



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 06:48 PM EDT

PDB ID : 2B4R / pdb_00002b4r
Title : Crystal structure of glyceraldehyde-3-phosphate dehydrogenase from Plasmodium falciparum at 2.25 Angstrom Resolution reveals intriguing extra electron density in the active site
Authors : Robien, M.A.; Bosch, J.; Hol, W.G.J.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)
Deposited on : 2005-09-26
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
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 2.25 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10700 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 glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	334	Total	C	N	O	S	58	0	0
			2551	1627	438	473	13			
1	P	334	Total	C	N	O	S	73	0	0
			2551	1627	438	473	13			
1	Q	334	Total	C	N	O	S	57	0	0
			2551	1627	438	473	13			
1	R	334	Total	C	N	O	S	47	0	0
			2551	1627	438	473	13			

There are 44 discrepancies between the modelled and reference sequences:

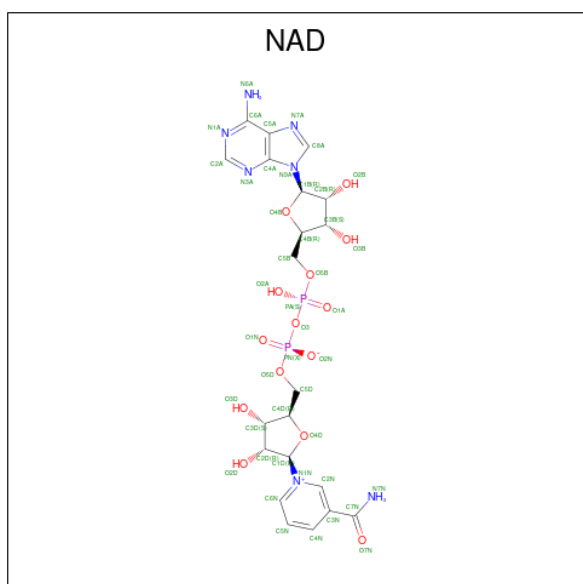
Chain	Residue	Modelled	Actual	Comment	Reference
O	-7	MET	-	cloning artifact	UNP Q8T6B1
O	-6	ALA	-	cloning artifact	UNP Q8T6B1
O	-5	HIS	-	expression tag	UNP Q8T6B1
O	-4	HIS	-	expression tag	UNP Q8T6B1
O	-3	HIS	-	expression tag	UNP Q8T6B1
O	-2	HIS	-	expression tag	UNP Q8T6B1
O	-1	HIS	-	expression tag	UNP Q8T6B1
O	0	HIS	-	expression tag	UNP Q8T6B1
O	3	ALA	VAL	engineered mutation	UNP Q8T6B1
O	336	THR	ASN	engineered mutation	UNP Q8T6B1
O	337	SER	ASN	engineered mutation	UNP Q8T6B1
P	-7	MET	-	cloning artifact	UNP Q8T6B1
P	-6	ALA	-	cloning artifact	UNP Q8T6B1
P	-5	HIS	-	expression tag	UNP Q8T6B1
P	-4	HIS	-	expression tag	UNP Q8T6B1
P	-3	HIS	-	expression tag	UNP Q8T6B1
P	-2	HIS	-	expression tag	UNP Q8T6B1
P	-1	HIS	-	expression tag	UNP Q8T6B1
P	0	HIS	-	expression tag	UNP Q8T6B1
P	3	ALA	VAL	engineered mutation	UNP Q8T6B1
P	336	THR	ASN	engineered mutation	UNP Q8T6B1

