



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:28 AM UTC

PDB ID : 1CER / pdb_00001cer
Title : DETERMINANTS OF ENZYME THERMOSTABILITY OBSERVED IN
THE MOLECULAR STRUCTURE OF THERMUS AQUATICUS D-GLYCE
RALDEHYDE-3-PHOSPHATE DEHYDROGENASE AT 2.5 ANGSTROMS
RESOLUTION
Authors : Tanner, J.J.; Hecht, R.M.; Krause, K.L.
Deposited on : 1995-11-11
Resolution : 2.50 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

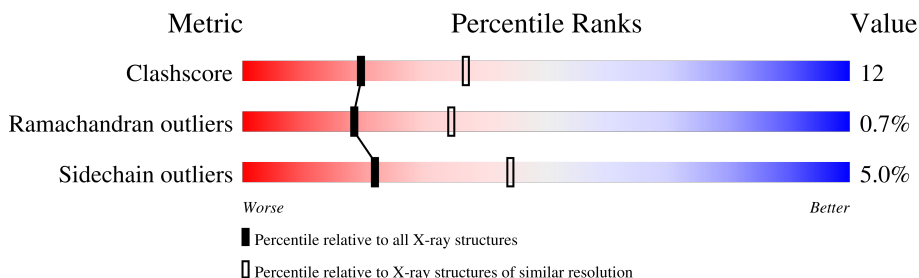
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	331	
1	B	331	
1	C	331	
1	D	331	
1	O	331	
1	P	331	
1	Q	331	
1	R	331	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20226 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 HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	331	Total	C	N	O	S	0	0	0
			2475	1572	430	466	7			
1	P	331	Total	C	N	O	S	0	0	0
			2496	1583	435	471	7			
1	Q	331	Total	C	N	O	S	0	0	0
			2487	1580	432	468	7			
1	R	331	Total	C	N	O	S	0	0	0
			2479	1575	431	466	7			
1	A	331	Total	C	N	O	S	0	0	0
			2475	1572	430	466	7			
1	B	331	Total	C	N	O	S	0	0	0
			2496	1583	435	471	7			
1	C	331	Total	C	N	O	S	0	0	0
			2487	1580	432	468	7			
1	D	331	Total	C	N	O	S	0	0	0
			2479	1575	431	466	7			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	P	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	Q	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	R	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

3 Residue-property plots

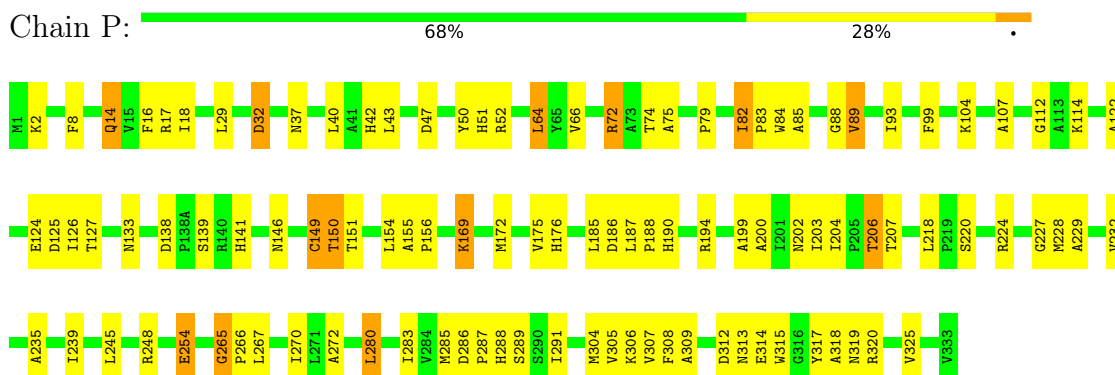
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

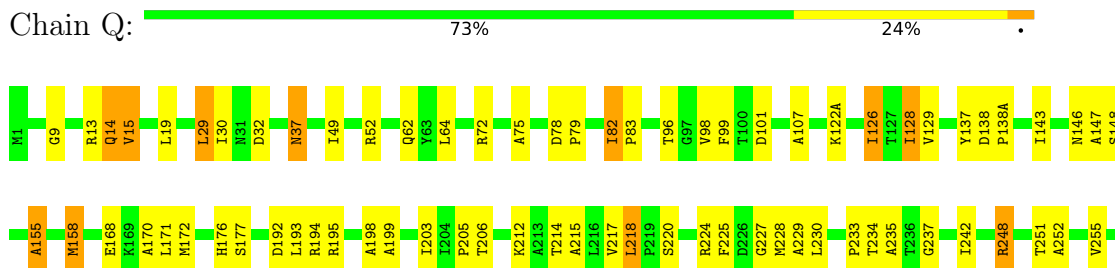
• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

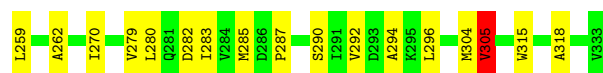


• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



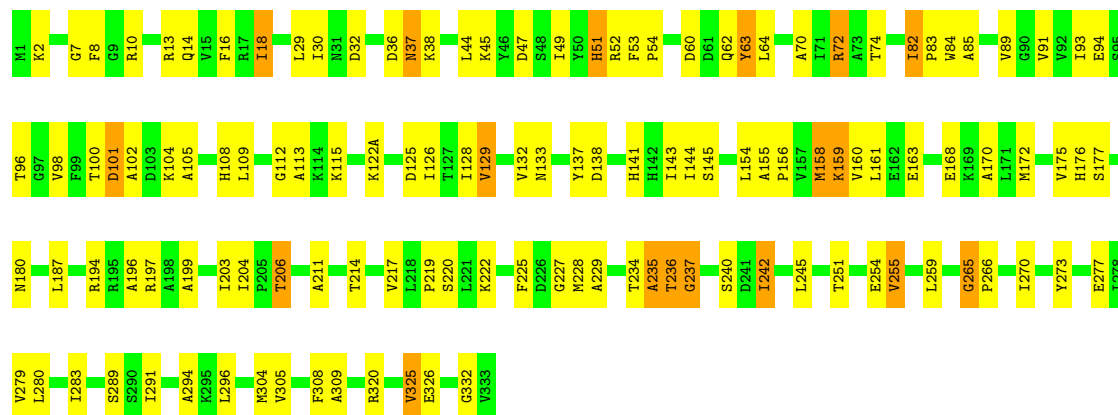
• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE





