Analýza výsledků

- ⇨ výpočet RMSd
- ⇨ výpočet průměrné struktury
- ⇨ analýza vzdáleností, úhlů, torzí
- ⇨ výpočet helikálních parametrů
- ⇨ výpočet interakčních energií
- ⇨ analýza hydratace a interakcí s ionty
- ⇨ MIP, MM-PBSA, PCA, entropie, atd.

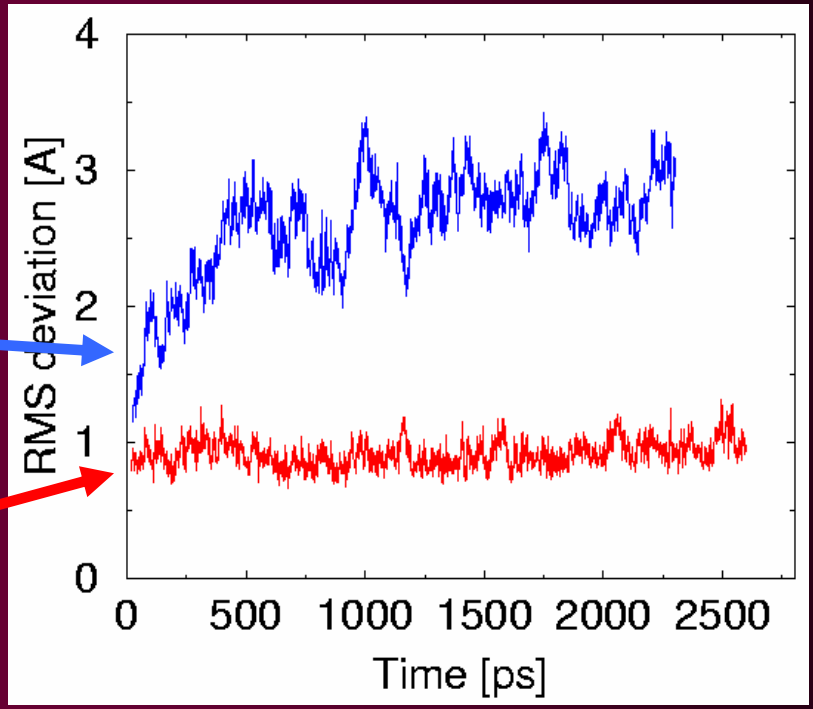
Analýza RMSd

⇨ RMSd = Root Mean Square deviation

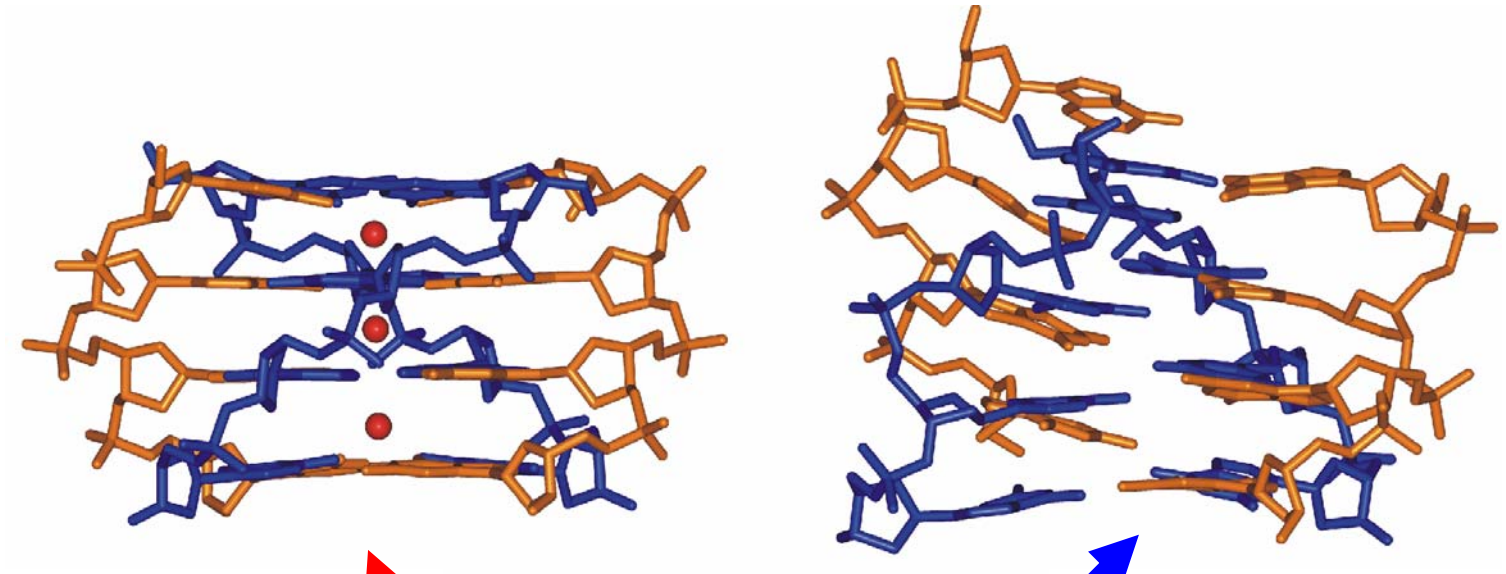
⇨ udává např., jak moc se liší studovaná molekula v simulacích MD od startovní struktury

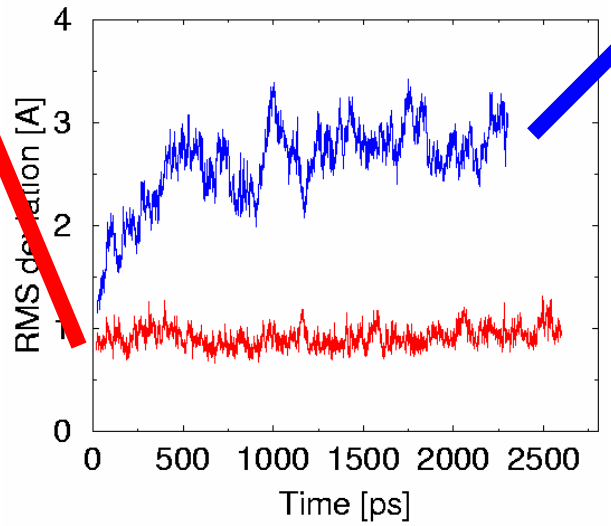
geometrie molekuly se v průběhu MD výrazně změnila

