



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:40 PM UTC

PDB ID : 1HWY / pdb_00001hwy
Title : BOVINE GLUTAMATE DEHYDROGENASE COMPLEXED WITH NAD
AND 2-OXOGLUTARATE
Authors : Smith, T.J.; Peterson, P.E.; Schmidt, T.; Fang, J.; Stanley, C.A.
Deposited on : 2001-01-10
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

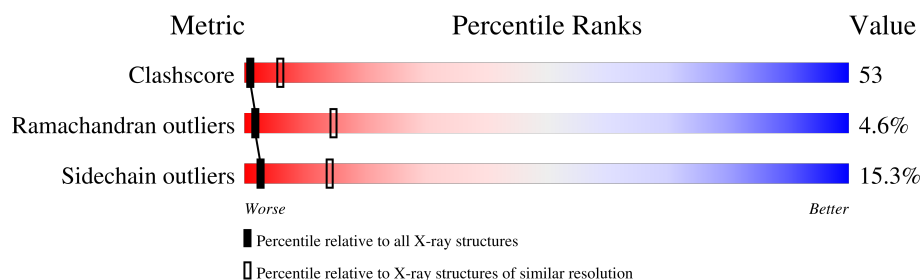
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	501	30% 54% 15% .
1	B	501	28% 55% 15% .
1	C	501	28% 55% 15% .
1	D	501	30% 54% 15% .
1	E	501	28% 55% 15% .
1	F	501	28% 55% 15% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	502	-	-	X	-
2	PO4	A	504	-	-	X	-
2	PO4	B	503	-	-	X	-
2	PO4	B	505	-	-	X	-
2	PO4	C	503	-	-	X	-
2	PO4	C	505	-	-	X	-
2	PO4	D	503	-	-	X	-
2	PO4	D	504	-	-	X	-
2	PO4	E	503	-	-	X	-
2	PO4	E	504	-	-	X	-
2	PO4	F	502	-	-	X	-
2	PO4	F	504	-	-	X	-
3	AKG	A	506	-	-	X	-
3	AKG	B	506	-	-	X	-
3	AKG	C	506	-	-	X	-
3	AKG	D	506	-	-	X	-
3	AKG	E	506	-	-	X	-
3	AKG	F	506	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24468 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	B	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	C	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	D	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	E	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	F	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			

There are 30 discrepancies between the modelled and reference sequences:

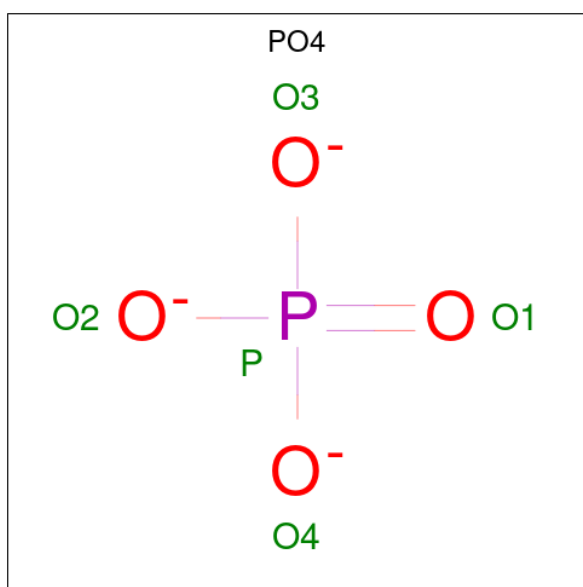
Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	LYS	SEE REMARK 999	UNP P00366
A	201	LYS	PRO	SEE REMARK 999	UNP P00366
A	202	PRO	GLY	SEE REMARK 999	UNP P00366
A	221	HIS	GLY	SEE REMARK 999	UNP P00366
A	222	GLY	HIS	SEE REMARK 999	UNP P00366
B	200	GLY	LYS	SEE REMARK 999	UNP P00366
B	201	LYS	PRO	SEE REMARK 999	UNP P00366
B	202	PRO	GLY	SEE REMARK 999	UNP P00366
B	221	HIS	GLY	SEE REMARK 999	UNP P00366
B	222	GLY	HIS	SEE REMARK 999	UNP P00366
C	200	GLY	LYS	SEE REMARK 999	UNP P00366
C	201	LYS	PRO	SEE REMARK 999	UNP P00366
C	202	PRO	GLY	SEE REMARK 999	UNP P00366
C	221	HIS	GLY	SEE REMARK 999	UNP P00366
C	222	GLY	HIS	SEE REMARK 999	UNP P00366
D	200	GLY	LYS	SEE REMARK 999	UNP P00366
D	201	LYS	PRO	SEE REMARK 999	UNP P00366

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Chain	Residue	Modelled	Actual	Comment	Reference
D	202	PRO	GLY	SEE REMARK 999	UNP P00366
D	221	HIS	GLY	SEE REMARK 999	UNP P00366
D	222	GLY	HIS	SEE REMARK 999	UNP P00366
E	200	GLY	LYS	SEE REMARK 999	UNP P00366
E	201	LYS	PRO	SEE REMARK 999	UNP P00366
E	202	PRO	GLY	SEE REMARK 999	UNP P00366
E	221	HIS	GLY	SEE REMARK 999	UNP P00366
E	222	GLY	HIS	SEE REMARK 999	UNP P00366
F	200	GLY	LYS	SEE REMARK 999	UNP P00366
F	201	LYS	PRO	SEE REMARK 999	UNP P00366
F	202	PRO	GLY	SEE REMARK 999	UNP P00366
F	221	HIS	GLY	SEE REMARK 999	UNP P00366
F	222	GLY	HIS	SEE REMARK 999	UNP P00366

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



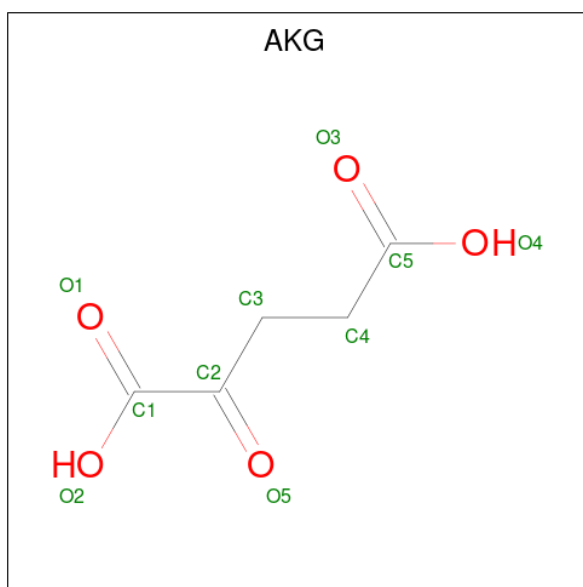
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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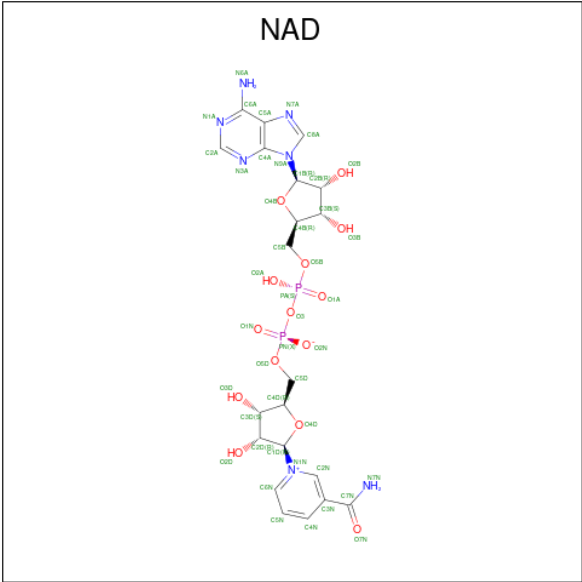
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	F	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	1
			88	42	14	28	4		

- Molecule 5 is water.

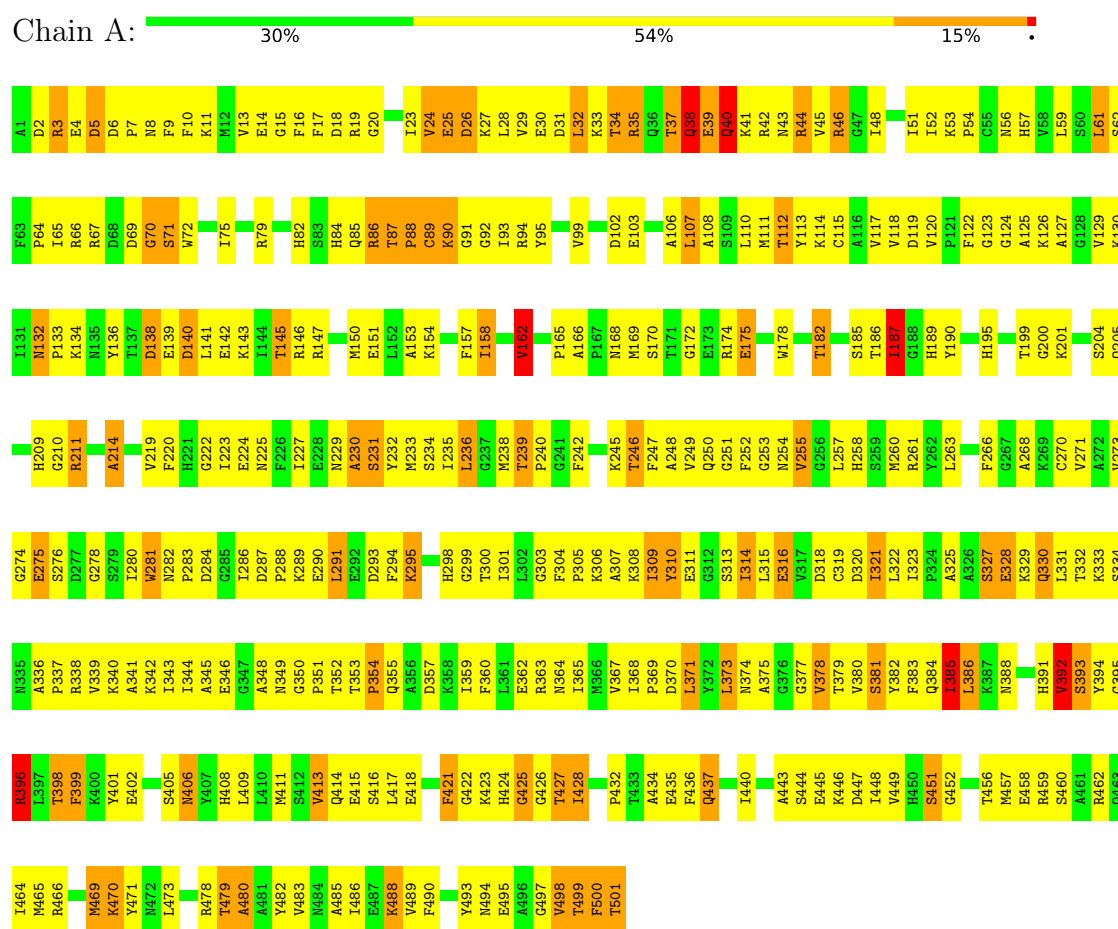
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	6	Total 6	O 6	0	0
5	C	6	Total 6	O 6	0	0
5	D	6	Total 6	O 6	0	0
5	E	6	Total 6	O 6	0	0
5	F	6	Total 6	O 6	0	0

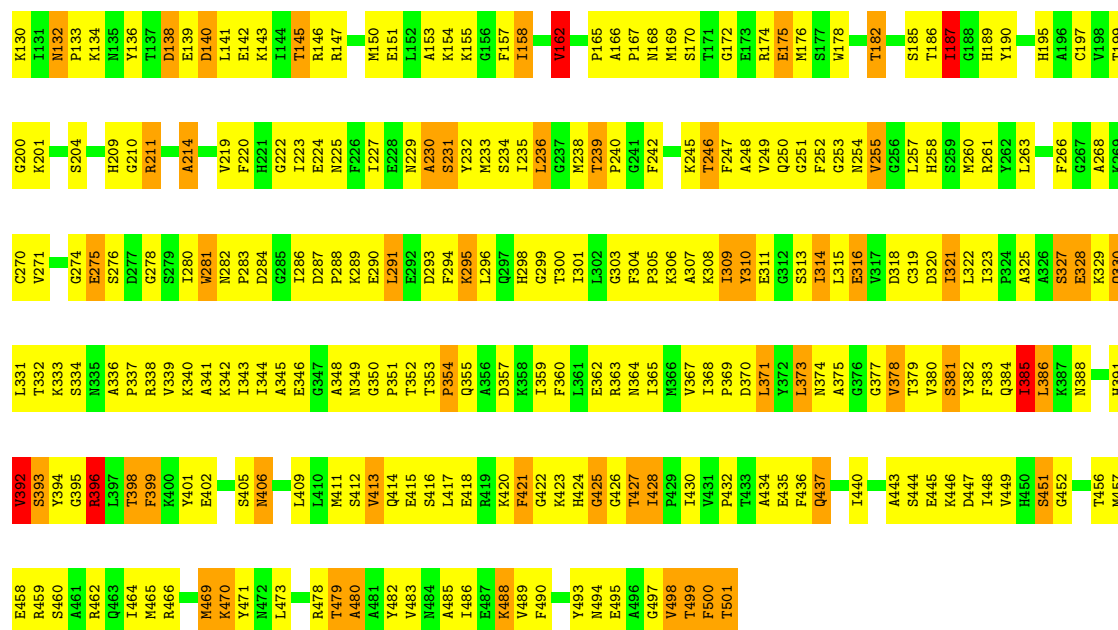
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