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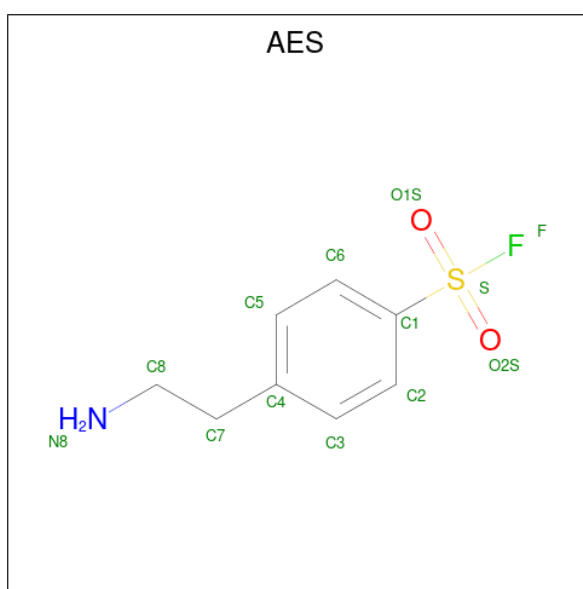
Chain	Residue	Modelled	Actual	Comment	Reference
P	337	SER	ASN	engineered mutation	UNP Q8T6B1
Q	-7	MET	-	cloning artifact	UNP Q8T6B1
Q	-6	ALA	-	cloning artifact	UNP Q8T6B1
Q	-5	HIS	-	expression tag	UNP Q8T6B1
Q	-4	HIS	-	expression tag	UNP Q8T6B1
Q	-3	HIS	-	expression tag	UNP Q8T6B1
Q	-2	HIS	-	expression tag	UNP Q8T6B1
Q	-1	HIS	-	expression tag	UNP Q8T6B1
Q	0	HIS	-	expression tag	UNP Q8T6B1
Q	3	ALA	VAL	engineered mutation	UNP Q8T6B1
Q	336	THR	ASN	engineered mutation	UNP Q8T6B1
Q	337	SER	ASN	engineered mutation	UNP Q8T6B1
R	-7	MET	-	cloning artifact	UNP Q8T6B1
R	-6	ALA	-	cloning artifact	UNP Q8T6B1
R	-5	HIS	-	expression tag	UNP Q8T6B1
R	-4	HIS	-	expression tag	UNP Q8T6B1
R	-3	HIS	-	expression tag	UNP Q8T6B1
R	-2	HIS	-	expression tag	UNP Q8T6B1
R	-1	HIS	-	expression tag	UNP Q8T6B1
R	0	HIS	-	expression tag	UNP Q8T6B1
R	3	ALA	VAL	engineered mutation	UNP Q8T6B1
R	336	THR	ASN	engineered mutation	UNP Q8T6B1
R	337	SER	ASN	engineered mutation	UNP Q8T6B1

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



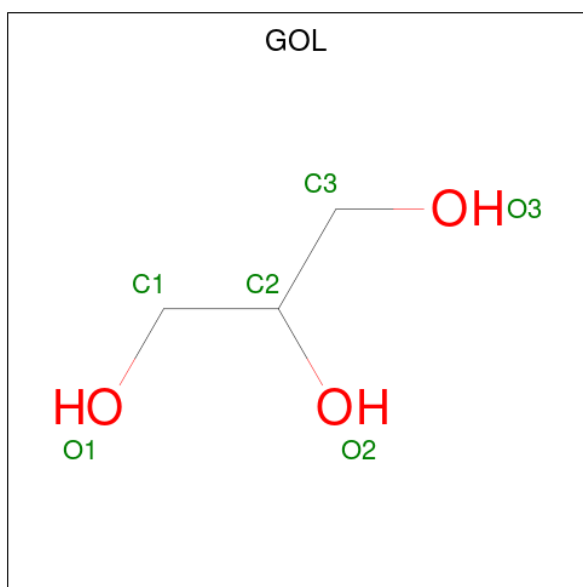
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (CCD ID: AES) (formula: $C_8H_{10}FNO_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	O	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
3	P	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
3	R	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	1	Total	C	O	0	0
			6	3	3		
4	P	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	63	Total	O	0	0
			63	63		
5	P	67	Total	O	0	0
			67	67		
5	Q	53	Total	O	0	0
			53	53		
5	R	74	Total	O	0	0
			74	74		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.33Å 104.58Å 90.84Å 90.00° 107.35° 90.00°	Depositor
Resolution (Å)	46.37 – 2.25	Depositor
% Data completeness (in resolution range)	96.9 (46.37-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.243	Depositor
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.149	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10700	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

