

# Supplementary Materials: Synthesis, Antiphospholipase A<sub>2</sub>, Antiprotease, Antibacterial Evaluation and Molecular Docking Analysis of Certain Novel Hydrazones

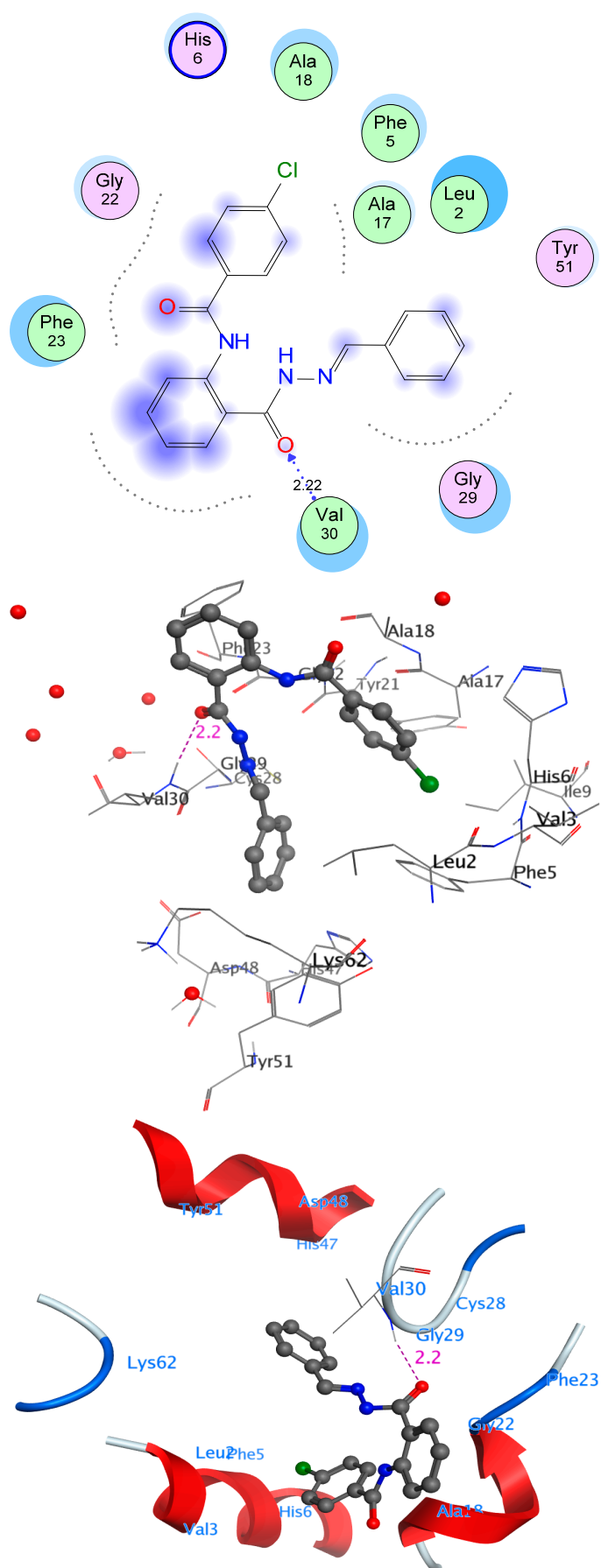
Nahed N. E. El-Sayed, Ahmed M. Alafeefy, Mohammed A. Bakht, Vijay H. Masand, Ali Aldalbahi, Nan Chen, Chunhai Fan and Abir Ben Bacha

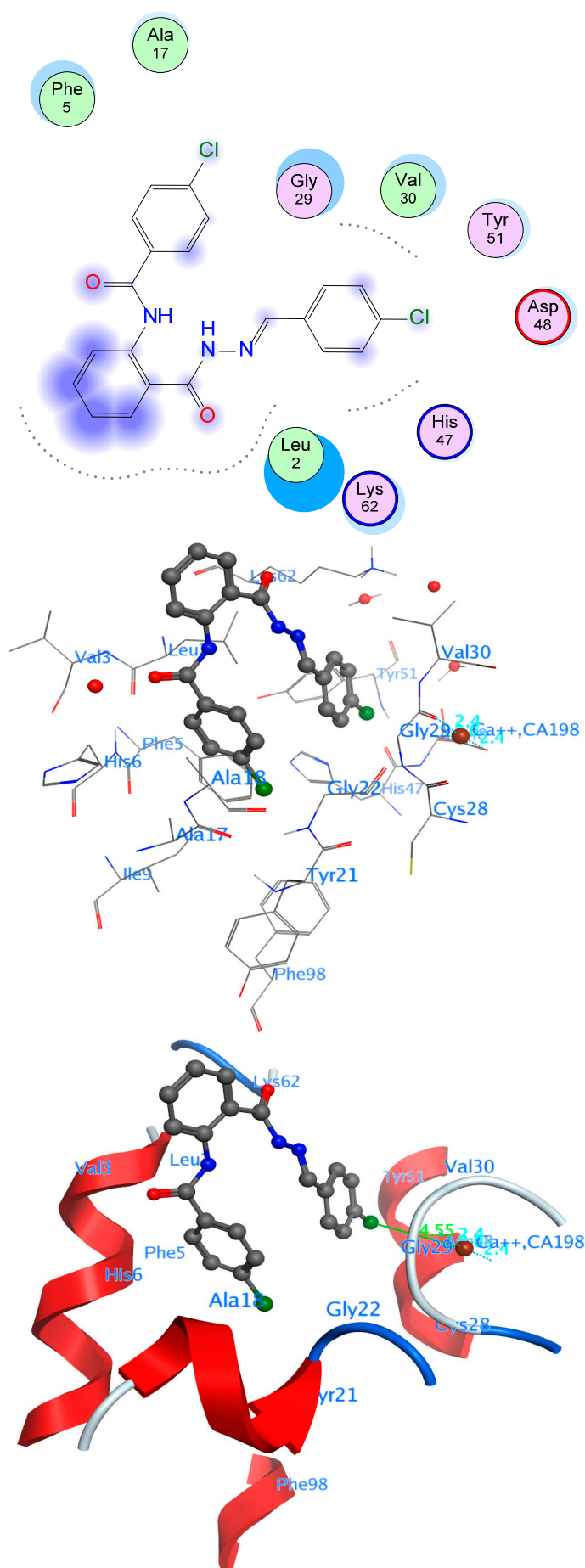
Table S1. Inhibitory activity of compounds 6a–o against sPLA<sub>2</sub> (hG-IIA and DrG-IB).

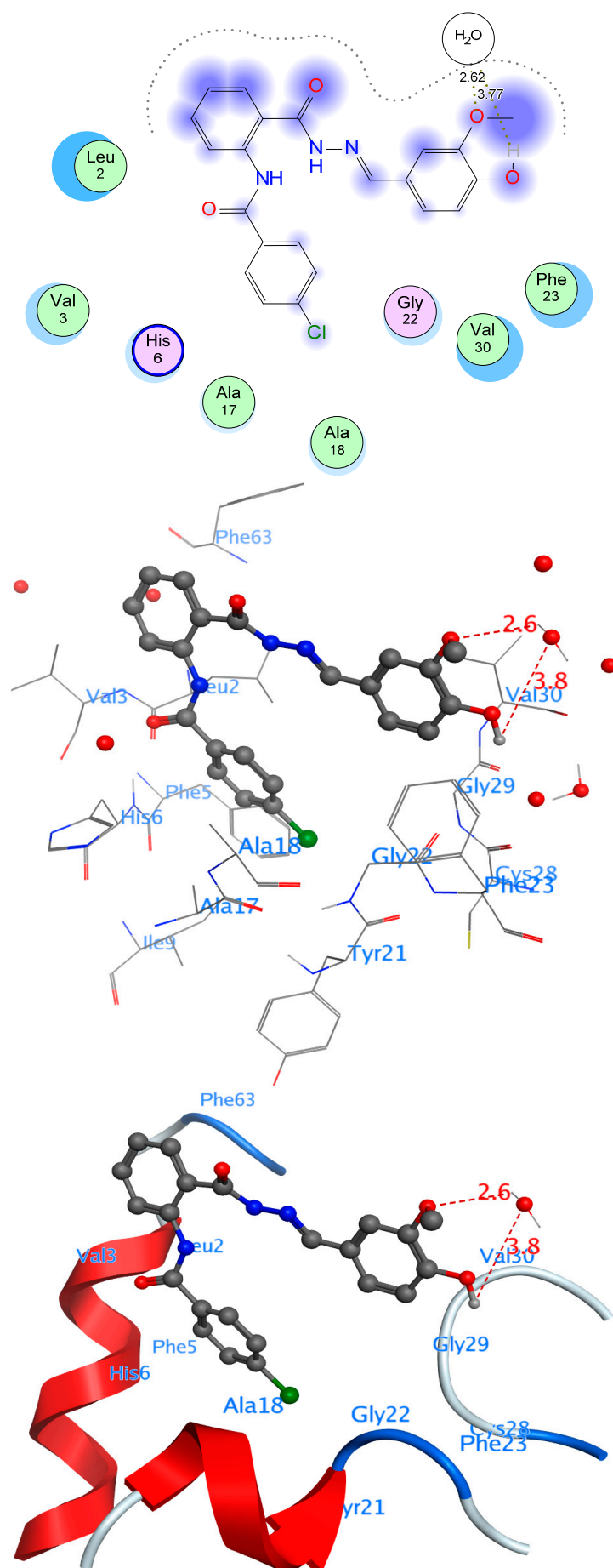
Compound	sPLA <sub>2</sub> Inhibitory Activity (%)	
	hG-IIA	DrG-IB
6a	39.67 ± 2.51	2.66 ± 2.51
6b	37.33 ± 4.04	11.67 ± 3.51
6c	50.67 ± 4.04	14.67 ± 2.51
6d	55.67 ± 4.72	10 ± 3.00
6e	72.67 ± 2.51	4.66 ± 0.57
6f	37.33 ± 3.51	6.33 ± 0.57
6g	10.67 ± 0.57	9 ± 1.73
6h	15.33 ± 2.51	8.33 ± 1.15
6i	26.67 ± 3.21	5.66 ± 1.52
6j	19.33 ± 2.08	6.66 ± 1.52
6k	35.33 ± 3.51	6.66 ± 2.08
6l	74.33 ± 3.21	11.33 ± 2.51
6m	17.67 ± 3.05	2.66 ± 1.15
6n	9 ± 2	4 ± 3.60
6o	12.67 ± 3.21	1.66 ± 1.15

Table S2. Antiprotease activity (%) of compounds 6a–o against different protease enzymes.