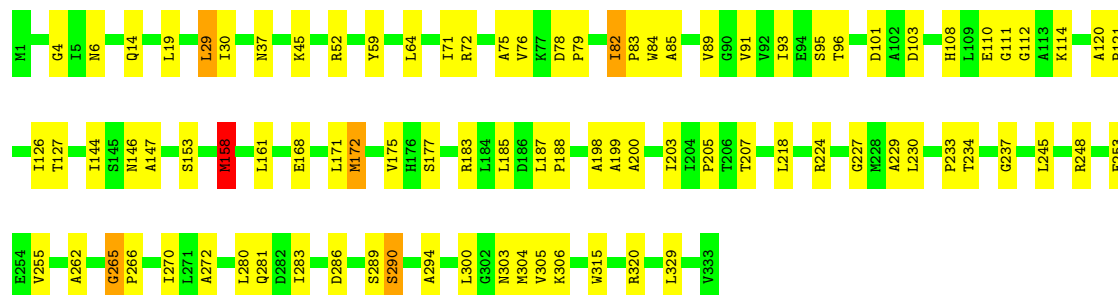
• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain R: 62% 33% 5%



• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain A: 73% 25% .



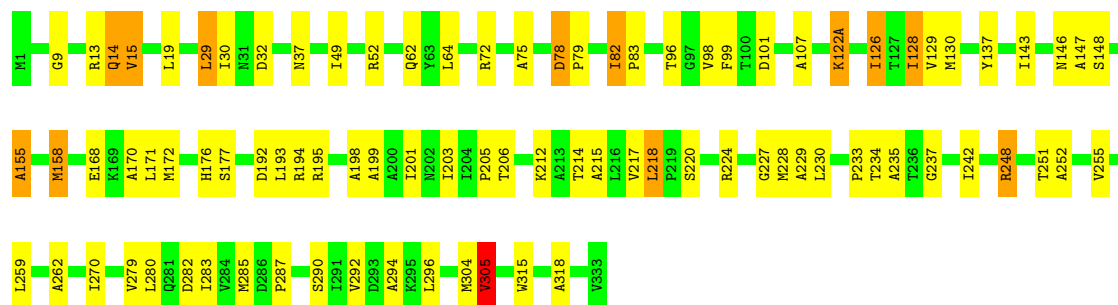
• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain B: 70% 26% .



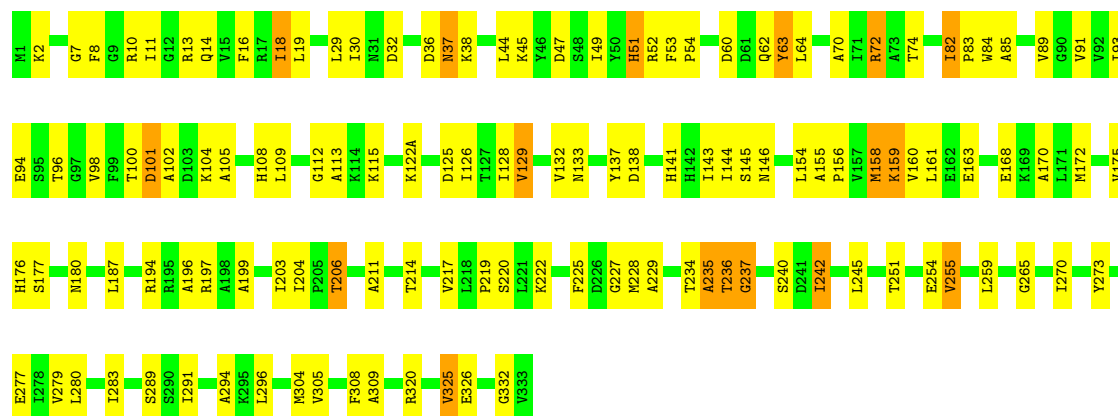
• Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain C: 73% 23% .



● Molecule 1: HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain D: 61% 34% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	144.77Å 148.77Å 149.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50	Depositor
% Data completeness (in resolution range)	72.0 (12.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.205 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20226	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: NAD

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	1.19	7/2519 (0.3%)	1.36	22/3429 (0.6%)
1	B	1.22	5/2540 (0.2%)	1.37	32/3453 (0.9%)
1	C	1.30	8/2531 (0.3%)	1.38	23/3442 (0.7%)
1	D	1.22	4/2523 (0.2%)	1.37	25/3433 (0.7%)
1	O	1.19	7/2519 (0.3%)	1.36	22/3429 (0.6%)
1	P	1.22	5/2540 (0.2%)	1.37	32/3453 (0.9%)
1	Q	1.30	8/2531 (0.3%)	1.38	23/3442 (0.7%)
1	R	1.22	4/2523 (0.2%)	1.37	25/3433 (0.7%)
All	All	1.23	48/20226 (0.2%)	1.37	204/27514 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	P	0	1
All	All	0	2

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	158	MET	SD-CE	-9.94	1.54	1.79
1	C	158	MET	SD-CE	-9.93	1.54	1.79
1	A	82	ILE	CA-CB	7.32	1.61	1.53
1	R	18	ILE	CA-CB	-7.31	1.45	1.54
1	D	18	ILE	CA-CB	-7.27	1.45	1.54

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ILE	CA-C-N	10.42	132.87	119.84
1	A	82	ILE	C-N-CA	10.42	132.87	119.84
1	O	82	ILE	CA-C-N	10.39	132.82	119.84
1	O	82	ILE	C-N-CA	10.39	132.82	119.84
1	C	82	ILE	CA-C-N	10.31	132.73	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	190	HIS	Sidechain
1	P	190	HIS	Sidechain

5.2 Too-close contacts

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	2475	0	2477	46	6
1	B	2496	0	2517	57	0
1	C	2487	0	2503	53	0
1	D	2479	0	2488	87	0
1	O	2475	0	2477	48	0
1	P	2496	0	2517	60	7
1	Q	2487	0	2503	52	1
1	R	2479	0	2488	87	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	O	44	0	26	1	0
2	P	44	0	26	0	0
2	Q	44	0	26	0	0
2	R	44	0	26	0	0
All	All	20226	0	20178	467	7

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 12.