11 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
4	GOL	P	703	-	5,5,5	0.40	0	5,5,5	0.25	0
3	AES	P	602	-	12,13,13	0.50	0	17,18,18	1.51	2 (11%)
4	GOL	R	503	-	5,5,5	0.35	0	5,5,5	0.33	0
2	NAD	P	701	-	46,48,48	1.76	6 (13%)	64,73,73	1.49	8 (12%)
4	GOL	O	804	-	5,5,5	0.37	0	5,5,5	0.24	0
2	NAD	R	901	-	46,48,48	1.74	6 (13%)	64,73,73	1.58	7 (10%)
3	AES	R	603	-	12,13,13	0.49	0	17,18,18	1.44	2 (11%)
3	AES	O	601	-	12,13,13	0.50	0	17,18,18	1.45	2 (11%)
2	NAD	O	801	-	46,48,48	1.70	5 (10%)	64,73,73	1.57	8 (12%)
2	NAD	Q	501	-	46,48,48	1.84	6 (13%)	64,73,73	1.56	8 (12%)
4	GOL	R	903	-	5,5,5	0.34	0	5,5,5	0.33	0

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	GOL	P	703	-	-	2/4/4/4	-
3	AES	P	602	-	-	7/9/9/9	0/1/1/1
4	GOL	R	503	-	-	2/4/4/4	-
2	NAD	P	701	-	-	6/30/62/62	0/5/5/5
4	GOL	O	804	-	-	4/4/4/4	-
2	NAD	R	901	-	-	7/30/62/62	0/5/5/5
3	AES	R	603	-	-	6/9/9/9	0/1/1/1
3	AES	O	601	-	-	7/9/9/9	0/1/1/1
2	NAD	O	801	-	-	7/30/62/62	0/5/5/5
2	NAD	Q	501	-	-	12/30/62/62	0/5/5/5
4	GOL	R	903	-	-	3/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	501	NAD	O7N-C7N	9.69	1.42	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	701	NAD	O7N-C7N	8.94	1.40	1.24
2	O	801	NAD	O7N-C7N	8.84	1.40	1.24
2	R	901	NAD	O7N-C7N	8.72	1.40	1.24
2	Q	501	NAD	C2A-N1A	2.98	1.39	1.33
2	P	701	NAD	C2N-N1N	2.98	1.38	1.35
2	O	801	NAD	C2A-N1A	2.95	1.39	1.33
2	Q	501	NAD	C2N-N1N	2.94	1.38	1.35
2	R	901	NAD	PN-O3	2.93	1.62	1.59
2	P	701	NAD	C2A-N1A	2.91	1.39	1.33
2	R	901	NAD	C2A-N3A	2.83	1.39	1.33
2	R	901	NAD	C2A-N1A	2.71	1.38	1.33
2	O	801	NAD	C2A-N3A	2.70	1.38	1.33
2	Q	501	NAD	C2A-N3A	2.69	1.38	1.33
2	P	701	NAD	C2A-N3A	2.61	1.38	1.33
2	P	701	NAD	PA-O3	2.50	1.62	1.59
2	Q	501	NAD	PN-O3	2.41	1.62	1.59
2	O	801	NAD	PN-O3	2.37	1.62	1.59
2	R	901	NAD	C8A-N7A	2.29	1.36	1.31
2	R	901	NAD	PA-O3	2.26	1.61	1.59
2	Q	501	NAD	C8A-N7A	2.22	1.36	1.31
2	P	701	NAD	C8A-N7A	2.21	1.35	1.31
2	O	801	NAD	C8A-N7A	2.11	1.35	1.31