MD geometrie ve velmi dobré shodě se startovní strukturou



Příklad – guaninový kvadruplex

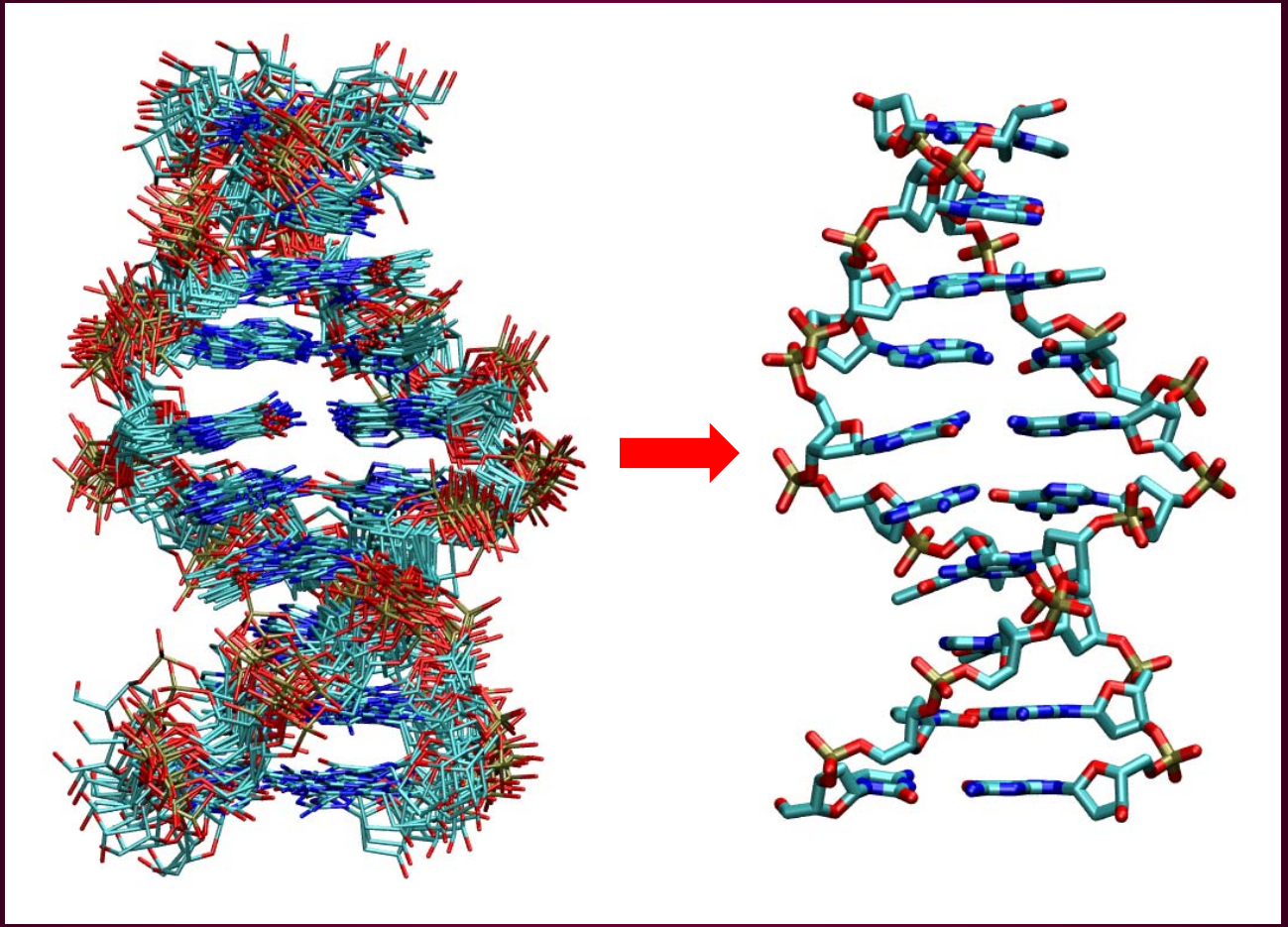




G-DNA s ionty v centrálním kanálu

G-DNA bez iontů v kanálu

Průměrná struktura

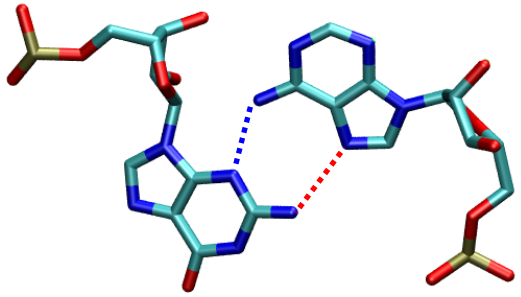


