



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:31 PM UTC

PDB ID : 1DFH / pdb_00001dfh
Title : X-RAY STRUCTURE OF ESCHERICHIA COLI ENOYL REDUCTASE
WITH BOUND NAD AND THIENO-DIAZABORINE
Authors : Baldock, C.; Rafferty, J.B.; Rice, D.W.
Deposited on : 1997-01-16
Resolution : 2.20 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	:	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

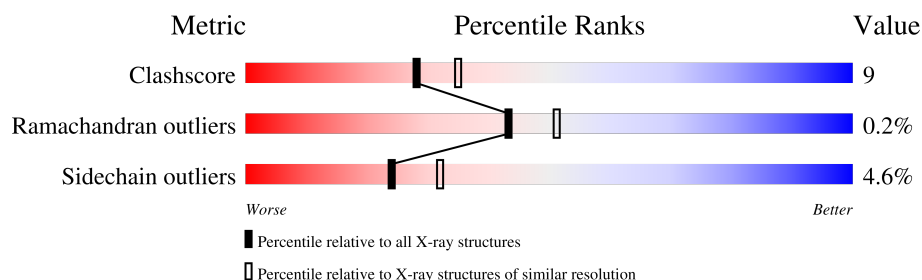
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	261	 76% 20% . .
1	B	261	 77% 19% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3936 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 ENOYL ACYL CARRIER PROTEIN REDUCTASE.

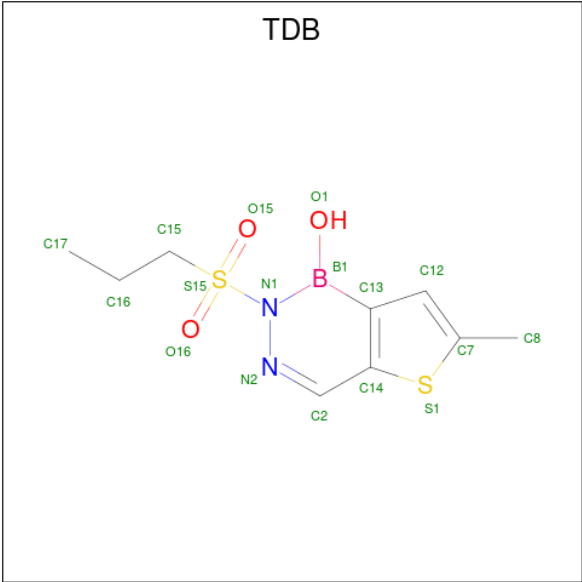
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1904	1200	327	364	13			
1	B	257	Total	C	N	O	S	0	0	0
			1910	1203	330	364	13			

- 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	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 6-METHYL-2(PROPANE-1-SULFONYL)-2H-THIENO[3,2-D][1,2,3]DIAZABORININ-1-OL (CCD ID: TDB) (formula: $C_9H_{13}BN_2O_3S_2$).



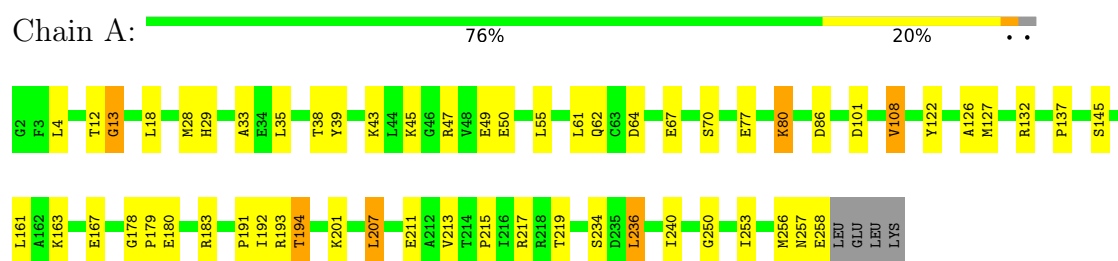
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	S	0	0
			17	1	9	2	3	2		
3	B	1	Total	B	C	N	O	S	0	0
			17	1	9	2	3	2		