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	501	NAD	N3A-C2A-N1A	-5.92	119.63	128.58
2	R	901	NAD	N3A-C2A-N1A	-5.82	119.77	128.58
2	O	801	NAD	N3A-C2A-N1A	-5.51	120.24	128.58
2	P	701	NAD	N3A-C2A-N1A	-5.49	120.27	128.58
3	P	602	AES	O2S-S-C1	-4.64	103.88	110.92
2	O	801	NAD	C5A-C4A-N3A	-4.44	120.61	126.72
2	R	901	NAD	C5A-C4A-N3A	-4.33	120.76	126.72
2	Q	501	NAD	C5A-C4A-N3A	-4.20	120.94	126.72
2	O	801	NAD	N9A-C8A-N7A	-4.11	108.11	113.94
2	P	701	NAD	C5A-C4A-N3A	-4.10	121.07	126.72
3	R	603	AES	O2S-S-C1	-4.04	104.79	110.92
2	R	901	NAD	N9A-C8A-N7A	-3.94	108.34	113.94
2	Q	501	NAD	N9A-C8A-N7A	-3.84	108.48	113.94
2	R	901	NAD	C5A-N7A-C8A	3.75	109.34	103.45
2	O	801	NAD	C5A-N7A-C8A	3.71	109.27	103.45
2	P	701	NAD	N9A-C8A-N7A	-3.67	108.73	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	601	AES	O2S-S-C1	-3.62	105.43	110.92
2	R	901	NAD	C2A-N3A-C4A	3.52	120.44	111.83
2	Q	501	NAD	C2A-N3A-C4A	3.43	120.22	111.83
3	O	601	AES	O1S-S-C1	-3.41	105.75	110.92
2	O	801	NAD	C2A-N3A-C4A	3.39	120.11	111.83
2	Q	501	NAD	C5A-N7A-C8A	3.37	108.75	103.45
2	R	901	NAD	C4A-C5A-N7A	-3.20	106.92	110.58
2	P	701	NAD	C5A-N7A-C8A	3.19	108.46	103.45
2	P	701	NAD	C2A-N3A-C4A	3.17	119.56	111.83
3	R	603	AES	O1S-S-C1	-3.01	106.35	110.92
2	O	801	NAD	C4A-C5A-N7A	-3.00	107.15	110.58
2	Q	501	NAD	N3A-C4A-N9A	2.92	132.13	127.17
2	O	801	NAD	N3A-C4A-N9A	2.81	131.95	127.17
2	P	701	NAD	N3A-C4A-N9A	2.63	131.65	127.17
2	R	901	NAD	N3A-C4A-N9A	2.49	131.40	127.17
2	P	701	NAD	C4A-C5A-N7A	-2.31	107.94	110.58
2	Q	501	NAD	C4A-C5A-N7A	-2.27	107.99	110.58
2	O	801	NAD	C4A-N9A-C8A	2.17	108.02	105.74
2	P	701	NAD	O4B-C1B-N9A	2.10	112.12	108.09
3	P	602	AES	O1S-S-C1	-2.04	107.83	110.92
2	Q	501	NAD	C4A-N9A-C8A	2.01	107.84	105.74

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	801	NAD	O4D-C1D-N1N-C2N
2	O	801	NAD	O4D-C1D-N1N-C6N
2	O	801	NAD	C2D-C1D-N1N-C2N
2	O	801	NAD	C2D-C1D-N1N-C6N
2	P	701	NAD	O4D-C1D-N1N-C2N
2	P	701	NAD	O4D-C1D-N1N-C6N
2	P	701	NAD	C2D-C1D-N1N-C2N
2	P	701	NAD	C2D-C1D-N1N-C6N
2	Q	501	NAD	C5D-O5D-PN-O2N
2	Q	501	NAD	O4D-C1D-N1N-C2N
2	Q	501	NAD	O4D-C1D-N1N-C6N
2	Q	501	NAD	C2D-C1D-N1N-C6N
2	R	901	NAD	O4D-C1D-N1N-C2N
2	R	901	NAD	O4D-C1D-N1N-C6N
2	R	901	NAD	C2D-C1D-N1N-C6N
3	O	601	AES	C2-C1-S-F

