

Supplementary data for the article:

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# Supporting Information

## Anion- $\pi$ interactions in complexes of proteins and halogen-containing amino acids

Sunčica Z. Borozan<sup>1</sup> · Mario V. Zlatović<sup>2</sup> · Srđan Đ. Stojanović<sup>3</sup>

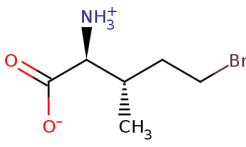
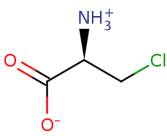
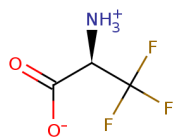
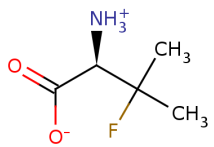
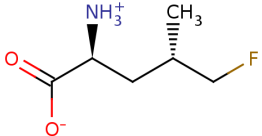
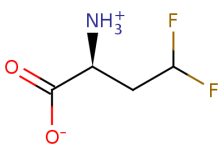
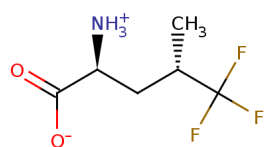
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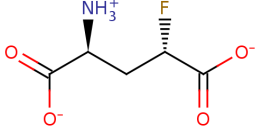
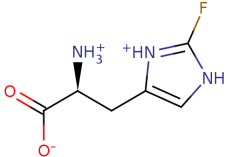
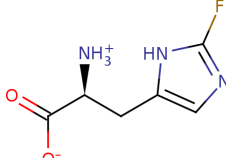
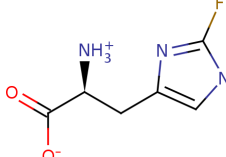
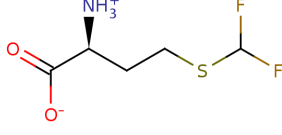
<sup>1</sup> Department of Chemistry, Faculty of Veterinary Medicine, University of Belgrade, Belgrade, Serbia

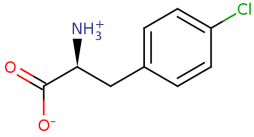
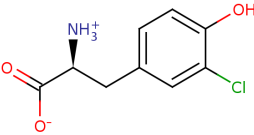
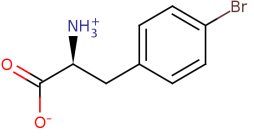
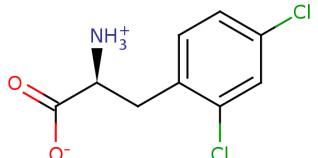
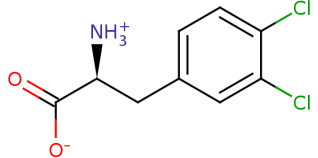
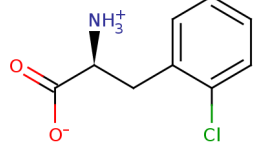
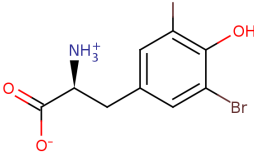
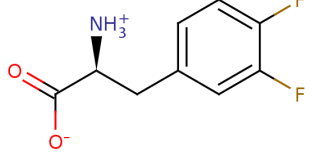
<sup>2</sup> Faculty of Chemistry, University of Belgrade, Belgrade, Serbia

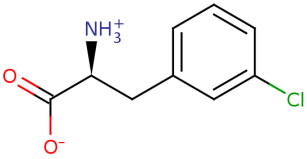
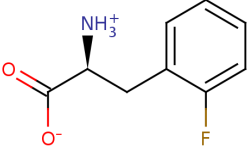
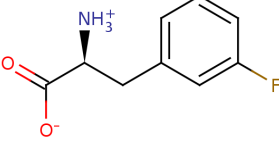
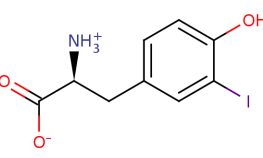
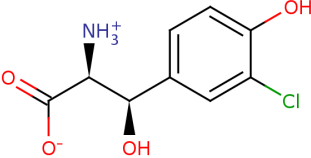
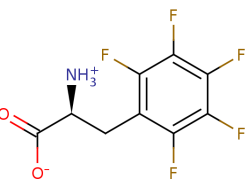
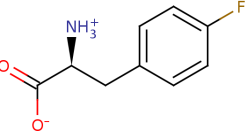
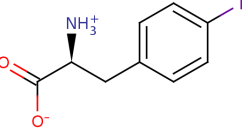
<sup>3</sup> ICTM - Department of Chemistry, University of Belgrade, Belgrade, Serbia