3 Residue-property plots [i](#)

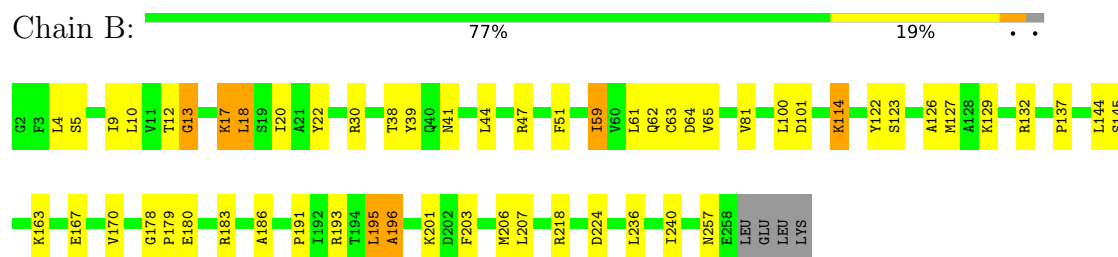
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ENOYL ACYL CARRIER PROTEIN REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	80.90Å 80.90Å 328.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	93.0 (10.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3936	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.94	0/1936	1.06	6/2616 (0.2%)
1	B	0.94	0/1942	1.12	4/2623 (0.2%)
All	All	0.94	0/3878	1.09	10/5239 (0.2%)

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	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	GLY	O-C-N	-16.46	105.75	122.54
1	A	13	GLY	O-C-N	-14.11	104.36	122.70
1	A	86	ASP	N-CA-C	5.85	119.73	112.59
1	B	9	ILE	N-CA-C	5.78	117.07	108.46
1	A	35	LEU	N-CA-C	5.70	119.02	109.95
1	A	108	VAL	N-CA-C	5.64	116.98	109.37
1	A	137	PRO	N-CA-C	-5.59	102.41	111.19
1	B	195	LEU	N-CA-C	-5.45	105.77	112.90
1	A	217	ARG	N-CA-C	5.38	119.13	112.24
1	B	137	PRO	N-CA-C	-5.36	102.78	111.19

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	GLY	Mainchain
1	B	13	GLY	Mainchain
1	B	257	ASN	Mainchain

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	1904	0	1887	38	0
1	B	1910	0	1898	30	0
2	A	44	0	24	2	0
2	B	44	0	24	2	0
3	A	17	0	13	1	0
3	B	17	0	13	1	0
All	All	3936	0	3859	69	0

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 9.