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Mol	Chain	Res	Type	Atoms
3	O	601	AES	C2-C1-S-O1S
3	O	601	AES	C6-C1-S-F
3	O	601	AES	C6-C1-S-O1S
3	O	601	AES	C4-C7-C8-N8
3	P	602	AES	C2-C1-S-F
3	P	602	AES	C6-C1-S-F
3	P	602	AES	C4-C7-C8-N8
3	R	603	AES	C2-C1-S-F
3	R	603	AES	C6-C1-S-F
4	P	703	GOL	O1-C1-C2-C3
4	R	903	GOL	O1-C1-C2-C3
4	P	703	GOL	O1-C1-C2-O2
4	R	903	GOL	O1-C1-C2-O2
2	Q	501	NAD	C4N-C3N-C7N-N7N
4	O	804	GOL	O1-C1-C2-C3
4	O	804	GOL	C1-C2-C3-O3
4	R	503	GOL	C1-C2-C3-O3
2	Q	501	NAD	C4N-C3N-C7N-O7N
4	R	503	GOL	O2-C2-C3-O3
2	O	801	NAD	O4B-C4B-C5B-O5B
3	O	601	AES	C2-C1-S-O2S
3	O	601	AES	C6-C1-S-O2S
3	P	602	AES	C2-C1-S-O1S
3	P	602	AES	C2-C1-S-O2S
3	P	602	AES	C6-C1-S-O2S
3	R	603	AES	C2-C1-S-O1S
3	R	603	AES	C2-C1-S-O2S
3	R	603	AES	C6-C1-S-O1S
3	R	603	AES	C6-C1-S-O2S
4	O	804	GOL	O2-C2-C3-O3
2	O	801	NAD	C3B-C4B-C5B-O5B
4	O	804	GOL	O1-C1-C2-O2
2	Q	501	NAD	C2N-C3N-C7N-N7N
2	Q	501	NAD	C5D-O5D-PN-O3
3	P	602	AES	C6-C1-S-O1S
2	Q	501	NAD	C2N-C3N-C7N-O7N
2	Q	501	NAD	C2D-C1D-N1N-C2N
2	R	901	NAD	C2D-C1D-N1N-C2N
2	Q	501	NAD	O4B-C4B-C5B-O5B
2	R	901	NAD	O4B-C4B-C5B-O5B
4	R	903	GOL	C1-C2-C3-O3
2	P	701	NAD	O4B-C4B-C5B-O5B