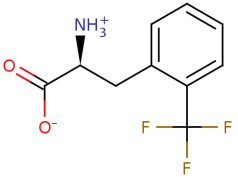
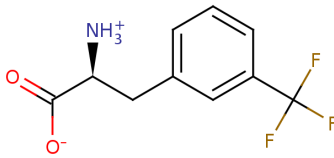
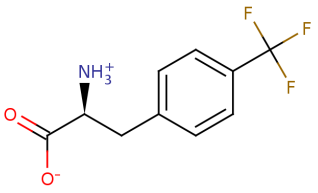
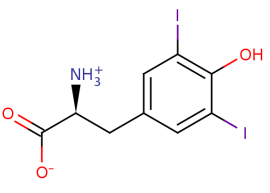
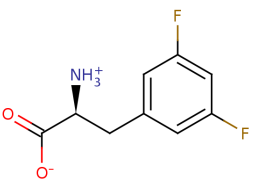
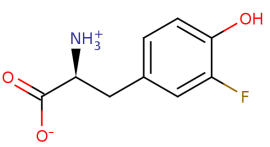
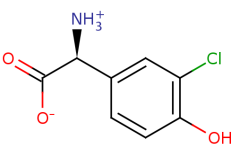
**Table S1:** Halogen-containing non-natural amino acids (SwissSidechain - <http://www.swissidechain.ch>)

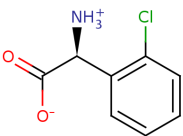
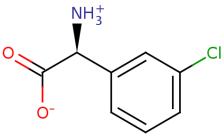
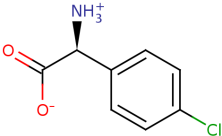
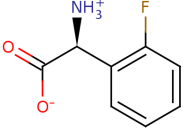
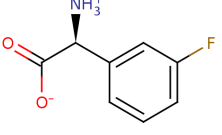
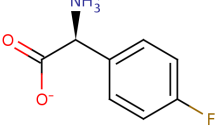
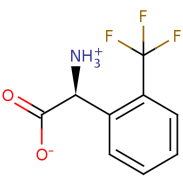
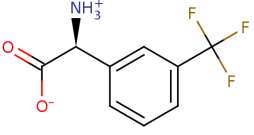
Alanine derivatives			
ID (D-form)	Full name	2D structure	PDB link
<a href="#">BIU</a>	5-bromo-l-isoleucine		<a href="#">PDB Ligand</a>
<a href="#">C2N</a>	3-chloro-l-alanine		<a href="#">PDB Ligand</a>
<a href="#">FLA</a>	Trifluoro-alanine		<a href="#">PDB Ligand</a>
<a href="#">FVAL</a>	3-Fluoro-valine		<a href="#">PDB Ligand</a>
<a href="#">LEF</a>	(4s)-5-fluoro-l-leucine		<a href="#">PDB Ligand</a>
<a href="#">OBF</a>	(2s)-2-amino-4,4-difluorobutanoic acid		<a href="#">PDB Ligand</a>
<a href="#">TFLE</a>	5,5,5-Trifluoro-leucine		<a href="#">PDB Ligand</a>

Aspartic derivatives			
ID (D-form)	Full name	2D structure	PDB link
<a href="#">FGA4</a>	4-Fluoro-glutamic acid		<a href="#">PDB Ligand</a>
Histidine derivatives			
ID (D-form)	Full name	2D structure	PDB link
<a href="#">2HF</a>	2-fluoro-l-histidine		<a href="#">PDB Ligand</a>
<a href="#">2HF1</a>	2-fluoro-l-histidine		<a href="#">PDB Ligand</a>
<a href="#">2HF2</a>	2-fluoro-l-histidine		<a href="#">PDB Ligand</a>
Methionine derivatives			
ID (D-form)	Full name	2D structure	PDB link
<a href="#">2FM</a>	s-(difluoromethyl)-homocysteine		<a href="#">PDB Ligand</a>
Phenylalanine derivatives			
ID (D-form)	Full name	2D structure	PDB link

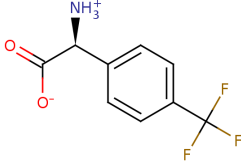
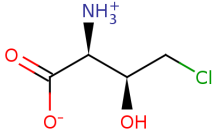
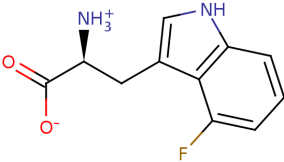
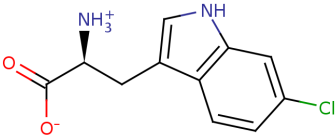
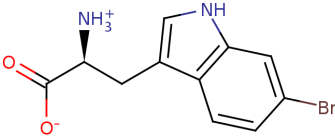
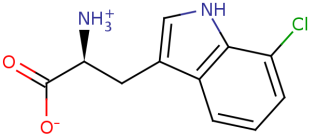
<a href="#">200</a>	4-chloro-Phenylalanine		PDB Ligand
<a href="#">3MY</a>	3-Chloro-tyrosine		PDB Ligand
<a href="#">4BF</a>	4-Bromo-phenylalanine		PDB Ligand
<a href="#">CP24</a>	2,4-dichloro-phenylalanine		PDB Ligand
<a href="#">CP34</a>	3,4-dichloro-phenylalanine		PDB Ligand
<a href="#">CPH2</a>	2-chloro-Phenylalanine		PDB Ligand
<a href="#">DBY</a>	3,5-dibromotyrosine		PDB Ligand
<a href="#">F2F</a>	3,4-Difluoro-phenylalanine		PDB Ligand

