.525
9	-6.0	1.908	3.561

Table S11. Molecular coupling results obtained from the 4XO9 code protein with the ligand b made in the AutoDock Vina software package.

Protein 4XO9			
Position s Ligand b	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.6	0.000	0.000
2	-6.6	0.050	1.144
3	-6.3	67.290	69.678
4	-6.0	2.167	3.980
5	-6.0	38.312	40.132
6	-5.9	1.852	5.723
7	-5.9	58.754	60.174
8	-5.9	36.749	38.576
9	-5.8	1.832	2.582

Table S12. Molecular coupling results obtained from the 4XO9 code protein with the ligand c made in the AutoDock Vina software package.

Protein 4XO9			
Position s Ligand c	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.9	0.000	0.000
2	-6.9	0.570	1.554
3	-6.5	1.390	1.995
4	-6.5	67.010	69.893
5	-6.3	2.213	3.964
6	-6.2	1.623	2.589
7	-6.2	2.017	6.040
8	-6.2	38.193	40.243
9	-6.1	38.360	40.410

Table S13. Molecular coupling results obtained from the 4XO9 code protein with the ligand d made in the AutoDock Vina software package.

Protein 4XO9			
Position s Ligand d	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.7	0.000	0.000
2	-6.4	1.826	2.232
3	-6.3	1.666	2.030
4	-6.2	67.289	69.356
5	-6.1	2.786	4.556
6	-6.1	2.550	6.132
7	-6.0	58.315	59.666
8	-6.0	36.846	38.540
9	-5.9	38.163	39.822

Table S14. Molecular coupling results obtained from the 4XO9 code protein with the ligand e made in the AutoDock Vina software package.

Protein 4XO9			
Position s Ligand e	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.9	0.000	0.000
2	-6.9	0.063	1.109
3	-6.8	0.981	1.531
4	-6.4	1.055	1.617
5	-6.4	67.657	69.915
6	-6.2	1.802	2.712
7	-6.1	38.501	40.246
8	-6.0	37.026	38.784
9	-5.9	58.652	60.016

Table S15. Molecular coupling results obtained from the 4XO9 code protein with the ligand f made in the AutoDock Vina software package.

Protein 4XO9			
Position s Ligand f	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.6	0.000	0.000
2	-6.6	0.159	1.125
3	-6.3	67.672	69.913
4	-6.1	1.035	1.595
5	-6.0	1.825	2.716
6	-6.0	38.537	40.228
7	-5.9	37.087	38.790
8	-5.8	58.725	60.055
9	-5.8	36.330	38.028

Table S16. Molecular coupling results obtained from the 4XO9 code protein with the ligand g made in the AutoDock Vina software package.

Protein 4XO9			
Position s Ligand g	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.8	0.000	0.000
2	-6.8	0.527	1.137
3	-6.6	37.106	39.006
4	-6.6	2.288	3.958
5	-6.5	67.156	70.265
6	-6.5	1.826	2.753
7	-6.5	2.389	6.714
8	-6.3	1.946	2.558
9	-6.3	66.606	69.742

Table S17. Molecular coupling results obtained from the 4XO9 code protein with the ligand h made in the AutoDock Vina software package.

Protein 4XO9			
Position s Ligand h	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.9	0.000	0.000
2	-6.7	2.328	6.856
3	-6.7	36.733	38.836
4	-6.7	66.856	70.107
5	-6.6	2.120	6.745
6	-6.5	2.292	6.551
7	-6.5	66.503	69.774
8	-6.5	1.710	2.410
9	-6.4	2.237	3.786

Table S18. Molecular coupling results obtained from the 4XO9 code protein with the ligand i made in the AutoDock Vina software package.

Protein 4XO9			
Position s Ligand i	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.8	0.000	0.000
2	-6.8	0.257	1.064
3	-6.8	0.767	1.122
4	-6.7	0.756	1.496
5	-6.2	1.694	2.517
6	-6.1	67.400	70.331
7	-5.9	37.168	38.872
8	-5.9	58.223	60.760
9	-5.9	38.353	40.057

Table S19. Molecular coupling results obtained from the 4XO9 code protein with the ligand j made in the AutoDock Vina software package.

Protein 4XO9			
Positions Ligand j	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-6.7	0.000	0.000
2	-6.7	0.293	3.726
3	-6.7	37.039	39.580
4	-6.6	37.027	39.782
5	-6.4	67.374	71.153
6	-6.4	67.396	71.111
7	-6.2	38.419	41.176
8	-6.2	38.324	40.951
9	-6.1	2.891	4.547

Table S20. Molecular coupling results obtained from the 4XO9 code protein with the ligand k made in the AutoDock Vina software package.

Protein 4XO9			
Positions Ligand k	Afinity (kcal/m ol)	Distance RMSD (Å)	Mode RMSD (Å)
1	-7.0	0.000	0.000
2	-6.4	67.649	70.133
3	-6.3	2.234	3.178
4	-6.3	59.324	60.659
5	-6.3	1.655	2.281
6	-6.3	1.872	2.302
7	-6.2	1.970	2.464
8	-6.1	2.321	3.177
9	-6.1	37.274	39.418

Table S21. Primers for classification of phylogenetic groups in *Escherichia coli*.

Gene	Sequence (5' to 3')	Amplicon size (bp)	Optimal Annealing Temperature (°C)	Reference
<i>chuA</i>	F: ATGGTACCGGACGAACCAAC R: TGCCGCCAGTACCAAAGACA	288		
<i>yjaA</i>	F: CAAACGTGAAGTGTCAGGAG R: AATGCGTTCCTCAACCTGTG	211		
TspE4.C2	F: CACTATTCGTAAGGTCATCC R: AGTTTATCGCTGCGGGTCGC	152	59	
<i>arpA</i>	F: AACGCTATTCGCCAGCTTGC R: TCTCCCCATACCGTACGCTA	400		[51]
<i>trpA</i>	F: AGTTTTATGCCCAGTGCGAG R: TCTGCGCCGGTCACGCCC	219		
<i>arpA</i>	F: GATTCCATCTTGTCAAAATATGCC R: GAAAAGAAAAAGAATTCCCAAGAG	301	57	
<i>trpA</i>	F: CGGCGATAAAGACATCTTCAC R: GCAACGCGGCCTGGCGGAAG	489		

Table S22. Primers for identification of virulence factors in uropathogenic UPEC strains.