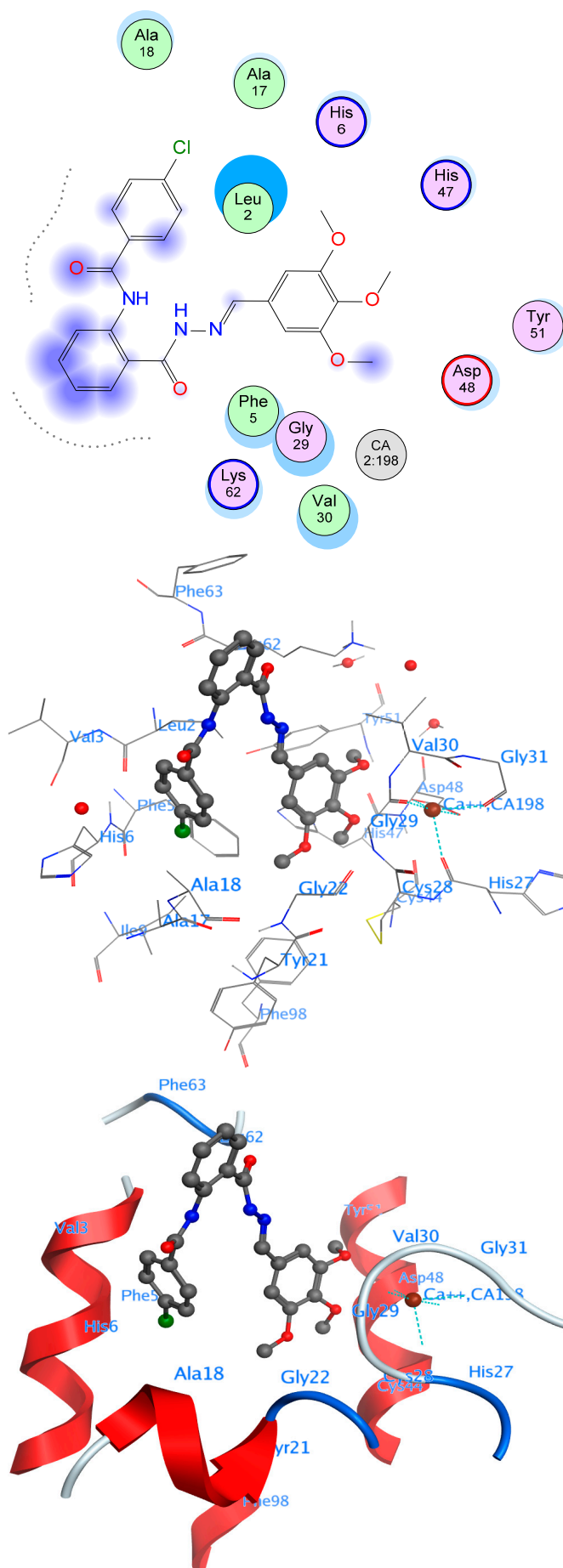
Compound	Anti-Protease Activity (%)		
	Proteinase K	Protease from <i>Bacillus sp.</i>	Esperase
6a	27.33 ± 2.51	40.66 ± 4.04	6.66 ± 1.52
6b	55.66 ± 5.03	72.33 ± 2.51	13 ± 2.00
6c	34.66 ± 2.51	51 ± 3.60	15 ± 3.00
6d	26.33 ± 3.21	38 ± 2.64	20.66 ± 3.05
6e	74.66 ± 2.51	57 ± 4.00	31.33 ± 6.02
6f	39 ± 4.58	44 ± 1.00	12.33 ± 2.08
6g	57.33 ± 2.51	72.33 ± 6.42	24 ± 3.60
6h	14.66 ± 3.51	7.66 ± 2.51	5 ± 1.00
6i	30.66 ± 5.50	42 ± 6.55	14 ± 2.64
6j	35 ± 3.60	48.33 ± 3.51	17.66 ± 3.51
6k	50.66 ± 4.04	62.33 ± 2.51	24.33 ± 4.04
6l	86 ± 2.64	74.66 ± 2.88	39.33 ± 3.21
6m	69 ± 4.58	56.33 ± 3.51	32.33 ± 2.08
6n	44.66 ± 6.50	50 ± 2.64	21.33 ± 3.51
6o	26 ± 4.58	41 ± 3.00	34.33 ± 3.05

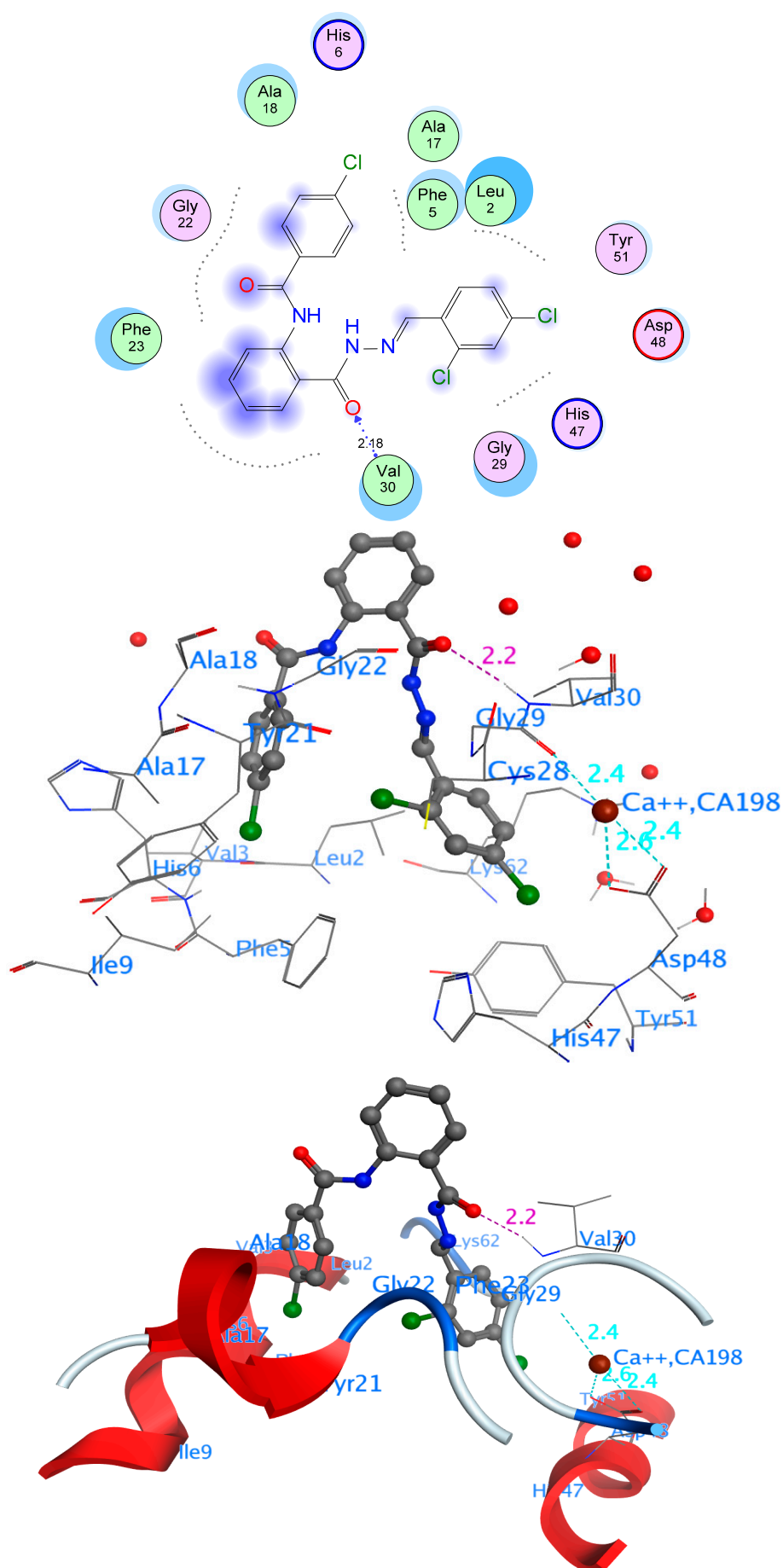
Docking Pose for Compound 6a in the Active Site of GIIAsPLA<sub>2</sub>

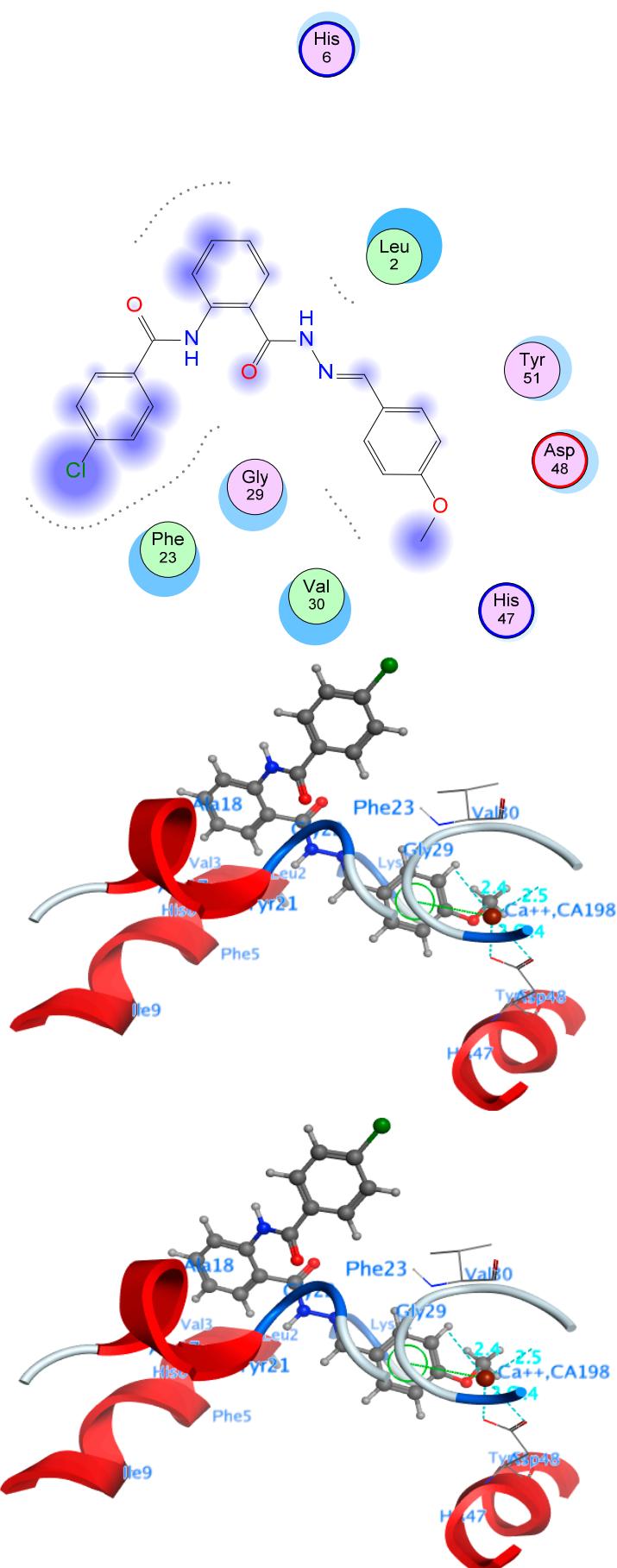
Docking pose for compound **6b** in the active site of GIIAsPLA<sub>2</sub>

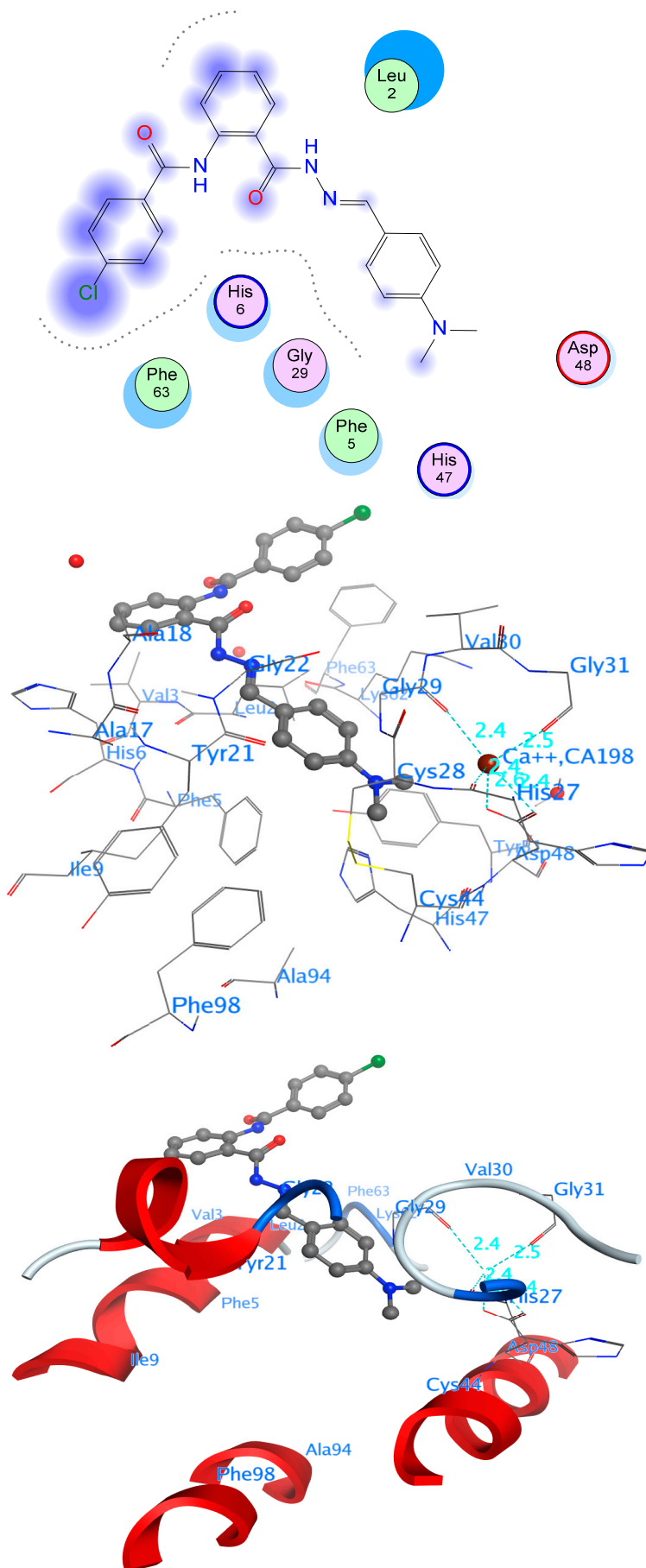
Docking pose for compound **6c** in the active site of GIIAsPLA<sub>2</sub>

