

Supplementary data for the article:

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Supporting Information

Anion- π interactions in complexes of proteins and halogen-containing amino acids

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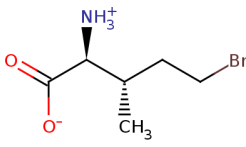
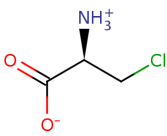
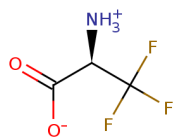
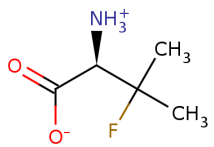
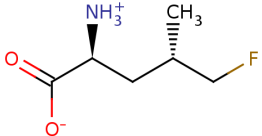
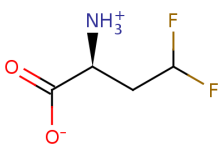
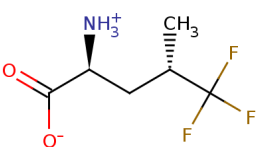
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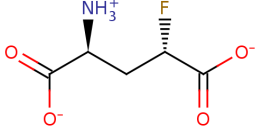
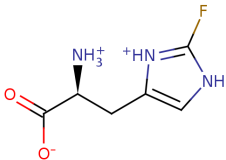
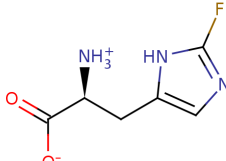
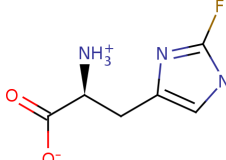
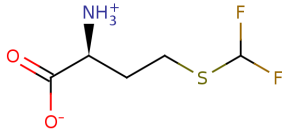
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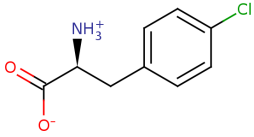
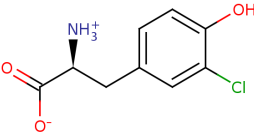
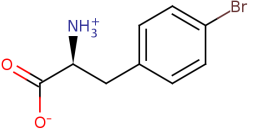
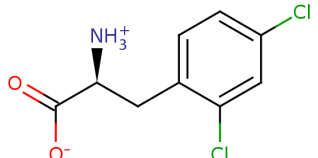
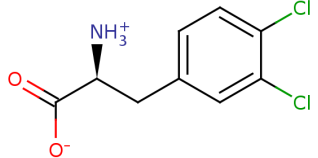
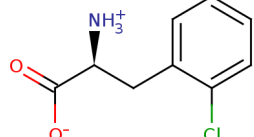
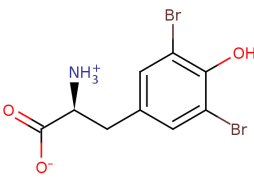
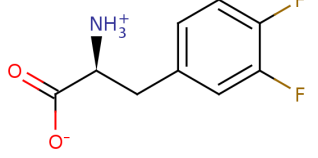
² Faculty of Chemistry, University of Belgrade, Belgrade, Serbia

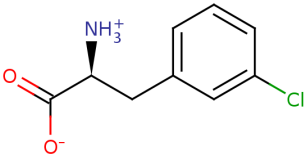
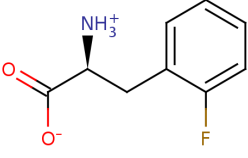
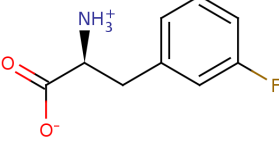
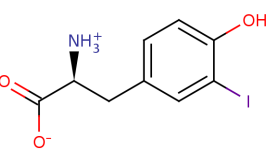
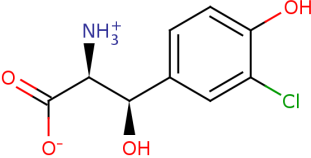
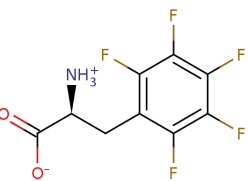
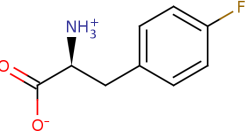
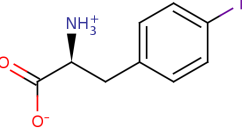
³ ICTM - Department of Chemistry, University of Belgrade, Belgrade, Serbia

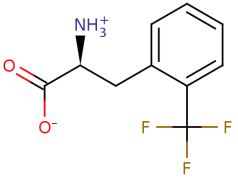
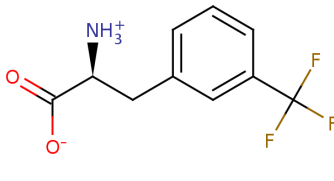
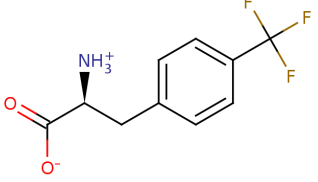
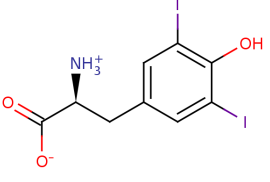
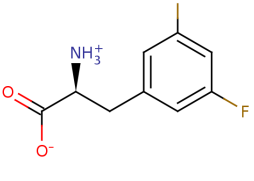
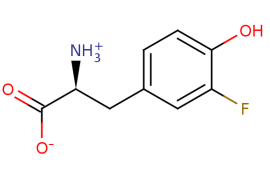
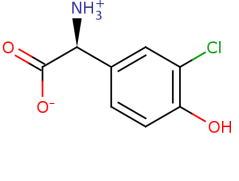
Table S1: Halogen-containing non-natural amino acids (SwissSidechain - <http://www.swissidechain.ch>)