Gene	Primer sequence (5' to 3')	Amplicon size (bp)	Reference
<i>KpsMT II F</i>	GCGCATTTGCTGATACTGTTG	272	
<i>KpsMT II R</i>	CATCCAGACGATAAGCATGAGCA		
<i>fimH F</i>	TGCAGAACGGATAAGCCGTGG	508	
<i>fimH R</i>	GCAGTCACCTGCCCTCCGGTA		
<i>PAI F</i>	GGACATCCTGTTACAGCGCGCA	930	[52]
<i>PAI R</i>	TCGCCACCAATCACAGCCGAAC		
<i>papAH F</i>	ATGGCAGTGGTGTCTTTTGGTG	720	
<i>papAH R</i>	CGTCCCACCATACGTGCTCTTC		
<i>fyuA F</i>	TGATTAACCCCGCGACGGGAA	880	
<i>fyuA R</i>	CGCAGTAGGCACGATGTTGTA		
<i>Usp F</i>	ATGCTACTGTTTCCGGGTAAGTGTGT	1000	[53]
<i>Usp R</i>	CATCATGTAGTCGGGGCGTAACAAT		

Table S23. Primers for identification of bacterial resistance genes.

Gene	Primer sequence (5' to 3')	Amplicon size (bp)	Reference
TEM-F	ATGAGTATTCAACATTTCGG	867	
TEM-R	CTGACAGTTACCAATGCTTA		
SHV-F	GGTTATGCGTTATATTCGCC	867	[60]
SHV-R	TTAGCGTTGCCAGTGCTC		
CTX-M-1F	ATGGTTAAAAAATCACTGCGYC	876	[61]
CTX-M-1R	TTA CAA ACC GTC GGT G		
OXA-F	ACACAATACATATCAACTTCGC	885	[60]
OXA-R	AGTGTGTTTAGAATGGTGATC		

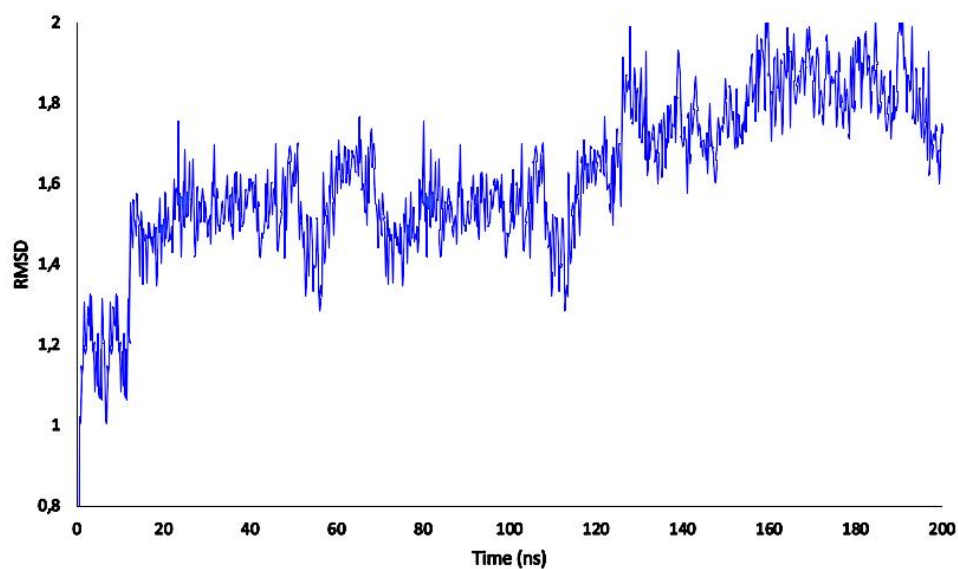


Figure S1. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand native.

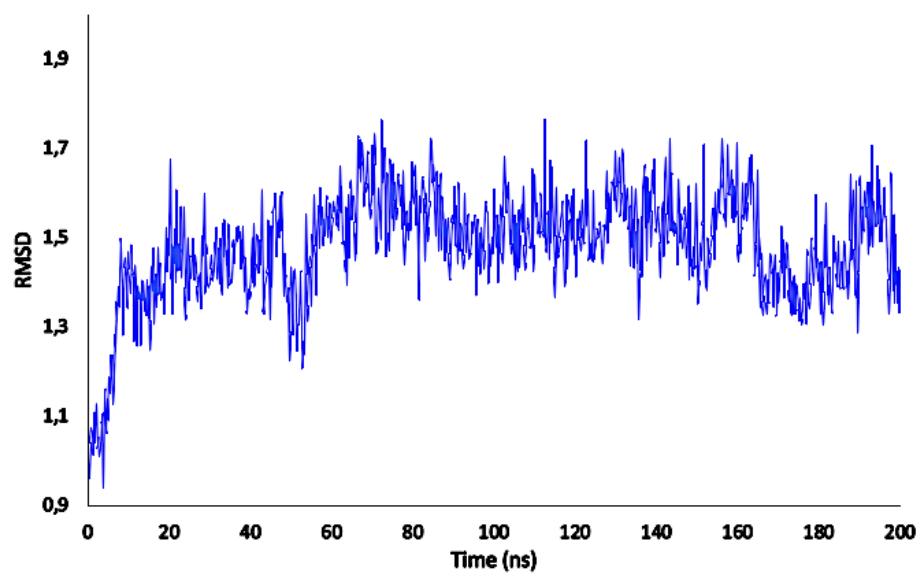


Figure S2. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand b.

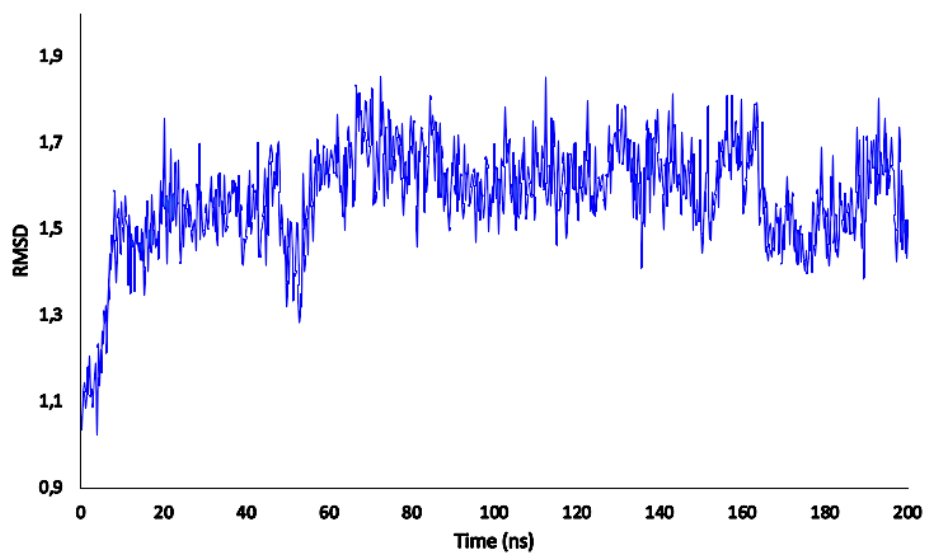


Figure S3. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand c.