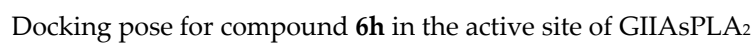


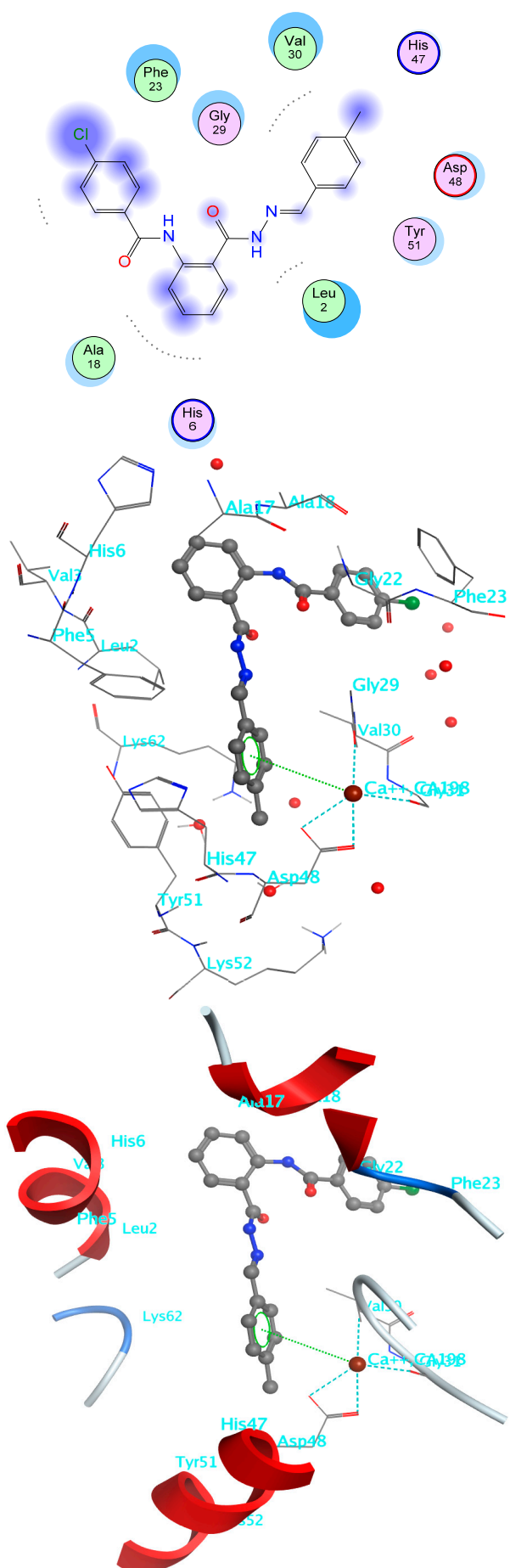
Docking pose for compound **6d** in the active site of GIIAsPLA<sub>2</sub>

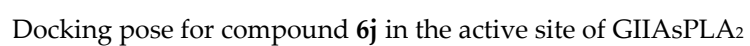
Docking pose for compound **6e** in the active site of GIIAsPLA2

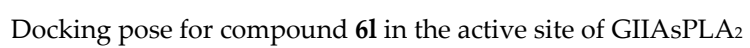
Docking pose for compound **6f** in the active site of GIIAsPLA<sub>2</sub>

Docking pose for compound **6g** in the active site of GIIAsPLA<sub>2</sub>

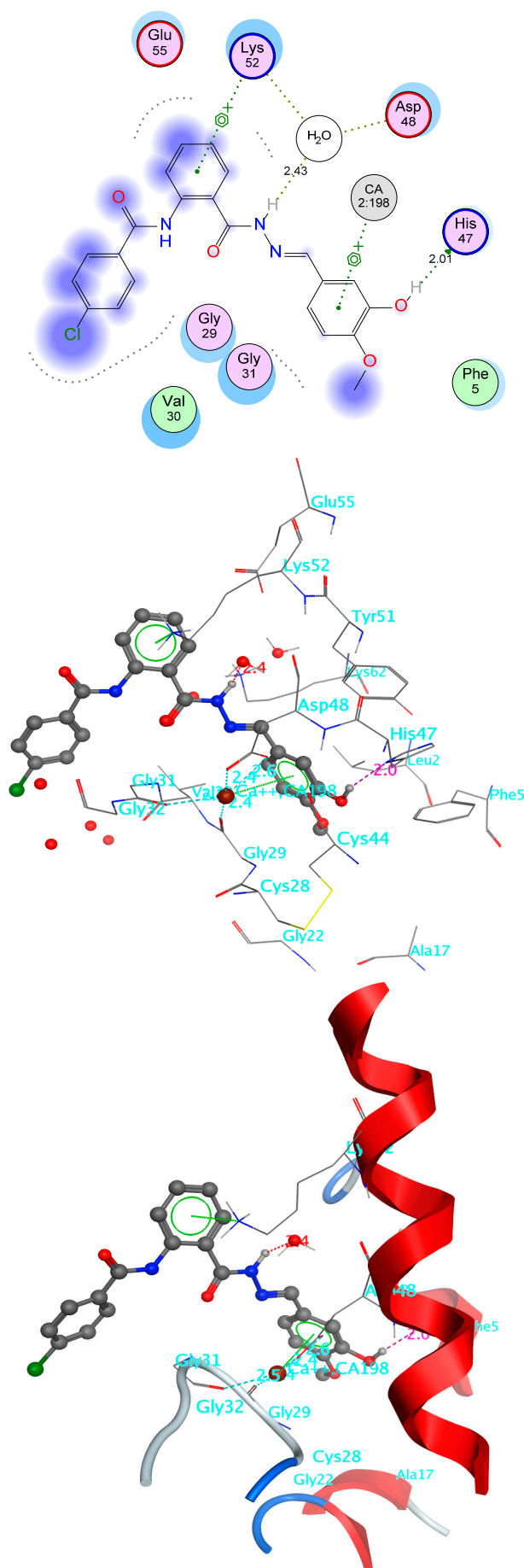


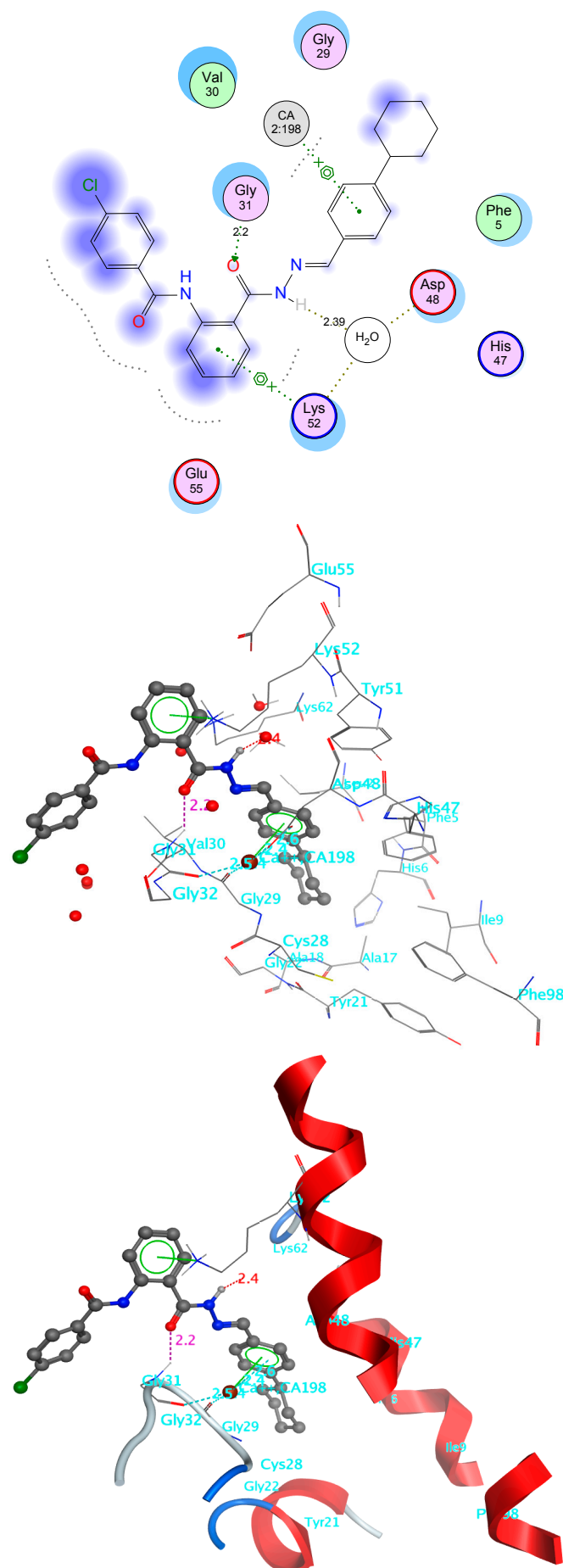
Docking pose for compound **6i** in the active site of GIIAsPLA<sub>2</sub>