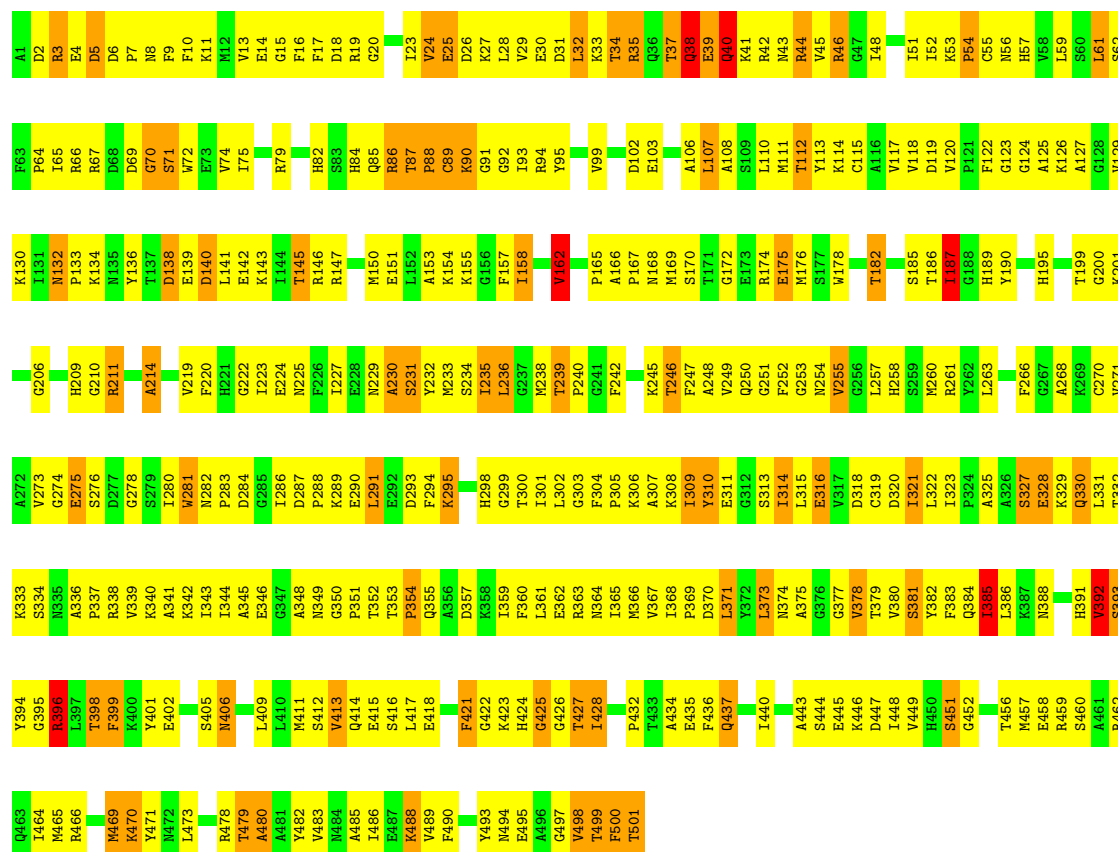
• Molecule 1: GLUTAMATE DEHYDROGENASE





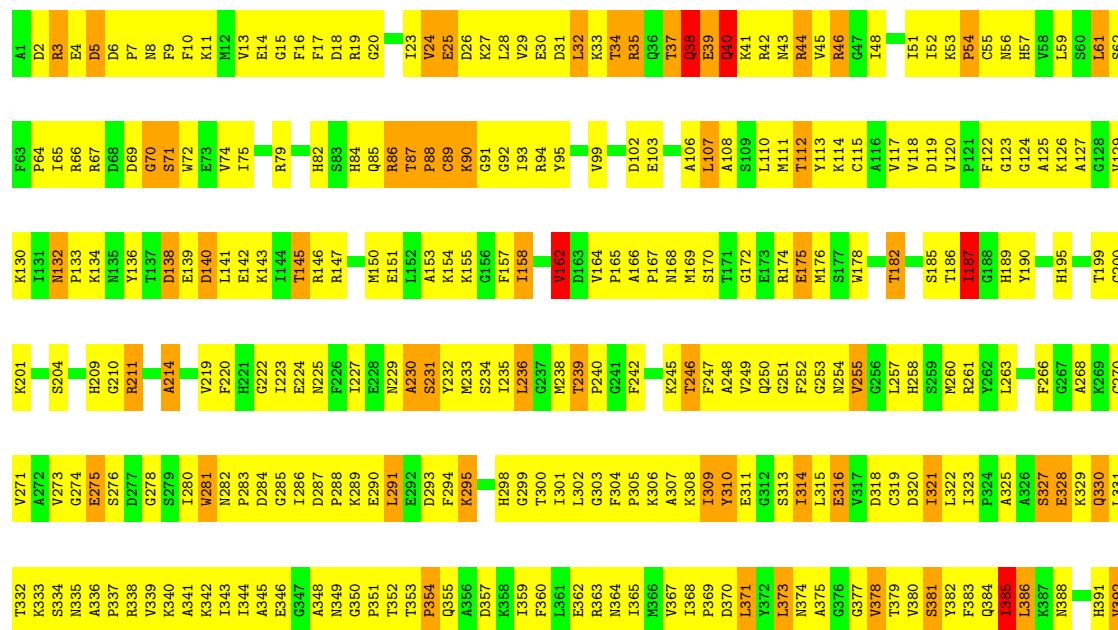
• Molecule 1: GLUTAMATE DEHYDROGENASE

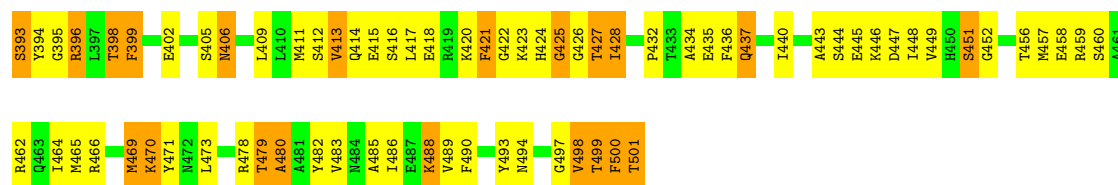
Chain C: 28% 55% 15%



• Molecule 1: GLUTAMATE DEHYDROGENASE

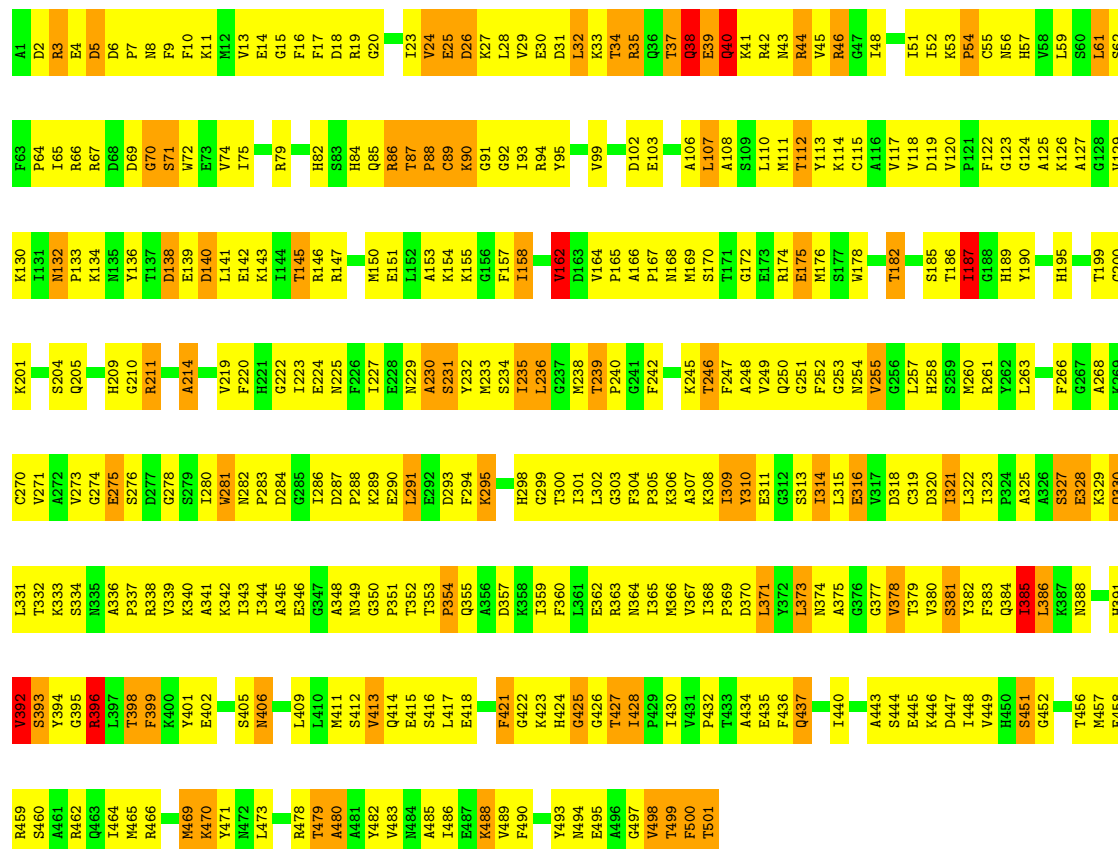
I464 I465 I466 M469 K470 Y471 M472 L473 R478 I479 A480 A481 Y482 Y483 M484 A485 I486 A487 K488 Y489 F490 Y493 N494 A495 A496 G497 Y498 F499 F500 T501	G395 R396 L397 T398 F399 E402 S403 M405 L409 L410 M411 S412 Y413 Q414 E415 L416 S417 A418 E419 K420 F421 G422 K423 H424 A425 G426 T427 I428	S334 G335 A336 P337 R338 V339 K340 A341 S342 K343 I344 A345 E346 G347 A348 R349 G350 P351 T352 L353 P354 Q355 K356 D357 K358 L359 F360 L361 E362 R363 S364 M366 K367 I368 A369 F370 L371 Y372 L373 K374 A375 E376 G377 F378 T379 K380 S381 Y382 F383 Q384 L385 L386 K387 N388 H391 V392 S393 R462 F463	V273 G274 E275 D276 G277 G278 S279 L280 N281 K282 P283 D284 E285 G286 T287 R288 G289 E290 L291 E292 D293 F294 K295 H298 G299 T300 L301 E302 R303 S304 M306 K307 I308 A309 Y310 E311 G312 S313 L314 A315 E316 G317 F318 T319 K320 S321 L322 P323 Q324 K325 L326 A327 E328 T329 R330 G331 F332 D333 N334 M335 S336 L337 K338 I339 A340 Y341 E342 G343 F344 T345 R346 D347 N348 M349 S350 L351 K352 I353 A354 Y355 E356 G357 F358 T359 R360 D361 N362 M363 S364 L365 K366 I367 A368 Y369 E370 G371 F372 T373 R374 D375 N376 M377 S378 L379 K380 I381 A382 Y383 E384 G385 F386 T387 R388 D389 N390 M391 S392 L393 K394 I395 A396 Y397 E398 G399 F400 T401 R402 D403 N404 M405 S406 L407 K408 I409 A410 Y411 E412 G413 F414 T415 R416 D417 N418 M419 S420 L421 K422 I423 A424 Y425 E426 G427 F428 T429 R430 D431 N432 M433 S434 L435 K436 I437 A438 Y439 E440 G441 F442 T443 R444 D445 N446 M447 S448 L449 K450 I451 A452 Y453 E454 G455 F456 T457 R458 D459 N460 M461 S462 L463 K464 I465 A466 Y467 E468 G469 F470 T471 R472 D473 N474 M475 S476 L477 K478 I479 A480 Y481 E482 G483 F484 T485 R486 D487 N488 M489 S490 L491 K492 I493 A494 Y495 E496 G497 F498 T499 R500 D501 N502 M503 S504 L505 K506 I507 A508 Y509 E509 G510 F511 T512 R513 D514 N515 M516 S517 L518 K519 I520 A521 Y522 E523 G524 F525 T526 R527 D528 N529 M530 S531 L532 K533 I534 A535 Y536 E537 G538 F539 T540 R541 D542 N543 M544 S545 L546 K547 I548 A549 Y550 E551 G552 F553 T554 R555 D556 N557 M558 S559 L560 K561 I562 A563 Y564 E565 G566 F567 T568 R569 D570 N571 M572 S573 L574 K575 I576 A577 Y578 E579 G580 F581 T582 R583 D584 N585 M586 S587 L588 K589 I590 A591 Y592 E593 G594 F595 T596 R597 D598 N599 M600 S601 L602 K603 I604 A605 Y606 E607 G608 F609 T610 R611 D612 N613 M614 S615 L616 K617 I618 A619 Y620 E621 G622 F623 T624 R625 D626 N627 M628 S629 L630 K631 I632 A633 Y634 E635 G636 F637 T638 R639 D640 N641 M642 S643 L644 K645 I646 A647 Y648 E649 G650 F651 T652 R653 D654 N655 M656 S657 L658 K659 I660 A661 Y662 E663 G664 F665 T666 R667 D668 N669 M670 S671 L672 K673 I674 A675 Y676 E677 G678 F679 T680 R681 D682 N683 M684 S685 L686 K687 I688 A689 Y690 E691 G692 F693 T694 R695 D696 N697 M698 S699 L700 K701 I702 A703 Y704 E705 G706 F707 T708 R709 D710 N711 M712 S713 L714 K715 I716 A717 Y718 E719 G720 F721 T722 R723 D724 N725 M726 S727 L728 K729 I730 A731 Y732 E733 G734 F735 T736 R737 D738 N739 M740 S741 L742 K743 I744 A745 Y746 E747 G748 F749 T750 R751 D752 N753 M754 S755 L756 K757 I758 A759 Y760 E761 G762 F763 T764 R765 D766 N767 M768 S769 L770 K771 I772 A773 Y774 E775 G776 F777 T778 R779 D780 N781 M782 S783 L784 K785 I786 A787 Y788 E789 G790 F791 T792 R793 D794 N795 M796 S797 L798 K799 I800 A801 Y802 E803 G804 F805 T806 R807 D808 N809 M810 S811 L812 K813 I814 A815 Y816 E817 G818 F819 T820 R821 D822 N823 M824 S825 L826 K827 I828 A829 Y830 E831 G832 F833 T8
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• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain F: 28% 55% 15% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.50Å 101.00Å 164.60Å 90.00° 102.20° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24468	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NAD, AKG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	0/3991	1.24	41/5384 (0.8%)
1	B	0.75	0/3991	1.24	41/5384 (0.8%)
1	C	0.75	0/3991	1.24	41/5384 (0.8%)
1	D	0.75	0/3991	1.24	41/5384 (0.8%)
1	E	0.75	0/3991	1.24	41/5384 (0.8%)
1	F	0.75	0/3991	1.24	41/5384 (0.8%)
All	All	0.75	0/23946	1.24	246/32304 (0.8%)

There are no bond length outliers.