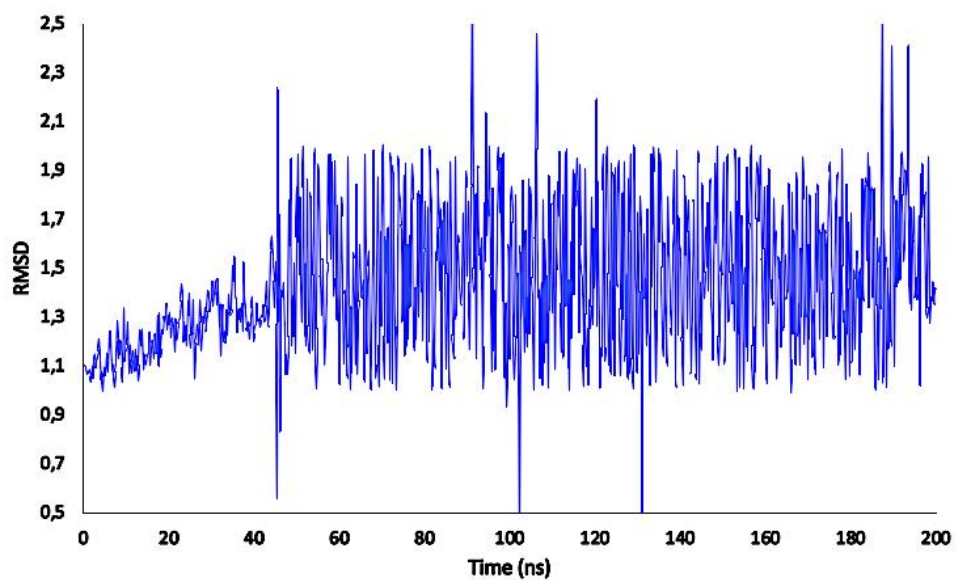


Figure S4. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand d.

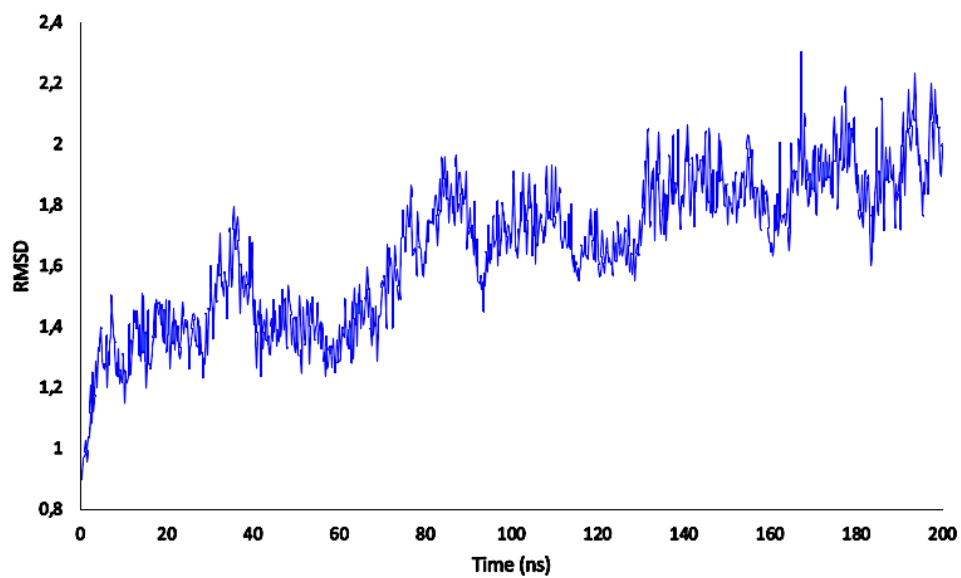


Figure S5. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand e.