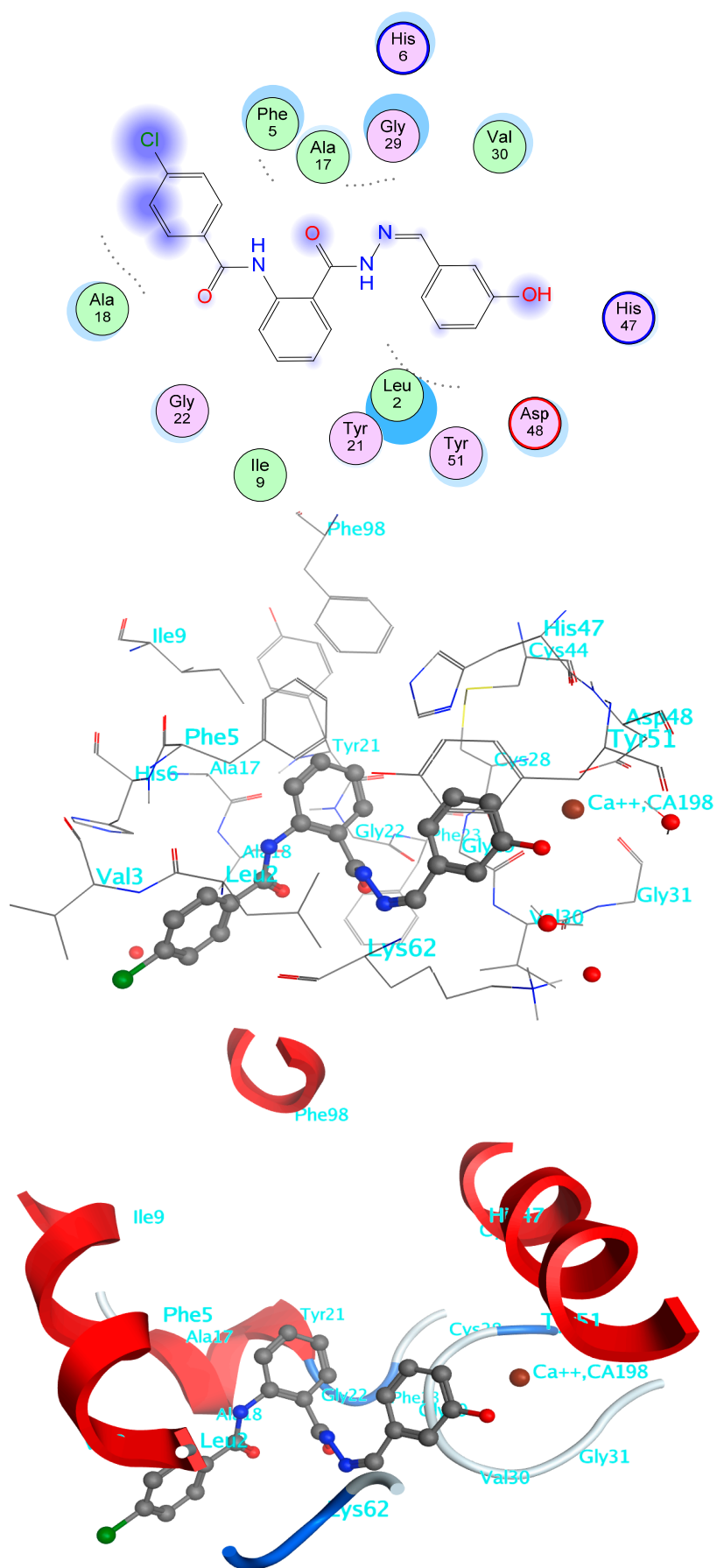






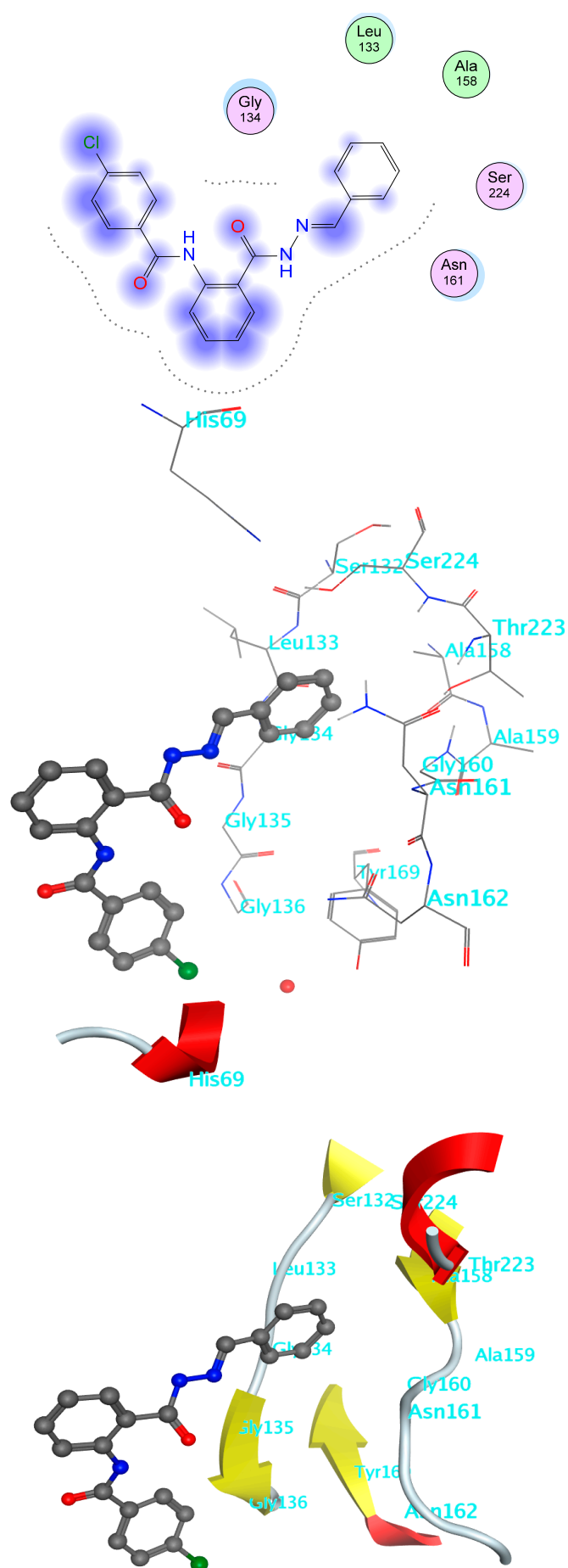
Docking pose for compound **6m** in the active site of GIIAsPLA<sub>2</sub>

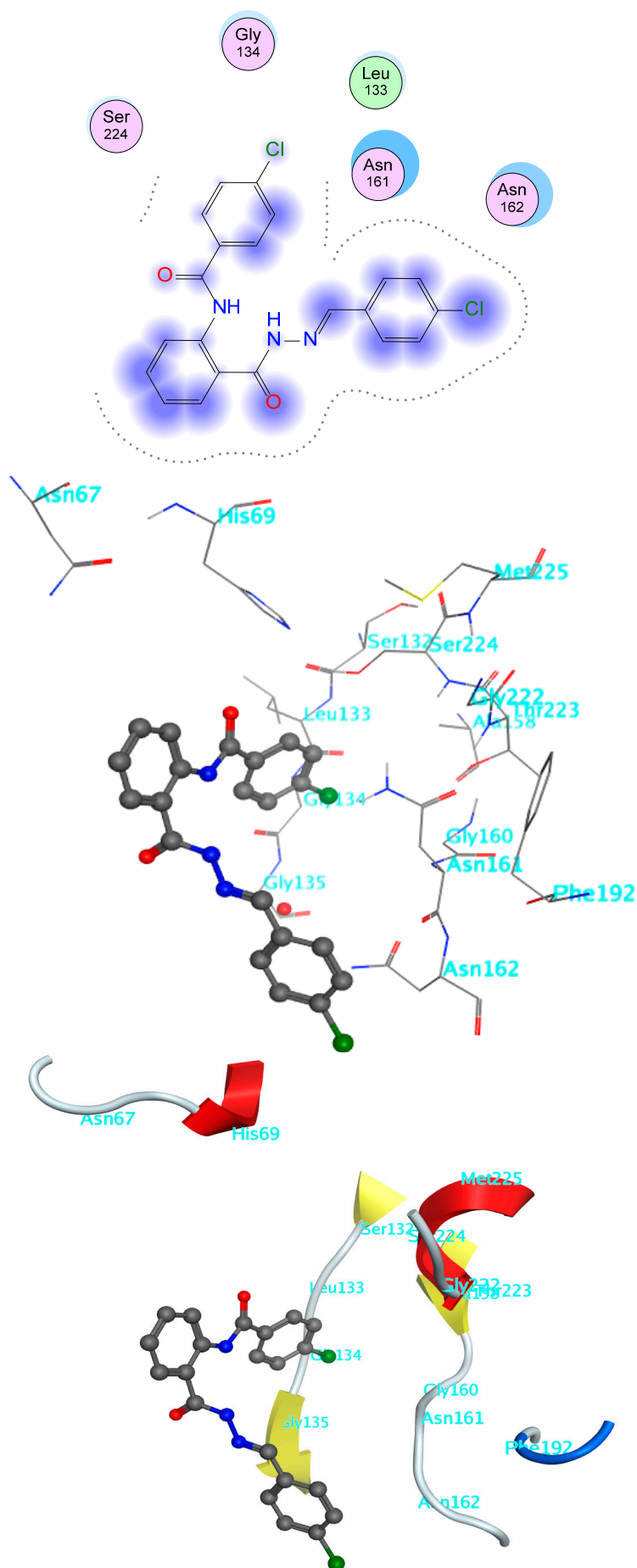
Docking pose for compound **6n** in the active site of GIIAsPLA<sub>2</sub>

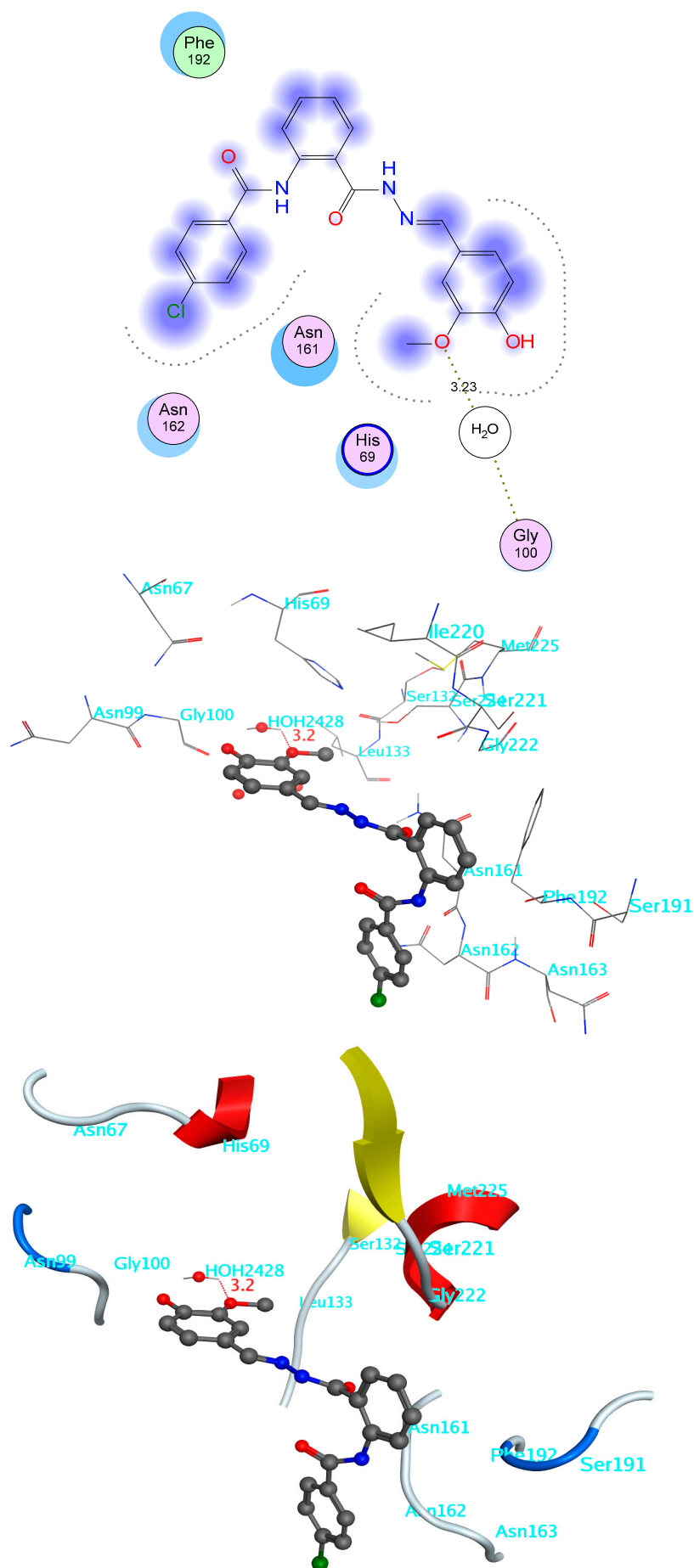


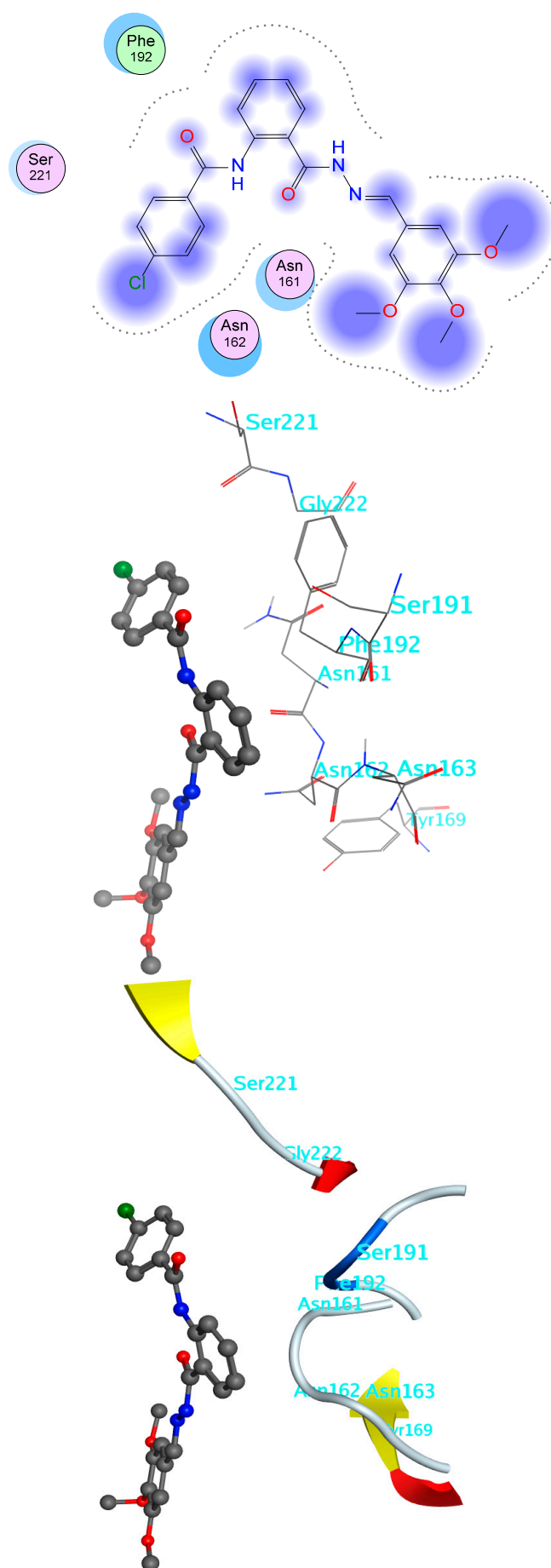
Docking pose for compound **60** in the active site of GIIAsPLA<sub>2</sub>