The worst 5 of 467 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:A:158:MET:HE2	1:A:158:MET:HA	1.45	0.98
1:O:158:MET:HA	1:O:158:MET:HE2	1.45	0.96
1:D:158:MET:HE2	1:D:158:MET:HA	1.49	0.94
1:Q:172:MET:HE3	1:Q:227:GLY:HA3	1.49	0.94
1:R:158:MET:HE2	1:R:158:MET:HA	1.49	0.93

The worst 5 of 7 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:P:138:ASP:CG	1:A:253:GLU:OE1[1_545]	1.58	0.62
1:P:138:ASP:OD1	1:A:253:GLU:OE2[1_545]	1.60	0.60
1:P:139:SER:OG	1:A:253:GLU:OE2[1_545]	1.64	0.56
1:P:254:GLU:OE2	1:Q:224:ARG:NH2[2_555]	1.65	0.55
1:P:138:ASP:OD1	1:A:253:GLU:CD[1_545]	1.76	0.44

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	329/331 (99%)	300 (91%)	25 (8%)	4 (1%)	10	20
1	B	329/331 (99%)	305 (93%)	24 (7%)	0	100	100
1	C	329/331 (99%)	303 (92%)	23 (7%)	3 (1%)	14	27
1	D	329/331 (99%)	291 (88%)	36 (11%)	2 (1%)	21	38
1	O	329/331 (99%)	300 (91%)	25 (8%)	4 (1%)	10	20
1	P	329/331 (99%)	305 (93%)	24 (7%)	0	100	100
1	Q	329/331 (99%)	303 (92%)	23 (7%)	3 (1%)	14	27
1	R	329/331 (99%)	291 (88%)	36 (11%)	2 (1%)	21	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2632/2648 (99%)	2398 (91%)	216 (8%)	18 (1%)	18	34

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	198	ALA
1	A	198	ALA
1	R	332	GLY
1	D	332	GLY
1	Q	147	ALA

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	251/265 (95%)	239 (95%)	12 (5%)	23	46
1	B	257/265 (97%)	244 (95%)	13 (5%)	21	43
1	C	254/265 (96%)	244 (96%)	10 (4%)	28	55
1	D	252/265 (95%)	237 (94%)	15 (6%)	17	36
1	O	251/265 (95%)	239 (95%)	12 (5%)	23	46
1	P	257/265 (97%)	244 (95%)	13 (5%)	21	43
1	Q	254/265 (96%)	243 (96%)	11 (4%)	26	51
1	R	252/265 (95%)	237 (94%)	15 (6%)	17	36
All	All	2028/2120 (96%)	1927 (95%)	101 (5%)	22	44

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	MET
1	B	206	THR
1	D	277	GLU
1	A	185	LEU
1	B	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	256	ASN
1	D	142	HIS
1	B	20	HIS
1	D	256	ASN
1	C	256	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	NAD	A	336	-	46,48,48	1.55	5 (10%)	64,73,73	2.31	21 (32%)
2	NAD	D	336	-	46,48,48	1.77	6 (13%)	64,73,73	2.50	25 (39%)
2	NAD	P	336	-	46,48,48	1.48	5 (10%)	64,73,73	2.44	27 (42%)
2	NAD	B	336	-	46,48,48	1.47	5 (10%)	64,73,73	2.44	27 (42%)
2	NAD	C	336	-	46,48,48	1.46	6 (13%)	64,73,73	2.23	19 (29%)
2	NAD	O	336	-	46,48,48	1.56	5 (10%)	64,73,73	2.31	21 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	Q	336	-	46,48,48	1.46	6 (13%)	64,73,73	2.23	19 (29%)
2	NAD	R	336	-	46,48,48	1.77	6 (13%)	64,73,73	2.50	25 (39%)

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
2	NAD	A	336	-	-	8/30/62/62	0/5/5/5
2	NAD	D	336	-	-	16/30/62/62	0/5/5/5
2	NAD	P	336	-	-	10/30/62/62	0/5/5/5
2	NAD	B	336	-	-	10/30/62/62	0/5/5/5
2	NAD	C	336	-	-	8/30/62/62	0/5/5/5
2	NAD	O	336	-	-	8/30/62/62	0/5/5/5
2	NAD	Q	336	-	-	8/30/62/62	0/5/5/5
2	NAD	R	336	-	-	16/30/62/62	0/5/5/5

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	336	NAD	C2N-N1N	6.91	1.42	1.35
2	D	336	NAD	C2N-N1N	6.90	1.42	1.35
2	R	336	NAD	PN-O3	-6.75	1.52	1.59
2	D	336	NAD	PN-O3	-6.73	1.52	1.59
2	O	336	NAD	C2N-N1N	6.38	1.42	1.35

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	336	NAD	N3A-C4A-N9A	6.72	138.59	127.17
2	O	336	NAD	N3A-C4A-N9A	6.68	138.52	127.17
2	B	336	NAD	N3A-C4A-N9A	6.64	138.46	127.17
2	P	336	NAD	N3A-C4A-N9A	6.64	138.46	127.17
2	P	336	NAD	C5A-C4A-N3A	-6.60	117.63	126.72