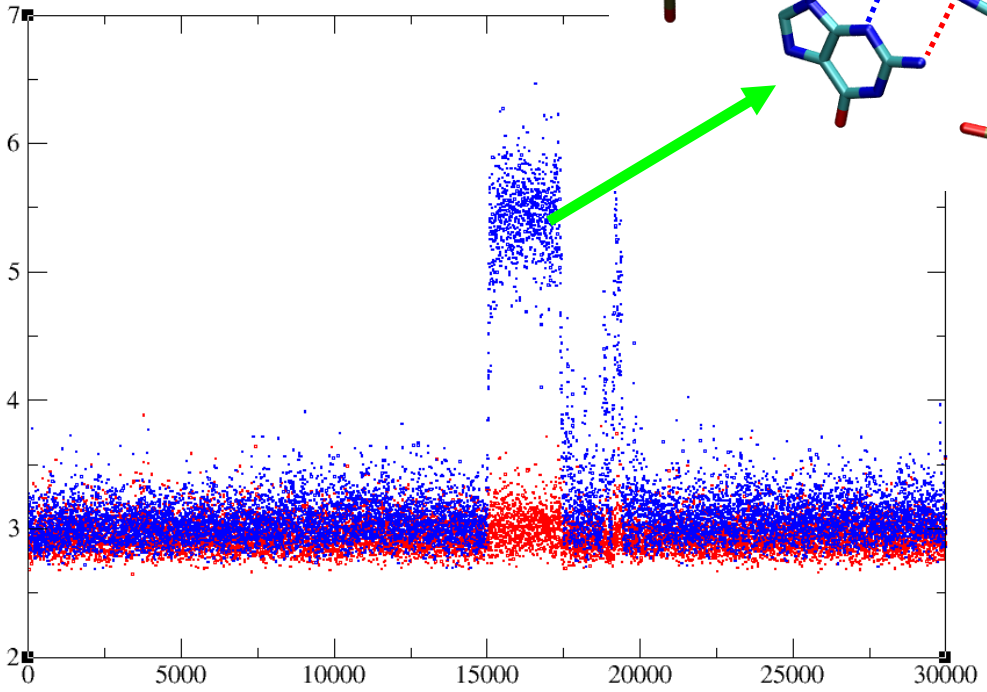
jednotlivé snímky
trajektorie MD

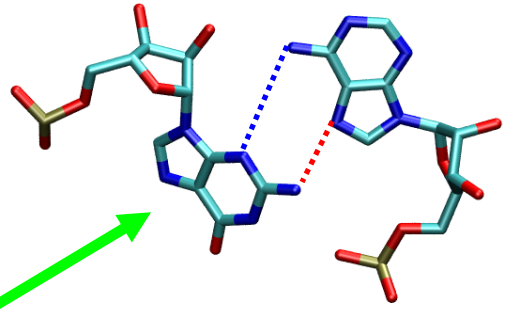
průměrná struktura

Analýza vzdáleností

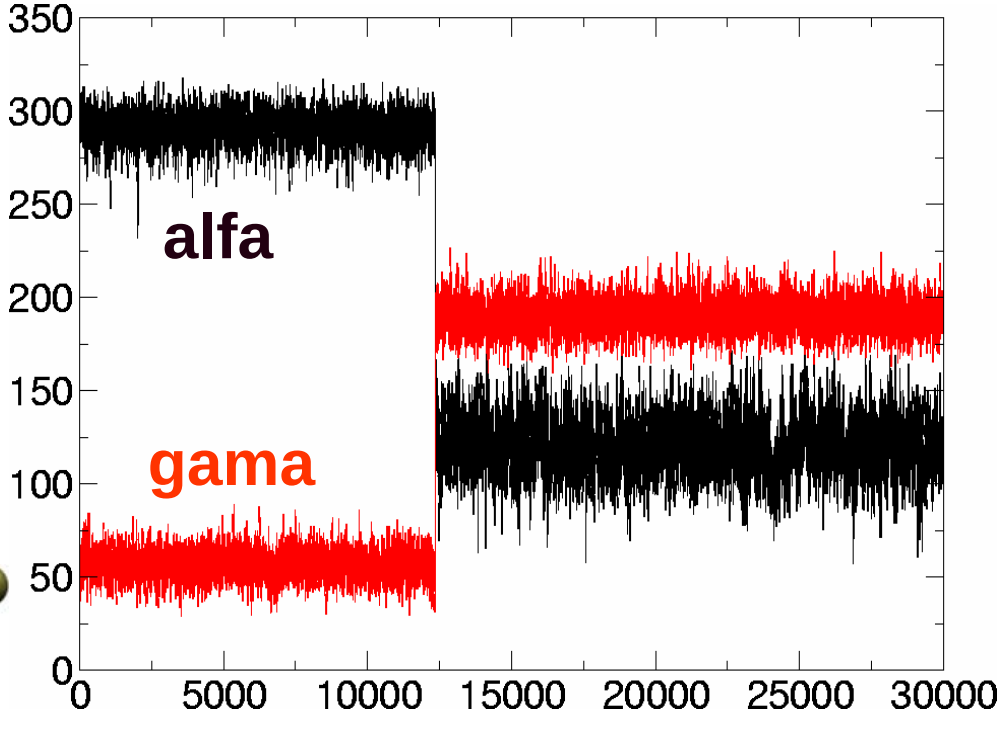
Příklad: změna geometrie páru A.G

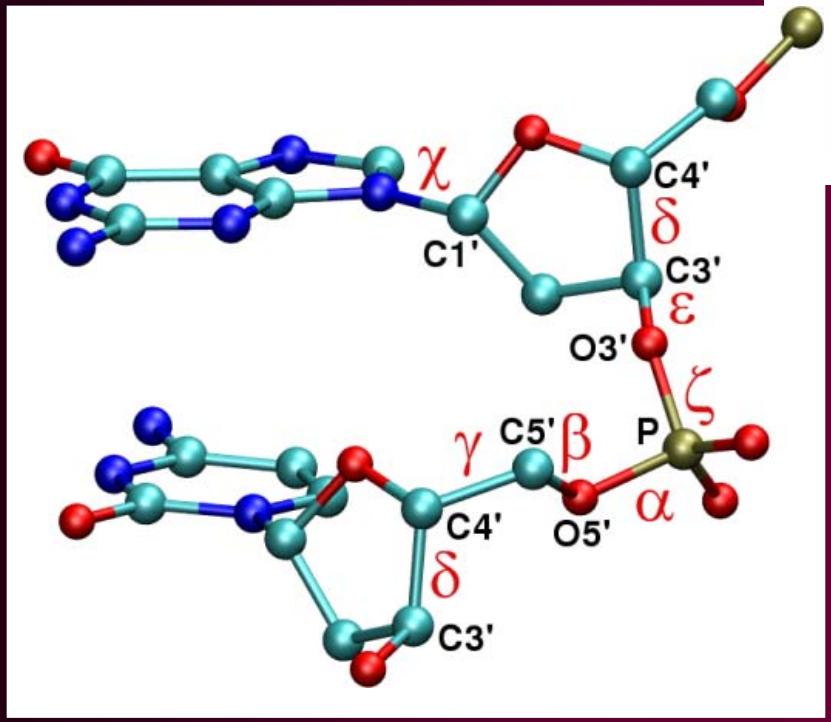