All (69) 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:B:218:ARG:NH2	1:B:224:ASP:OD2	2.04	0.90
1:B:59:ILE:HD13	1:B:81:VAL:HG21	1.57	0.86
1:A:258:GLU:HG3	1:A:258:GLU:O	1.82	0.78
1:A:132:ARG:NH2	1:A:180:GLU:OE2	2.14	0.76
1:B:38:THR:HA	1:B:61:LEU:O	1.88	0.72
1:A:193:ARG:HG3	1:A:207:LEU:HD21	1.72	0.72
1:A:108:VAL:O	1:B:129:LYS:HE3	1.89	0.72
1:B:193:ARG:HA	1:B:207:LEU:HD11	1.81	0.62
1:A:193:ARG:HA	1:A:207:LEU:HD21	1.82	0.62
1:A:193:ARG:HG3	1:A:207:LEU:CD2	2.28	0.61
1:A:39:TYR:CZ	1:A:62:GLN:HB2	2.39	0.57
1:B:12:THR:HG21	1:B:127:MET:HE1	1.87	0.57
1:A:101:ASP:OD1	1:A:101:ASP:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:NAD:C2D	3:A:0:TDB:N1	2.67	0.56
1:A:38:THR:HA	1:A:61:LEU:O	2.06	0.56
1:B:10:LEU:HD11	1:B:38:THR:HG23	1.88	0.55
1:B:17:LYS:HG3	1:B:22:TYR:CE2	2.40	0.55
1:A:122:TYR:CE2	1:A:126:ALA:HB2	2.41	0.55
1:B:39:TYR:CZ	1:B:62:GLN:HB2	2.42	0.54
1:A:193:ARG:CG	1:A:207:LEU:HD21	2.38	0.54
1:A:77:GLU:O	1:A:80:LYS:HB2	2.08	0.53
1:B:122:TYR:CE2	1:B:126:ALA:HB2	2.44	0.53
2:B:501:NAD:H2D	3:B:0:TDB:N1	2.23	0.53
1:A:45:LYS:HE2	1:A:49:GLU:OE2	2.09	0.52
1:A:64:ASP:OD1	1:A:64:ASP:C	2.52	0.52
1:A:183:ARG:HD2	1:A:240:ILE:O	2.10	0.51
1:A:234:SER:OG	1:A:236:LEU:HB2	2.11	0.51
1:A:18:LEU:HD13	1:A:194:THR:HG22	1.91	0.51
1:A:258:GLU:O	1:A:258:GLU:CG	2.52	0.49
1:B:101:ASP:OD1	1:B:201:LYS:HD3	2.12	0.49
1:B:62:GLN:HG2	1:B:63:CYS:N	2.26	0.49
1:A:47:ARG:O	1:A:50:GLU:HB2	2.13	0.49
1:B:132:ARG:NH2	1:B:180:GLU:OE2	2.43	0.49
1:A:29:HIS:CG	1:A:55:LEU:HD12	2.47	0.49
1:A:145:SER:O	2:A:501:NAD:H6N	2.14	0.48
1:B:59:ILE:HD13	1:B:81:VAL:CG2	2.37	0.47
1:B:145:SER:O	2:B:501:NAD:H6N	2.14	0.47
1:A:29:HIS:CD2	1:A:55:LEU:O	2.68	0.47
1:B:170:VAL:HG21	1:B:186:ALA:HB2	1.97	0.47
1:A:256:MET:C	1:A:258:GLU:H	2.22	0.47
1:B:163:LYS:O	1:B:167:GLU:HG3	2.14	0.47
1:A:250:GLY:O	1:A:253:ILE:HG13	2.15	0.47
1:B:203:PHE:HA	1:B:206:MET:HE3	1.96	0.46
1:B:64:ASP:OD1	1:B:64:ASP:C	2.58	0.46
1:B:191:PRO:HB2	1:B:207:LEU:HD23	1.98	0.46
1:B:195:LEU:C	1:B:196:ALA:O	2.56	0.46
1:A:4:LEU:HB3	1:A:33:ALA:HB2	1.97	0.45
1:B:41:ASN:OD1	1:B:41:ASN:C	2.59	0.45
1:A:191:PRO:HB2	1:A:207:LEU:HD12	1.97	0.45
1:B:114:LYS:HB2	1:B:114:LYS:HE3	1.57	0.45
1:A:257:ASN:O	1:A:258:GLU:C	2.59	0.44
1:B:47:ARG:HG3	1:B:51:PHE:CE2	2.53	0.44
1:A:67:GLU:HB2	1:A:70:SER:CB	2.48	0.43
1:B:30:ARG:O	1:B:30:ARG:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LYS:NZ	1:B:17:LYS:HB2	2.34	0.43
1:B:178:GLY:N	1:B:179:PRO:CD	2.82	0.43
1:A:43:LYS:HG2	1:A:43:LYS:O	2.18	0.43
1:B:183:ARG:HD2	1:B:240:ILE:O	2.19	0.43
1:A:193:ARG:CB	1:A:207:LEU:HD21	2.49	0.42
1:A:178:GLY:N	1:A:179:PRO:CD	2.83	0.42
1:A:4:LEU:HD12	1:A:28:MET:HA	2.02	0.42
1:B:65:VAL:HB	1:B:123:SER:HB2	2.02	0.41
1:A:257:ASN:HD22	1:A:257:ASN:HA	1.56	0.41
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.81	0.41
1:A:12:THR:HG21	1:A:127:MET:HE1	2.03	0.41
1:A:211:GLU:HG2	1:A:219:THR:HG23	2.03	0.40
1:A:163:LYS:O	1:A:167:GLU:HG3	2.21	0.40
1:A:213:VAL:HB	1:A:257:ASN:HB2	2.03	0.40
1:A:161:LEU:HD12	1:A:161:LEU:N	2.37	0.40

There are no symmetry-related clashes.

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	255/261 (98%)	243 (95%)	12 (5%)	0	100	100
1	B	255/261 (98%)	247 (97%)	7 (3%)	1 (0%)	30	34
All	All	510/522 (98%)	490 (96%)	19 (4%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	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	195/200 (98%)	188 (96%)	7 (4%)	31	42
1	B	196/200 (98%)	185 (94%)	11 (6%)	19	24
All	All	391/400 (98%)	373 (95%)	18 (5%)	24	32

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	192	ILE
1	A	194	THR
1	A	201	LYS
1	A	207	LEU
1	A	215	PRO
1	A	236	LEU
1	B	4	LEU
1	B	5	SER
1	B	17	LYS
1	B	18	LEU
1	B	20	ILE
1	B	44	LEU
1	B	59	ILE
1	B	100	LEU
1	B	114	LYS
1	B	144	LEU
1	B	236	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	257	ASN
1	B	40	GLN
1	B	54	GLN

5.3.3 RNA [i](#)

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](#)

