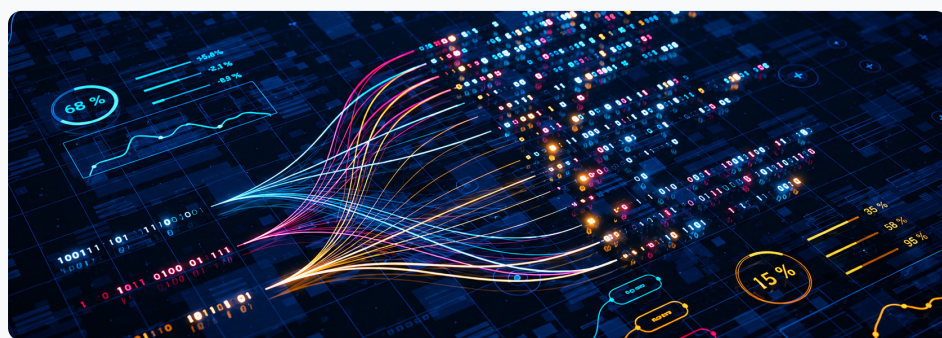


Discover, target, and focus on new interactions

Formerly known as ViewContacts:
the gold standard for non-bonded
interaction analysis and visualisation.



Raptor



A data-driven and rule-based algorithmic framework

The absolute reliability of Raptor stems from a superior, rule-based algorithm developed from the latest findings in structural biology, molecular modelling, molecular recognition, and database mining. The software automatically assigns SMARTS-based atom types and employs an extensive range of rigorously tested chemical and geometric rules to ensure that every non-covalent contact is accurately identified and classified.

This high-performance methodology allows for the comprehensive detection of a wide variety of interaction types, ranging from standard hydrogen bonds, van der Waals, metal bonding, and ionic pairs to less commonly flagged close contacts.

Raptor maps out the complete environment of the binding site, capturing:

- Hydrogen bonding and ionic polar pairs.
- van der Waals and pi-p apolar pairs.
- Cation-pi, h₂donor-pi, and hydrogen bonding directly to pi-systems.
- Halogen bonding arising from σ -hole bonds.
- Different pi-pi stacking, and pi-edge-to-face contacts.
- Dipolar antiperiplanar interactions, cation-dipole pairs, and orthogonal dipolar alignments.
- Weak hydrogen bonding involving aliphatic CH groups.



Deep qualitative understanding of molecular recognition

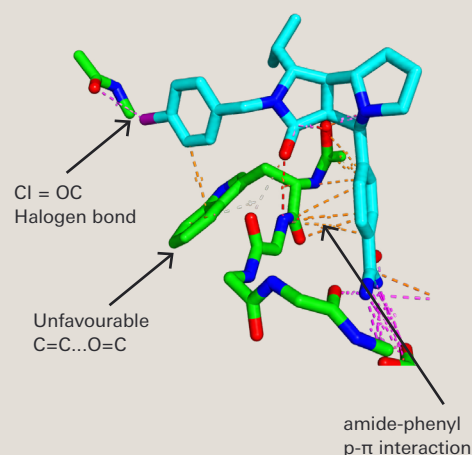
Raptor is state-of-the-art analysis software designed to provide a superior, comprehensive understanding of both favourable and unfavourable non-covalent interactions within protein-ligand complexes, in protein complexes with antibodies, and any protein assembly. While non-covalent bonds are weak by nature, they are the primary mechanism through which drugs bind to their targets, and are essential for maintaining the three-dimensional structure of proteins.

By accurately identifying, classifying, and visualising these interactions, Raptor offers chemists, modellers, crystallographers, and other scientists the precise structural insights needed to best optimise targeted drug design and decode the subtle processes through which proteins recognise and bind to small molecules and other proteins.

Pair interaction definitions

Raptor automatically identifies both favourable and unfavourable interactions using chemical rules and distance and angle constraints. The system categorises the following contact types:

- Hydrogen bonding.
- Metal bonding.
- Ionic interactions.
- Cation-dipole.
- Cation-pi.
- Dipolar alignments.
- σ -hole (halogen) bonds
- Hydrogen donor-pi contacts.
- pi-pi packing interactions.
- van der Waals interactions.
- Unfavourable electrostatic repulsions and clashing pairs.
- Polar and non-polar steric clashes.
- Polar-nonpolar desolvation penalties.



Example: 2cf8 (Thrombin)

Raptor creates PyMOL scripts that allows fast and easy exploration of the key protein-ligand interaction determining binding affinity.

Strategic handling of solvation and the math of water replacement

A critical component of effective ligand design is the ability to strategically characterise binding site water molecules and pinpoint precisely any desolvation penalties that might be detrimental to binding affinity.