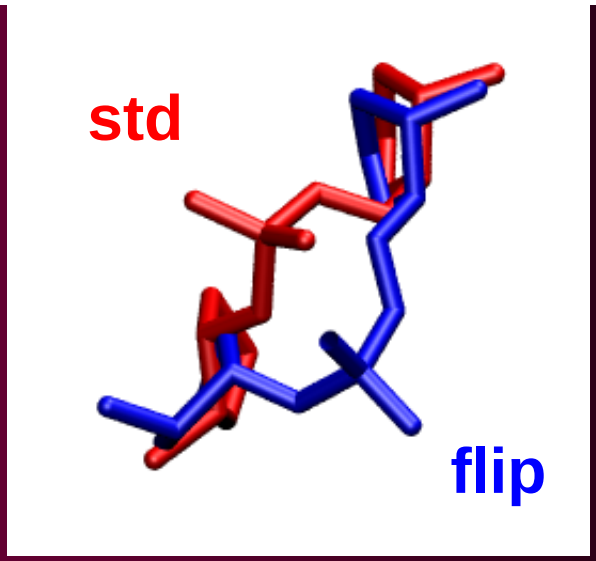


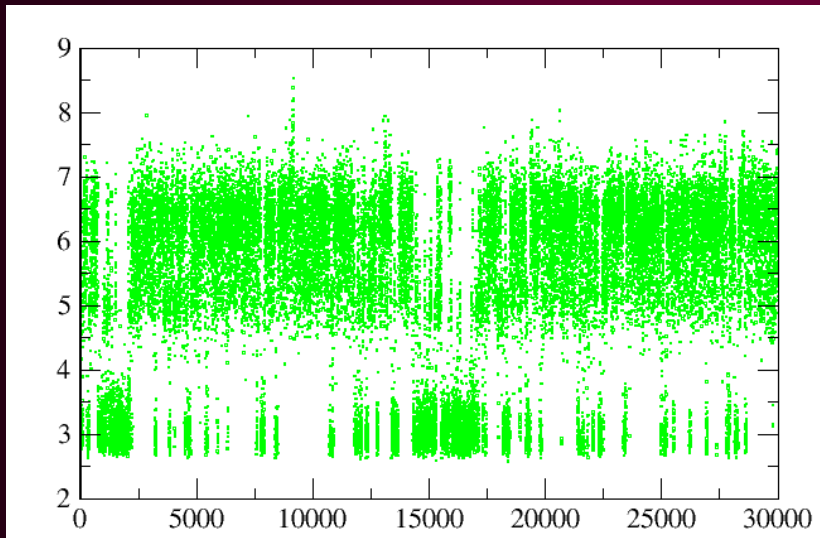


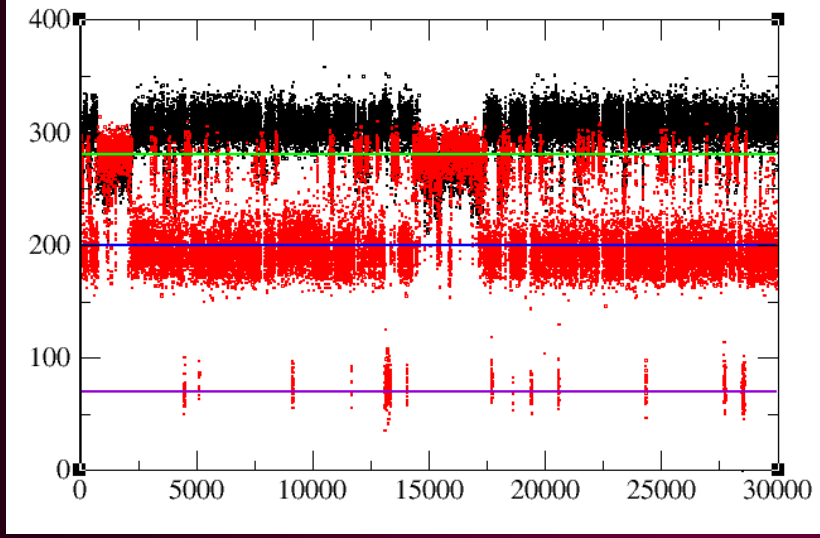
Analýza torzních úhlů páteře



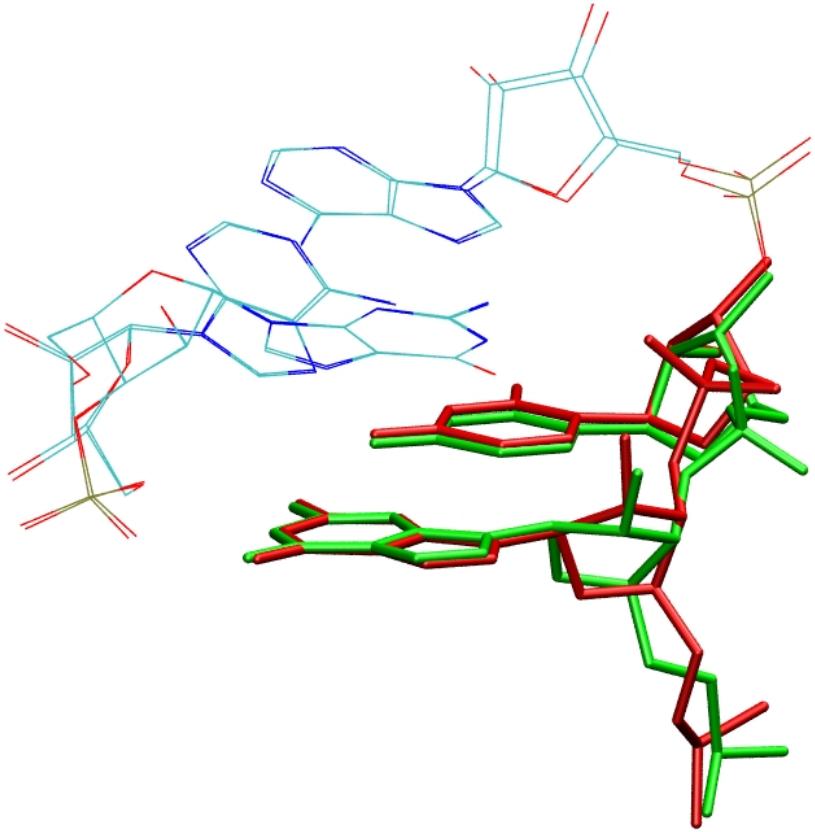




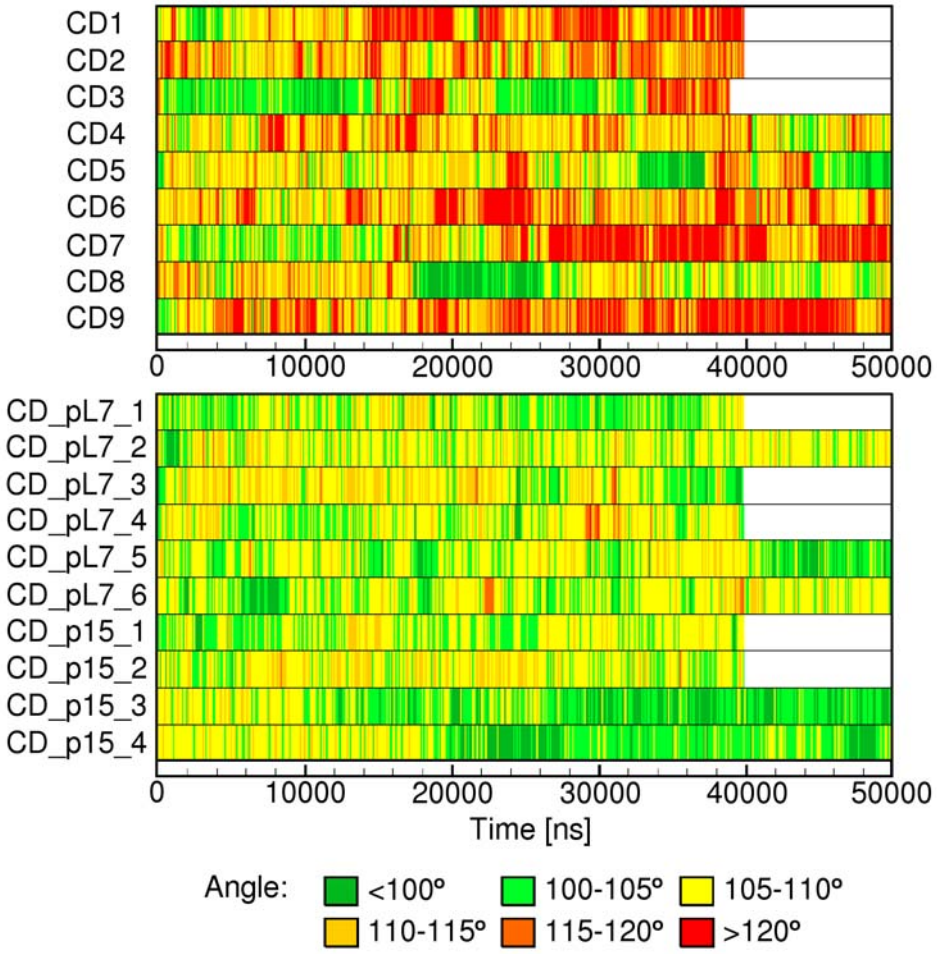