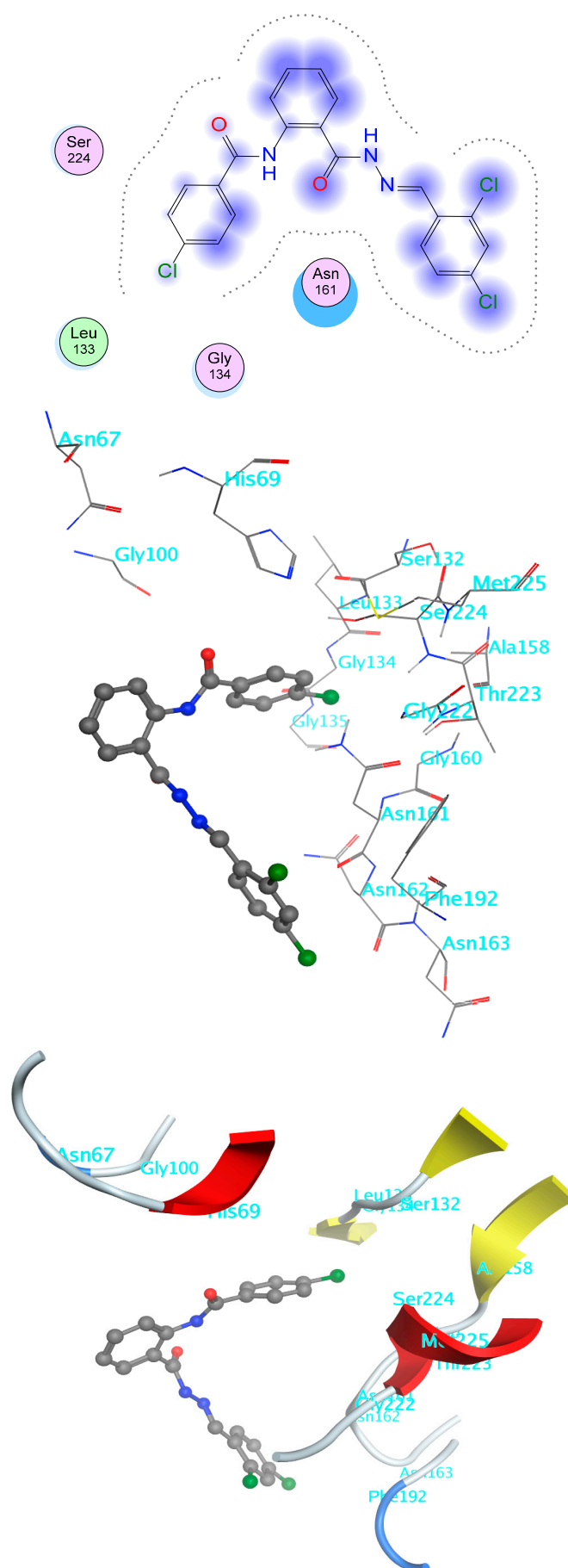
**Figures S1.** Docking poses of compounds **6a–o** in active site of GIIAsPLA<sub>2</sub>.

Docking pose for compound **6a** in the active site of Proteinase K

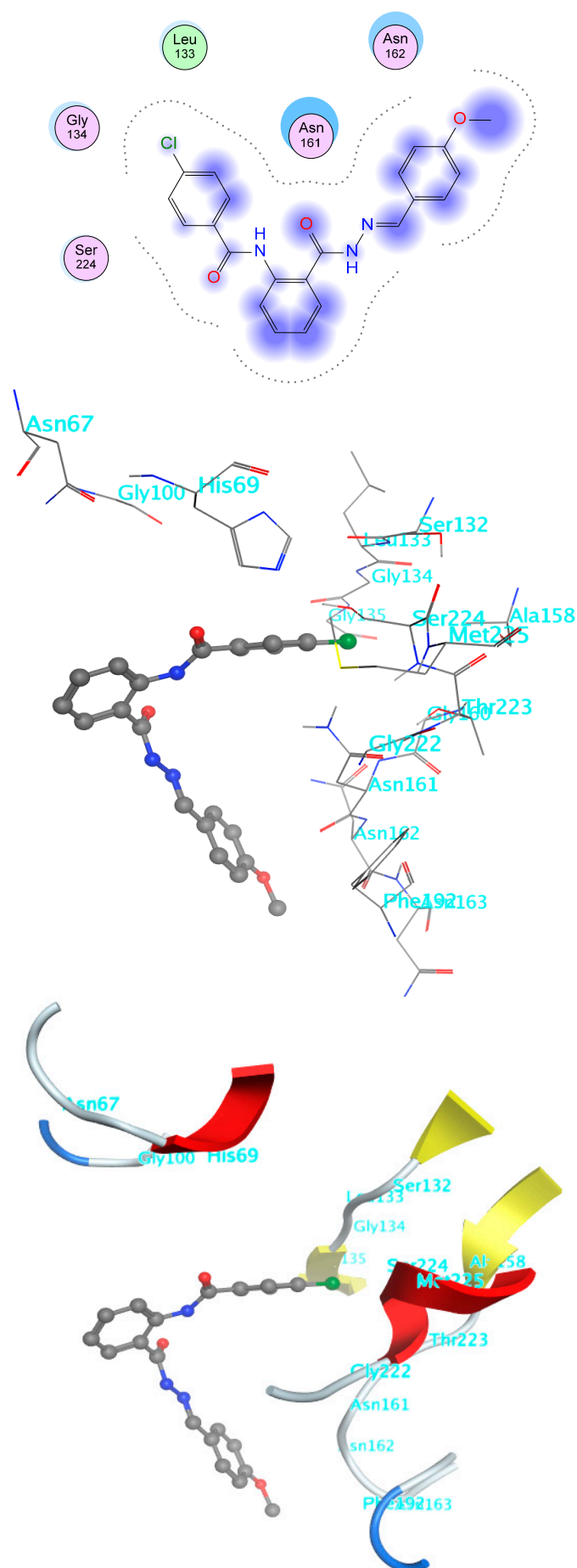
Docking pose for compound **6b** in the active site of Proteinase K

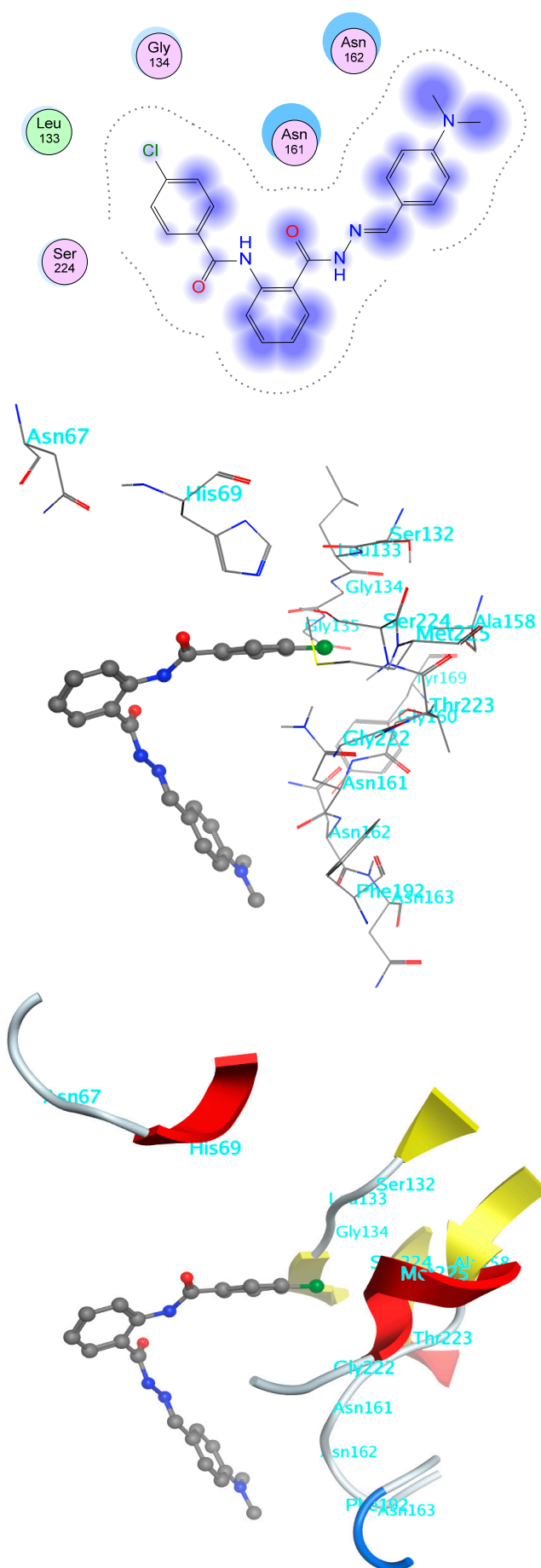
Docking pose for compound **6c** in the active site of Proteinase K

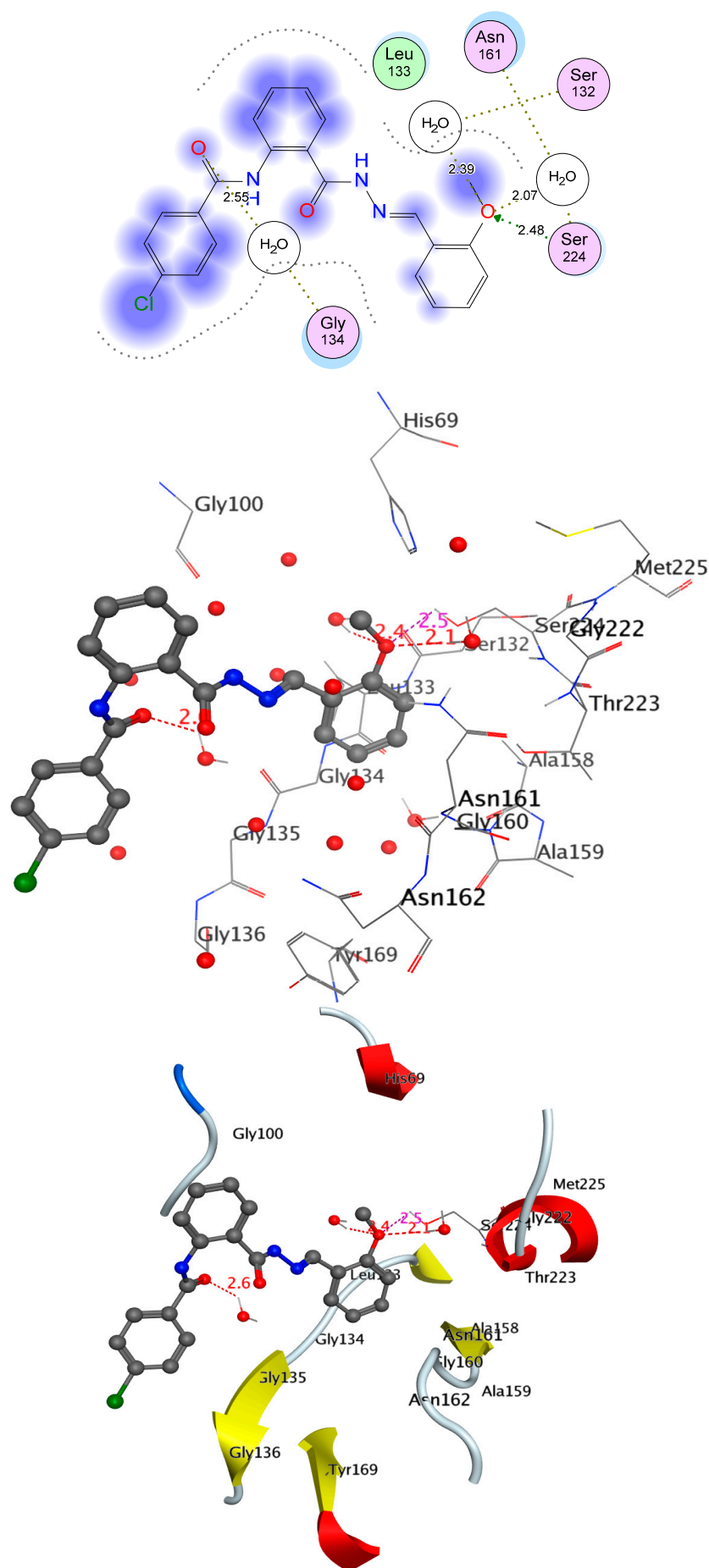
Docking pose for compound **6d** in the active site of Proteinase K

