PyMOL Selection Operator/Modifier Table

From https://pymolwiki.org/index.php/Selection_Algebra

Selection operators and modifiers are listed below. The dummy variables *s1* and *s2* stand for selection-expressions such as "chain a" or "hydro."

Operator	Description
Generic	
all	All atoms currently loaded into PyMOL
none	Empty selection
enabled	Atoms from enabled objects
Named selections	
sele	Named selection or object "sele", but only if it doesn't conflict with the name of another operator
%sele	Named selection or object "sele" Recommended, avoids ambiguity
?sele	Named selection or object "sele", or empty selection if "sele" doesn't exist
Logical	
not S1	Inverts selection
S1 and S2	Atoms included in both S1 and S2
S1 or S2	Atoms included in either S1 or S2
S1 S2	implicit or
S1 and (S2 or S3)	Parentheses for evaluation order control
first S1	First atom in S1 (single atom selection)
last S1	Last atom in S1 (single atom selection)
Identifiers (see also Selection Macros)	
model 1ubq	Atoms from object "1ubq"
chain C	Chain identifier "C"
segi S	Segment identifier "S" (label_asym_id from mmCIF)
resn ALA	Residue name "ALA"
resi 100-200	Residue identifier between 100 and 200
name CA	Atom name "CA"
alt A	Alternate location "A"
index 123	Internal per-object atom index (changes with sorting)
id 123	ID column from PDB file
rank 123	Per-object atom index at load time (see also retain_order)
pepseq ACDEF	Protein residue sequence with one-letter code "ACDEF" (see also FindSeq)
label "Hello World"	Atoms with label "Hello World" (new in PyMOL 1.9)

Identifier matching	
S1 in S2	Atoms in S1 whose identifiers name, resi, resn, chain and segi all match atoms in S2
S1 like S2	Atoms in S1 whose identifiers name and resi match atoms in S2
Entity expansion	
Important: All "by"-operators have a weak priority, so (byres S1 or S2) is actually identical to (byres (S1 or S2)) and not to ((byres S1) or S2)	
byobject S1	Expands S1 to complete objects
bysegi S1	Expands S1 to complete segments
bychain S1	Expands S1 to complete chains
byres S1	Expands S1 to complete residues
bycalpha S1	CA atoms of residues with at least one atom in S1
bymolecule S1	Expands S1 to complete molecules (connected with bonds)
byfragment S1	
byring S1	All rings of size ≤ 7 which have at least one atom in S1 (new in PyMOL 1.8.2)
bycell S1	Expands selection to unit cell
Bond expansion	
bound_to S1	Atoms directly bonded to S1, may include S1
neighbor S1	Atoms directly bonded to S1, excludes S1
S1 extend 3	Expands S1 by 3 bonds connected to atoms in S1
Proximity (see also comparison of distance operators)	
S1 within 12.3 of S2	Atoms in S1 that are within 12.3 Angstroms of any atom in S2
S1 around 12.3	Atoms with centers within 12.3 Angstroms of the center of any atom in S1
S1 expand 12.3	Expands S1 by atoms within 12.3 Angstroms of the center of any atom in S1

S1 gap 1.2	Atoms whose VDW radii are separated from the VDW radii of S1 by a minimum of 1.2 Angstroms.
S1 near_to 12.3 of S2	Same as within, but excludes S2 from the selection (and thus is identical to S1 and S2 around 12.3)
S1 beyond 12.3 of S2	Atoms in S1 that are at least 12.3 Anstroms away from S2

Properties	
partial_charge < 1.2	
formal_charge = 1	
b < 100.0	B-factor less than 100.0
q < 1.0	Occupancy less than 1.0
ss H+S	Atoms with secondary structure H (helix) or S (sheet)
elem C	Atoms of element C (carbon)
p.foo = 12	
p.foo < 12.3	
p.foo in 12+34	
stereo R	Chiral R/S stereo center with label R (only Incentive PyMOL 1.4-1.8)
Flags	
bonded	Atoms which have at least one bond
protected	see protect
fixed	see flag
restrained	see flag
masked	see mask
flag 25	Atoms with flag 25, see flag
Chemical classes	
organic	Non-polymer organic compounds (e.g. ligands, buffers)
inorganic	Non-polymer inorganic atoms/ions
solvent	Water molecules
polymer	Protein or Nucleic Acid
polymer.protein	Protein (New in PyMOL 2.1)
polymer.nucleic	Nucleic Acid (New in PyMOL 2.1)
guide	Protein CA and nucleic acid C4*/C4'
hetatm	Atoms loaded from PDB HETATM records
hydrogens	Hydrogen atoms
backbone	Polymer backbone atoms (new in PyMOL 1.6.1)
sidechain	Polymer non-backbone atoms (new in PyMOL 1.6.1)
metals	Metal atoms (new in PyMOL 1.6.1)
donors	Hydrogen bond donor atoms
acceptors	Hydrogen bond acceptor atoms
Style	
visible	Atoms in enabled objects with at least one visible representation
rep cartoon	Atoms with cartoon representation
color blue	Atoms with atom-color blue (by color index)
cartoon_color blue	Atoms with atom-level cartoon_color setting (by color index)
ribbon_color blue	Atoms with atom-level ribbon_color setting (by color index)
Non molecular	
center	Pseudo-atom at the center of the scene
origin	Pseudo-atom at the origin of rotation
Coordinates	
state 123	Atoms with coordinates in state 123
present	Atoms with coordinates in the current state
x < 12.3	Atoms with model-space x coordinate less than 12.3
y < 12.3	Atoms with model-space y coordinate less than 12.3
z > 12.3	Atoms with model-space z coordinate greater than 12.3