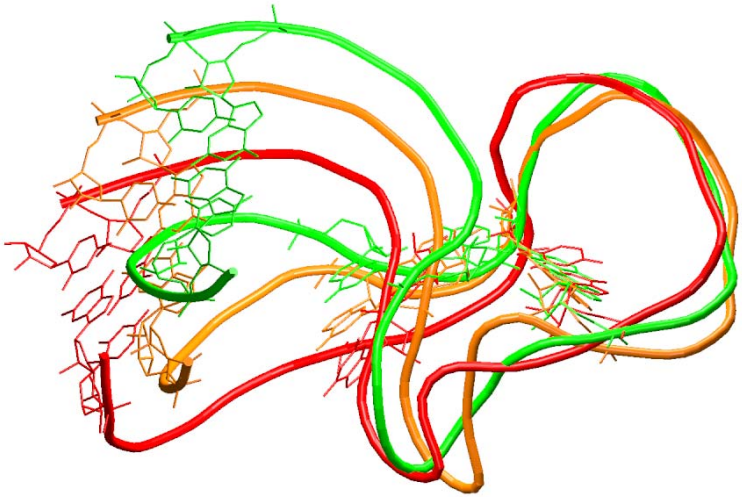


zeleně – vzdálenost N1-O2P
červeně – torzní úhel alfa
černě – úhel chi

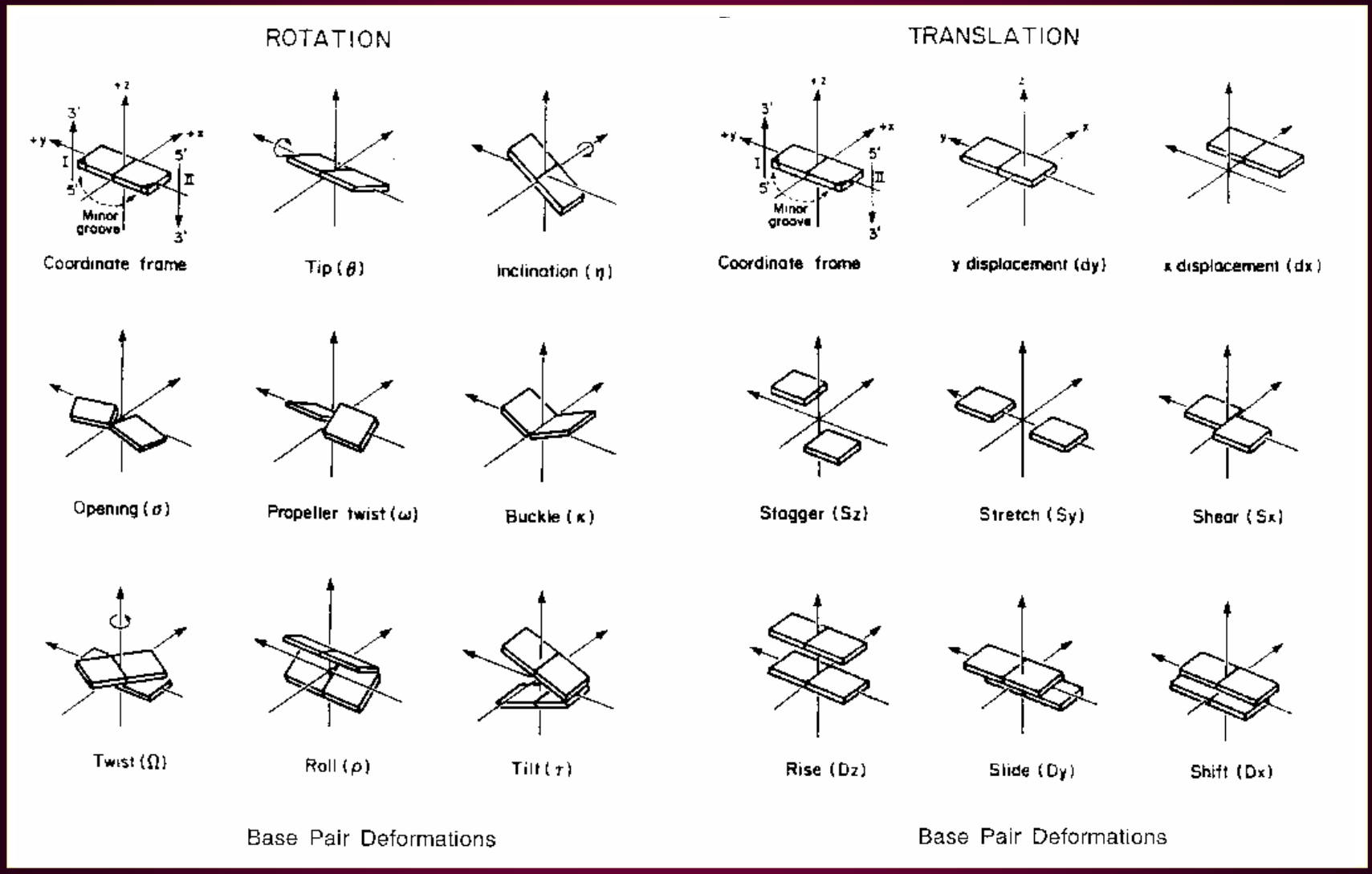


Interhelikální úhel



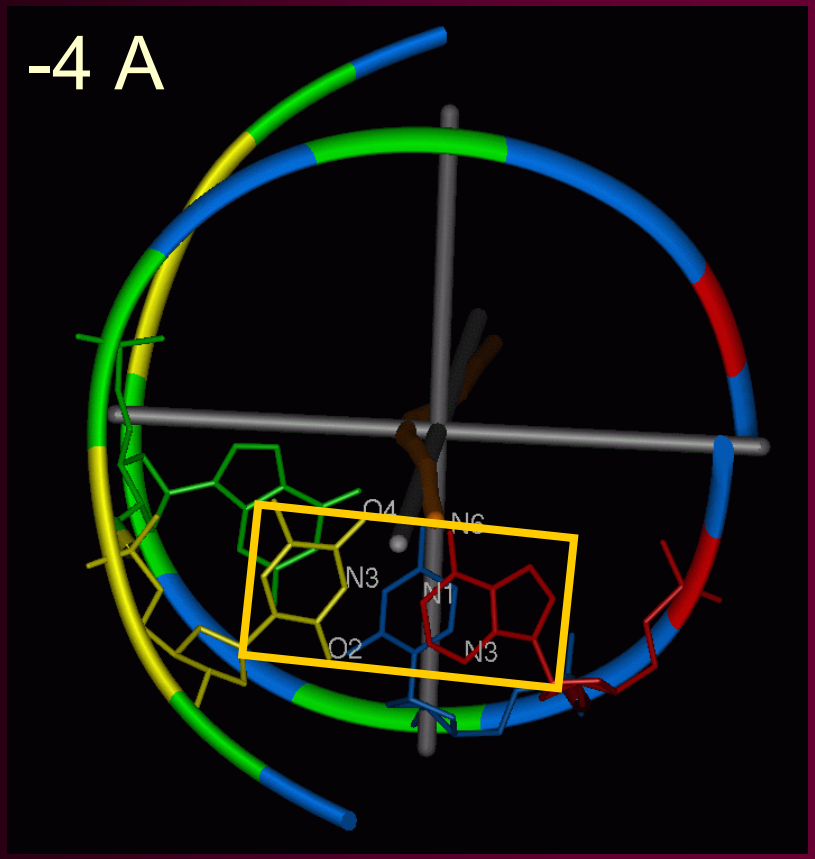


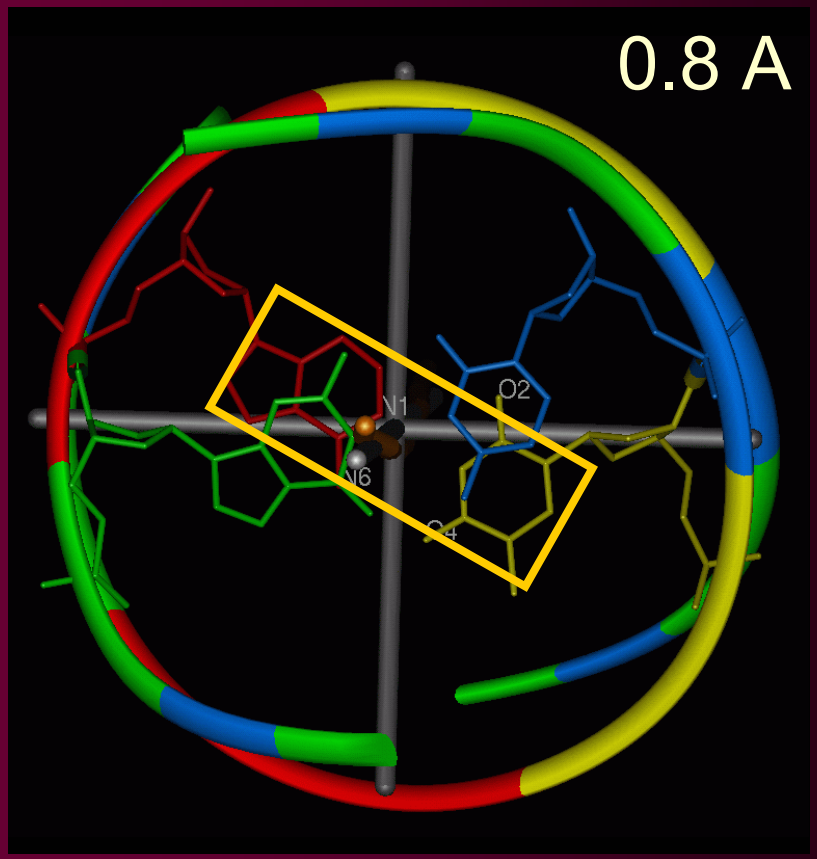
Helikální parametry