4 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	$\# Z > 2$
3	TDB	B	0	2	14,18,18	4.80	11 (78%)	17,27,27	8.06	14 (82%)
3	TDB	A	0	2	14,18,18	5.47	11 (78%)	17,27,27	10.56	13 (76%)
2	NAD	A	501	3	46,48,48	1.82	12 (26%)	64,73,73	2.32	22 (34%)
2	NAD	B	501	3	46,48,48	2.03	14 (30%)	64,73,73	2.49	17 (26%)

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
3	TDB	B	0	2	-	1/4/23/23	0/1/2/2
3	TDB	A	0	2	-	2/4/23/23	0/1/2/2
2	NAD	A	501	3	-	9/30/62/62	0/5/5/5
2	NAD	B	501	3	-	12/30/62/62	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	0	TDB	B1-O1	12.97	1.56	1.36
3	A	0	TDB	B1-O1	12.56	1.55	1.36
3	A	0	TDB	O15-S15	9.19	1.53	1.43
3	A	0	TDB	O16-S15	7.77	1.52	1.43
3	A	0	TDB	C14-S1	-6.01	1.60	1.73
3	B	0	TDB	C14-S1	-5.74	1.61	1.73
3	B	0	TDB	O16-S15	5.56	1.49	1.43
3	B	0	TDB	C15-S15	5.18	1.83	1.78
2	A	501	NAD	C3N-C7N	5.12	1.58	1.50
3	A	0	TDB	C8-C7	-4.82	1.39	1.50
2	B	501	NAD	C2N-N1N	4.73	1.40	1.35
2	B	501	NAD	O2B-C2B	-4.33	1.32	1.43
3	B	0	TDB	C2-N2	4.19	1.34	1.29
2	B	501	NAD	C5A-N7A	-4.10	1.31	1.39
2	A	501	NAD	PN-O3	4.09	1.63	1.59
3	A	0	TDB	C7-S1	-4.00	1.62	1.72
2	A	501	NAD	C5A-N7A	-3.86	1.32	1.39
2	B	501	NAD	PN-O3	3.78	1.63	1.59
2	B	501	NAD	C3N-C7N	3.48	1.55	1.50
2	B	501	NAD	O4D-C4D	3.36	1.52	1.45
2	A	501	NAD	O4D-C4D	3.20	1.52	1.45
3	B	0	TDB	C8-C7	-3.14	1.43	1.50
2	A	501	NAD	O3B-C3B	3.14	1.50	1.43
2	B	501	NAD	O4B-C4B	3.02	1.51	1.45
3	A	0	TDB	C12-C7	2.91	1.43	1.36
2	B	501	NAD	C4A-N9A	2.90	1.43	1.37
3	B	0	TDB	N1-N2	-2.77	1.32	1.39
3	B	0	TDB	C12-C7	2.73	1.43	1.36
2	A	501	NAD	O2B-C2B	-2.66	1.36	1.43
3	A	0	TDB	N1-N2	-2.66	1.32	1.39
2	A	501	NAD	PN-O1N	-2.62	1.41	1.50
2	B	501	NAD	PN-O1N	-2.61	1.41	1.50
3	A	0	TDB	C16-C15	-2.57	1.38	1.51
2	B	501	NAD	C2A-N1A	-2.55	1.29	1.33
3	B	0	TDB	C7-S1	-2.52	1.66	1.72
2	A	501	NAD	C2A-N1A	-2.48	1.29	1.33
2	A	501	NAD	C2N-N1N	2.45	1.37	1.35
3	B	0	TDB	O15-S15	2.42	1.46	1.43
3	A	0	TDB	C15-S15	2.41	1.80	1.78
2	B	501	NAD	O3B-C3B	2.34	1.48	1.43
2	B	501	NAD	C6A-N6A	-2.23	1.28	1.34
2	A	501	NAD	O3D-C3D	-2.15	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	C3D-C4D	2.13	1.58	1.53
3	A	0	TDB	C2-N2	2.12	1.32	1.29
2	B	501	NAD	C2A-N3A	2.12	1.37	1.33
2	A	501	NAD	C5D-C4D	-2.10	1.45	1.51
2	B	501	NAD	C5N-C4N	2.08	1.42	1.38
3	B	0	TDB	B1-N1	-2.06	1.43	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	0	TDB	O16-S15-O15	27.13	146.31	118.99
3	A	0	TDB	C7-C12-C13	-25.02	103.35	114.97
3	B	0	TDB	C7-C12-C13	-20.72	105.35	114.97
3	A	0	TDB	C12-C13-C14	17.75	117.52	110.78
3	B	0	TDB	C12-C13-C14	16.19	116.93	110.78
3	B	0	TDB	O16-S15-C15	-11.21	89.55	107.97
3	B	0	TDB	O16-S15-O15	10.72	129.78	118.99