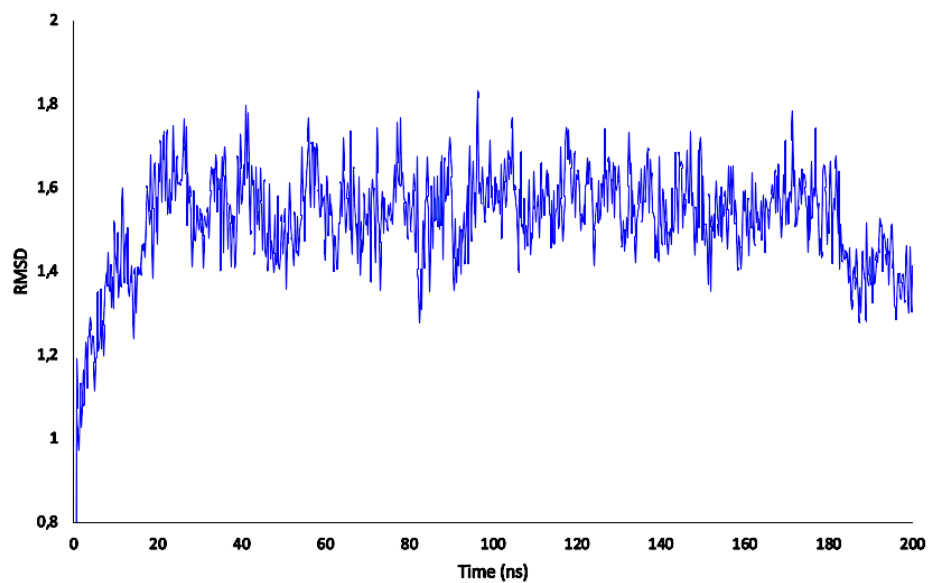


Figure S6. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand f

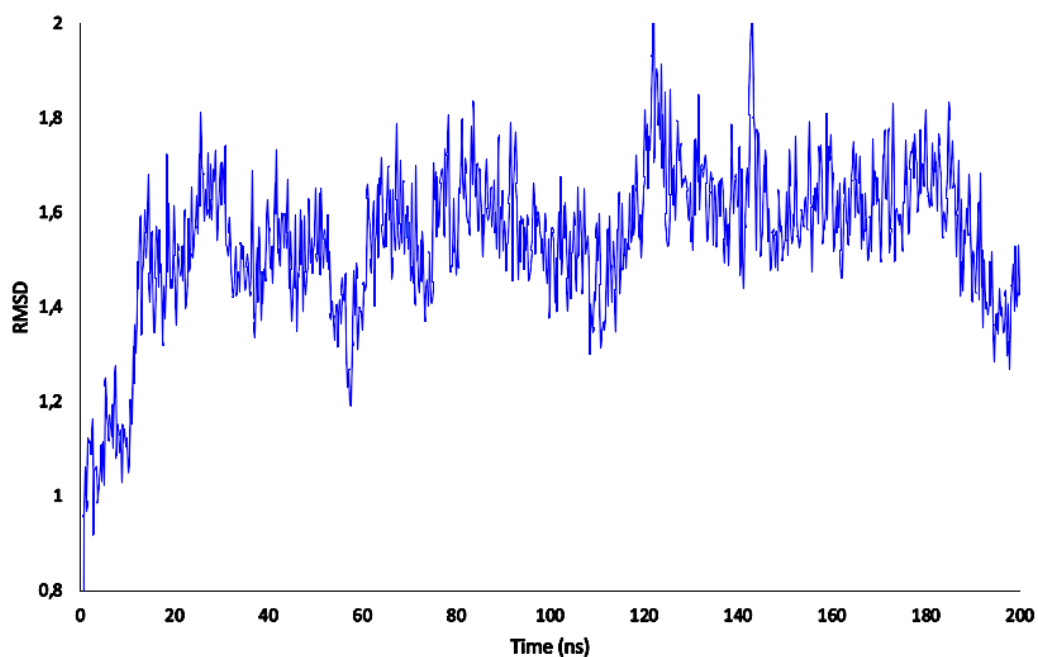


Figure S7. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand g.

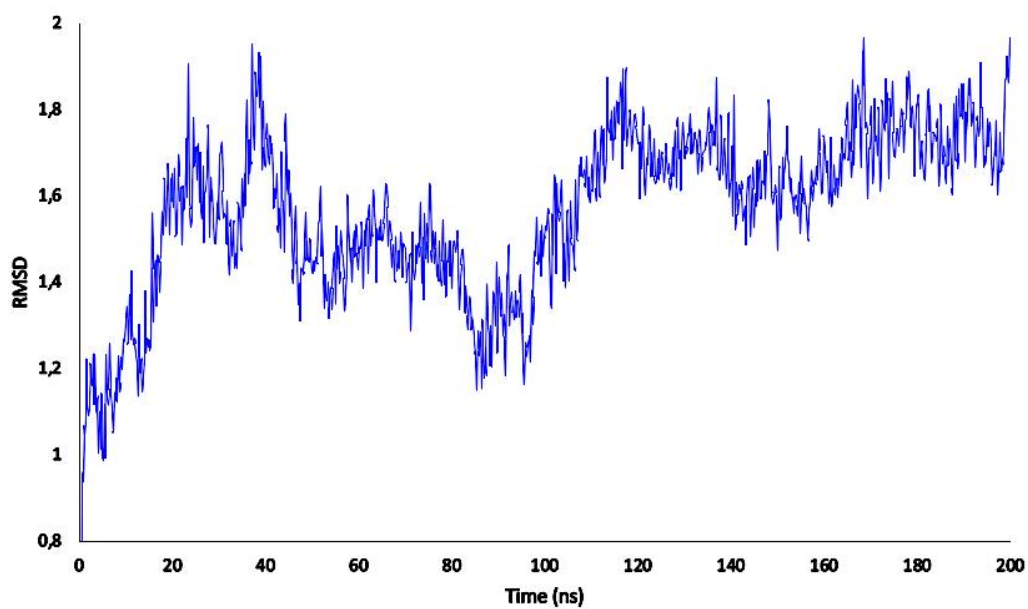


Figure S8. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand h.

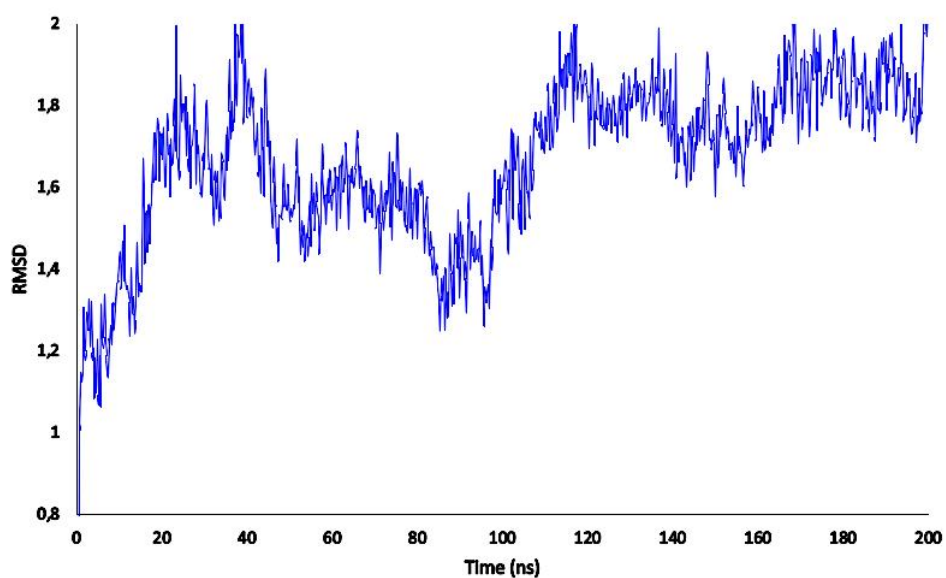


Figure S9. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand i.

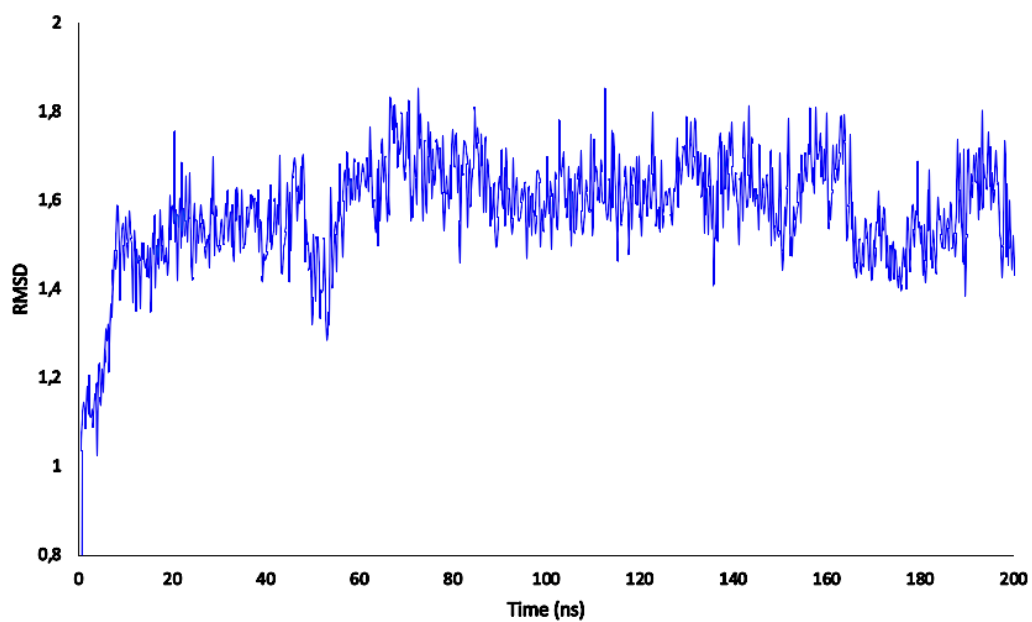


Figure S10. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand j.