A-DNA x B-DNA

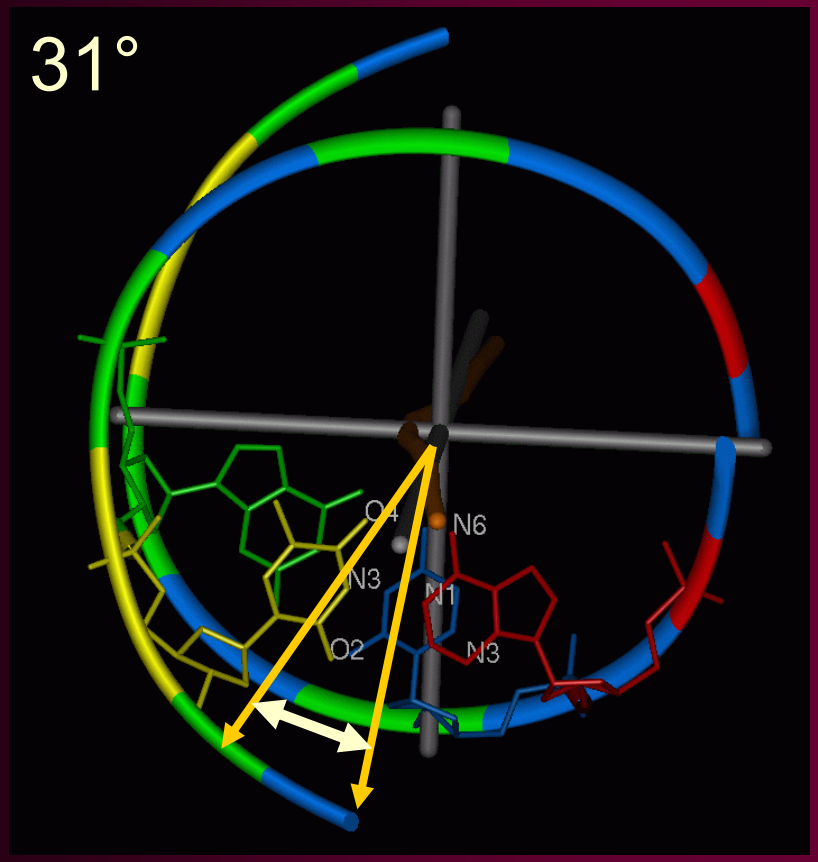
X-displacement

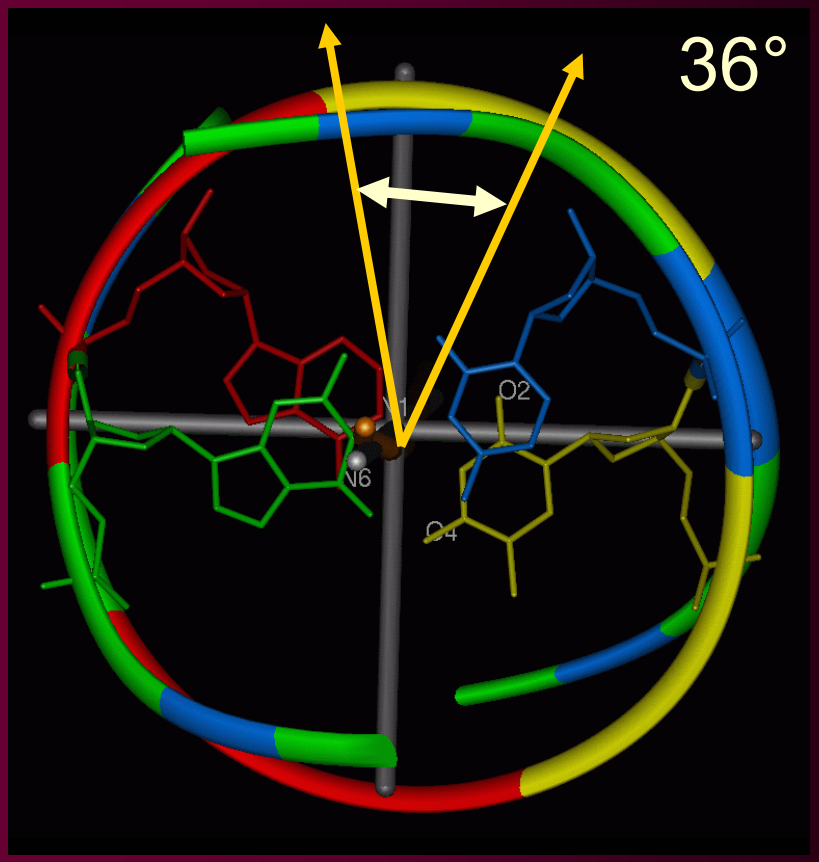




A-DNA x B-DNA

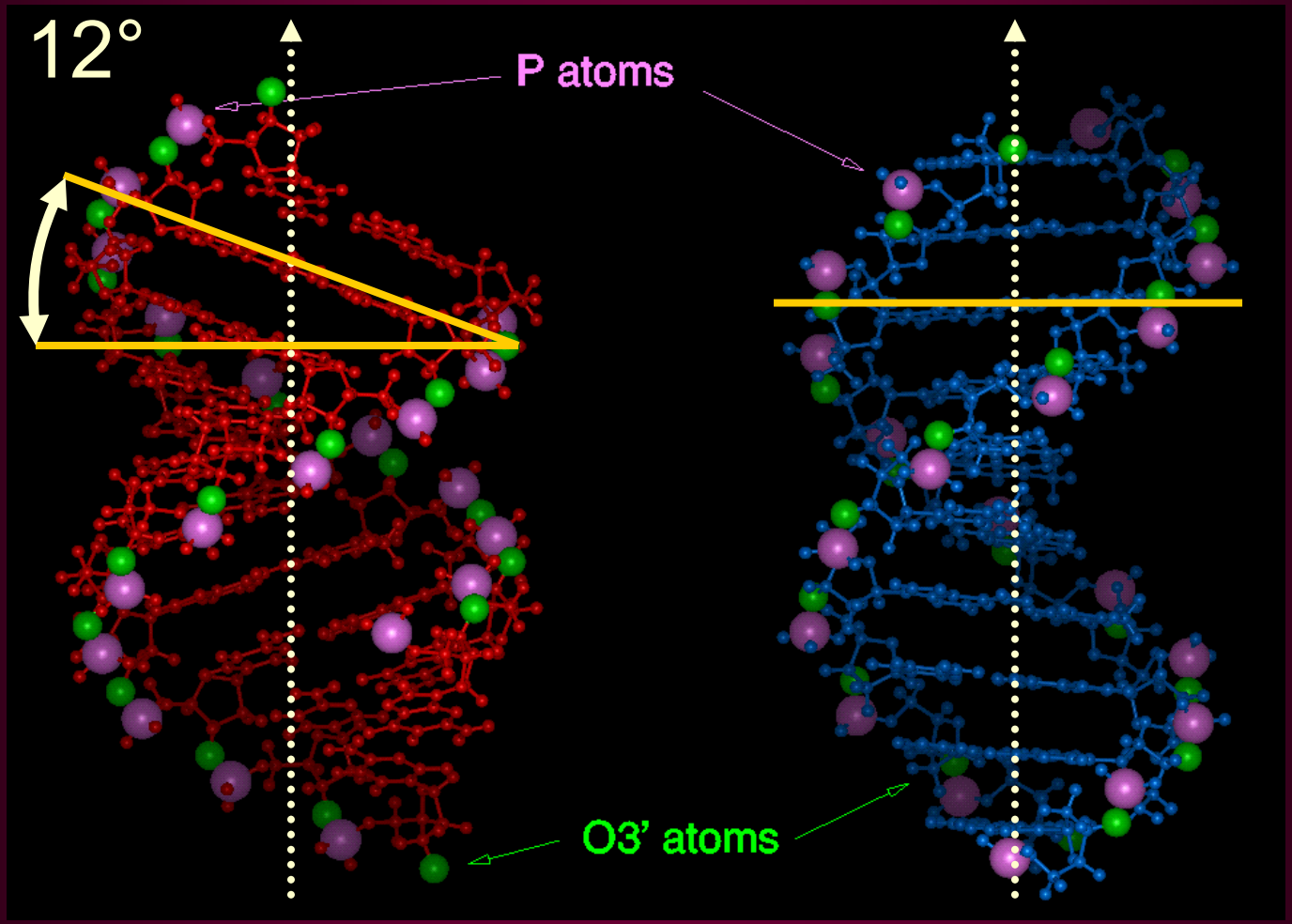
Helikální twist



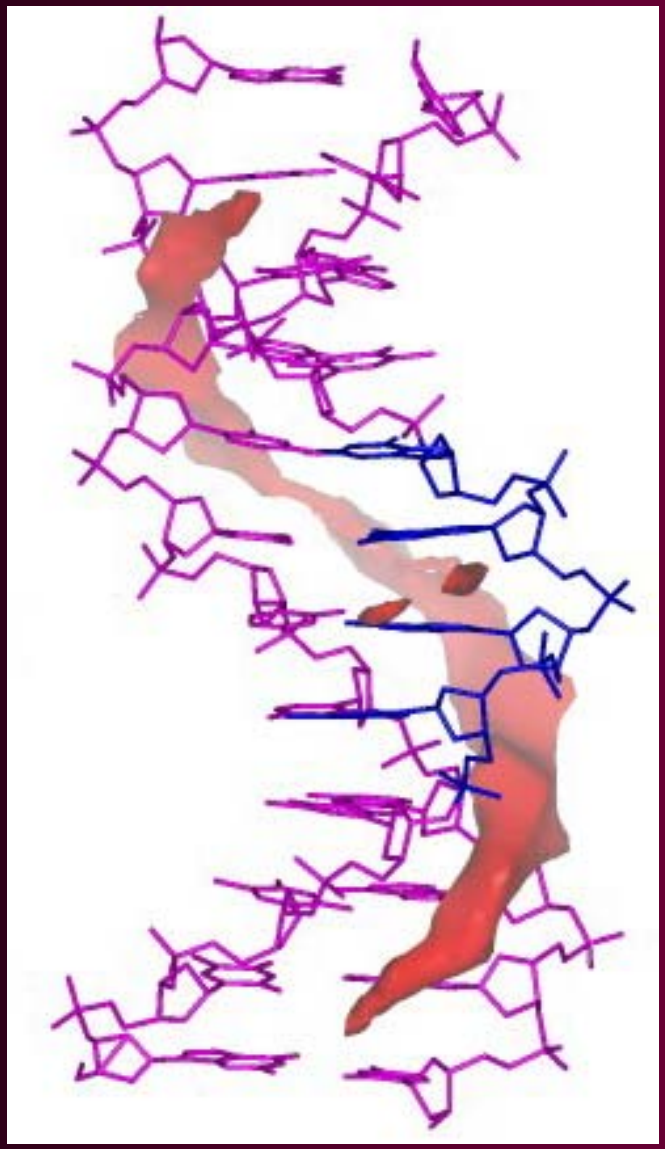


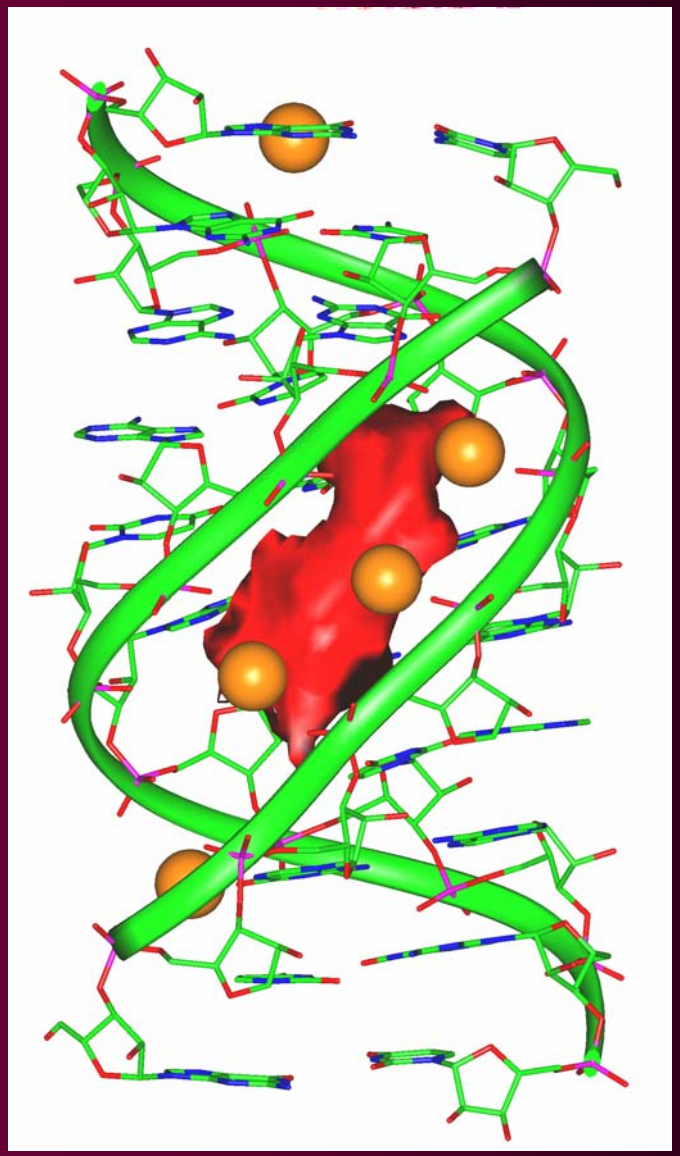