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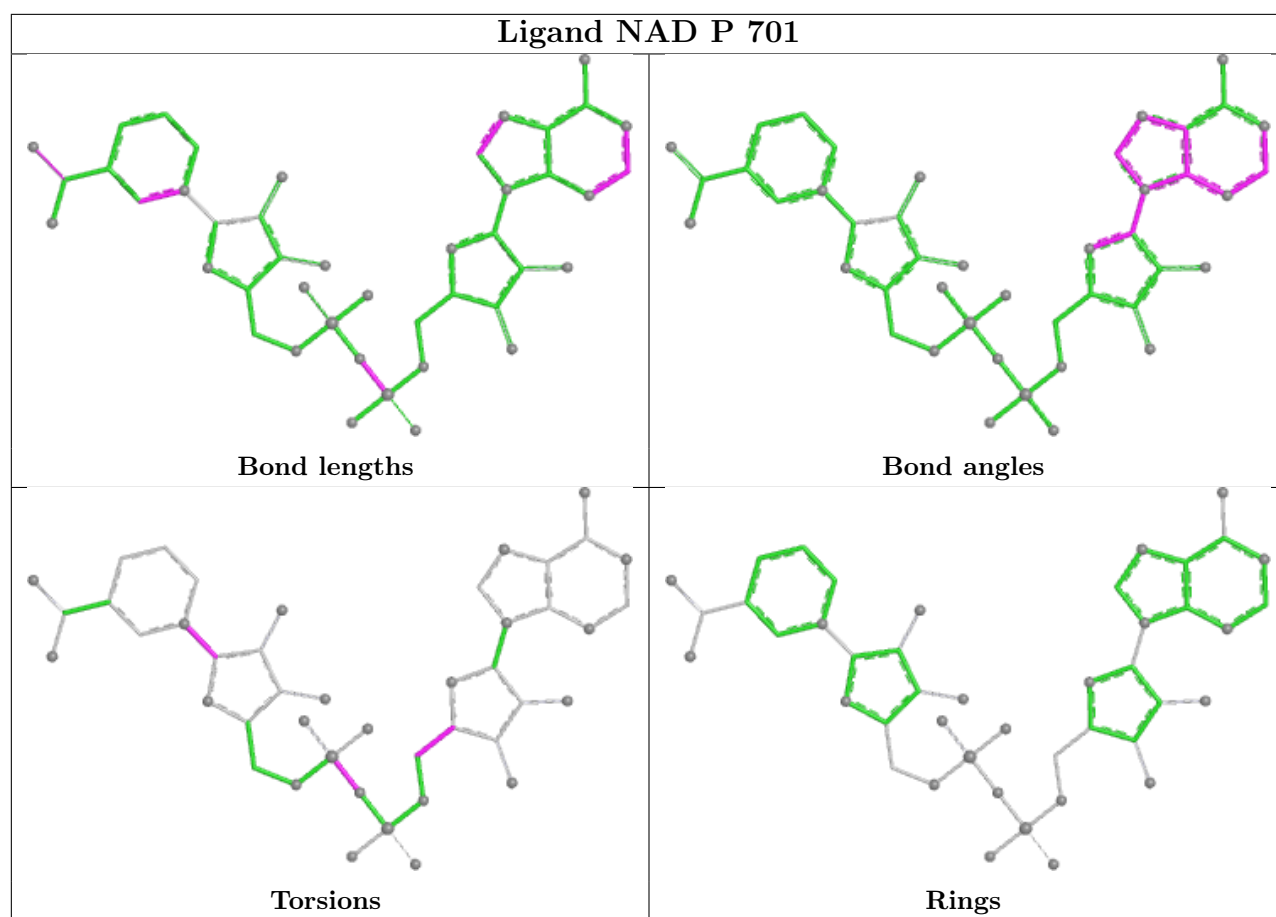
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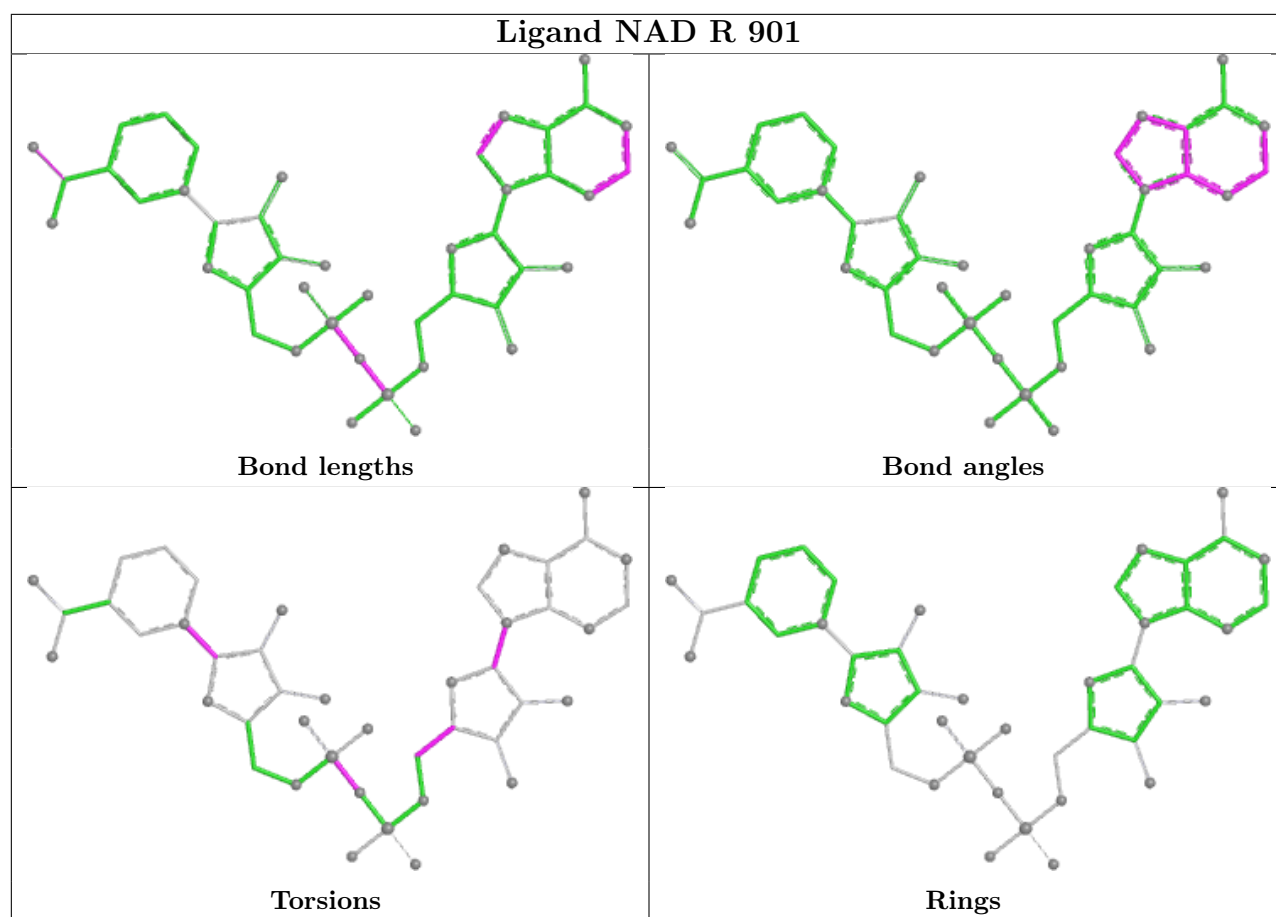
Mol	Chain	Res	Type	Atoms
2	O	801	NAD	PA-O3-PN-O1N
2	Q	501	NAD	PA-O3-PN-O1N
2	R	901	NAD	C2B-C1B-N9A-C8A
2	P	701	NAD	PA-O3-PN-O1N
2	R	901	NAD	PA-O3-PN-O1N