The worst 5 of 246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	40	GLN	N-CA-C	-12.84	97.36	111.36
1	D	40	GLN	N-CA-C	-12.83	97.38	111.36
1	F	40	GLN	N-CA-C	-12.82	97.38	111.36
1	C	40	GLN	N-CA-C	-12.81	97.39	111.36
1	A	40	GLN	N-CA-C	-12.81	97.40	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3910	0	3888	444	1
1	B	3910	0	3888	469	2
1	C	3910	0	3888	445	2
1	D	3910	0	3888	435	0
1	E	3910	0	3888	451	1
1	F	3910	0	3888	465	0
2	A	20	0	0	6	0
2	B	20	0	0	6	0
2	C	20	0	0	6	0
2	D	20	0	0	6	0
2	E	20	0	0	6	0
2	F	20	0	0	6	0
3	A	10	0	4	6	0
3	B	10	0	4	7	0
3	C	10	0	4	7	0
3	D	10	0	4	7	0
3	E	10	0	4	6	0
3	F	10	0	4	7	0
4	A	132	0	78	33	0
4	B	132	0	78	36	0
4	C	132	0	78	39	0
4	D	132	0	77	35	0
4	E	132	0	77	31	0
4	F	132	0	77	34	0
5	A	6	0	0	4	0
5	B	6	0	0	4	0
5	C	6	0	0	4	0
5	D	6	0	0	5	0
5	E	6	0	0	4	0
5	F	6	0	0	4	0
All	All	24468	0	23817	2569	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

The worst 5 of 2569 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:HIS:CA	4:D:507[A]:NAD:O3D	1.66	1.41
1:F:391:HIS:CA	4:F:508[A]:NAD:O3D	1.66	1.41
1:B:391:HIS:CA	4:B:507[A]:NAD:O3D	1.69	1.40
1:C:391:HIS:CA	4:C:507[A]:NAD:O3D	1.70	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:HIS:CA	4:A:507[A]:NAD:O3D	1.69	1.38

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:CZ	1:E:298:HIS:NE2[2_556]	2.14	0.06
1:B:309:ILE:CG1	1:C:284:ASP:OD1[2_545]	2.14	0.06
1:B:69:ASP:O	1:C:3:ARG:NH2[2_545]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2	15
1	B	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2	15
1	C	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2	15
1	D	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2	15
1	E	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2	15
1	F	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2	15
All	All	2994/3006 (100%)	2502 (84%)	354 (12%)	138 (5%)	2	15

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	35	ARG
1	A	70	GLY
1	B	5	ASP
1	B	35	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	B	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	C	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	D	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	E	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	F	417/417 (100%)	353 (85%)	64 (15%)	3	14
All	All	2502/2502 (100%)	2118 (85%)	384 (15%)	3	14

5 of 384 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	371	LEU
1	E	295	LYS
1	D	393	SER
1	E	40	GLN
1	E	386	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	450	HIS
1	F	168	ASN
1	D	254	ASN
1	F	132	ASN
1	F	282	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	F	503	-	4,4,4	1.25	1 (25%)	6,6,6	0.92	0
2	PO4	B	505	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
2	PO4	D	503	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
4	NAD	D	508	-	46,48,48	2.47	14 (30%)	64,73,73	2.10	16 (25%)
2	PO4	A	502	-	4,4,4	1.26	1 (25%)	6,6,6	0.92	0
2	PO4	C	503	-	4,4,4	1.26	1 (25%)	6,6,6	0.92	0
3	AKG	C	506	-	9,9,9	1.76	2 (22%)	11,11,11	3.30	5 (45%)
4	NAD	C	508	-	46,48,48	2.48	15 (32%)	64,73,73	2.09	16 (25%)
4	NAD	E	507[A]	-	46,48,48	2.57	14 (30%)	64,73,73	2.21	18 (28%)
4	NAD	B	508	-	46,48,48	2.47	15 (32%)	64,73,73	2.09	16 (25%)
3	AKG	B	506	-	9,9,9	1.75	2 (22%)	11,11,11	3.30	5 (45%)
4	NAD	E	507[B]	-	46,48,48	2.69	15 (32%)	64,73,73	1.95	17 (26%)
2	PO4	B	504	-	4,4,4	1.99	1 (25%)	6,6,6	0.90	0
4	NAD	C	507[A]	-	46,48,48	2.58	14 (30%)	64,73,73	2.22	18 (28%)
2	PO4	A	504	-	4,4,4	1.26	1 (25%)	6,6,6	0.91	0
2	PO4	E	502	-	4,4,4	1.24	1 (25%)	6,6,6	0.91	0
2	PO4	E	505	-	4,4,4	1.99	1 (25%)	6,6,6	0.90	0
4	NAD	C	507[B]	-	46,48,48	2.68	15 (32%)	64,73,73	1.95	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAD	F	508[A]	-	46,48,48	2.57	14 (30%)	64,73,73	2.21	18 (28%)
4	NAD	F	508[B]	-	46,48,48	2.68	15 (32%)	64,73,73	1.95	17 (26%)
3	AKG	D	506	-	9,9,9	1.75	2 (22%)	11,11,11	3.31	5 (45%)
2	PO4	C	502	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
2	PO4	B	502	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
2	PO4	A	503	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
4	NAD	A	508	-	46,48,48	2.47	15 (32%)	64,73,73	2.09	16 (25%)
2	PO4	C	504	-	4,4,4	2.00	1 (25%)	6,6,6	0.90	0
2	PO4	D	505	-	4,4,4	1.98	1 (25%)	6,6,6	0.90	0
4	NAD	F	507	-	46,48,48	2.48	15 (32%)	64,73,73	2.09	16 (25%)
2	PO4	D	504	-	4,4,4	1.26	1 (25%)	6,6,6	0.91	0
2	PO4	F	505	-	4,4,4	1.99	1 (25%)	6,6,6	0.90	0
2	PO4	C	505	-	4,4,4	1.25	1 (25%)	6,6,6	0.92	0
2	PO4	F	504	-	4,4,4	1.27	1 (25%)	6,6,6	0.92	0
2	PO4	E	504	-	4,4,4	1.26	1 (25%)	6,6,6	0.91	0
4	NAD	E	508	-	46,48,48	2.48	15 (32%)	64,73,73	2.10	16 (25%)
3	AKG	A	506	-	9,9,9	1.75	2 (22%)	11,11,11	3.30	5 (45%)
3	AKG	F	506	-	9,9,9	1.76	2 (22%)	11,11,11	3.30	5 (45%)
2	PO4	B	503	-	4,4,4	1.26	1 (25%)	6,6,6	0.92	0
2	PO4	E	503	-	4,4,4	1.27	1 (25%)	6,6,6	0.92	0
4	NAD	A	507[A]	-	46,48,48	2.58	14 (30%)	64,73,73	2.22	18 (28%)
2	PO4	D	502	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
2	PO4	F	502	-	4,4,4	1.27	1 (25%)	6,6,6	0.92	0
4	NAD	D	507[A]	-	46,48,48	2.57	14 (30%)	64,73,73	2.21	18 (28%)
3	AKG	E	506	-	9,9,9	1.76	2 (22%)	11,11,11	3.29	5 (45%)
4	NAD	A	507[B]	-	46,48,48	2.69	15 (32%)	64,73,73	1.96	17 (26%)
4	NAD	D	507[B]	-	46,48,48	2.68	15 (32%)	64,73,73	1.95	17 (26%)
2	PO4	A	505	-	4,4,4	1.99	1 (25%)	6,6,6	0.90	0
4	NAD	B	507[A]	-	46,48,48	2.57	14 (30%)	64,73,73	2.21	18 (28%)
4	NAD	B	507[B]	-	46,48,48	2.68	15 (32%)	64,73,73	1.95	18 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	D	508	-	-	11/30/62/62	0/5/5/5
4	NAD	C	508	-	-	11/30/62/62	0/5/5/5
4	NAD	E	507[A]	-	-	9/30/62/62	0/5/5/5
3	AKG	C	506	-	-	4/9/9/9	-
4	NAD	B	508	-	-	11/30/62/62	0/5/5/5
3	AKG	B	506	-	-	4/9/9/9	-
4	NAD	E	507[B]	-	-	10/30/62/62	0/5/5/5
4	NAD	C	507[A]	-	-	9/30/62/62	0/5/5/5
4	NAD	C	507[B]	-	-	10/30/62/62	0/5/5/5
4	NAD	F	508[A]	-	-	9/30/62/62	0/5/5/5
4	NAD	F	508[B]	-	-	10/30/62/62	0/5/5/5
3	AKG	D	506	-	-	4/9/9/9	-
4	NAD	A	508	-	-	11/30/62/62	0/5/5/5
4	NAD	F	507	-	-	11/30/62/62	0/5/5/5
4	NAD	E	508	-	-	11/30/62/62	0/5/5/5
3	AKG	A	506	-	-	4/9/9/9	-
3	AKG	F	506	-	-	4/9/9/9	-
4	NAD	A	507[A]	-	-	9/30/62/62	0/5/5/5
4	NAD	D	507[A]	-	-	9/30/62/62	0/5/5/5
3	AKG	E	506	-	-	4/9/9/9	-
4	NAD	A	507[B]	-	-	10/30/62/62	0/5/5/5
4	NAD	D	507[B]	-	-	10/30/62/62	0/5/5/5
4	NAD	B	507[A]	-	-	9/30/62/62	0/5/5/5
4	NAD	B	507[B]	-	-	10/30/62/62	0/5/5/5

The worst 5 of 299 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	507[A]	NAD	PN-O3	8.78	1.69	1.59
4	A	507[A]	NAD	PN-O3	8.75	1.68	1.59
4	D	507[A]	NAD	PN-O3	8.74	1.68	1.59
4	F	508[A]	NAD	PN-O3	8.73	1.68	1.59
4	E	507[A]	NAD	PN-O3	8.71	1.68	1.59

The worst 5 of 337 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	506	AKG	O1-C1-C2	-6.87	113.27	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	506	AKG	O1-C1-C2	-6.87	113.27	121.81
3	F	506	AKG	O1-C1-C2	-6.85	113.29	121.81
3	A	506	AKG	O1-C1-C2	-6.84	113.30	121.81
3	C	506	AKG	O1-C1-C2	-6.84	113.31	121.81

There are no chirality outliers.

5 of 204 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	AKG	C1-C2-C3-C4
3	B	506	AKG	C1-C2-C3-C4
3	C	506	AKG	C1-C2-C3-C4
3	D	506	AKG	C1-C2-C3-C4
3	E	506	AKG	C1-C2-C3-C4

There are no ring outliers.