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

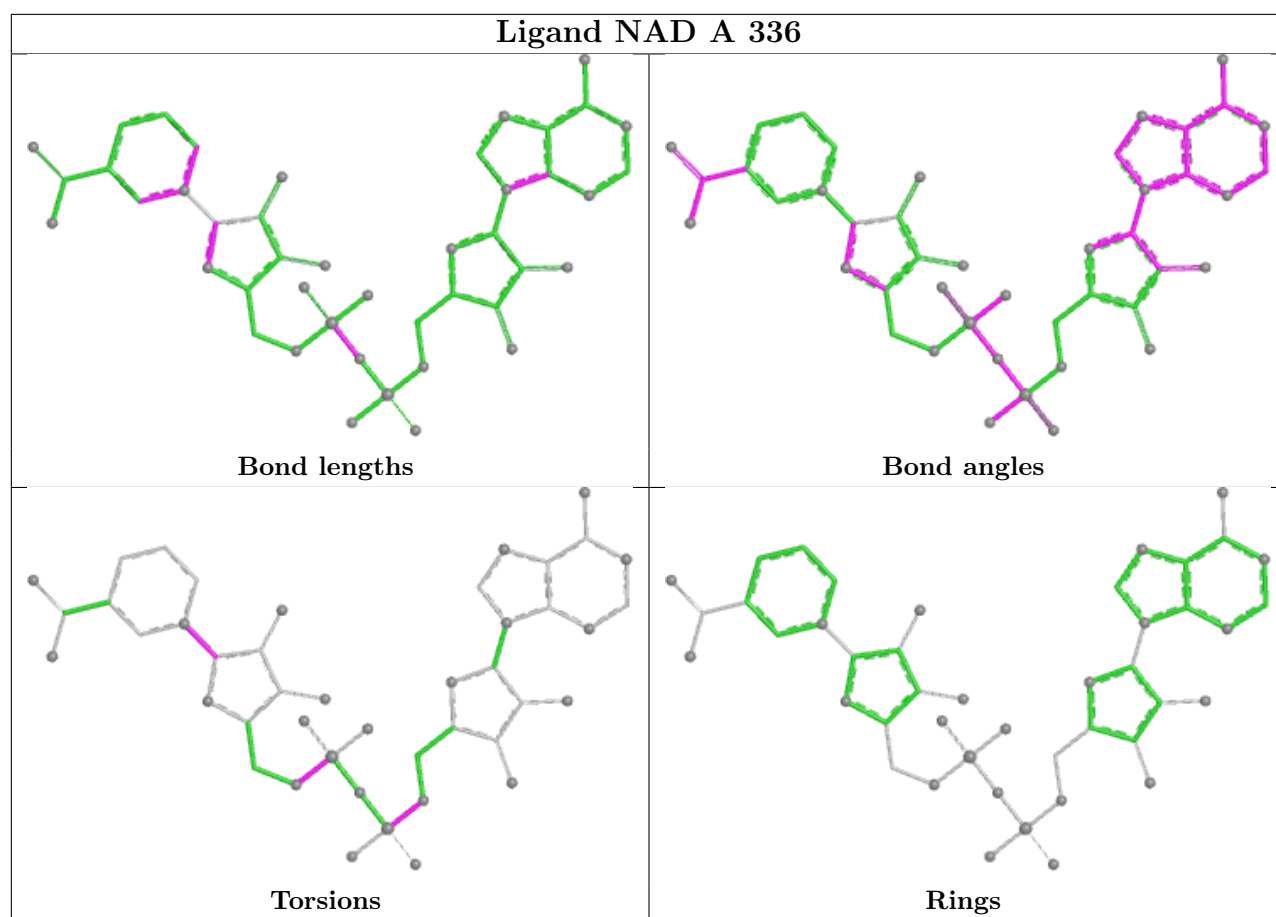
Mol	Chain	Res	Type	Atoms
2	O	336	NAD	C5B-O5B-PA-O1A
2	O	336	NAD	C5D-O5D-PN-O2N
2	O	336	NAD	O4D-C1D-N1N-C2N
2	O	336	NAD	O4D-C1D-N1N-C6N
2	O	336	NAD	C2D-C1D-N1N-C2N

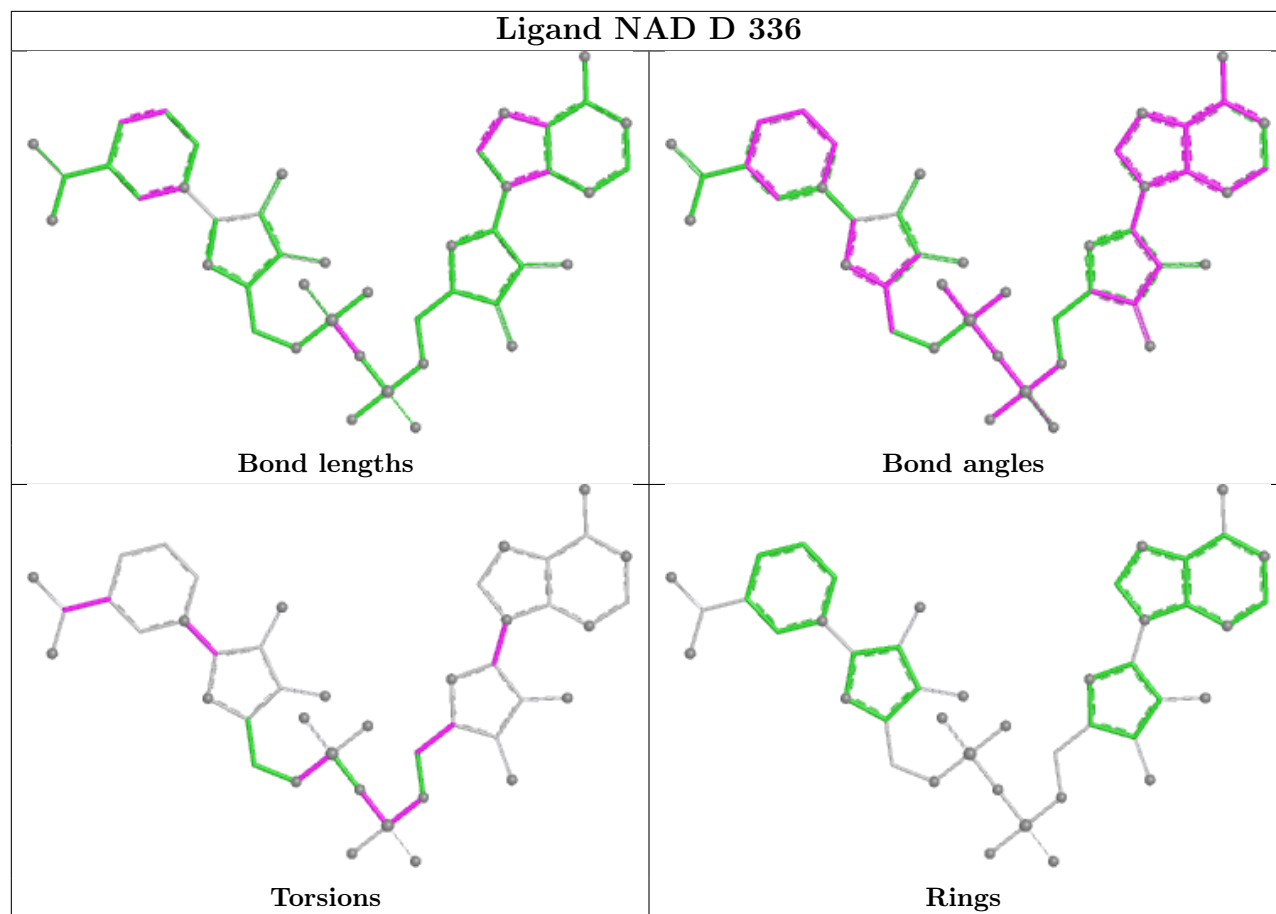
There are no ring outliers.