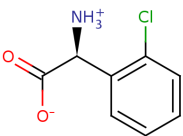
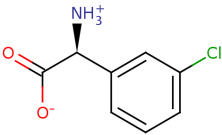
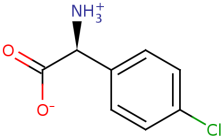
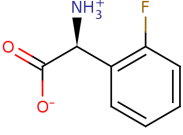
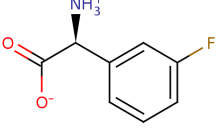
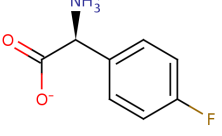
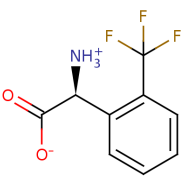
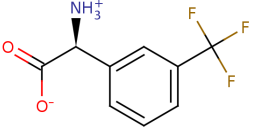
Alanine derivatives			
ID (D-form)	Full name	2D structure	PDB link
BIU	5-bromo-l-isoleucine		PDB Ligand
C2N	3-chloro-l-alanine		PDB Ligand
FLA	Trifluoro-alanine		PDB Ligand
FVAL	3-Fluoro-valine		PDB Ligand
LEF	(4s)-5-fluoro-l-leucine		PDB Ligand
OBF	(2s)-2-amino-4,4-difluorobutanoic acid		PDB Ligand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

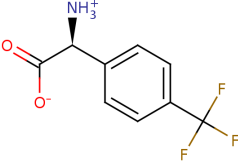
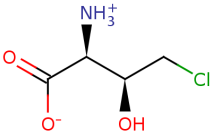
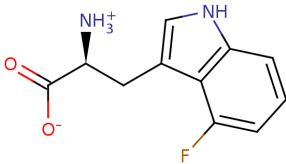
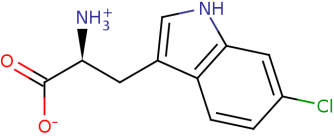
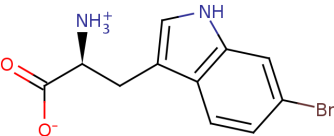
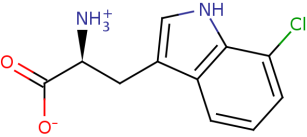
Aspartic derivatives			
ID (D-form)	Full name	2D structure	PDB link
FGA4	4-Fluoro-glutamic acid		PDB Ligand
Histidine derivatives			
ID (D-form)	Full name	2D structure	PDB link
2HF	2-fluoro-l-histidine		PDB Ligand
2HF1	2-fluoro-l-histidine		PDB Ligand
2HF2	2-fluoro-l-histidine		PDB Ligand
Methionine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

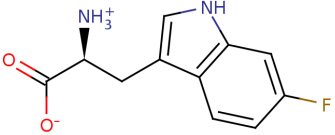
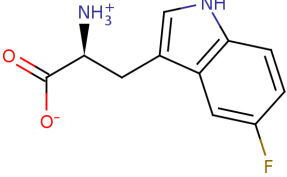
200	4-chloro-Phenylalanine		PDB Ligand
3MY	3-Chloro-tyrosine		PDB Ligand
4BF	4-Bromo-phenylalanine		PDB Ligand
CP24	2,4-dichloro-phenylalanine		PDB Ligand
CP34	3,4-dichloro-phenylalanine		PDB Ligand
CPH2	2-chloro-Phenylalanine		PDB Ligand
DBY	3,5-dibromotyrosine		PDB Ligand
F2F	3,4-Difluoro-phenylalanine		PDB Ligand

FCL	3-chloro-Phenylalanine		PDB Ligand
FPH2	2-Fluoro-Phenylalanine		PDB Ligand
FPH3	3-Fluoro-Phenylalanine		PDB Ligand
IYR	3-iodo-tyrosine		PDB Ligand
OMY	(betar)-3-chloro-beta-hydroxy-L-tyrosine		PDB Ligand
PF5	pentafluoro-phenylalanine		PDB Ligand
PFF	4-Fluoro-Phenylalanine		PDB Ligand
PHI	4-Iodo-Phenylalanine		PDB Ligand

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

CPG2	2-Chloro-phenylglycine		PDB Ligand
CPG3	3-Chloro-phenylglycine		PDB Ligand
CPG4	4-Chloro-phenylglycine		PDB Ligand
FPG2	2-Fluoro-phenylglycine		PDB Ligand
FPG3	3-Fluoro-phenylglycine		PDB Ligand
FPG4	4-Fluoro-phenylglycine		PDB Ligand
TFG2	2-(Trifluoromethyl)-phenylglycine		PDB Ligand
TFG3	3-(Trifluoromethyl)-phenylglycine		PDB Ligand

TFG4	4-(Trifluoromethyl)-phenylglycine		PDB Ligand
Serine derivatives			
ID (D-form)	Full name	2D structure	PDB link
CTH	4-chloro-threonine		PDB Ligand
Tryptophan derivatives			
ID (D-form)	Full name	2D structure	PDB link
4FW	4-fluoro-tryptophan		PDB Ligand
6CW	6-chloro-l-tryptophan		PDB Ligand
BTR	6-bromo-tryptophan		PDB Ligand
CTE	7-chloro-tryptophan		PDB Ligand

<p>FT6</p>	<p>6-fluoro-l-tryptophan</p>		<p>PDB Ligand</p>
<p>FTR</p>	<p>5-Fluoro-tryptophan</p>		<p>PDB Ligand</p>