48 monomers are involved in 262 short contacts:

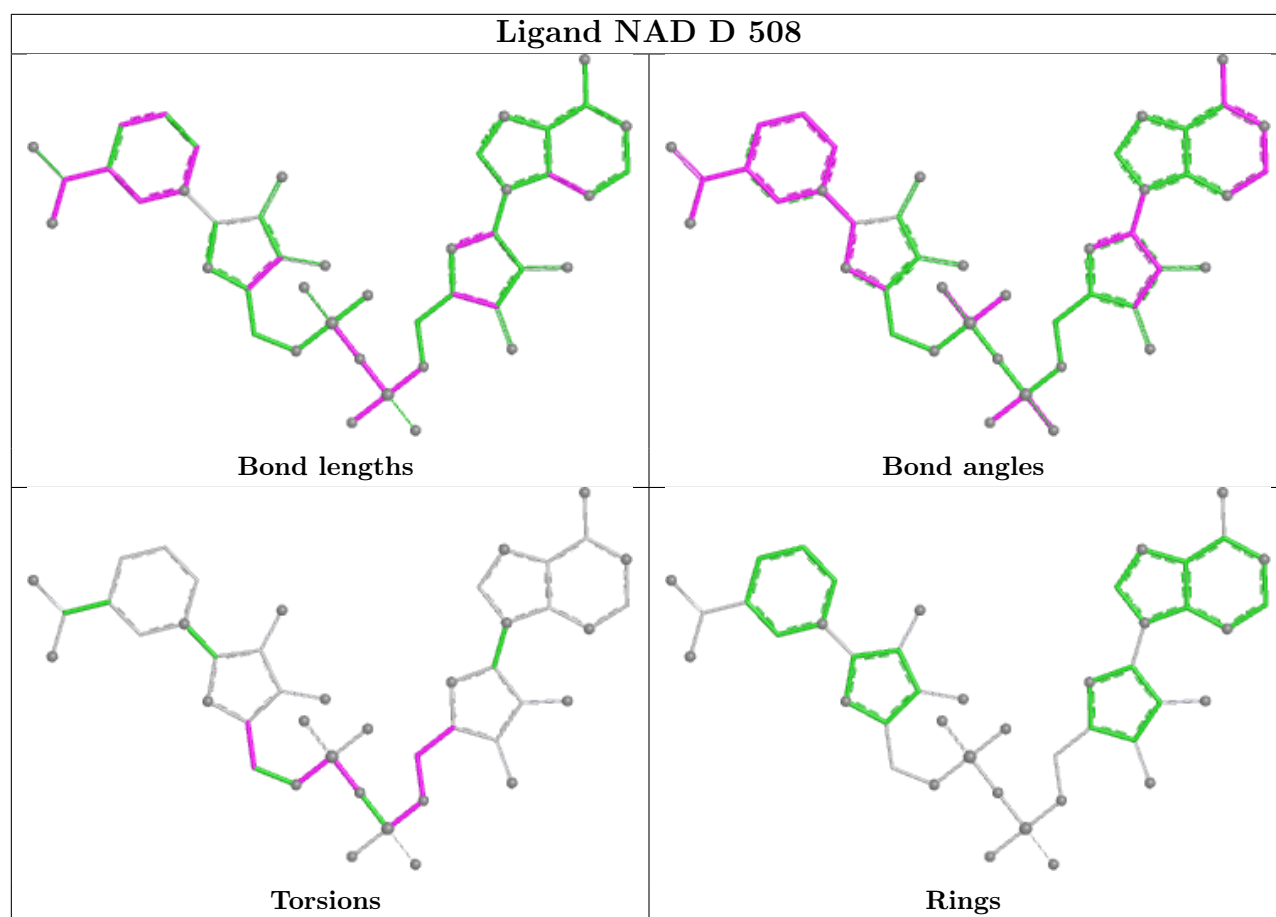
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	503	PO4	1	0
2	B	505	PO4	2	0
2	D	503	PO4	2	0
4	D	508	NAD	12	0
2	A	502	PO4	2	0
2	C	503	PO4	2	0
3	C	506	AKG	7	0
4	C	508	NAD	13	0
4	E	507[A]	NAD	12	0
4	B	508	NAD	12	0
3	B	506	AKG	7	0
4	E	507[B]	NAD	7	0
2	B	504	PO4	1	0
4	C	507[A]	NAD	19	0
2	A	504	PO4	2	0
2	E	502	PO4	1	0
2	E	505	PO4	1	0
4	C	507[B]	NAD	7	0
4	F	508[A]	NAD	14	0
4	F	508[B]	NAD	7	0
3	D	506	AKG	7	0
2	C	502	PO4	1	0

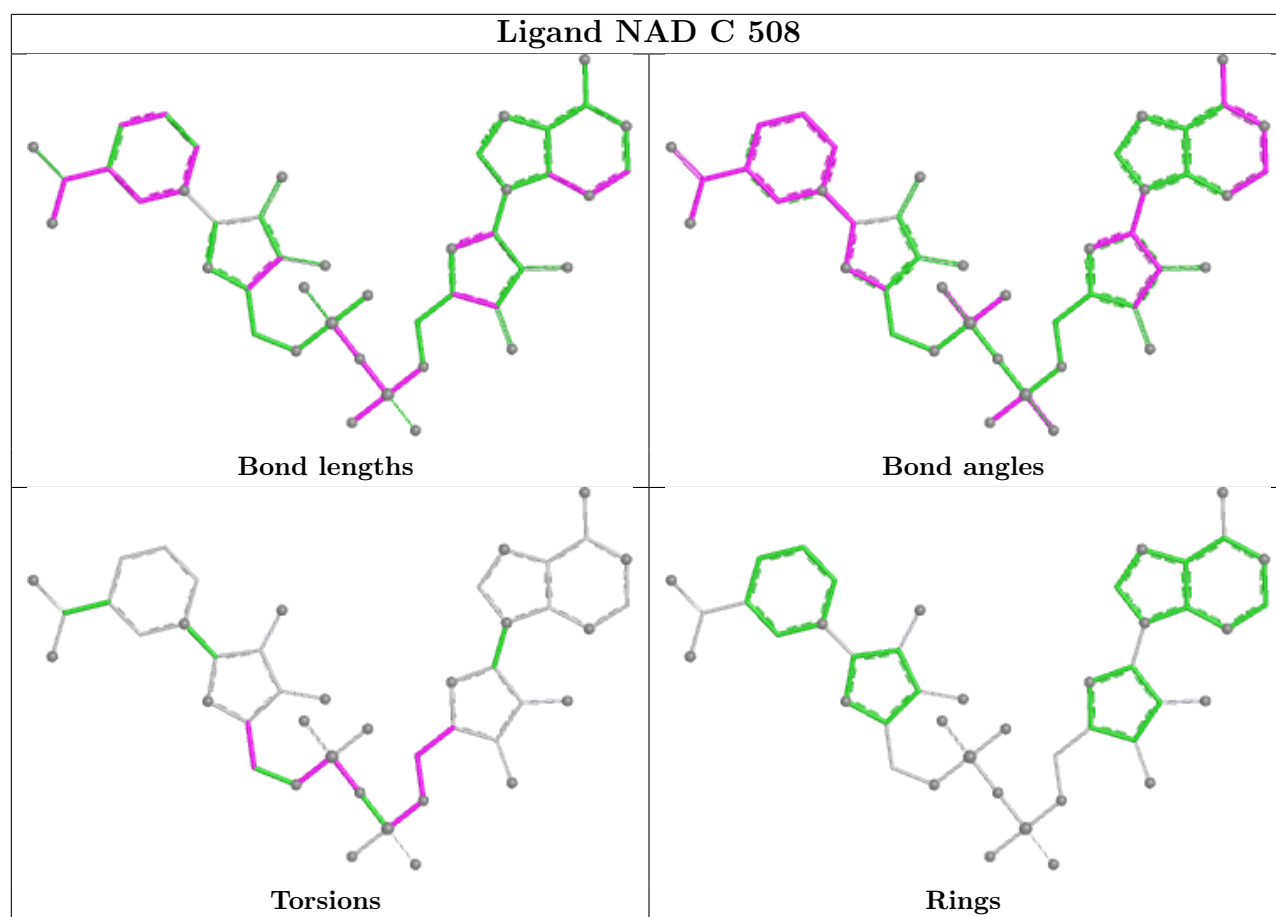
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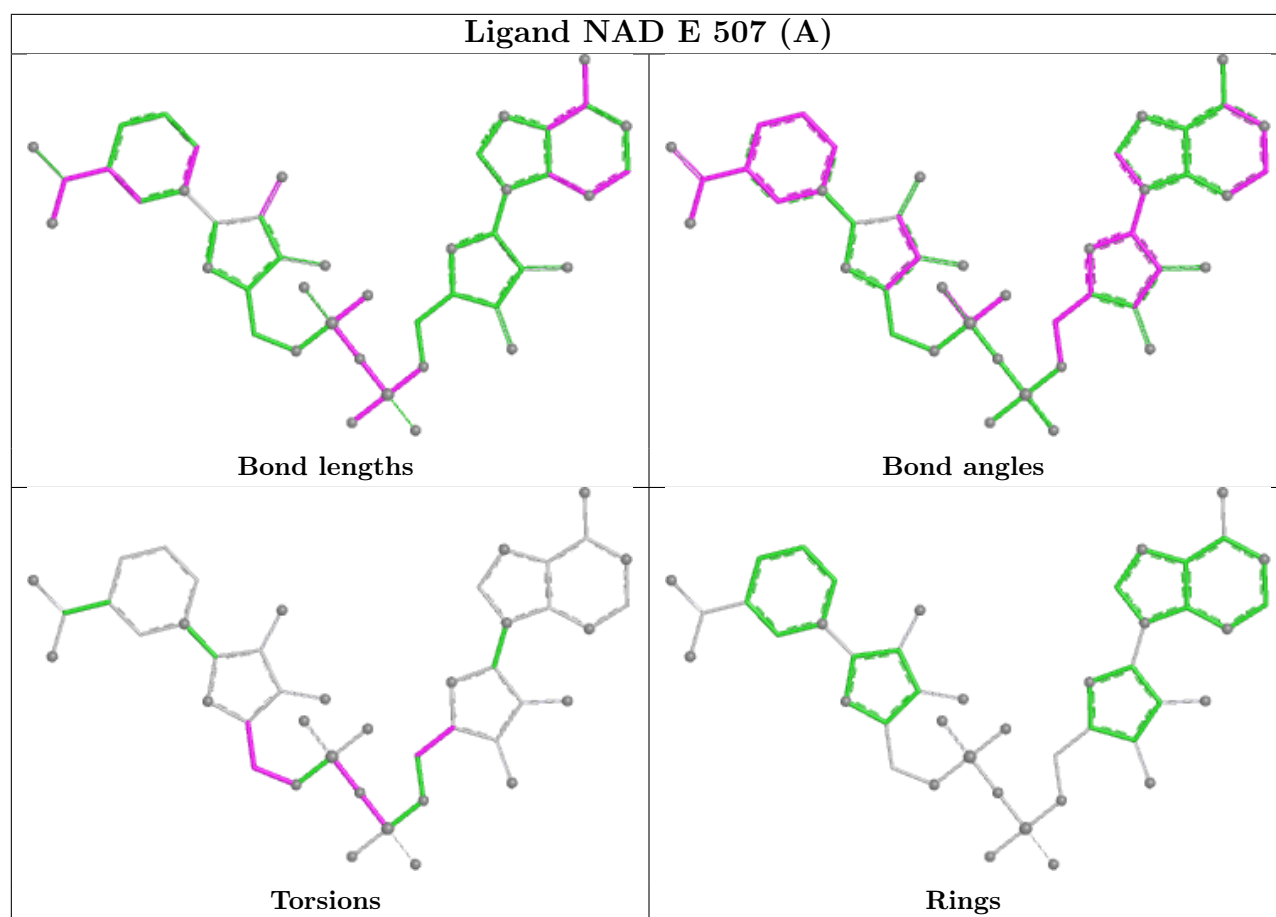
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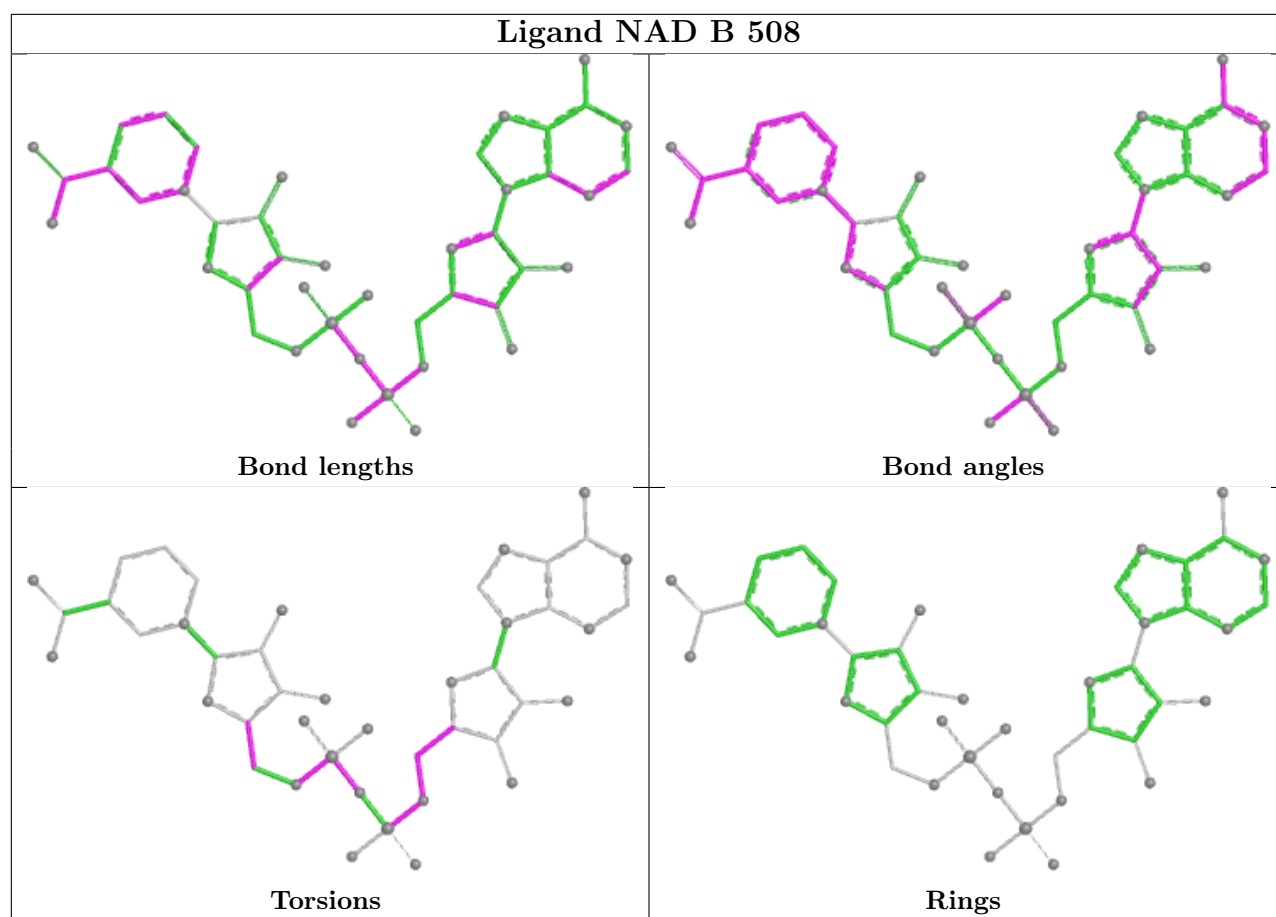
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	PO4	1	0
2	A	503	PO4	1	0
4	A	508	NAD	11	0
2	C	504	PO4	1	0
2	D	505	PO4	1	0
4	F	507	NAD	13	0
2	D	504	PO4	2	0
2	F	505	PO4	1	0
2	C	505	PO4	2	0
2	F	504	PO4	2	0
2	E	504	PO4	2	0
4	E	508	NAD	12	0
3	A	506	AKG	6	0
3	F	506	AKG	7	0
2	B	503	PO4	2	0
2	E	503	PO4	2	0
4	A	507[A]	NAD	16	0
2	D	502	PO4	1	0
2	F	502	PO4	2	0
4	D	507[A]	NAD	16	0
3	E	506	AKG	6	0
4	A	507[B]	NAD	6	0
4	D	507[B]	NAD	7	0
2	A	505	PO4	1	0
4	B	507[A]	NAD	17	0
4	B	507[B]	NAD	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