2	B	501	NAD	C2N-C3N-C4N	8.71	128.39	118.26
2	A	501	NAD	C2N-C3N-C4N	8.56	128.22	118.26
2	B	501	NAD	C5N-C4N-C3N	-8.12	112.38	120.36
3	A	0	TDB	O16-S15-C15	-7.75	95.23	107.97
2	A	501	NAD	C5N-C4N-C3N	-7.42	113.07	120.36
3	A	0	TDB	C7-S1-C14	6.84	97.73	92.61
3	B	0	TDB	C7-S1-C14	6.56	97.52	92.61
3	B	0	TDB	O15-S15-C15	6.54	118.71	107.97
3	A	0	TDB	O15-S15-C15	-6.38	97.48	107.97
2	B	501	NAD	C4A-N9A-C8A	-5.49	99.97	105.74
2	B	501	NAD	C6N-N1N-C2N	5.39	126.46	121.88
3	B	0	TDB	C16-C15-S15	5.37	134.89	114.16
2	A	501	NAD	C2A-N1A-C6A	4.98	126.91	118.73
3	A	0	TDB	C16-C15-S15	4.79	132.63	114.16
2	B	501	NAD	C5A-C4A-N3A	-4.69	120.26	126.72
2	A	501	NAD	C6N-N1N-C2N	4.43	125.65	121.88
2	B	501	NAD	C2A-N1A-C6A	4.31	125.81	118.73
2	A	501	NAD	N3A-C2A-N1A	-3.99	122.55	128.58
2	B	501	NAD	C6N-N1N-C1D	-3.93	112.02	119.73
3	A	0	TDB	C13-C14-S1	-3.88	107.73	111.73
2	B	501	NAD	O3D-C3D-C4D	-3.82	100.11	111.08
2	A	501	NAD	C5A-C4A-N3A	-3.51	121.89	126.72
2	A	501	NAD	C4A-N9A-C8A	-3.45	102.11	105.74
3	B	0	TDB	C13-C14-S1	-3.35	108.27	111.73
2	A	501	NAD	O3D-C3D-C4D	-3.32	101.54	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	0	TDB	C8-C7-C12	-3.20	121.36	128.40
2	A	501	NAD	C6N-N1N-C1D	-3.17	113.50	119.73
2	A	501	NAD	C2N-C3N-C7N	-3.10	110.50	119.46
2	B	501	NAD	C6A-C5A-C4A	3.10	121.41	117.18
2	B	501	NAD	N3A-C2A-N1A	-3.00	124.05	128.58
2	B	501	NAD	C5A-C4A-N9A	2.86	108.92	105.81
3	B	0	TDB	C8-C7-S1	2.77	126.74	121.03
3	B	0	TDB	C17-C16-C15	2.70	120.19	112.41
2	A	501	NAD	C6A-C5A-C4A	2.69	120.85	117.18
2	B	501	NAD	C2N-C3N-C7N	-2.67	111.74	119.46
3	A	0	TDB	C17-C16-C15	2.51	119.63	112.41
2	B	501	NAD	C6N-C5N-C4N	2.44	122.97	119.45
3	A	0	TDB	C12-C7-S1	2.40	113.65	110.43
2	A	501	NAD	O4D-C4D-C3D	-2.39	100.41	105.15
2	A	501	NAD	C3B-C2B-C1B	-2.37	96.98	101.46
3	B	0	TDB	C2-C14-S1	2.33	127.69	120.55
2	A	501	NAD	C2B-C3B-C4B	2.29	107.03	102.61
2	B	501	NAD	O2B-C2B-C3B	2.27	119.09	111.82
2	B	501	NAD	C5A-N7A-C8A	2.26	107.00	103.45
2	A	501	NAD	C2D-C3D-C4D	2.24	106.94	102.61
2	A	501	NAD	O2N-PN-O1N	2.22	122.76	112.44
2	A	501	NAD	C4B-O4B-C1B	-2.21	104.59	109.47
3	B	0	TDB	C2-N2-N1	2.21	119.83	117.71
3	A	0	TDB	C2-C14-S1	2.18	127.21	120.55
3	A	0	TDB	C2-N2-N1	2.16	119.79	117.71
2	A	501	NAD	C6N-C5N-C4N	2.15	122.55	119.45
2	B	501	NAD	O7N-C7N-C3N	-2.14	116.97	119.60
2	B	501	NAD	N3A-C4A-N9A	2.09	130.72	127.17
3	B	0	TDB	O1-B1-N1	-2.05	117.84	122.57
2	A	501	NAD	O2N-PN-O3	2.05	112.82	107.27
2	A	501	NAD	N3A-C4A-N9A	2.04	130.64	127.17
3	A	0	TDB	O1-B1-N1	-2.04	117.89	122.57
2	A	501	NAD	O2B-C2B-C3B	2.02	118.31	111.82
2	A	501	NAD	C5A-C6A-N1A	-2.01	112.40	117.51