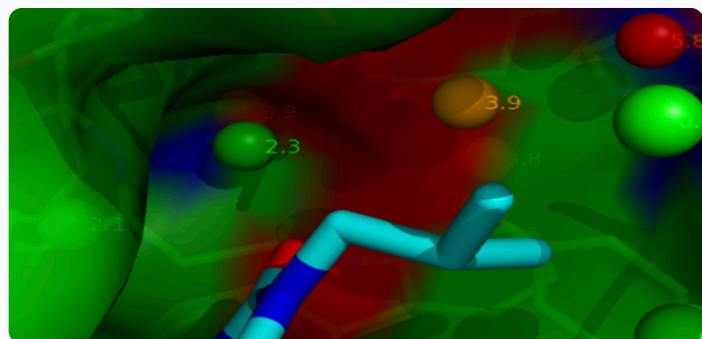
Raptor features a mathematically rigorous method for scoring bound water molecules based on their exact deviation from ideal tetrahedral coordination as observed in ice. The system evaluates the solvation environment using the following derived function:

$$Rank = \sum_n \left\{ \left(2.80 A / r_n \right) + \left[\sum_m \cos(\Theta_{Td} - \Theta_{ymn}) \right] / 6 \right\}$$

During calculation, a maximum of four protein contacts are counted (≤ 2 donors and ≤ 2 acceptors), and any overlapping contact angle less than 60° is automatically rejected by the engine. This rank score maps directly onto an intuitive green-to-red visual shorthand in your visualisation environment, identifying clear targets for ligand design experiments:

Example: 2r8q (PDE-B1)

Raptor ranks scores to provide easy identification of bound water molecules that can be targeted in ligand design experiments.



Colour	Score	Meaning
Green	2.3 – 4.0	Easy to replace
Amber	2.3 – 4.0	Possible to replace with suitable polar functionalities
Red	4.0 – 6.0	Unlikely to replace

Furthermore, Raptor excels at detecting potential desolvation penalties and other unfavourable contact pairs resulting from repulsive electrostatic forces, or short contact distances. The software can identify whether a polar atom would be strongly preferred at the location of an apolar atom, or vice versa, highlighting hidden chemical structure changes that could impact affinity.

Core technical features



LIGAND BINDING

Explores any HET group in any domain of any protein structure file with fully customisable binding site sizes.



DATA SEGMENTATION

Categorises interactions cleanly into weak or strong and allows for the separate viewing of protein-ligand contacts, contacts within a protein, and contacts between proteins.



SOLVATION HIGHLIGHTS

Automatically tracks and highlights water-mediated hydrogen bonds alongside geometric water rank scores.



ENTERPRISE DATA LINK

Links seamlessly with the Proasis enterprise protein structure database and visualisation systems for a completely unified research pipeline.



COMPREHENSIVE ATOM AND BOND TYPE DETERMINATION

Automatically detects correct bond orders from input .pdb files.



DOCKING STUDY INGESTION

Reads docking results with ease, processing multiple poses stored directly within input SDF files.



CUSTOMISABLE CONSTRAINTS

Allows users to extend or customise underlying SMARTS definitions, angle constraints, and distance parameters to match custom research targets.



TAUTOMER MANAGEMENT

Advanced SMARTS definitions natively handle complex ligand tautomers during input processing.



Automated PyMOL, MOE, and graphics scripting

Raptor removes the manual overhead of scene setup by automatically generating tailored visualisation scripts. These automated scripts create a highly optimised environments within PyMOL, MOE, or Benchware 3D, providing:

- Automated rendering of the molecular surface and solvent-excluded surface.
- One-click shortcuts for viewing temperature factors and occupancy.
- Immediate visual mapping of the key non-covalent interactions driving ligand affinity.

Hardware and software requirements

SERVER INFRASTRUCTURE

Raptor server software runs natively under Linux environments and requires RHEL 8 (or equivalent) or above.

FILE CONVERSION UTILITIES

OpenBabel is used to execute automated PDB to MOL file format conversions on the host machine.

VISUALIZATION SUPPORT

Built-in script deployment targets are fully supported for Proasis, PyMOL, MOE, and Benchware 3D.

FLEXIBLE CROSS-PLATFORM CLIENT ACCESS

Users interacting with the engine via the api resources can operate seamlessly on Microsoft Windows, Apple Mac, or Linux systems.



Raptor
by DesertSci

See your structural data with absolute clarity.

To establish an evaluation licence or arrange a technical walk-through of the Raptor interaction analysis engine, contact our expert team.

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