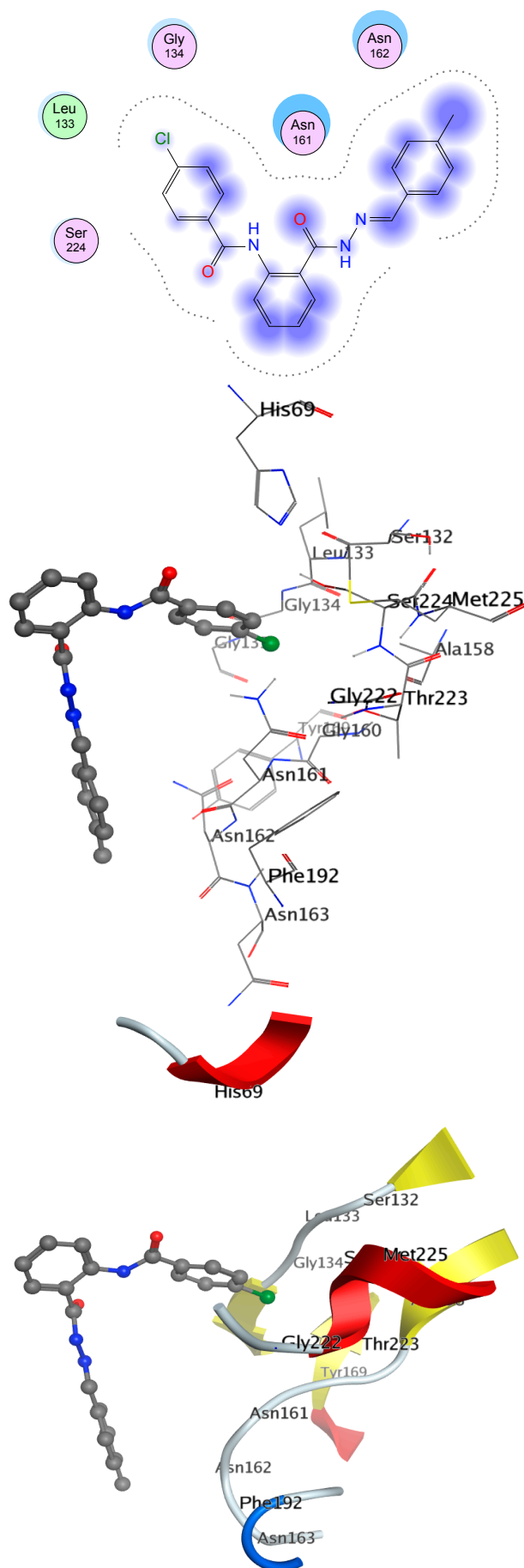
Docking pose for compound **6e** in the active site of Proteinase K

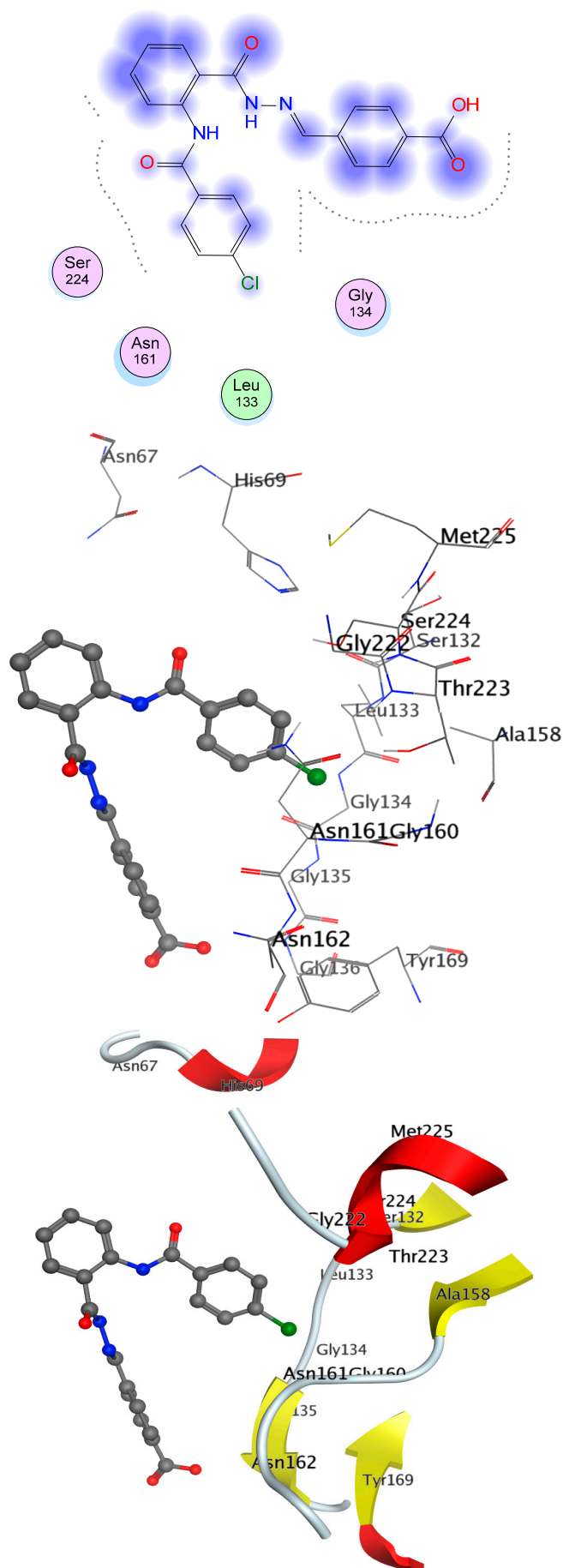


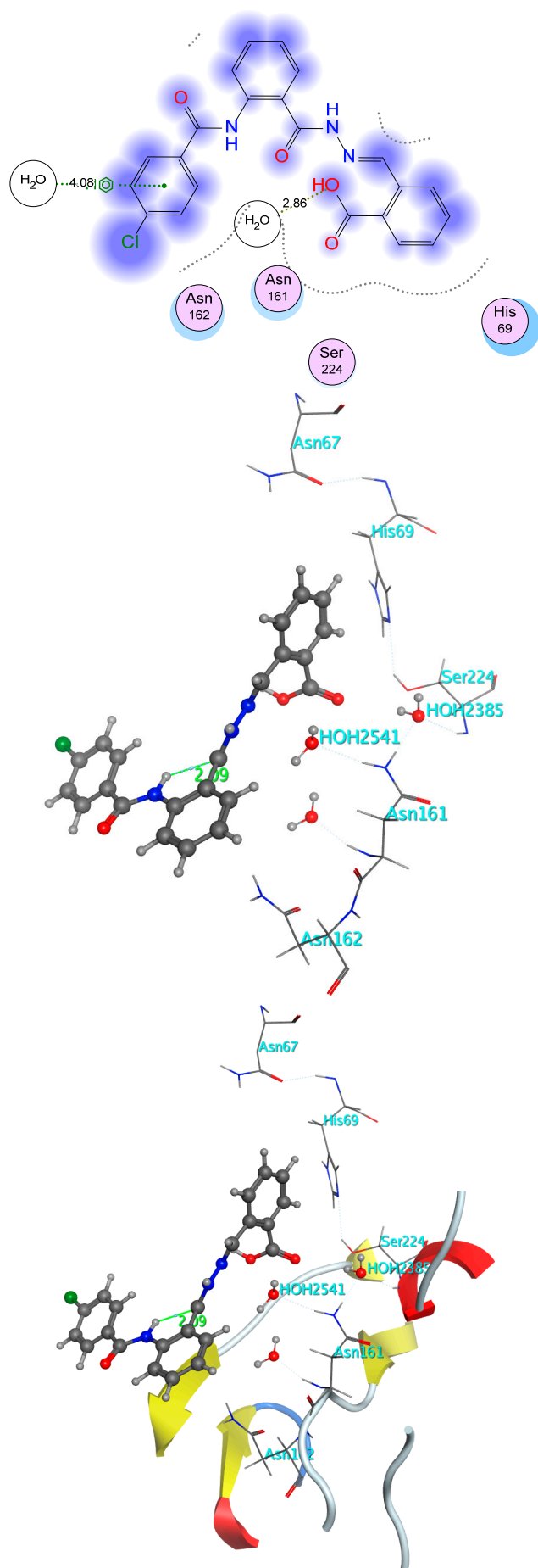
Docking pose for compound **6f** in the active site of Proteinase K

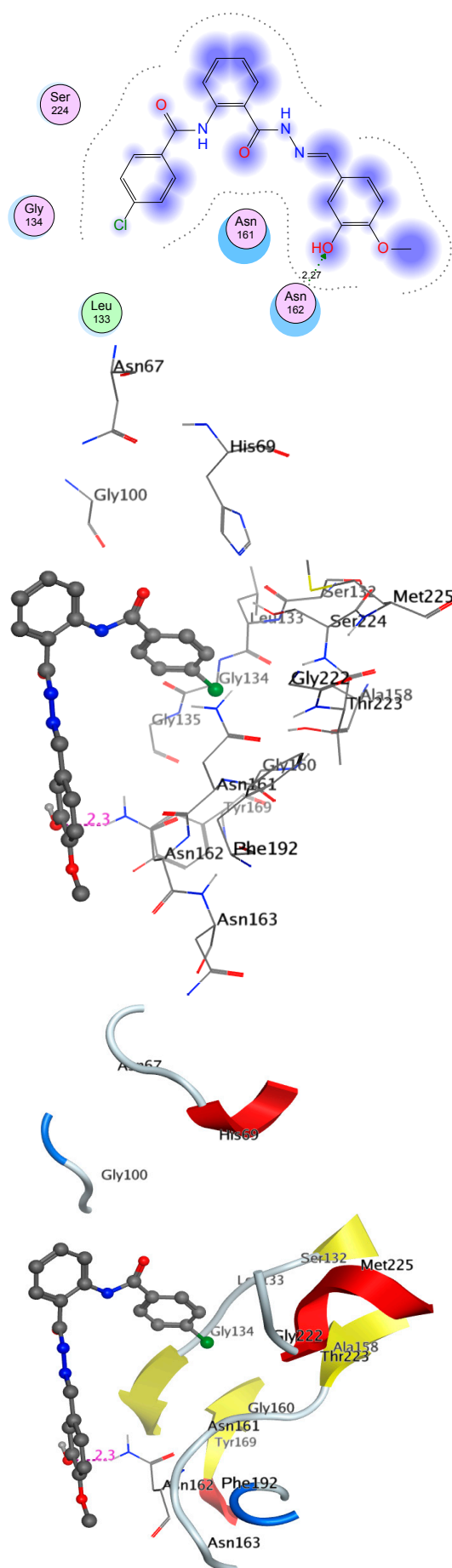
Docking pose for compound **6g** in the active site of Proteinase K