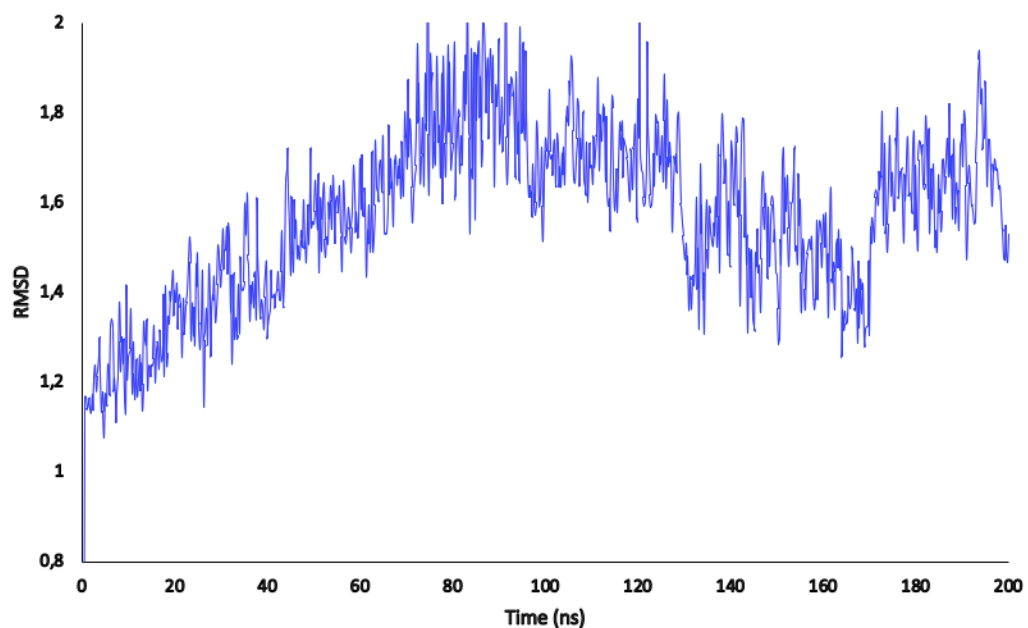


Figure S11. Visualization of root-mean-square deviation (RMSD) of the 4X5P protein with the ligand k.

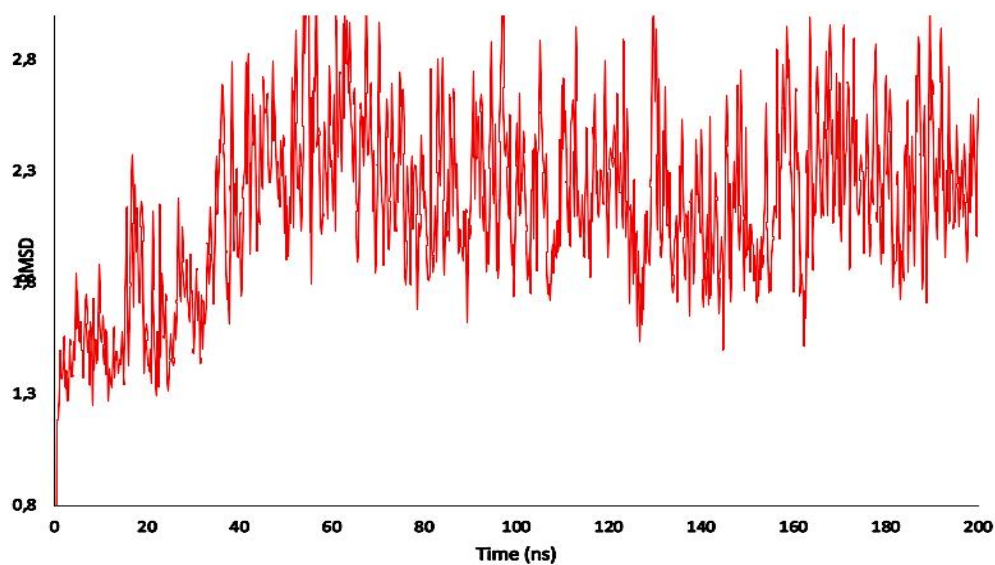


Figure S12. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand native.

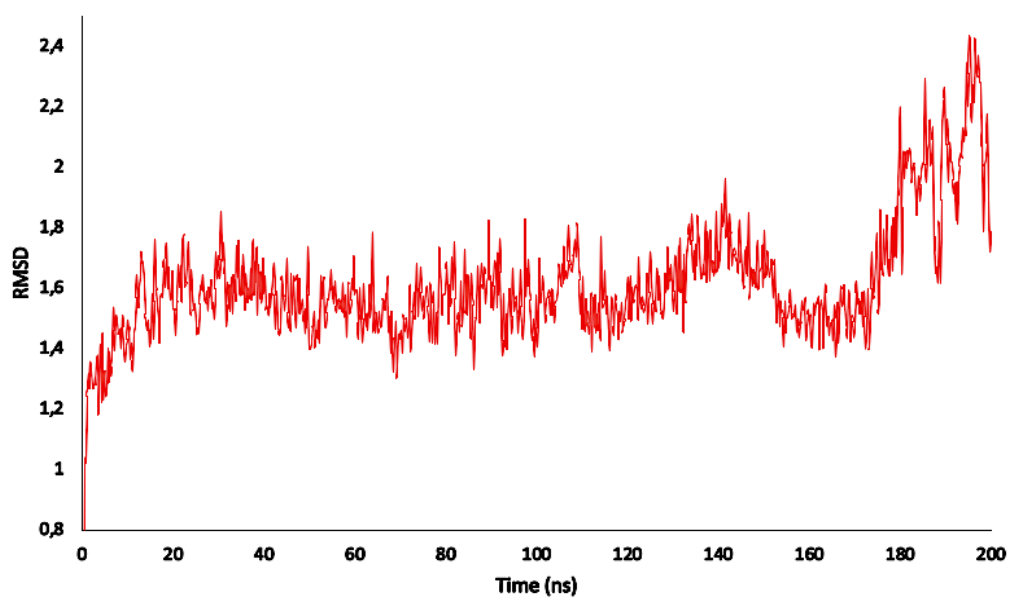


Figure S13. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand b.