A-DNA x B-DNA

inclination

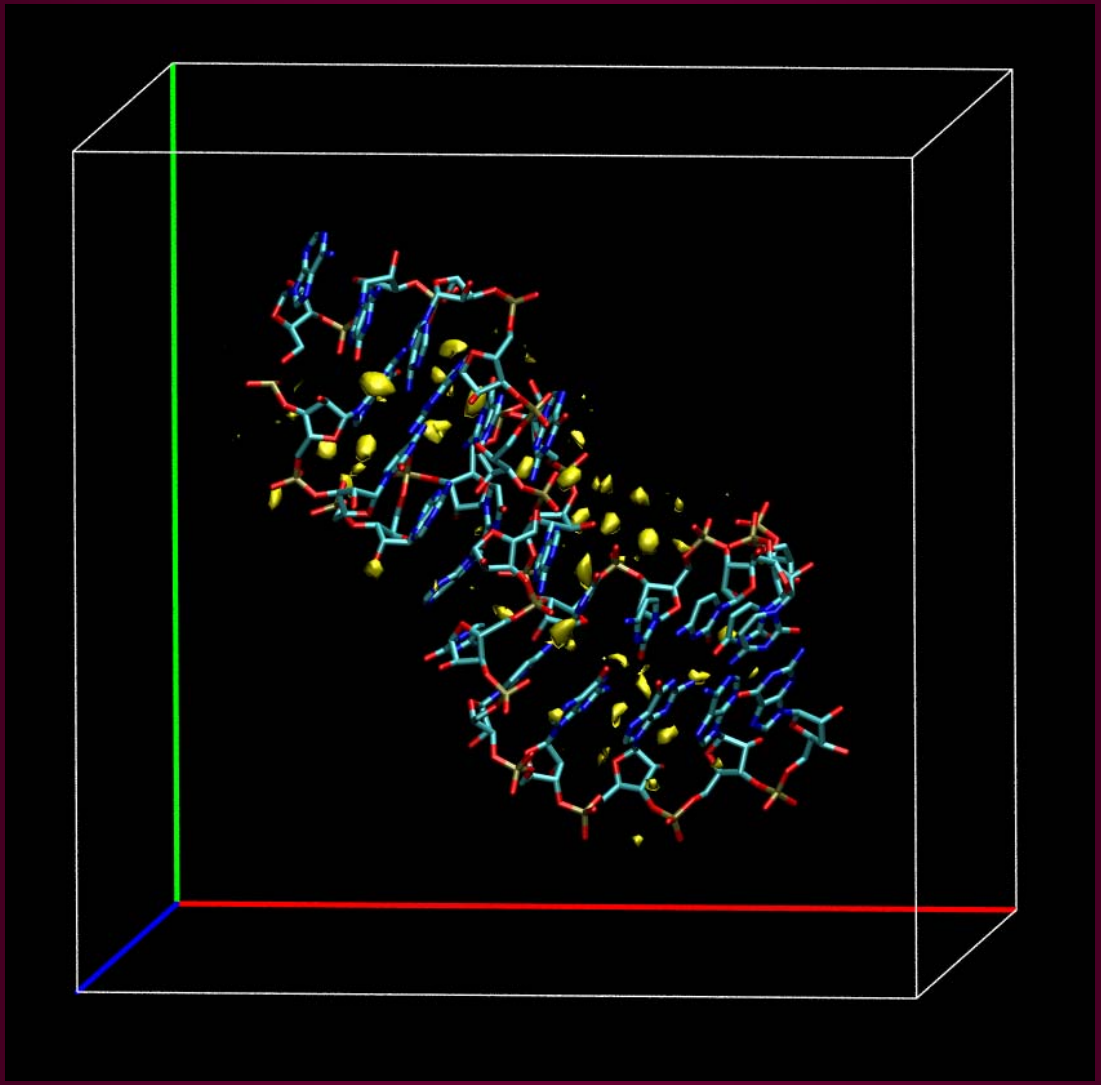


Molekulový interakční potenciál

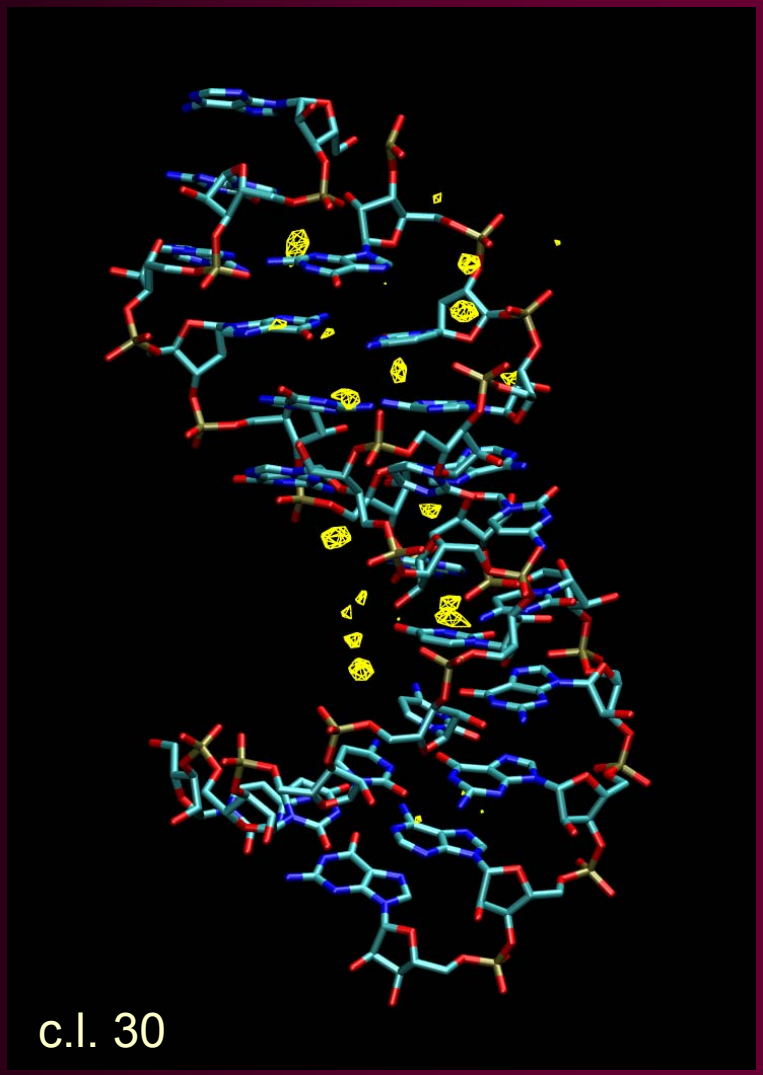


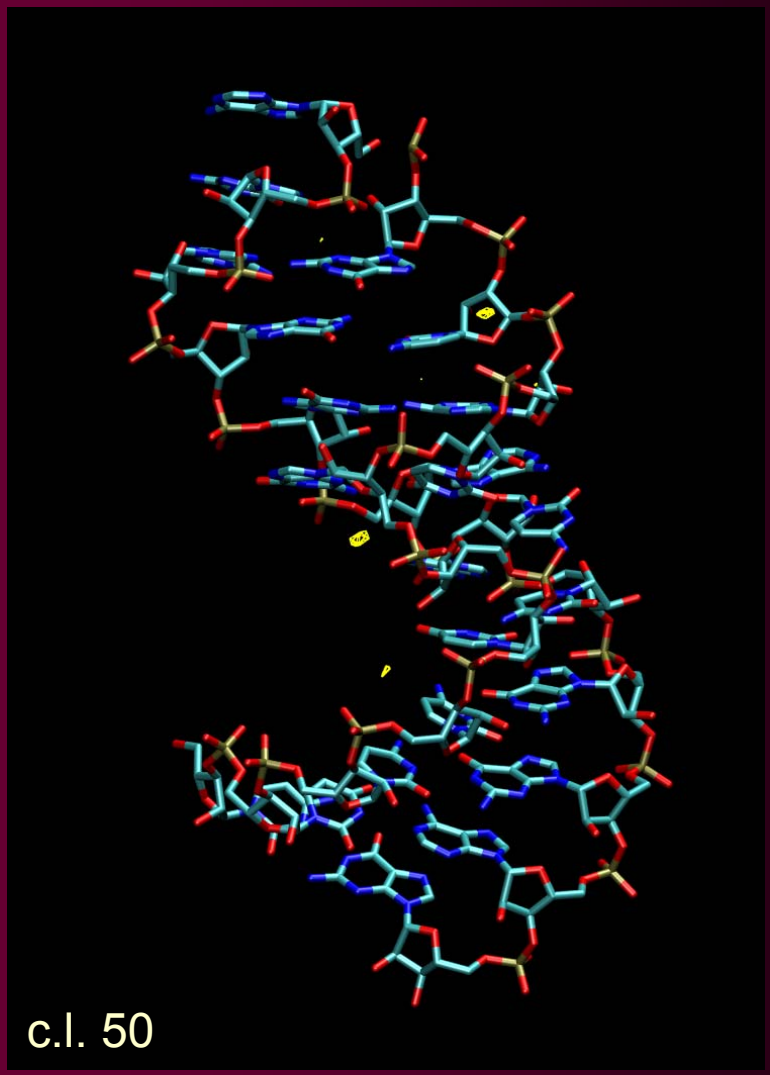


Analýza hydratace

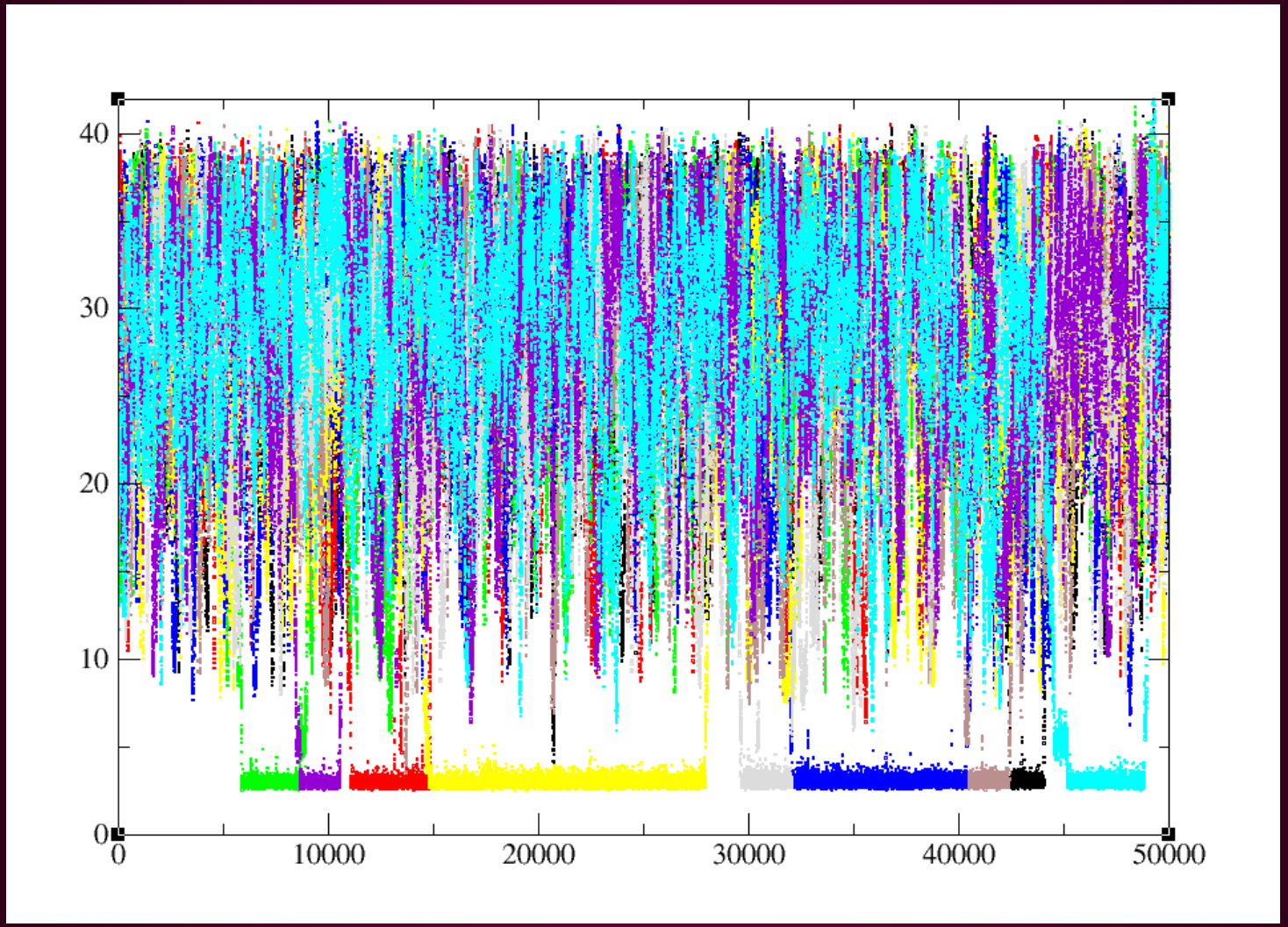