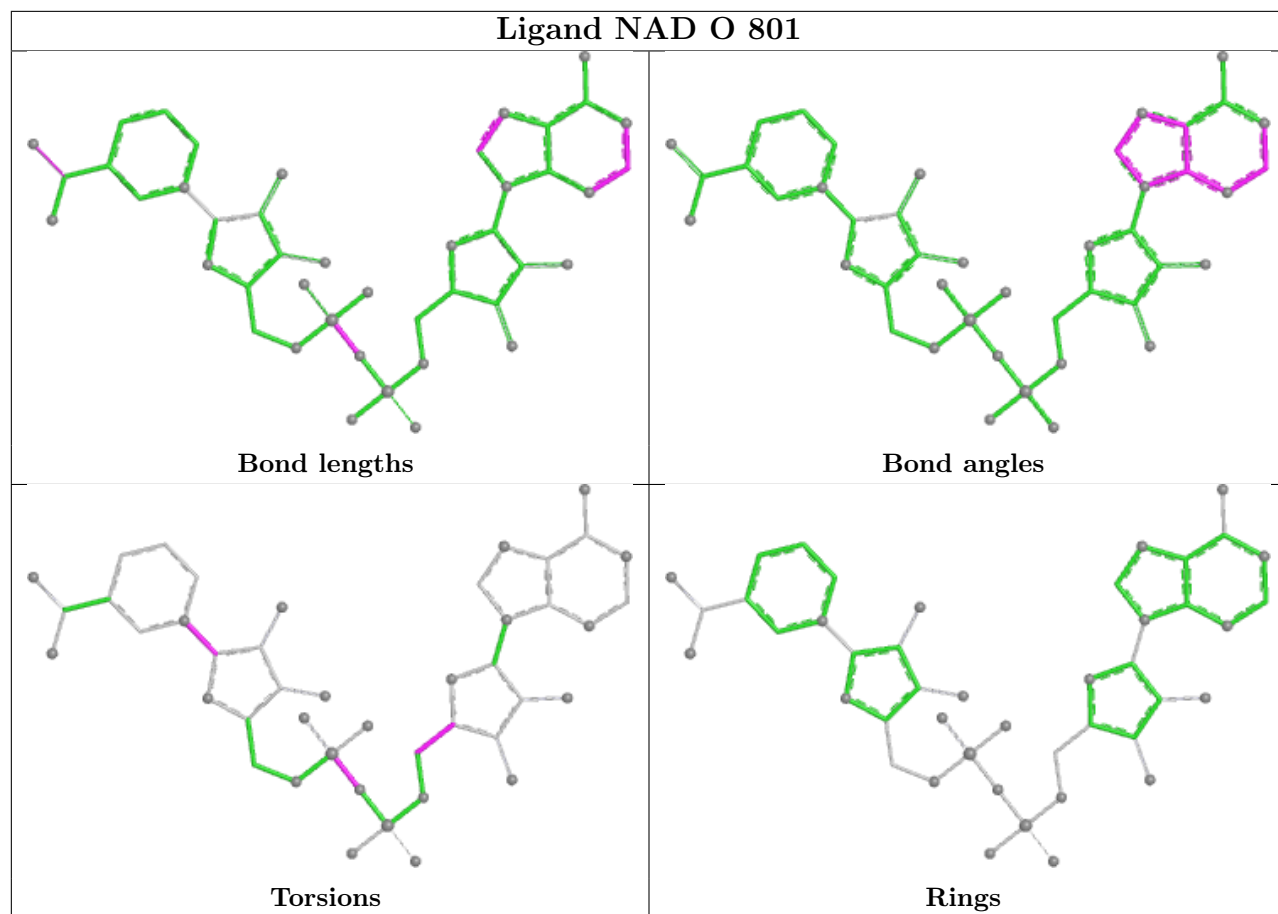
There are no ring outliers.