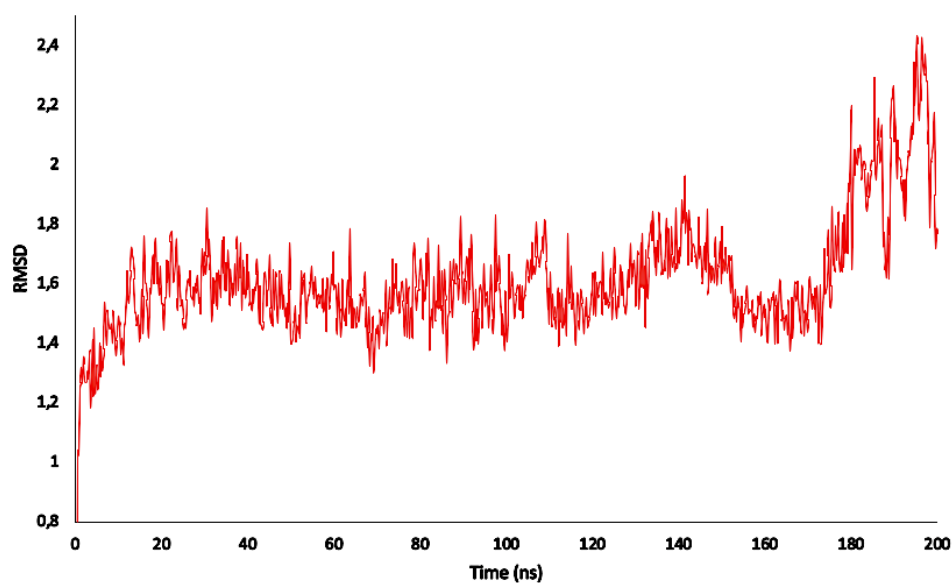


Figure S14. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand c.

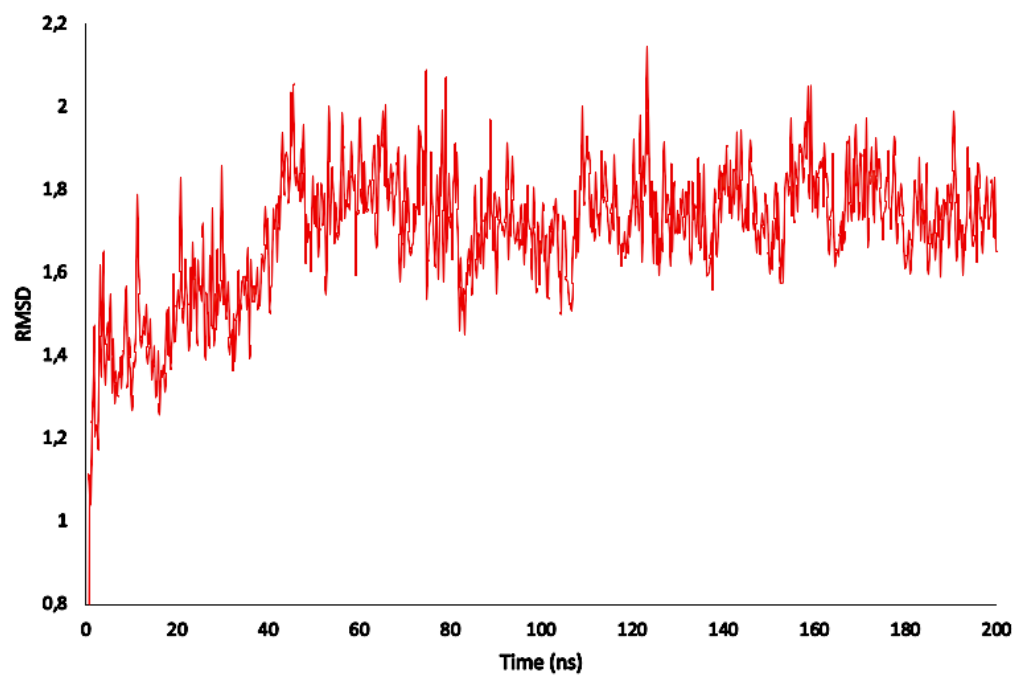


Figure S15. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand d.

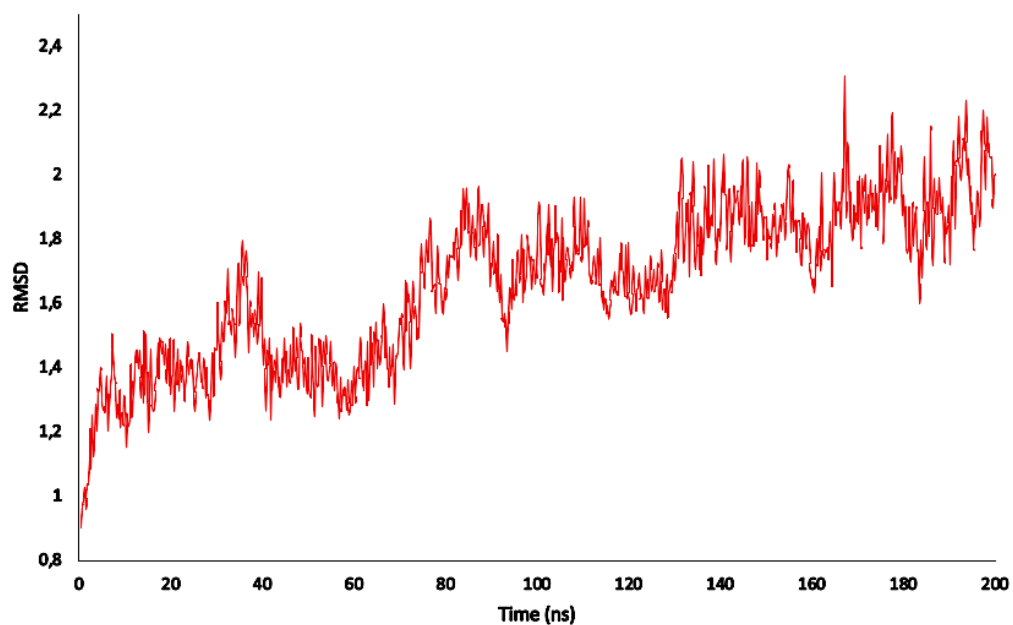


Figure S16. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand e.