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	C5D-O5D-PN-O3
2	A	501	NAD	C5D-O5D-PN-O1N
2	A	501	NAD	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	C5B-O5B-PA-O1A
2	B	501	NAD	C5D-O5D-PN-O3
2	B	501	NAD	C5D-O5D-PN-O1N
2	B	501	NAD	O4D-C1D-N1N-C2N
3	A	0	TDB	S15-C15-C16-C17
2	B	501	NAD	C3D-C4D-C5D-O5D
2	A	501	NAD	C3D-C4D-C5D-O5D
2	B	501	NAD	C5B-O5B-PA-O2A
2	B	501	NAD	C5B-O5B-PA-O3
2	A	501	NAD	PA-O3-PN-O1N
2	A	501	NAD	PA-O3-PN-O2N
2	B	501	NAD	PA-O3-PN-O1N
2	A	501	NAD	C2D-C1D-N1N-C2N
3	A	0	TDB	C16-C15-S15-O15
2	A	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	O4D-C4D-C5D-O5D
3	B	0	TDB	S15-C15-C16-C17
2	B	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	PA-O3-PN-O2N

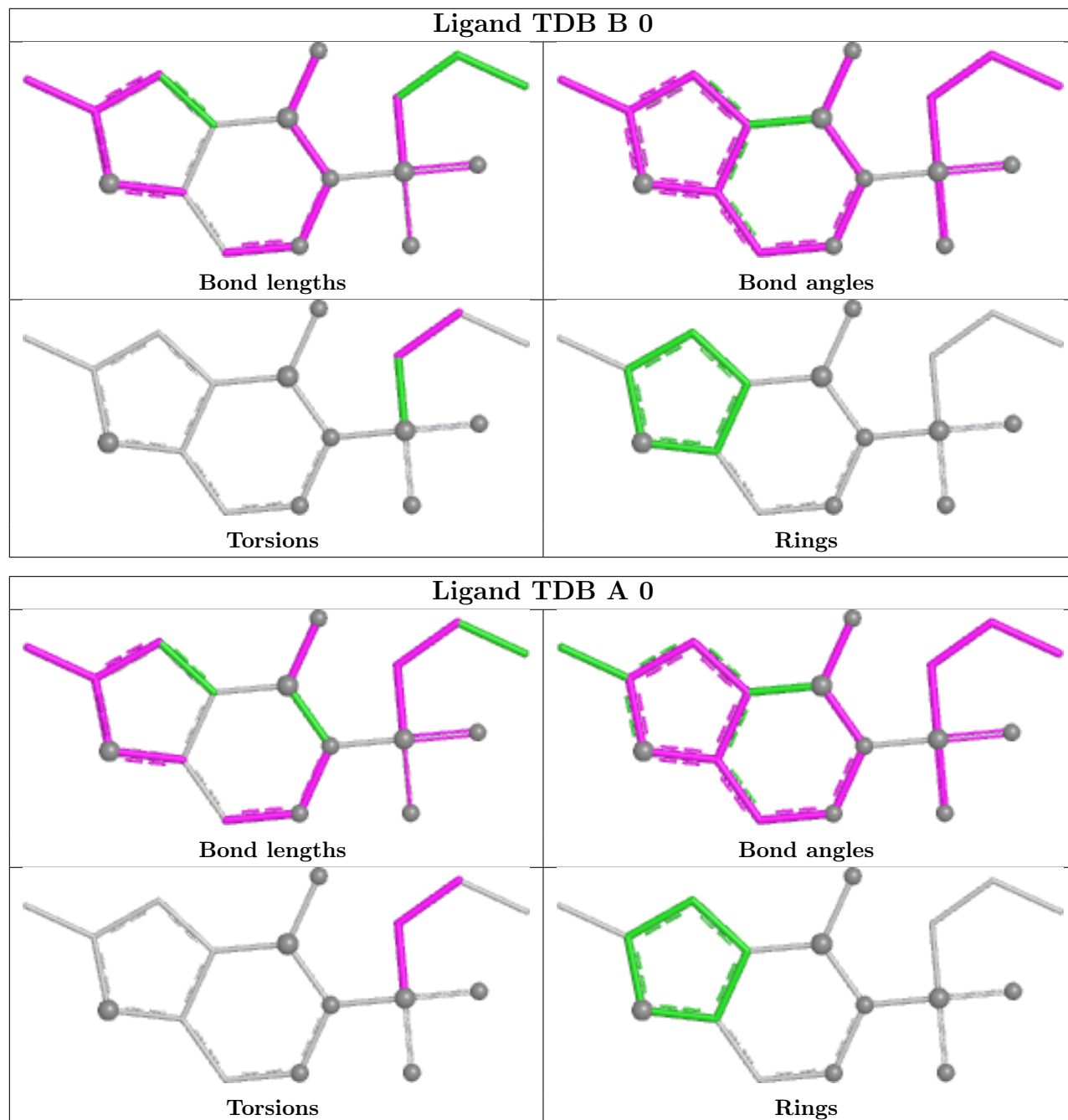
There are no ring outliers.