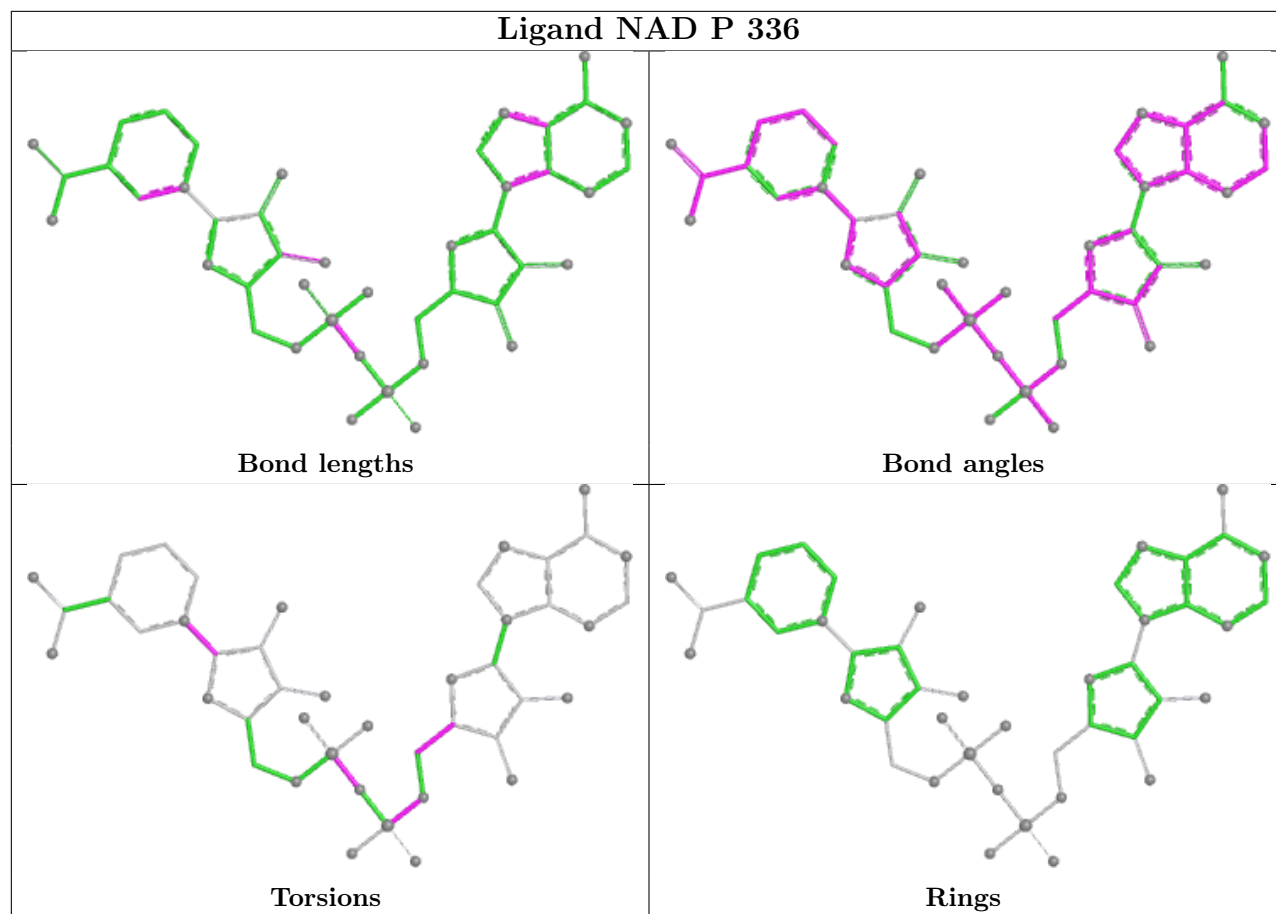
2 monomers are involved in 2 short contacts:

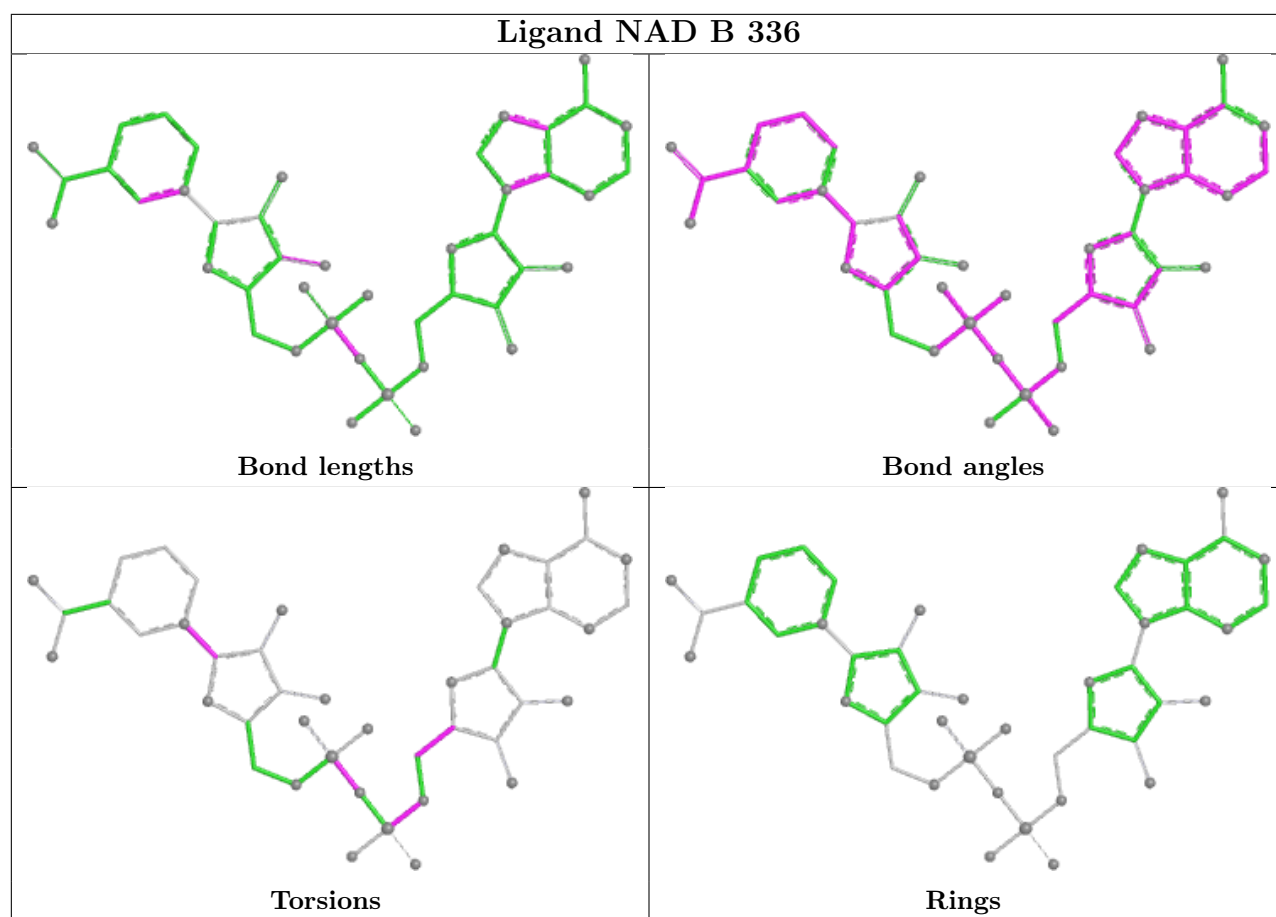
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	336	NAD	1	0
2	O	336	NAD	1	0

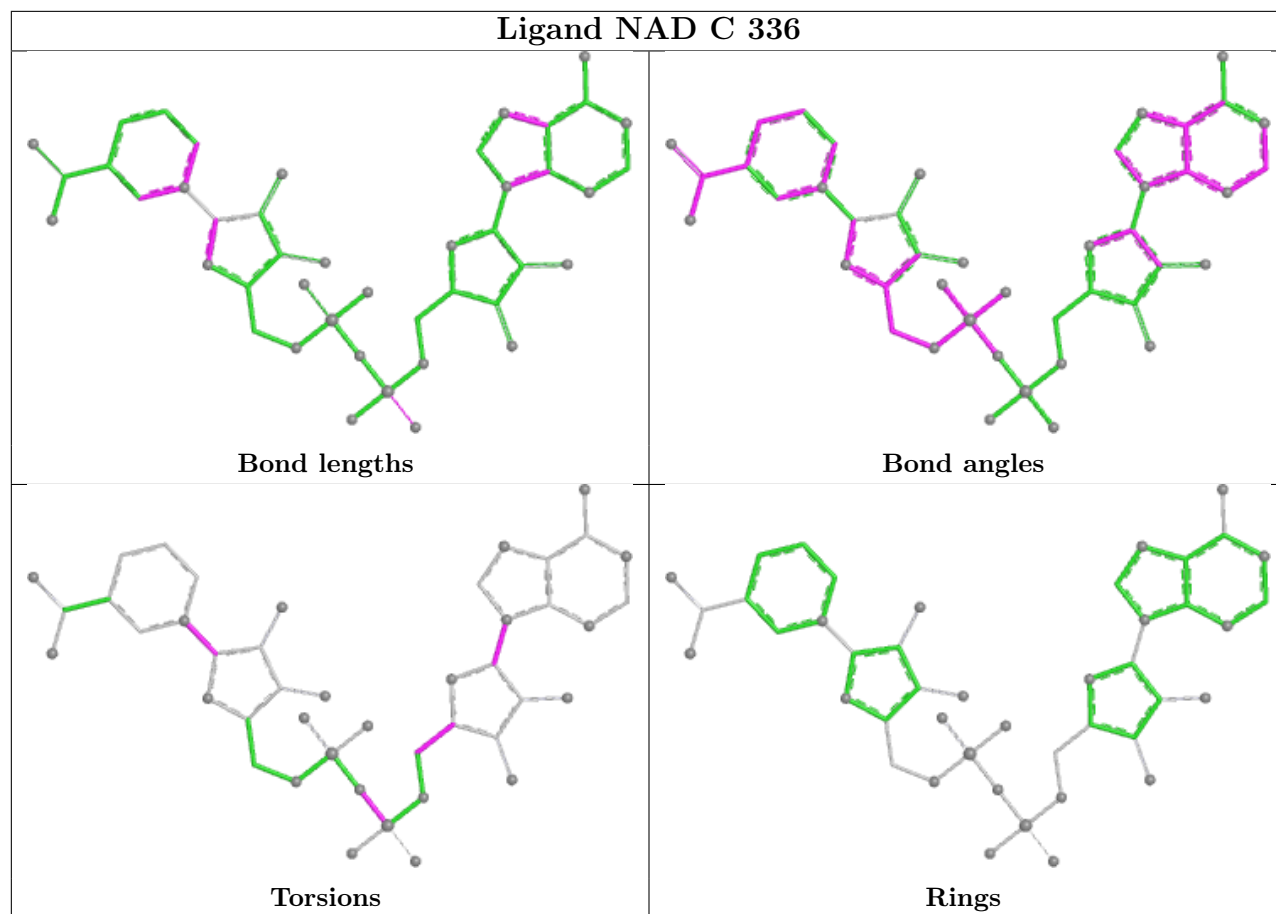
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