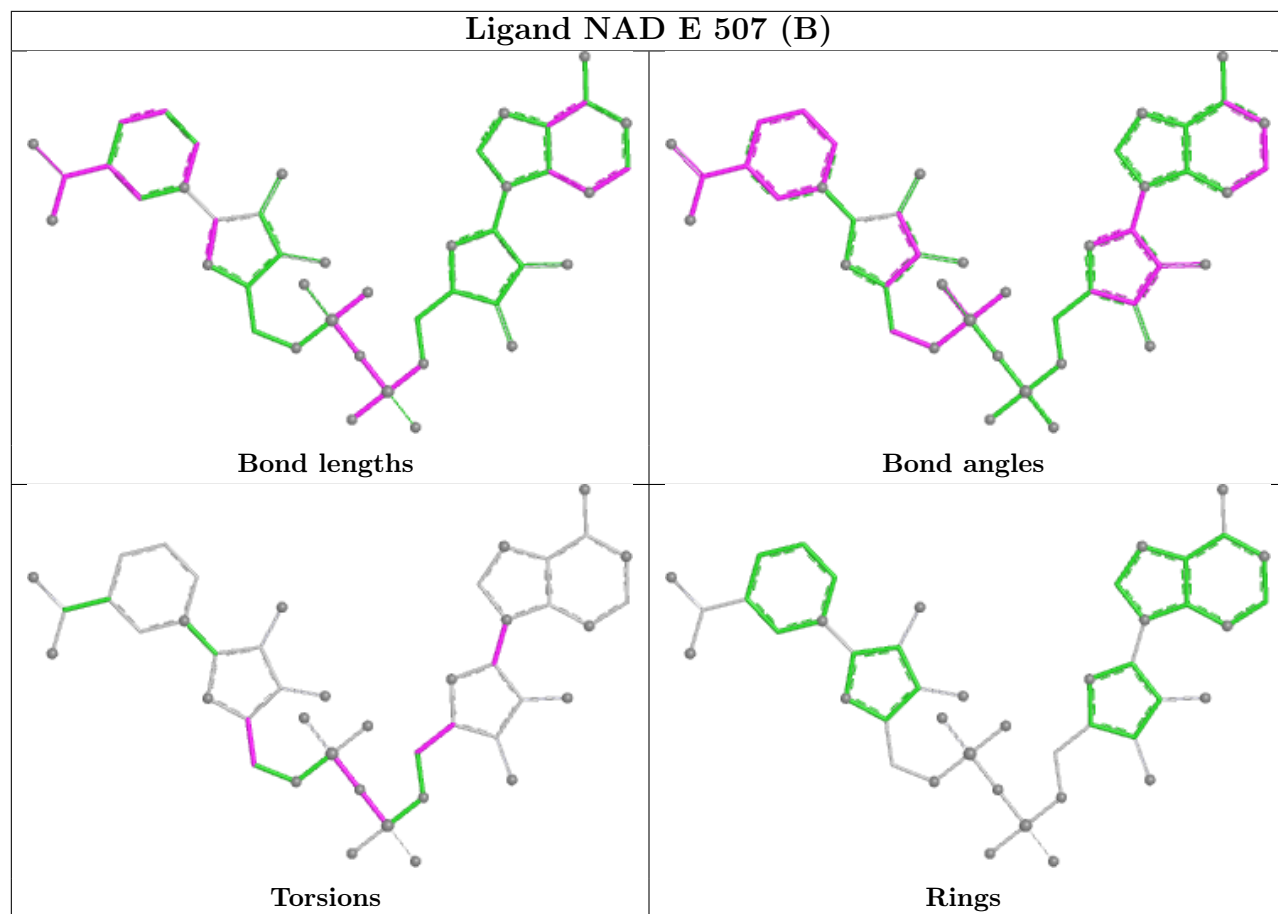


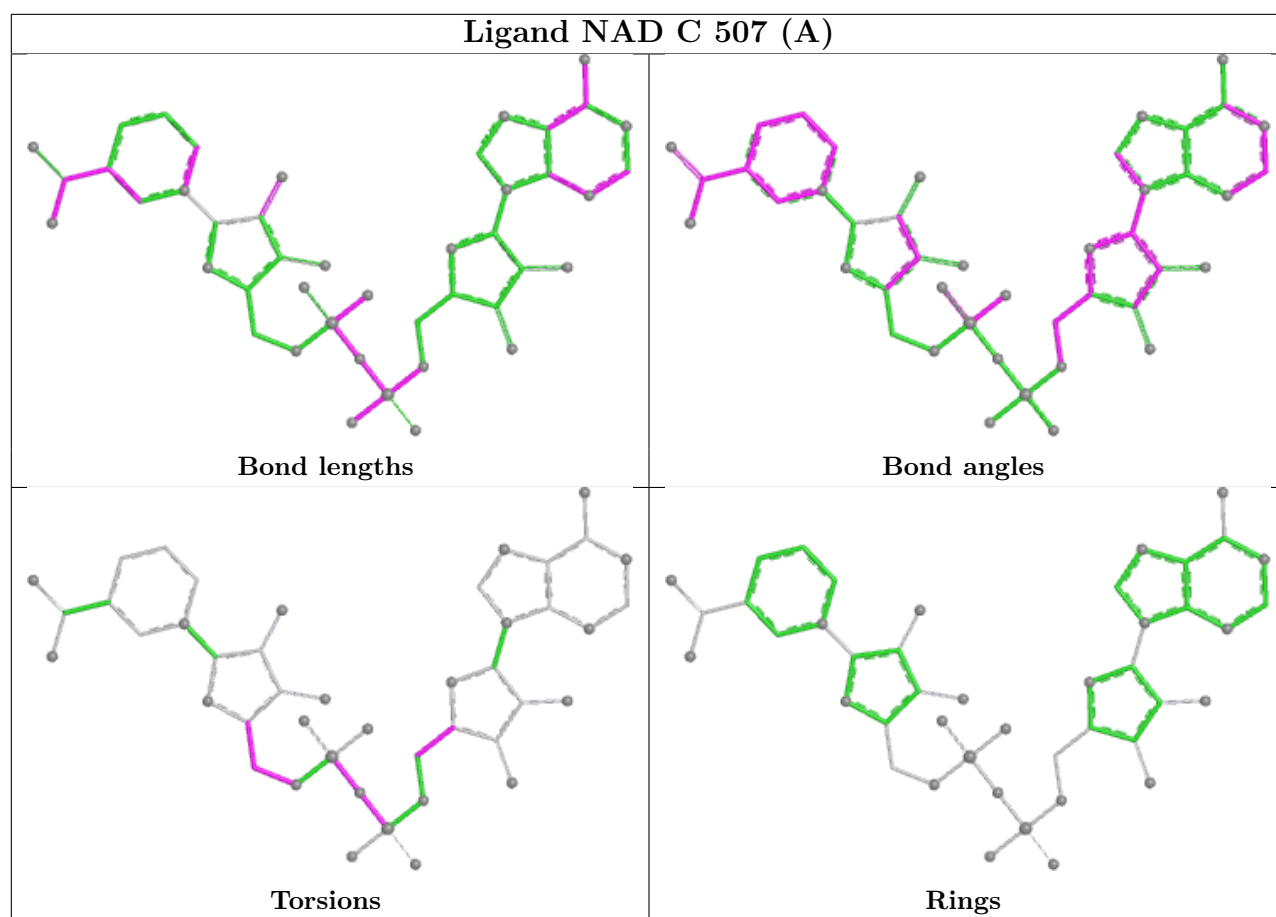




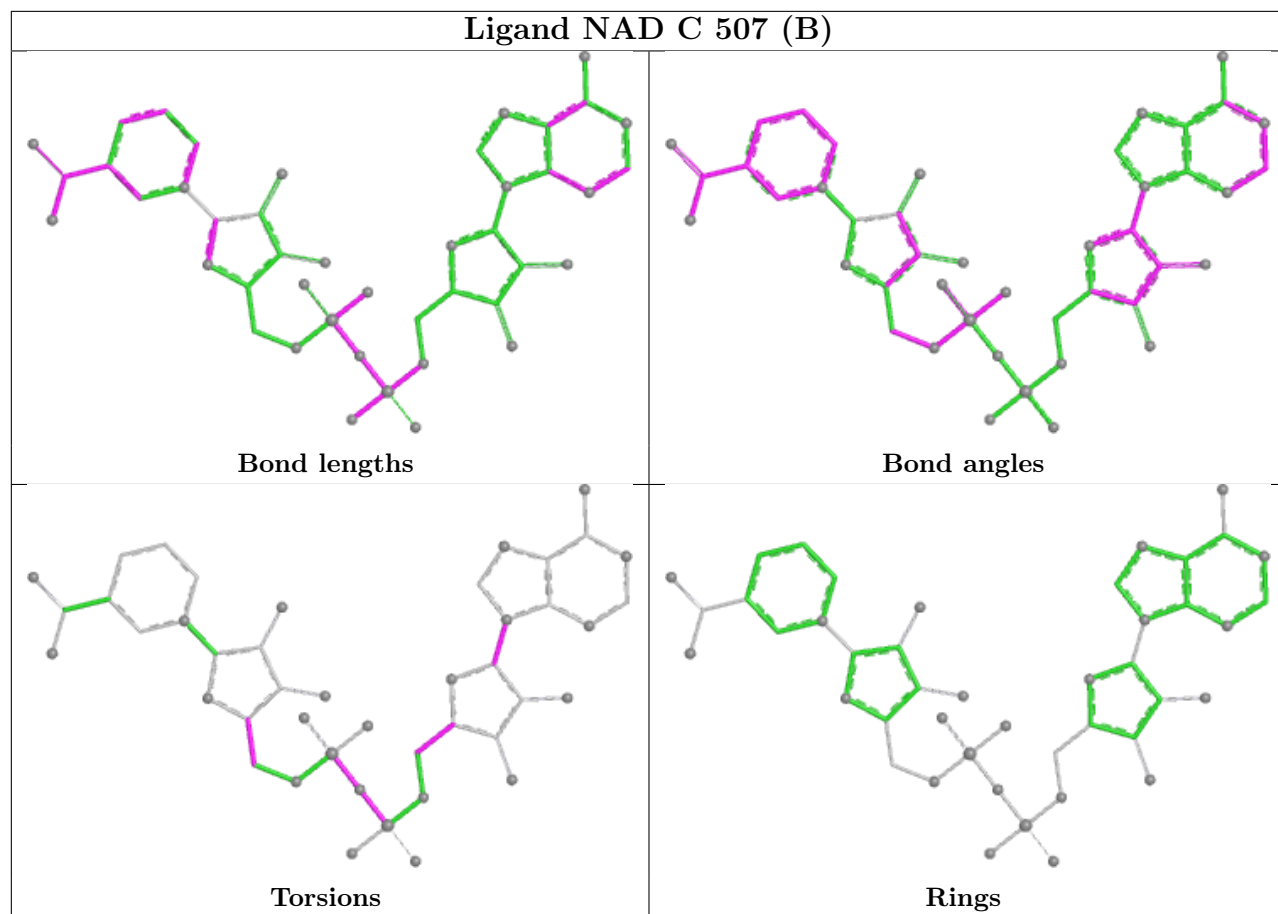


Ligand NAD E 507 (B)