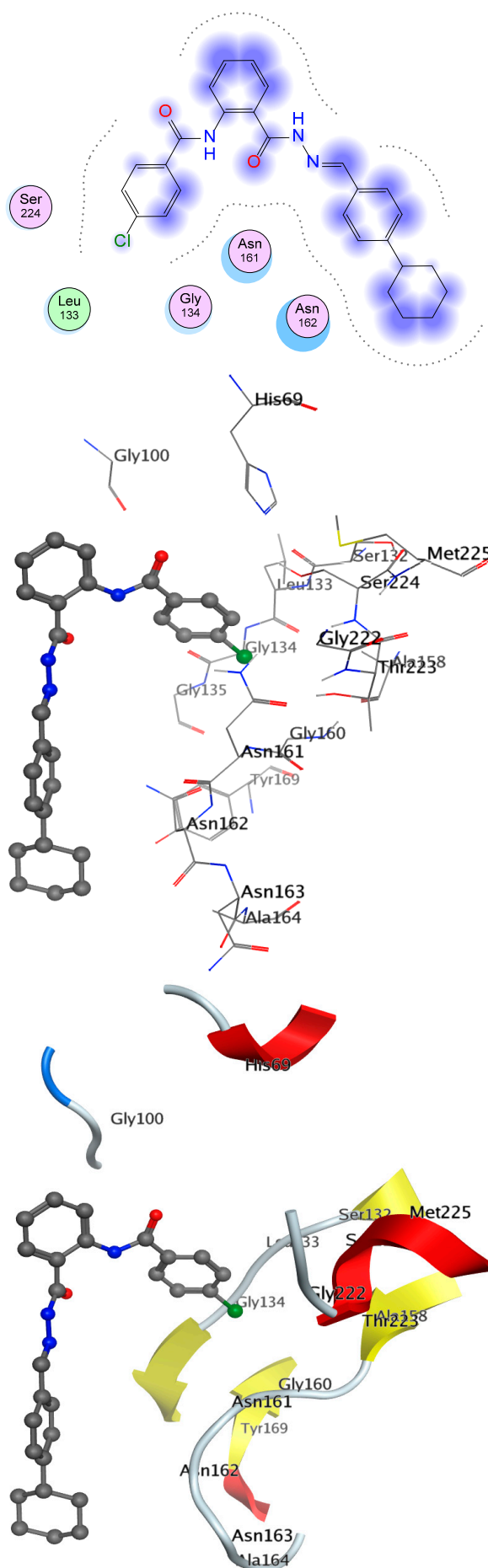
Docking pose for compound **6h** in the active site of Proteinase K

Docking pose for compound **6i** in the active site of Proteinase K

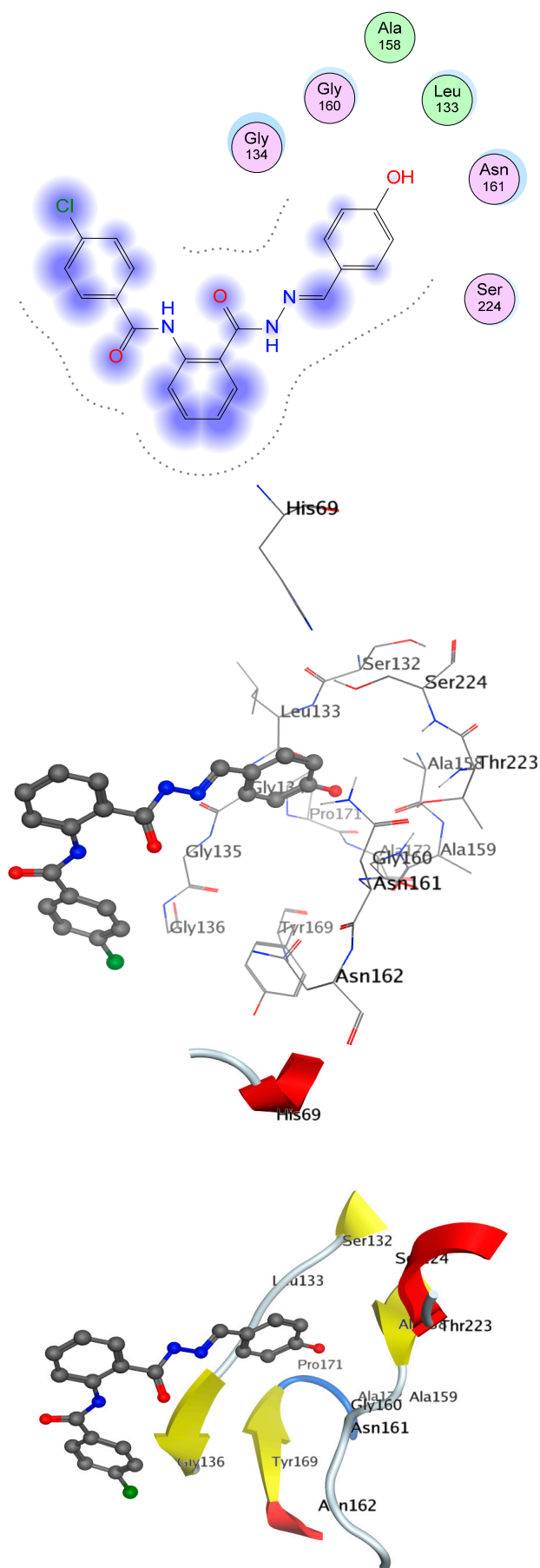
Docking pose for compound **6j** in the active site of Proteinase K

Docking pose for compound **61** in the active site of Proteinase K

Docking pose for compound **6m** in the active site of Proteinase K

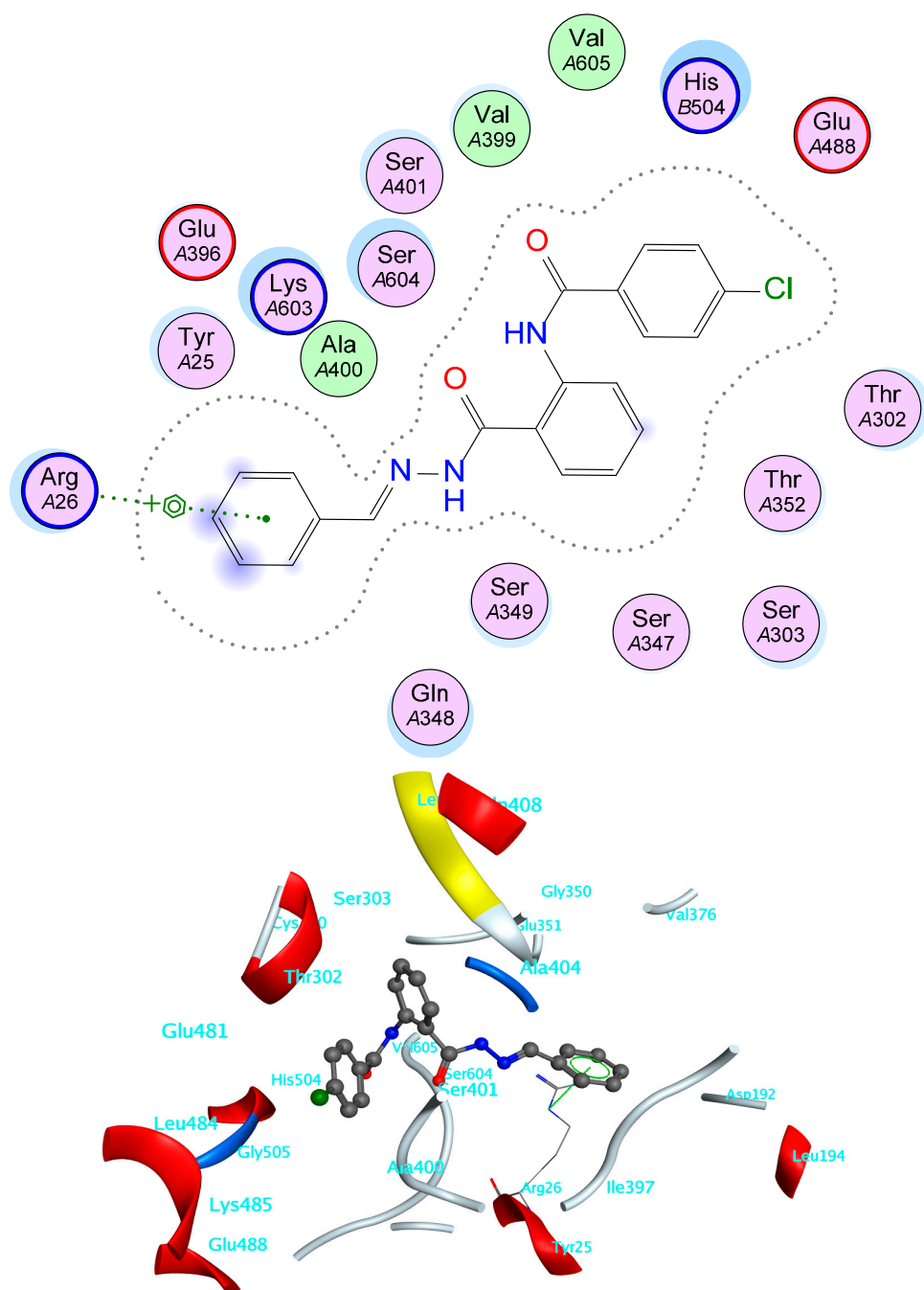
Docking pose for compound **6n** in the active site of Proteinase K