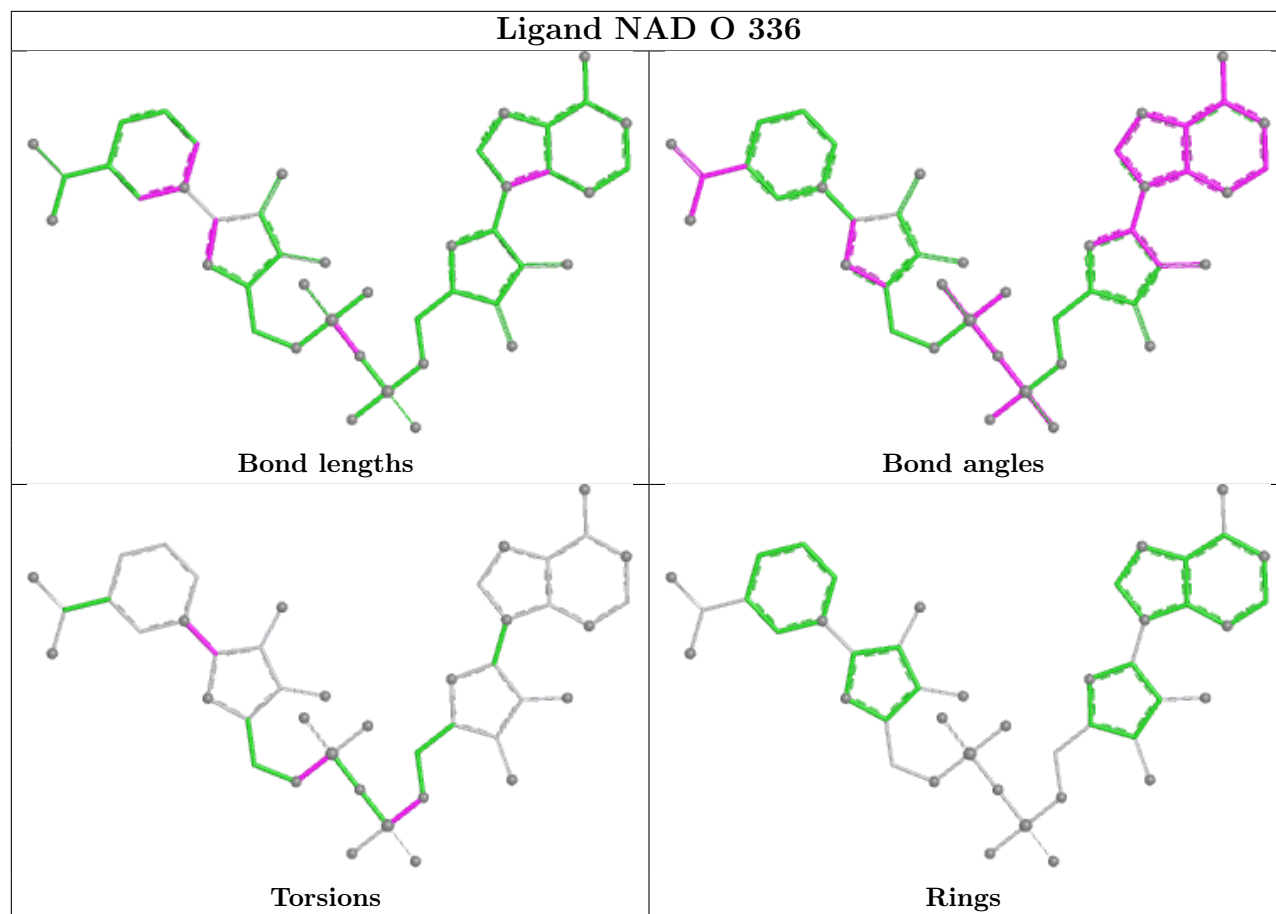


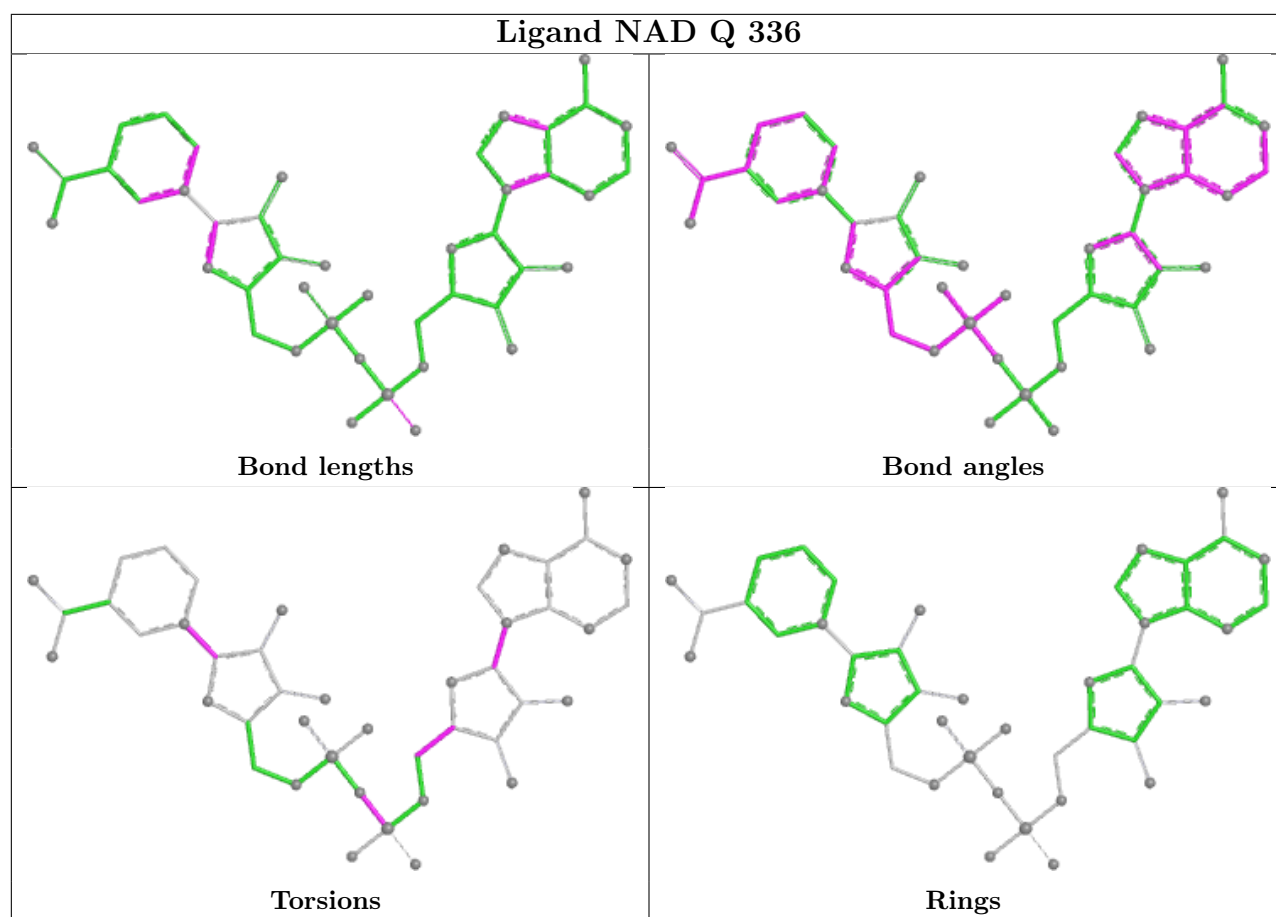