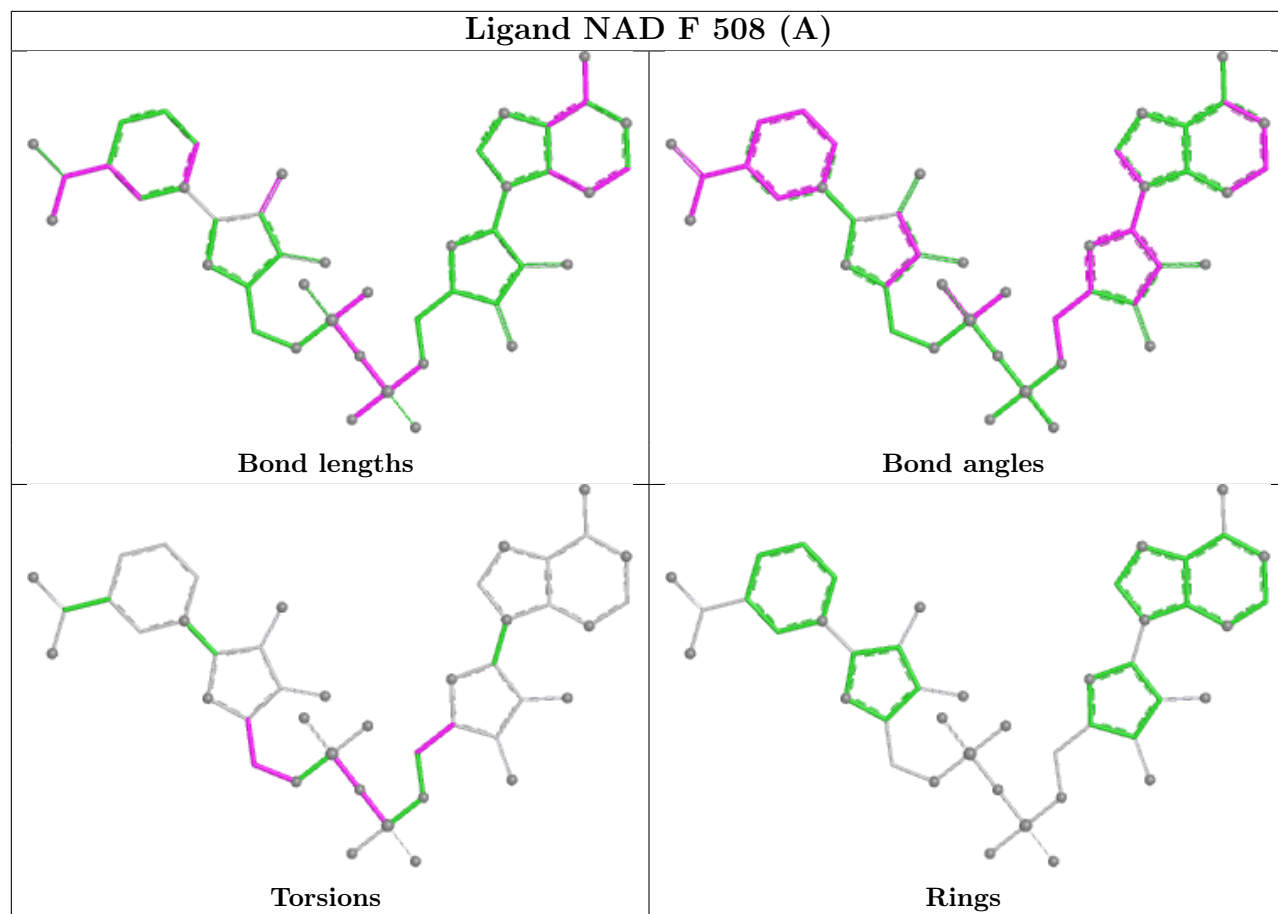




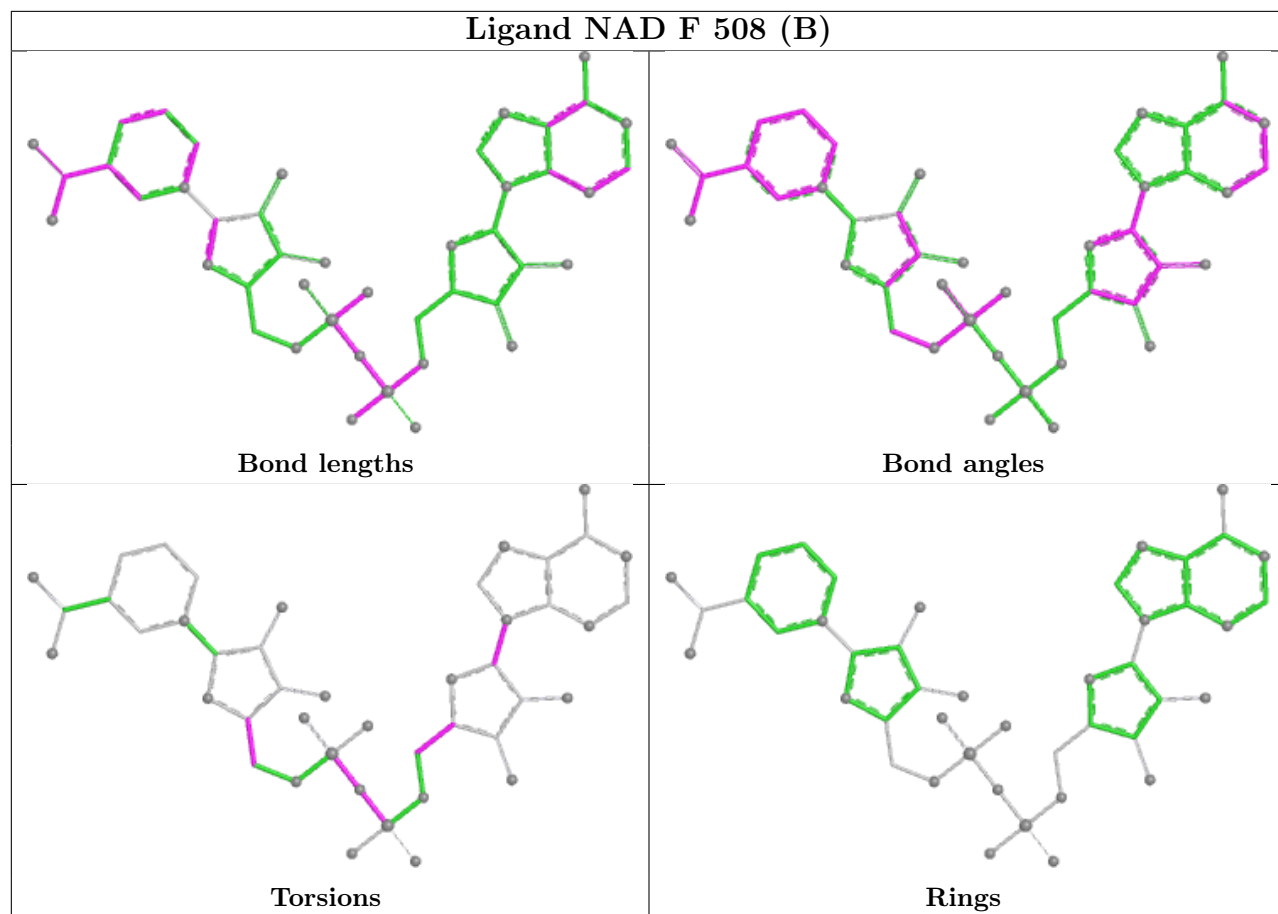
Ligand NAD C 507 (B)

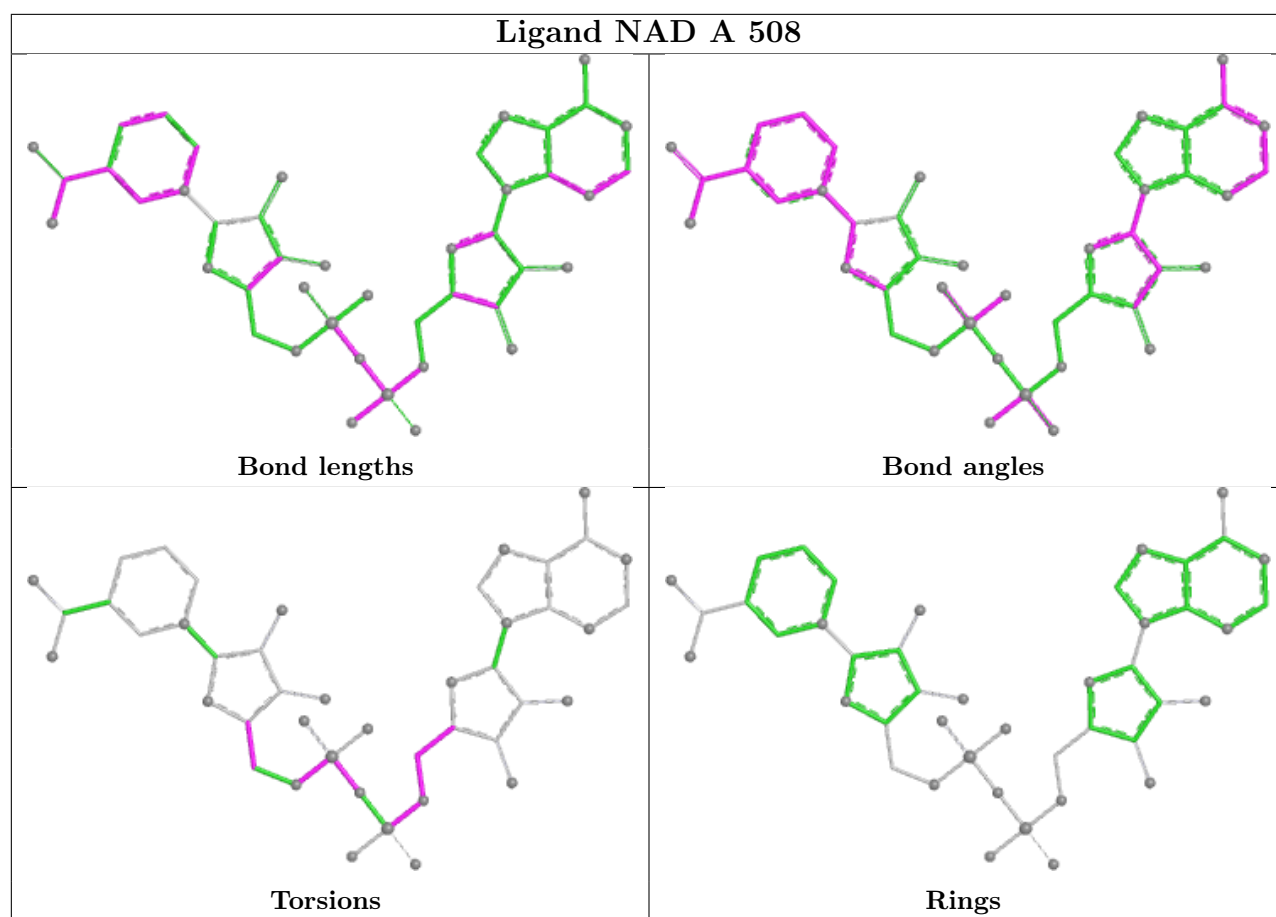


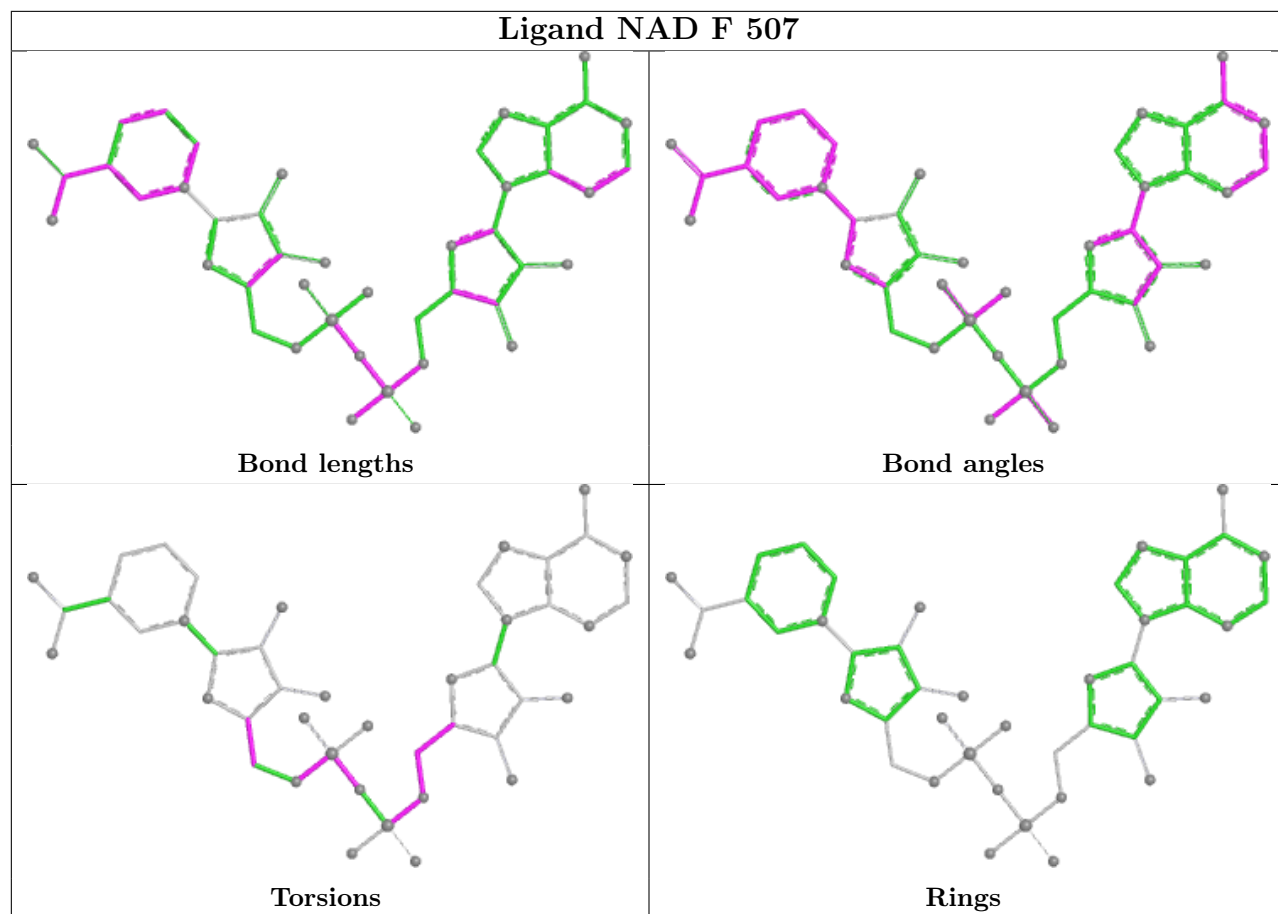
Ligand NAD F 508 (A)