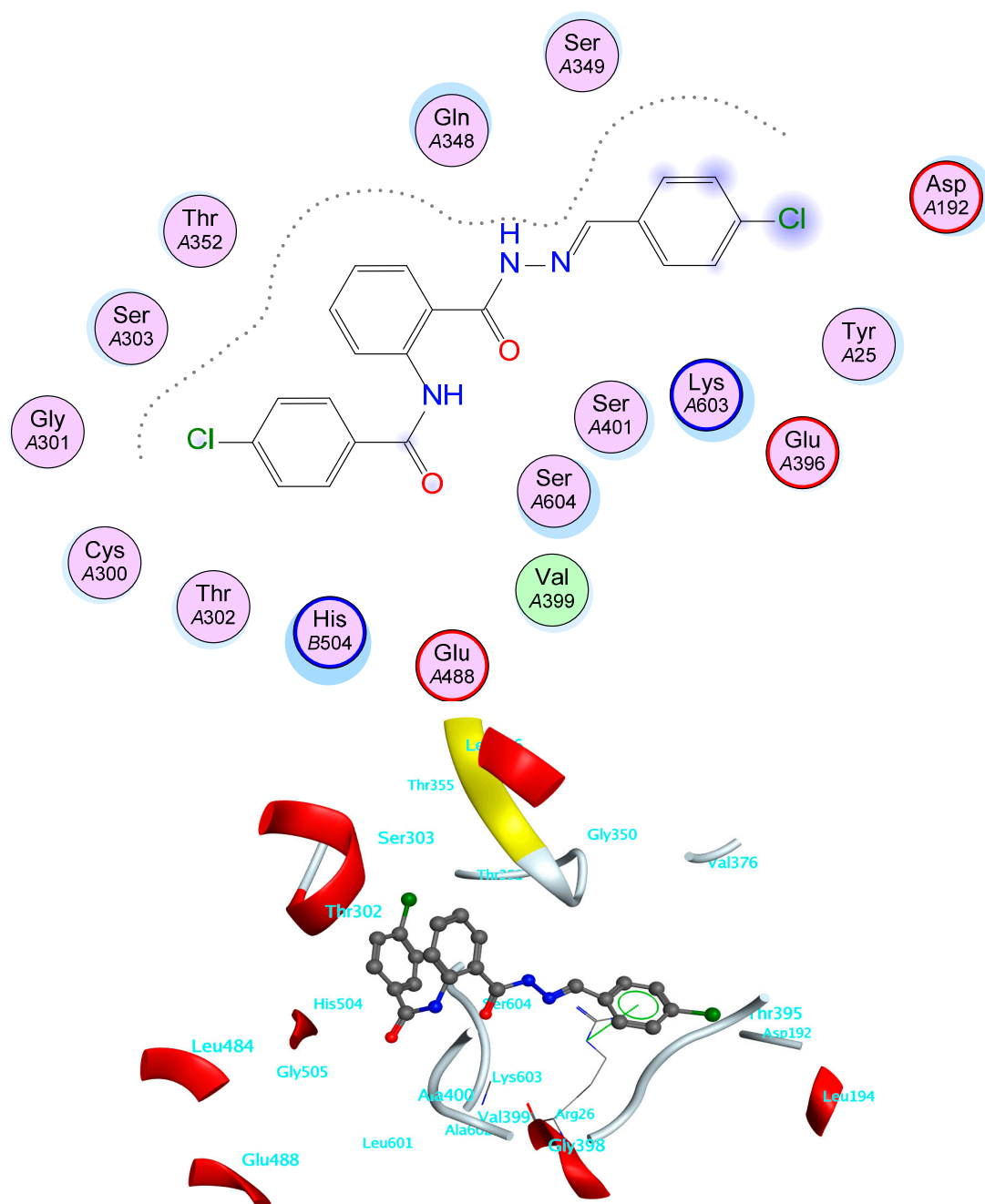


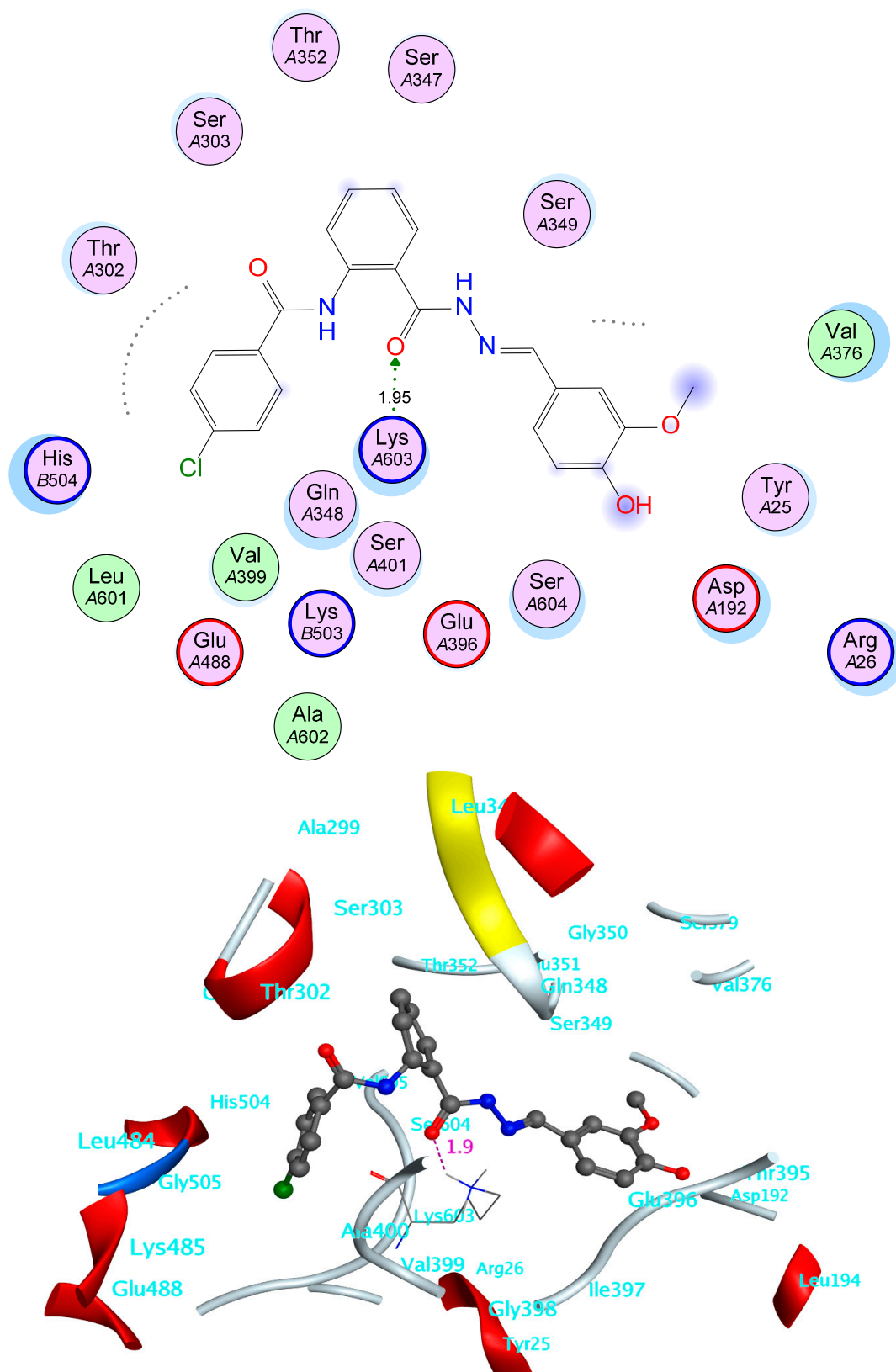
Docking pose for compound **60** in the active site of Proteinase K

**Figures S2.** Docking poses of compounds **6a–o** in active site of Proteinase K.

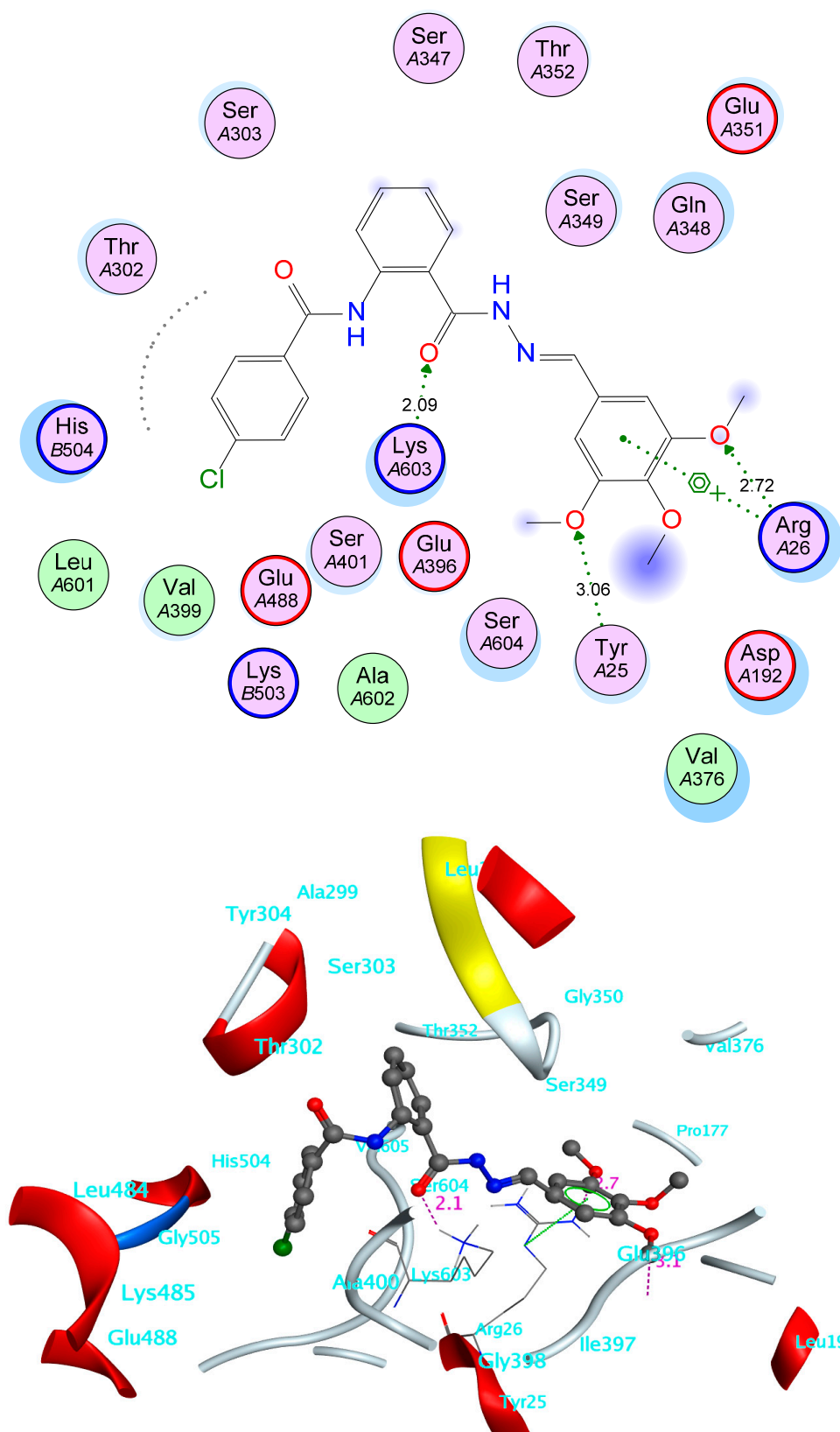


Docking pose in of **6a** in glucosamine-6-phosphate (GlcN6P) synthase

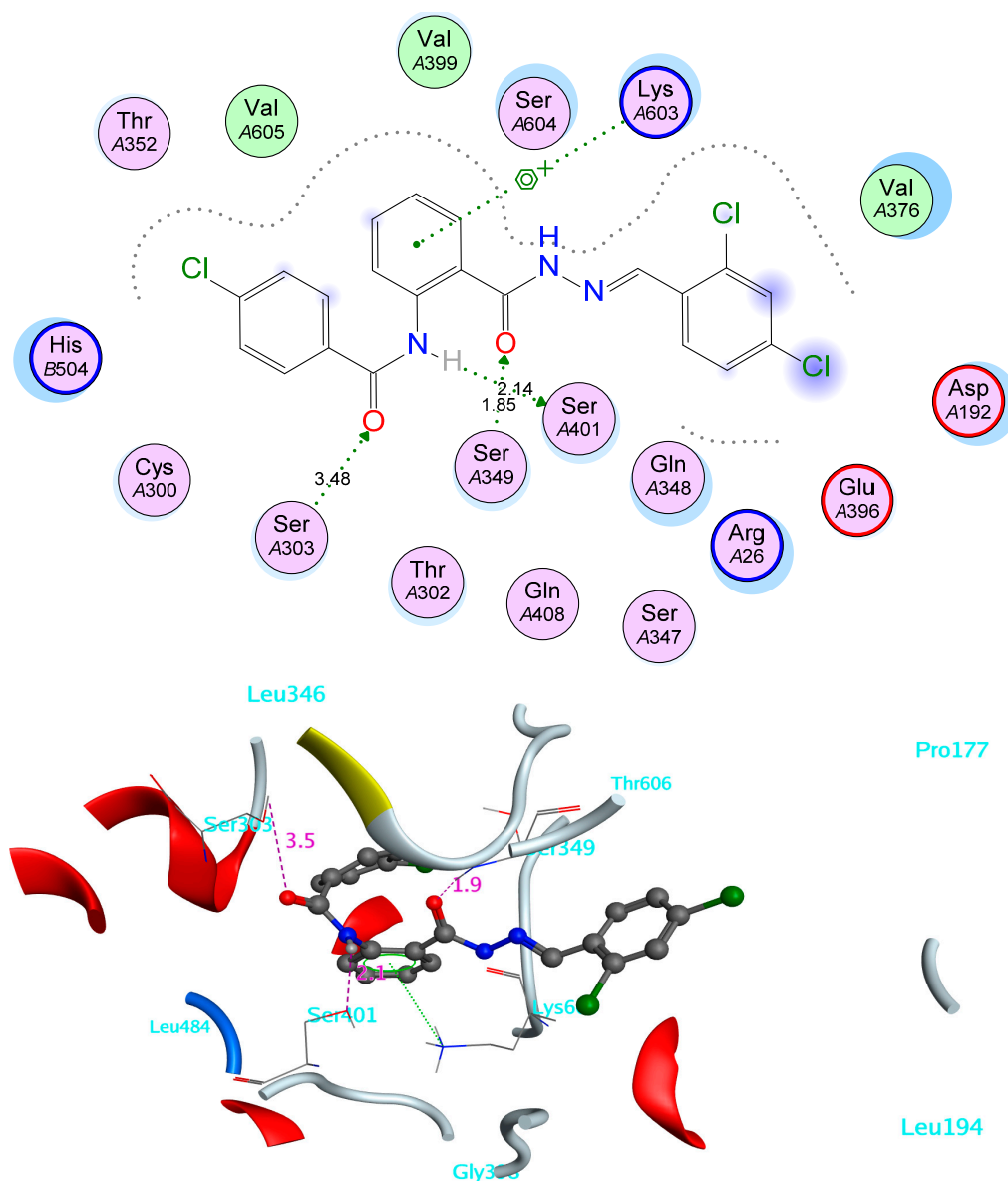
Docking pose in of **6b** in glucosamine-6-phosphate (GlcN6P) synthase



Docking pose in of **6c** in glucosamine-6-phosphate (GlcN6P) synthase



Docking pose in of **6d** in glucosamine-6-phosphate (GlcN6P) synthase



Docking pose in of **6e** in glucosamine-6-phosphate (GlcN6P) synthase

**Figures S3.** Docking poses of compounds **6a–e** in active site of glucosamine-6-phosphate (GlcN6P) synthase.