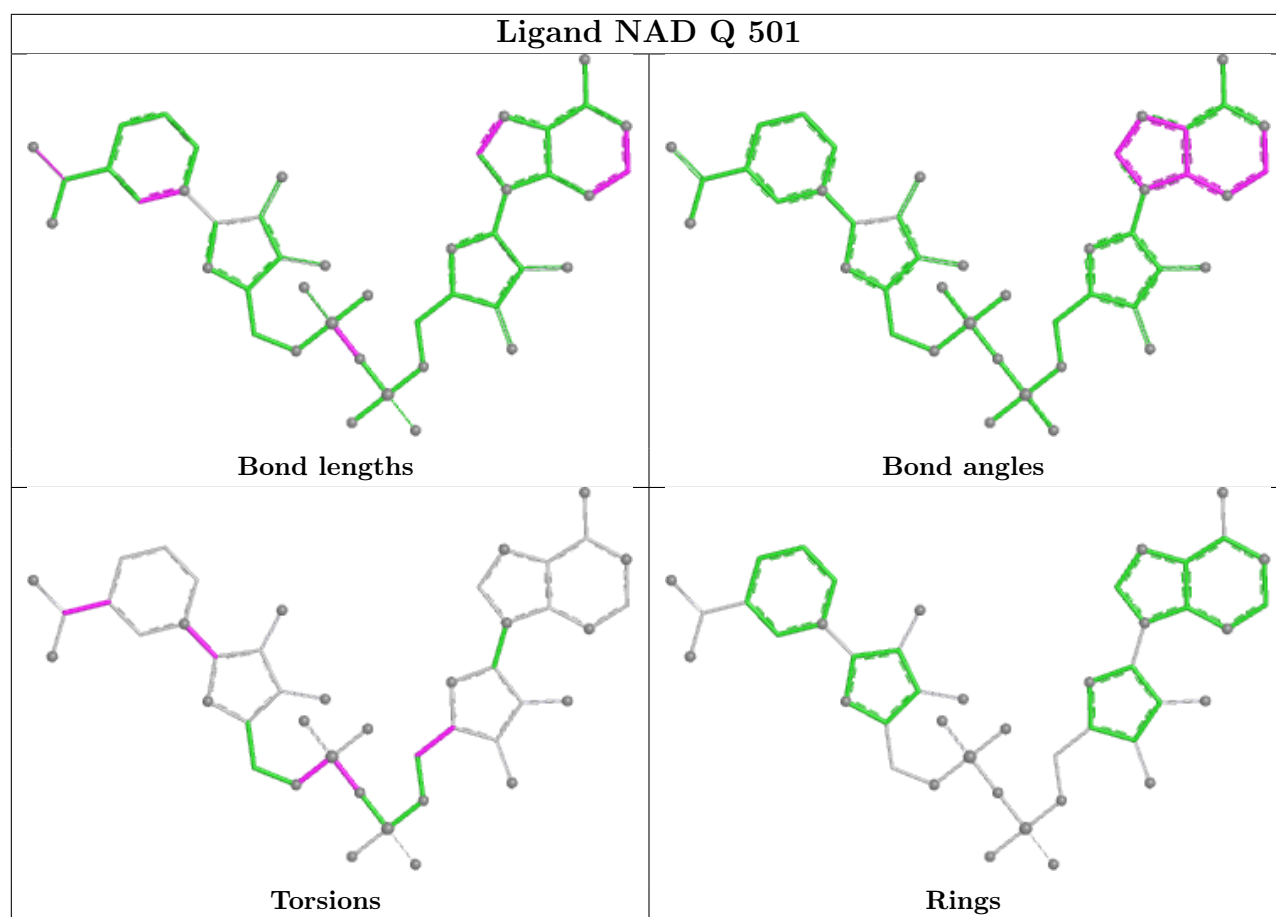
No monomer is involved in short contacts.

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.









4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.