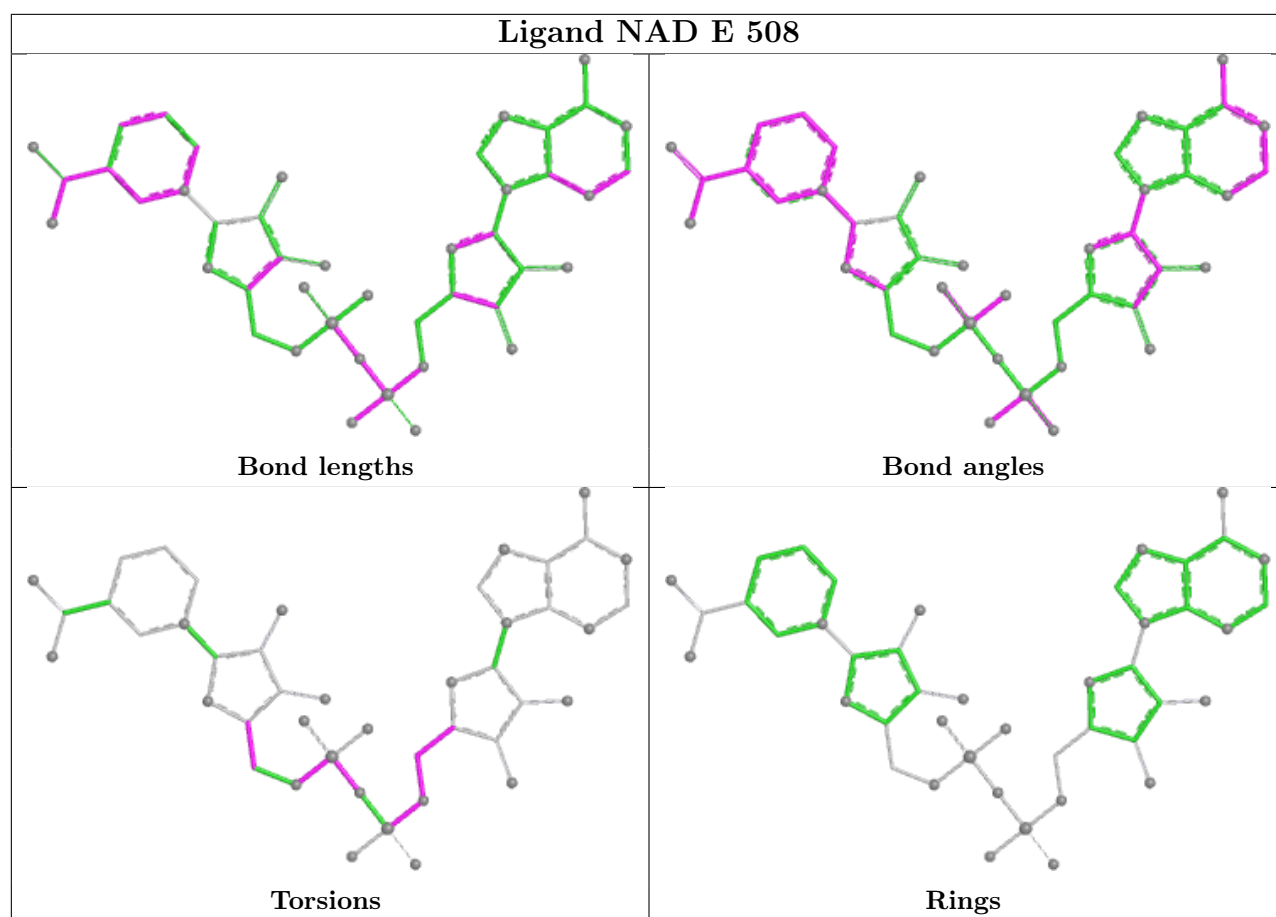


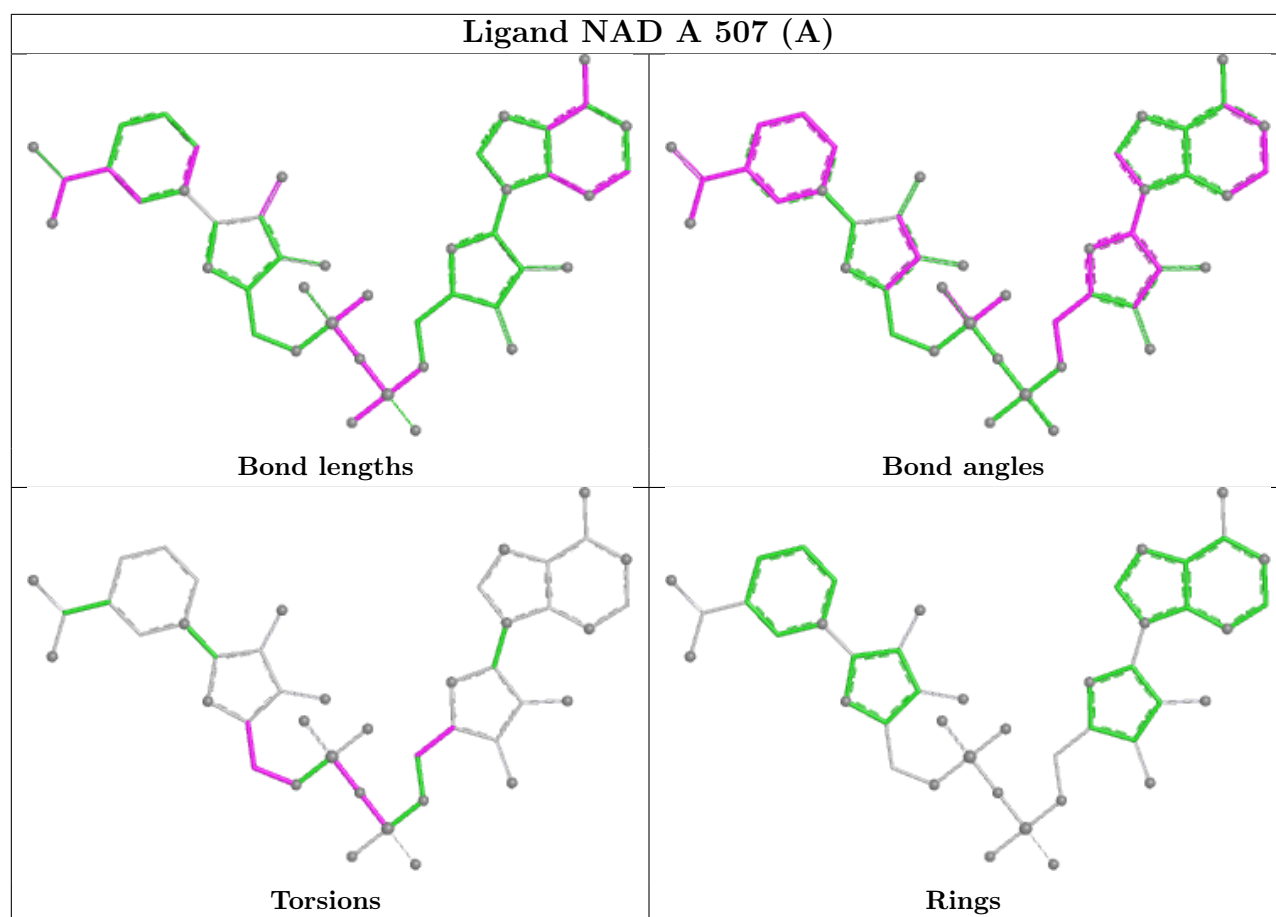
Ligand NAD F 508 (B)