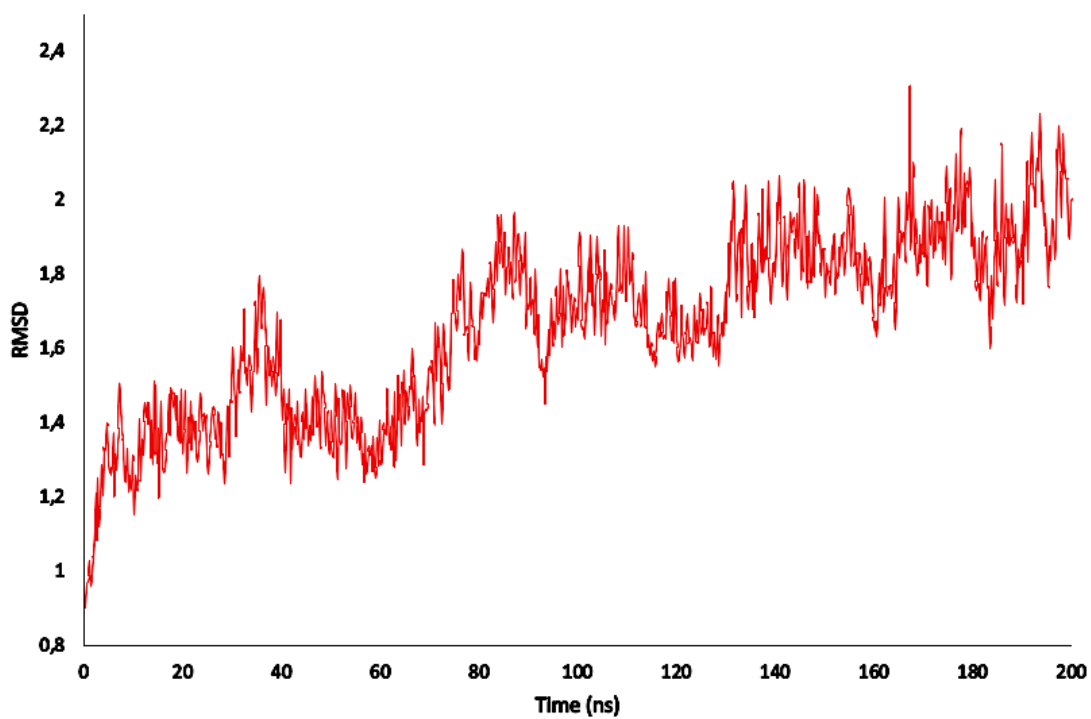


Figure S17. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand f.

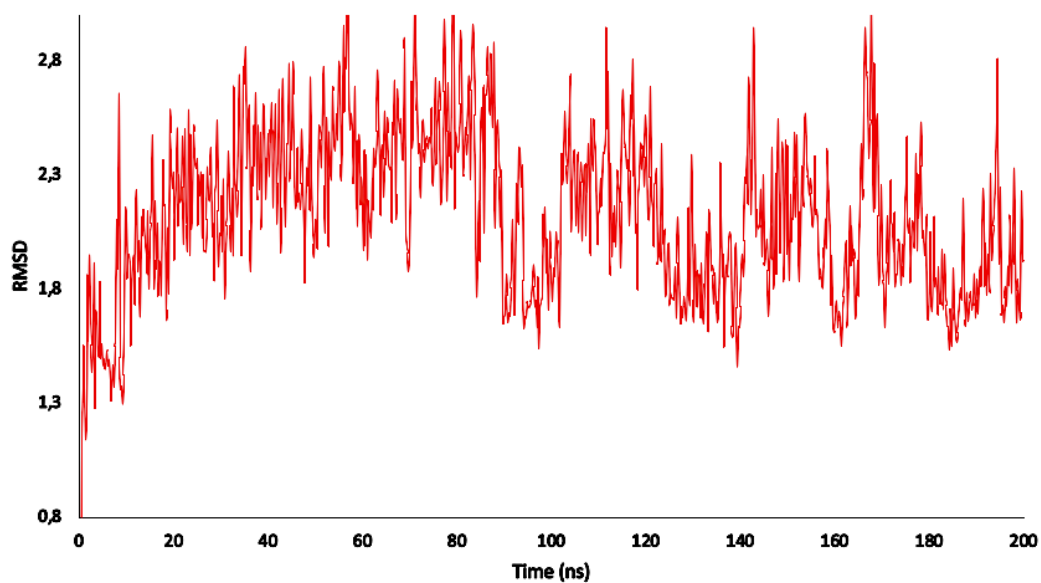


Figure S18. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand g.

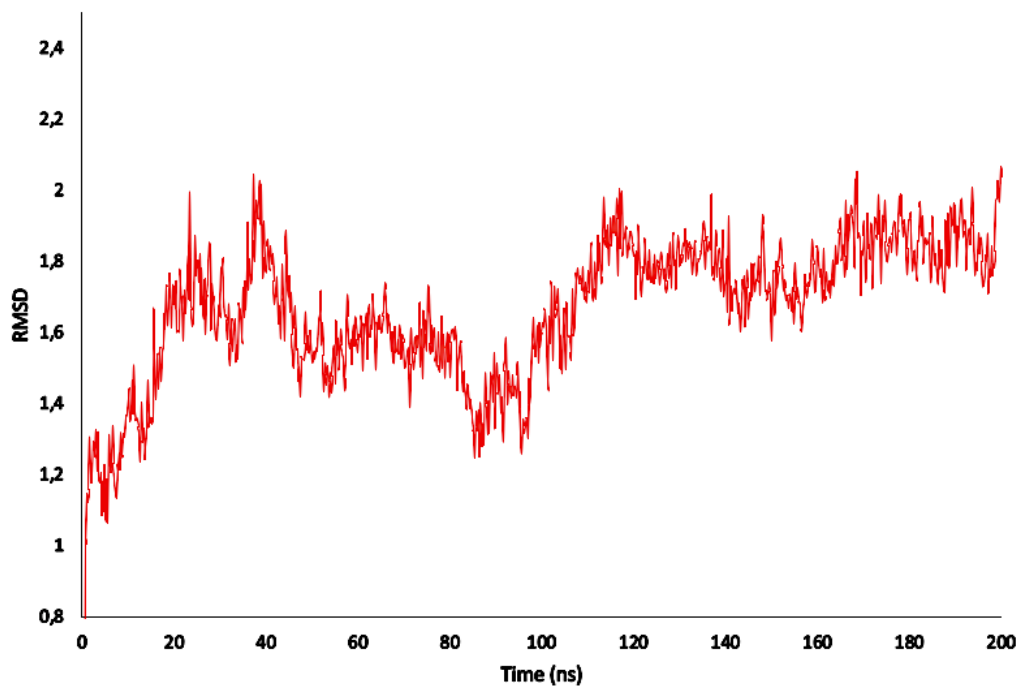


Figure S19. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand h.