Hydratační mapy

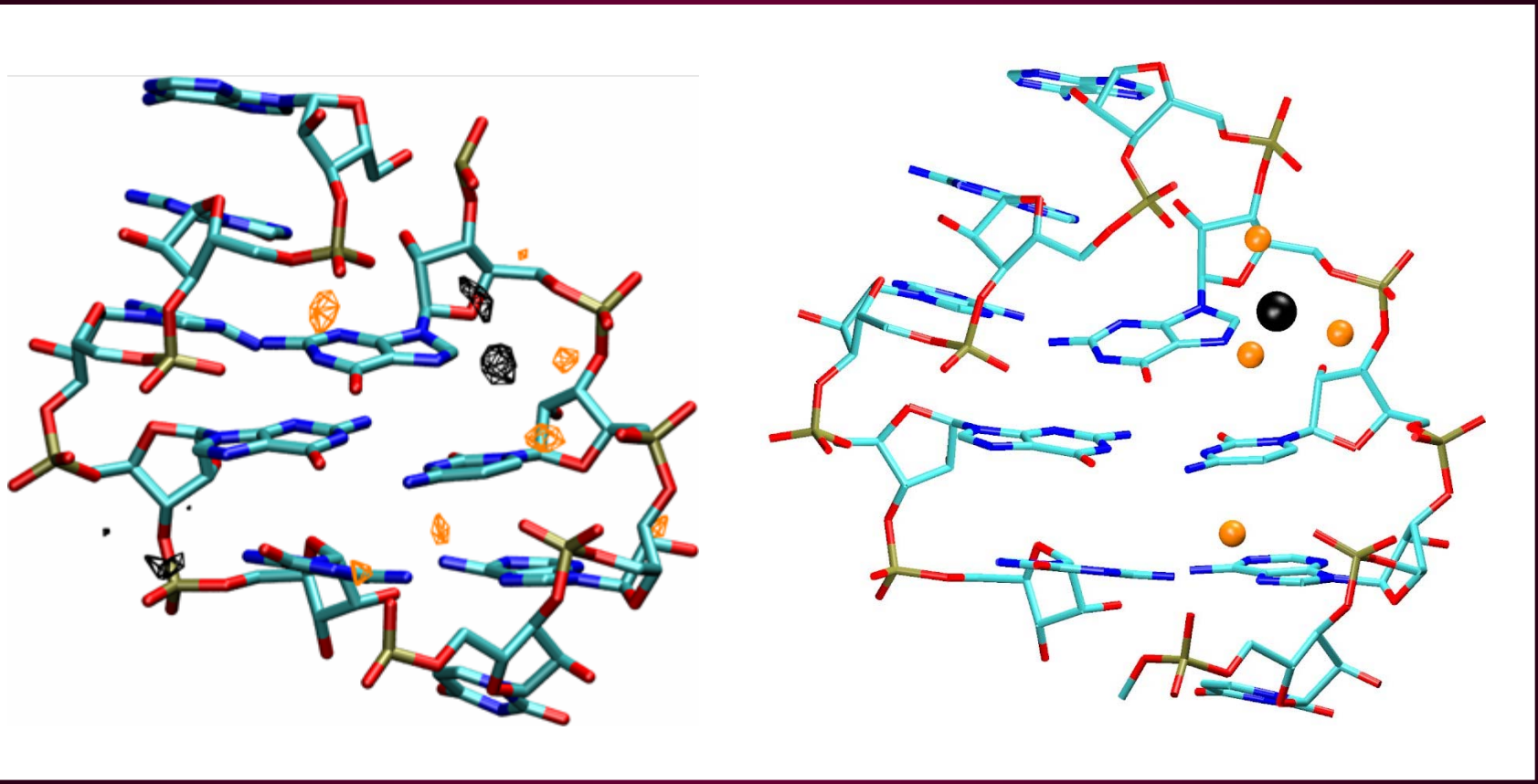




Vzdálenost jednotlivých vod od určitého atomu



Nalezení poloh jednotlivých vod na základě hydratační mapy



Výpočet interakční energie

Využití: např. sledování míry vertikální interakce (stackingu)