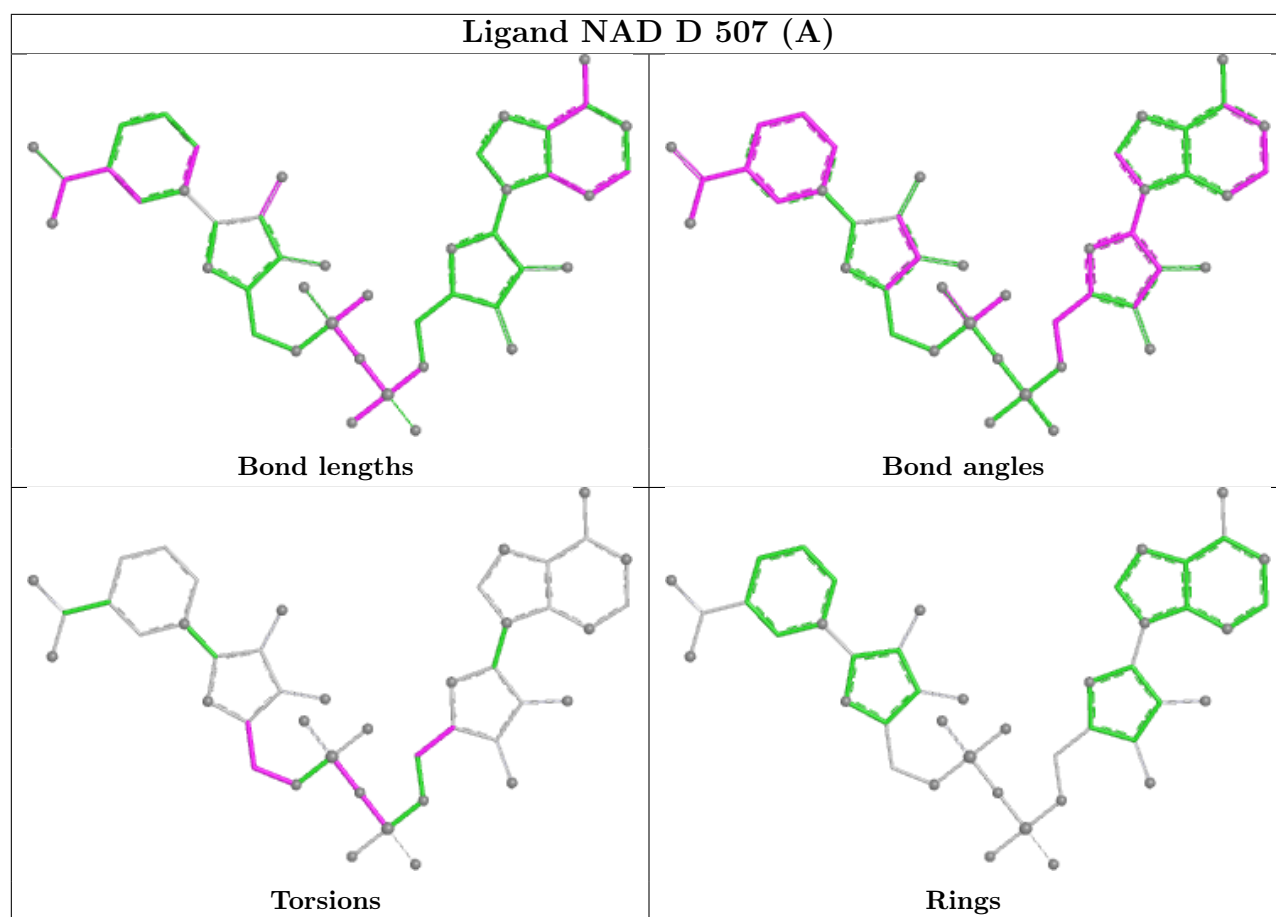




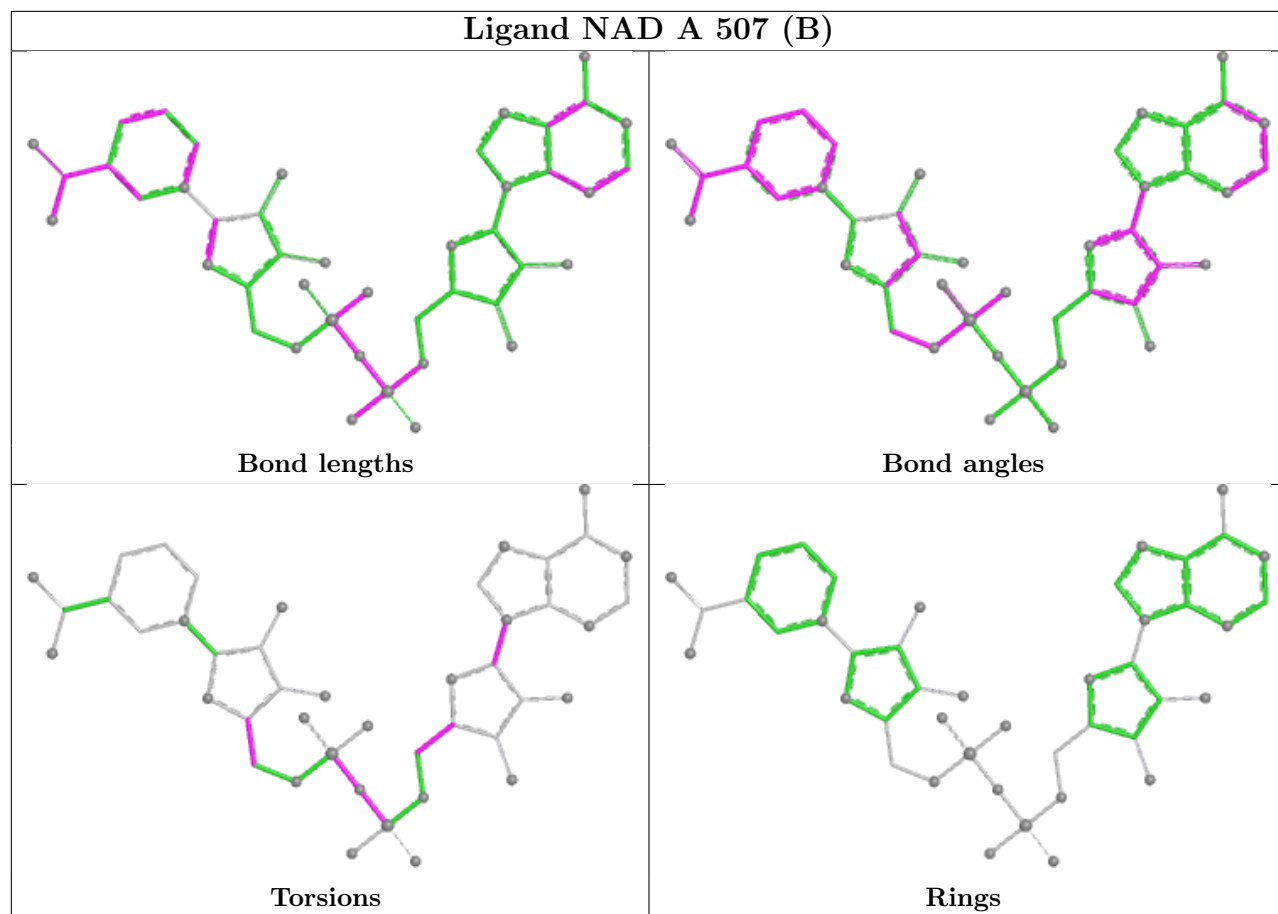




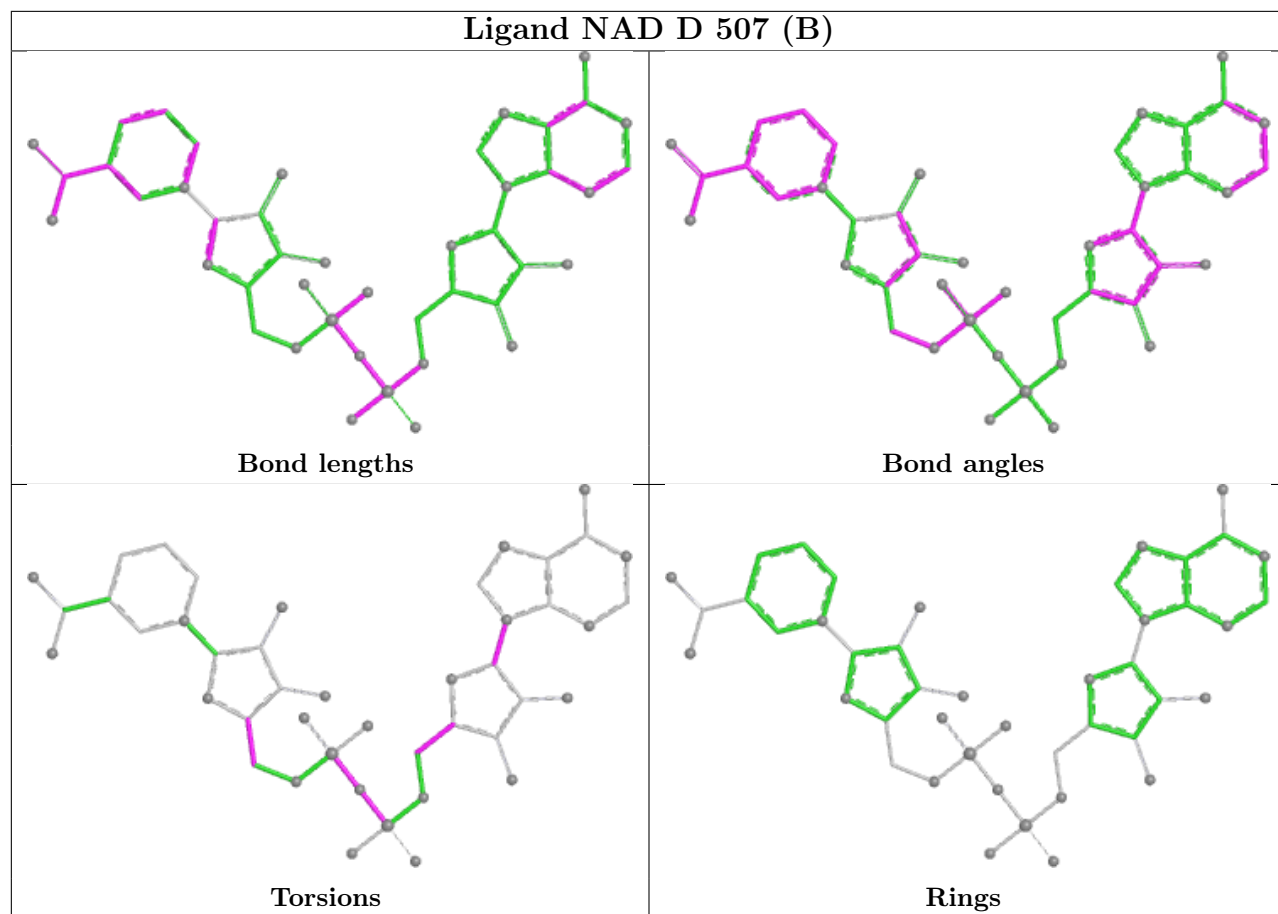


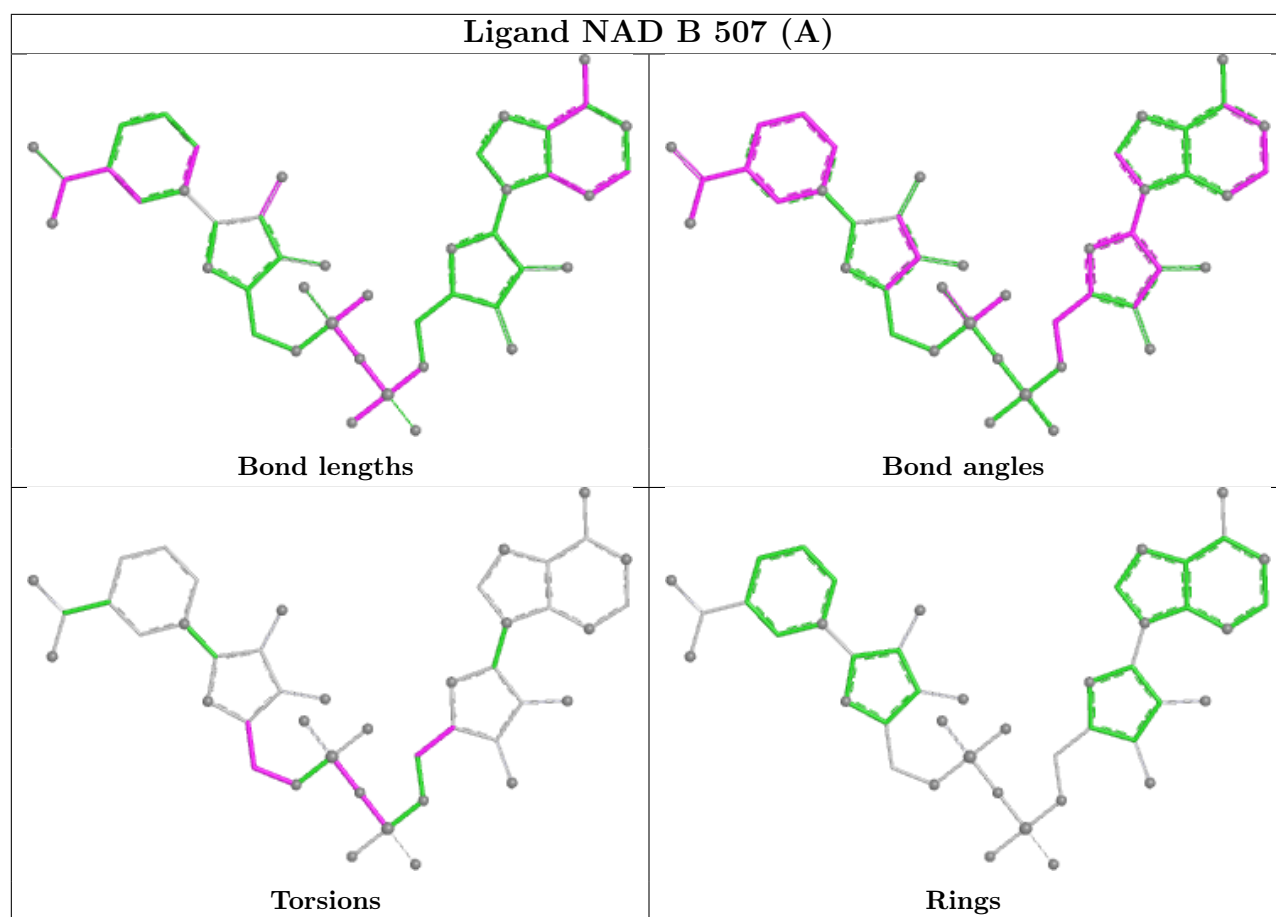


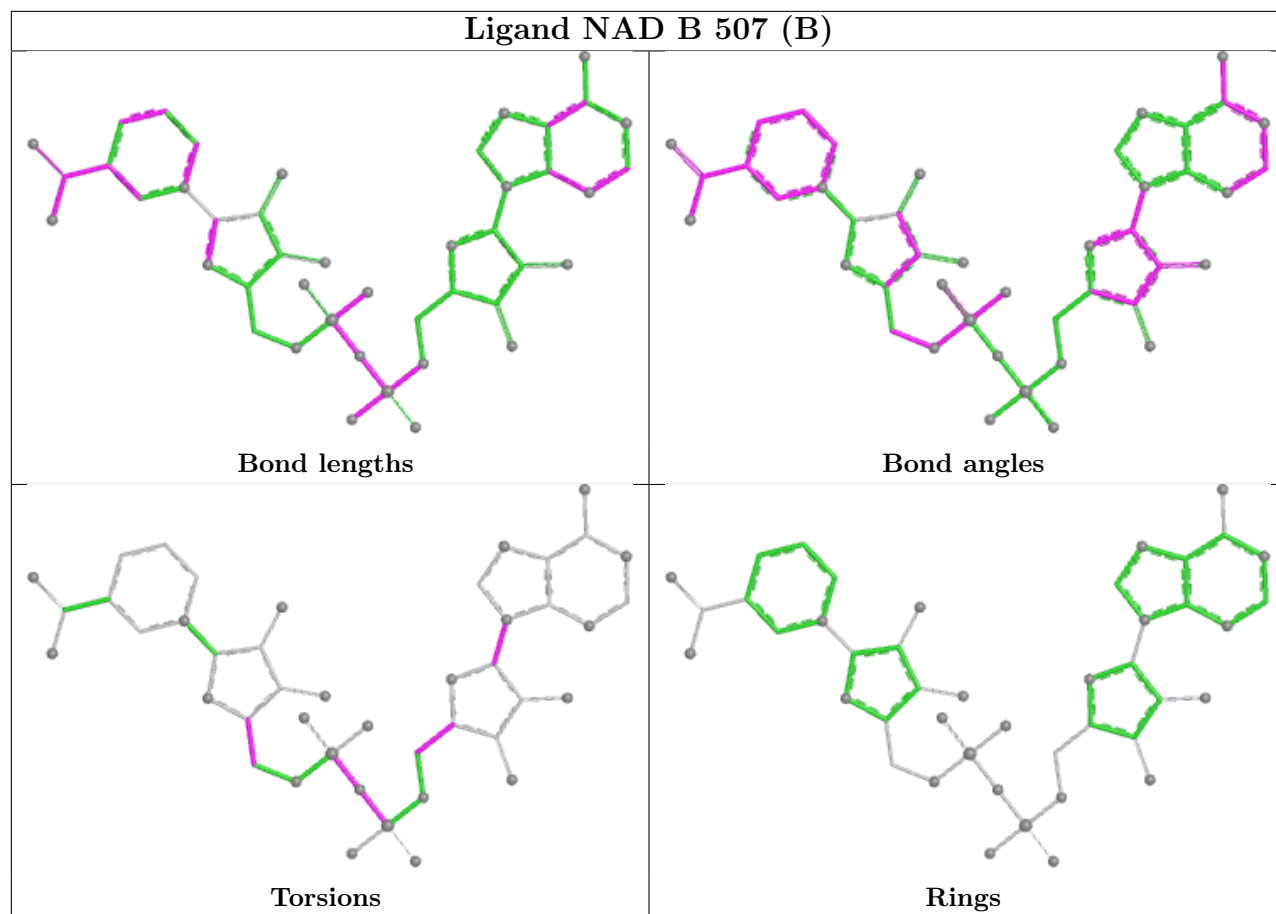
Ligand NAD A 507 (B)



Ligand NAD D 507 (B)







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.