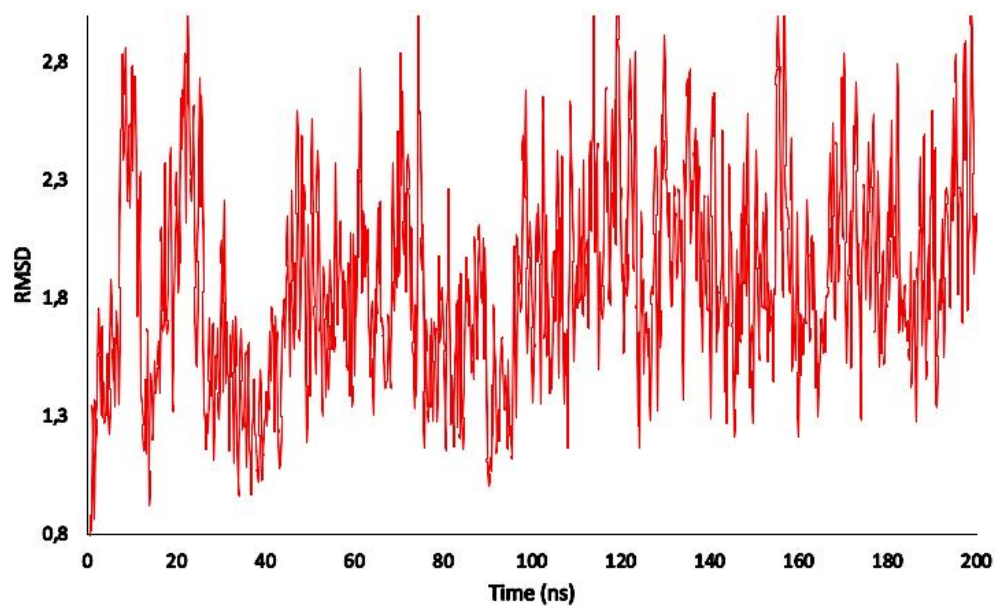


Figure S20. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand i.

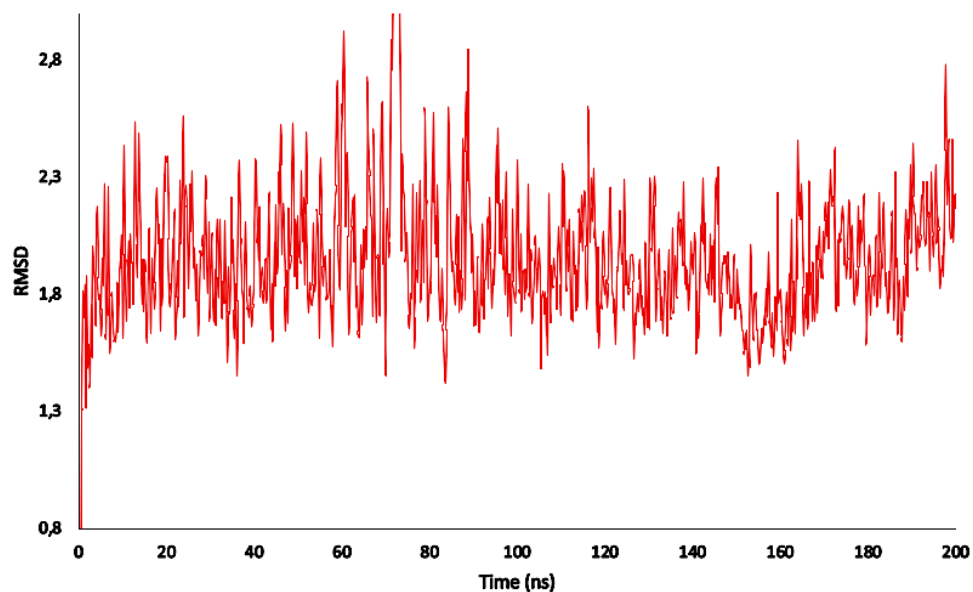


Figure S21. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand j.

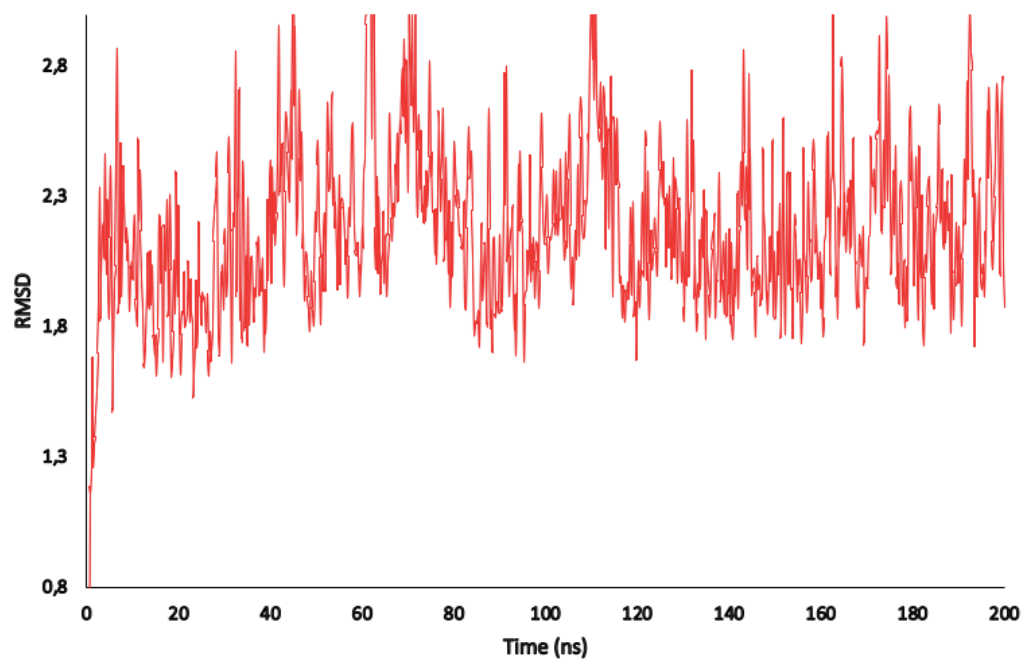


Figure S22. Visualization of root-mean-square deviation (RMSD) of the 4XO9 protein with the ligand k.