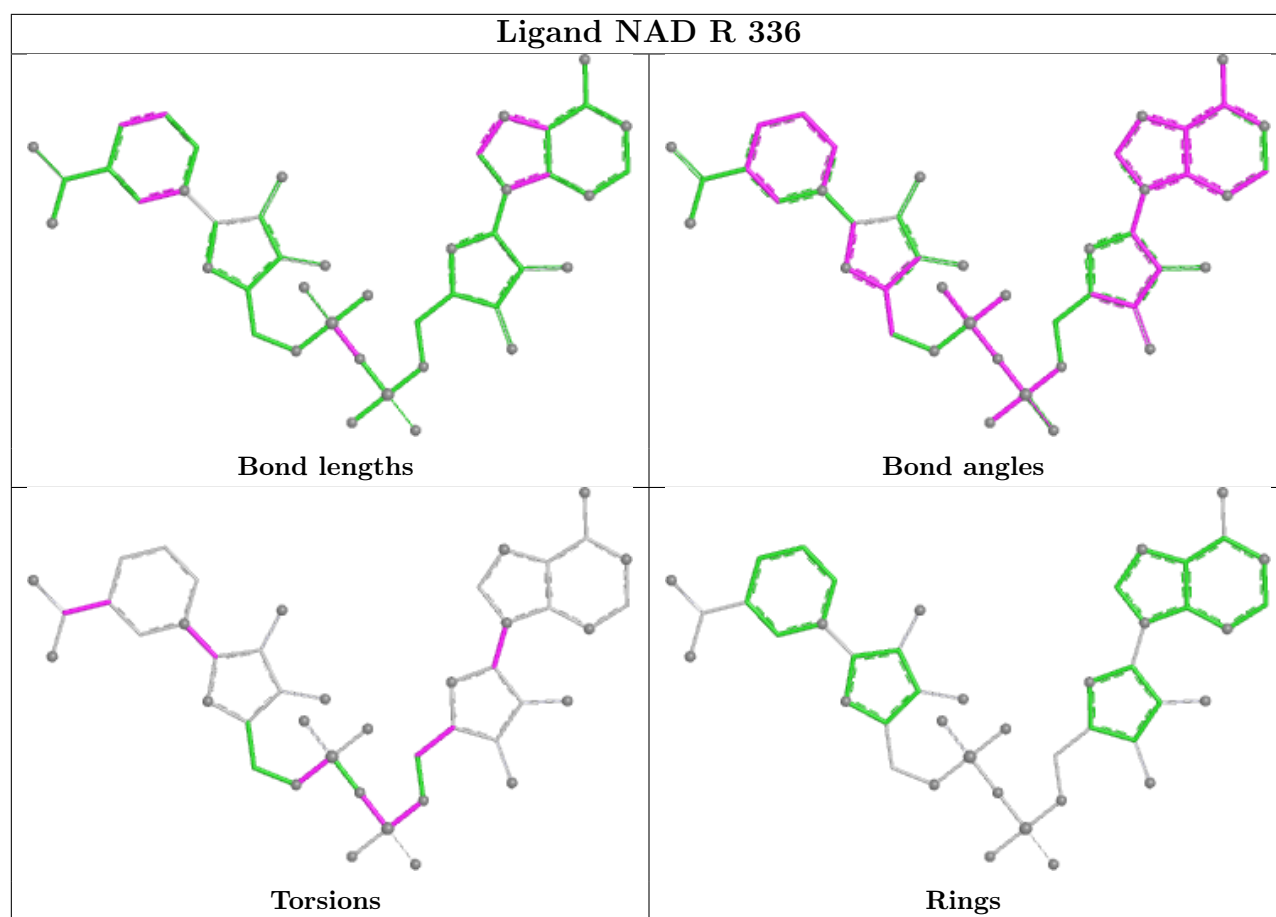












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.