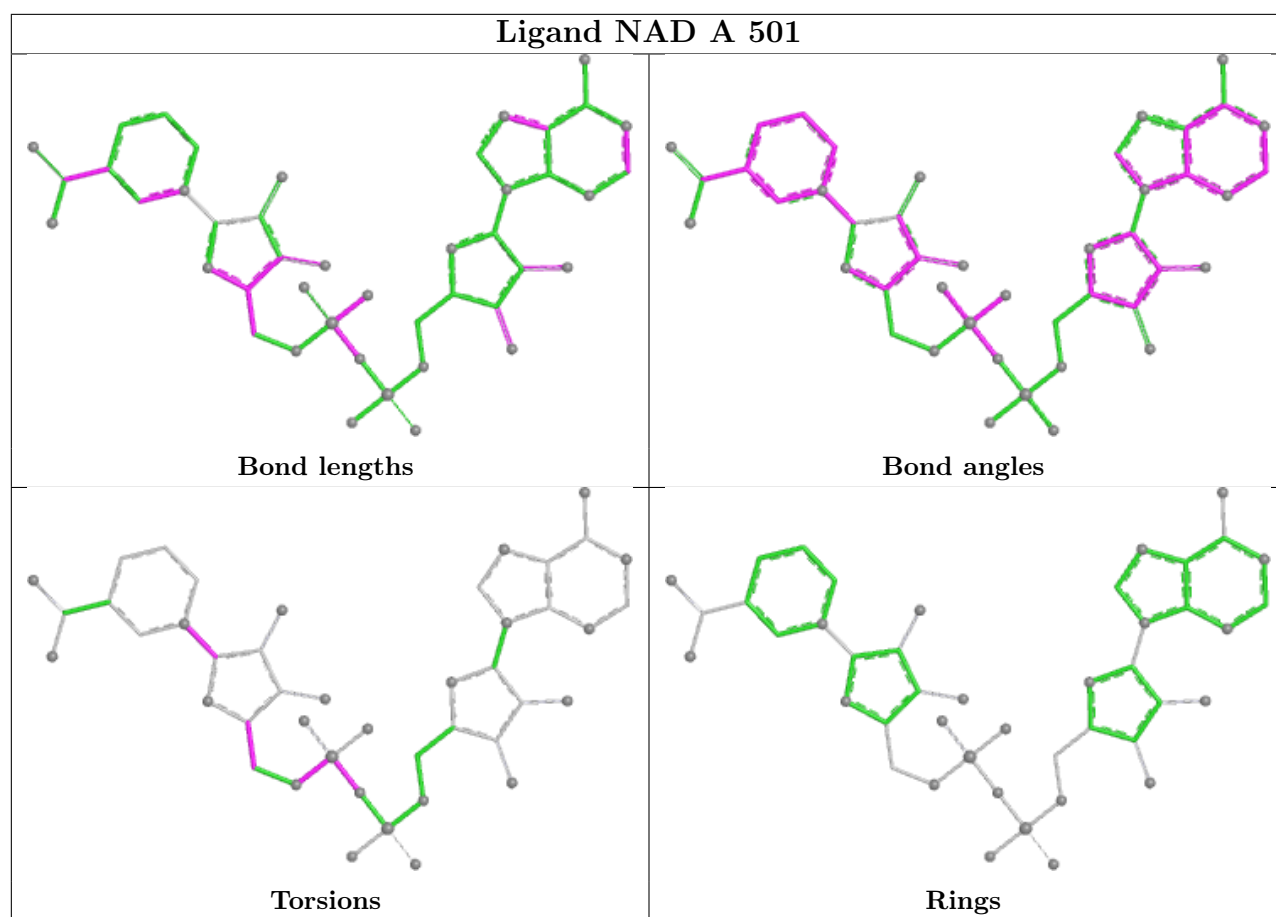
4 monomers are involved in 4 short contacts:

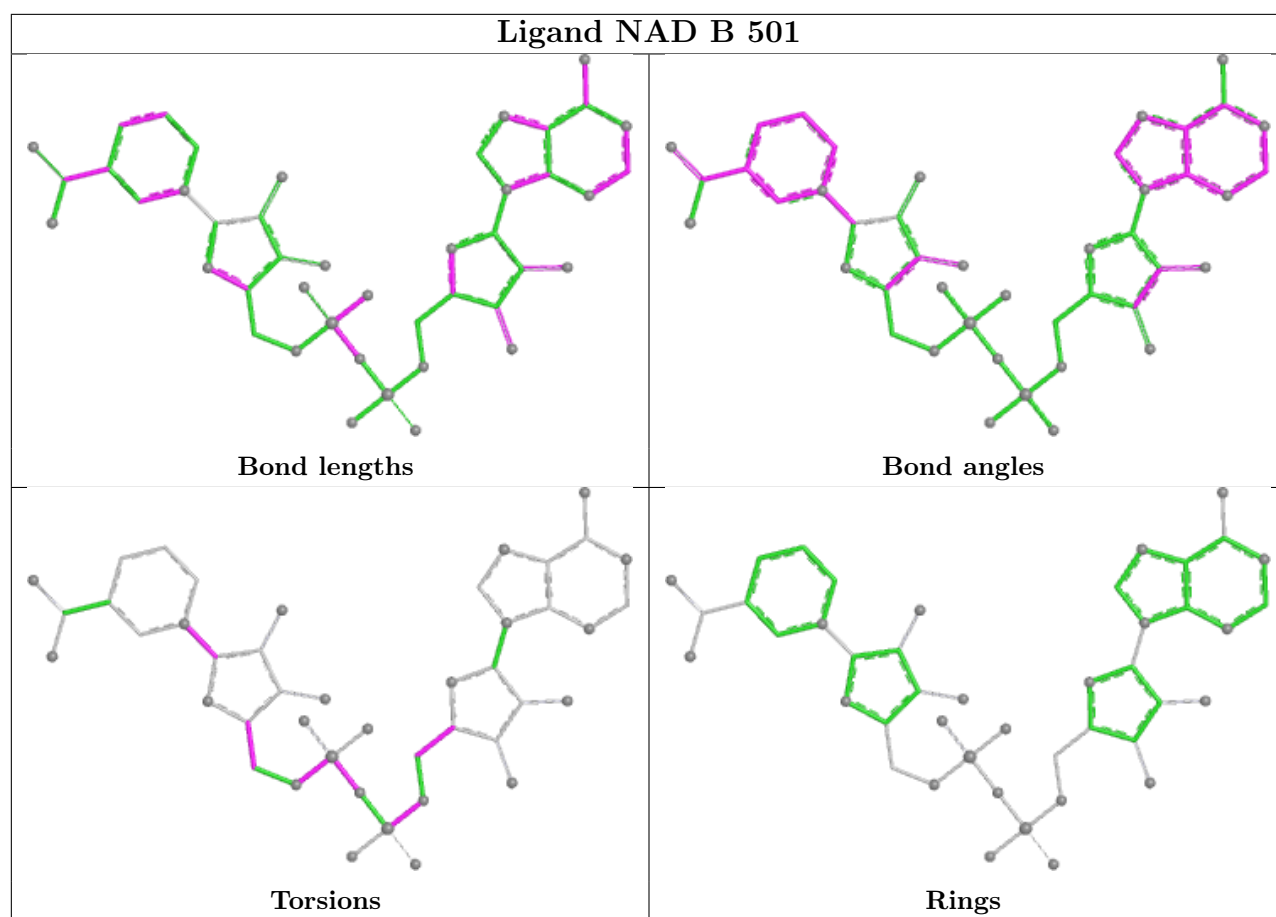
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	0	TDB	1	0
3	A	0	TDB	1	0
2	A	501	NAD	2	0
2	B	501	NAD	2	0

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.