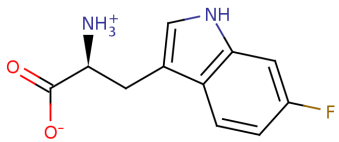
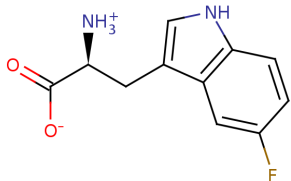
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<a href="#">FPH2</a>	2-Fluoro-Phenylalanine		PDB Ligand
<a href="#">FPH3</a>	3-Fluoro-Phenylalanine		PDB Ligand
<a href="#">IYR</a>	3-iodo-tyrosine		PDB Ligand
<a href="#">OMY</a>	(betar)-3-chloro-beta-hydroxy-L-tyrosine		PDB Ligand
<a href="#">PF5</a>	pentafluoro-phenylalanine		PDB Ligand
<a href="#">PFF</a>	4-Fluoro-Phenylalanine		PDB Ligand
<a href="#">PHI</a>	4-Iodo-Phenylalanine		PDB Ligand

<a href="#">TFP2</a>	2-(Trifluoromethyl)-phenylalanine		<a href="#">PDB Ligand</a>
<a href="#">TFP3</a>	3-(Trifluoromethyl)-phenylalanine		<a href="#">PDB Ligand</a>
<a href="#">TFP4</a>	4-(Trifluoromethyl)-phenylalanine		<a href="#">PDB Ligand</a>
<a href="#">TYI</a>	3,5-diiodotyrosine		<a href="#">PDB Ligand</a>
<a href="#">WFP</a>	3,5-Difluoro-phenylalanine		<a href="#">PDB Ligand</a>
<a href="#">YOF</a>	3-fluorotyrosine		<a href="#">PDB Ligand</a>
Phenylglycine derivatives			
ID (D-form)	Full name	2D structure	PDB link
<a href="#">CHP</a>	3-chloro-4-hydroxy-phenylglycine		<a href="#">PDB Ligand</a>

<a href="#">CPG2</a>	2-Chloro-phenylglycine		PDB Ligand
<a href="#">CPG3</a>	3-Chloro-phenylglycine		PDB Ligand
<a href="#">CPG4</a>	4-Chloro-phenylglycine		PDB Ligand
<a href="#">FPG2</a>	2-Fluoro-phenylglycine		PDB Ligand
<a href="#">FPG3</a>	3-Fluoro-phenylglycine		PDB Ligand
<a href="#">FPG4</a>	4-Fluoro-phenylglycine		PDB Ligand
<a href="#">TFG2</a>	2-(Trifluoromethyl)-phenylglycine		PDB Ligand
<a href="#">TFG3</a>	3-(Trifluoromethyl)-phenylglycine		PDB Ligand



<a href="#">TFG4</a>	4-(Trifluoromethyl)-phenylglycine		<a href="#">PDB Ligand</a>
<b>Serine derivatives</b>			
<b>ID (D-form)</b>	<b>Full name</b>	<b>2D structure</b>	<b>PDB link</b>
<a href="#">CTH</a>	4-chloro-threonine		<a href="#">PDB Ligand</a>
<b>Tryptophan derivatives</b>			
<b>ID (D-form)</b>	<b>Full name</b>	<b>2D structure</b>	<b>PDB link</b>
<a href="#">4FW</a>	4-fluoro-tryptophan		<a href="#">PDB Ligand</a>
<a href="#">6CW</a>	6-chloro-l-tryptophan		<a href="#">PDB Ligand</a>
<a href="#">BTR</a>	6-bromo-tryptophan		<a href="#">PDB Ligand</a>
<a href="#">CTE</a>	7-chloro-tryptophan		<a href="#">PDB Ligand</a>

<a href="#">FT6</a>	6-fluoro-l-tryptophan	 <p>The structure shows the L-tryptophan side chain with a fluorine atom at the 6-position of the indole ring. The amino group is shown as NH<sub>3</sub><sup>+</sup> and the carboxylate group as COO<sup>-</sup>.</p>	PDB Ligand
<a href="#">FTR</a>	5-Fluoro-tryptophan	 <p>The structure shows the L-tryptophan side chain with a fluorine atom at the 5-position of the indole ring. The amino group is shown as NH<sub>3</sub><sup>+</sup> and the carboxylate group as COO<sup>-</sup>.</p>	PDB Ligand