



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:46 am BST

PDB ID : 1LXC
Title : Crystal Structure of E. Coli Enoyl Reductase-NAD⁺ with a Bound Acrylamide Inhibitor
Authors : Miller, W.H.; Seefeld, M.A.; Newlander, K.A.; Uzinskas, I.N.; Burgess, W.J.; Heerding, D.A.; Yuan, C.C.K.; Head, M.S.; Payne, D.J.; Rittenhouse, S.F.; Moore, T.D.; Pearson, S.C.; Dewolf, V.; Berry, W.E.; Keller, P.M.; Polizzi, B.J.; Qiu, X.; Janson, C.A.; Huffman, W.F.
Deposited on : 2002-06-05
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

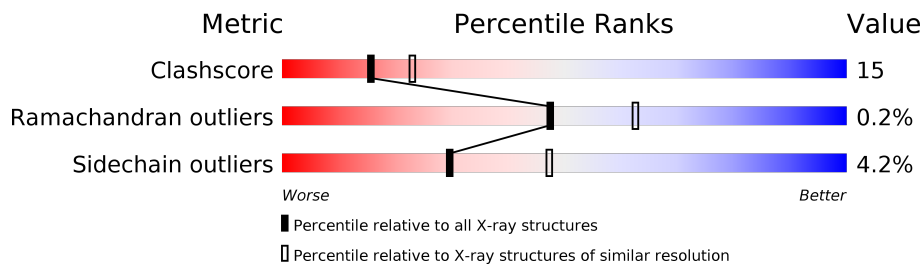
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 on 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	262	
1	B	262	

2 Entry composition i

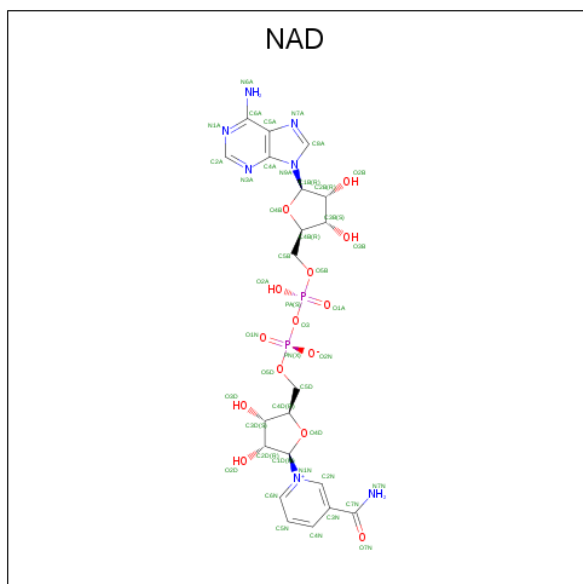
There are 4 unique types of molecules in this entry. The entry contains 4165 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 [NADH].

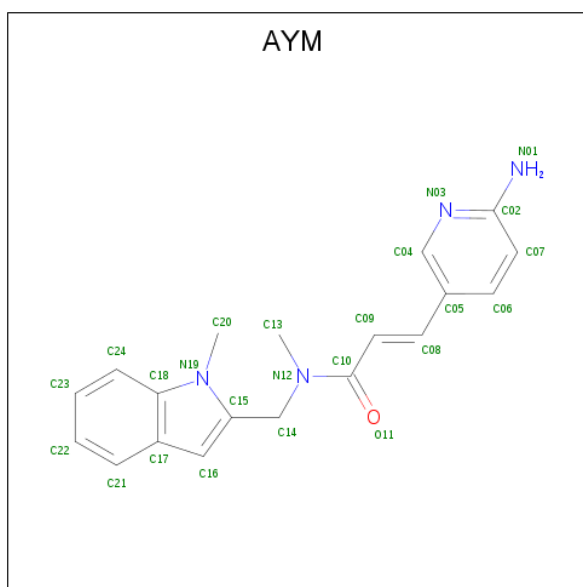
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	Total	C	N	O	S	0	0	0
			1866	1176	322	355	13			
1	B	251	Total	C	N	O	S	0	0	0
			1863	1176	319	355	13			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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 3-(6-AMINOPYRIDIN-3-YL)-N-METHYL-N-[(1-METHYL-1H-INDOL-2-YL)METHYL]ACRYLAMIDE (three-letter code: AYM) (formula: C₁₉H₂₀N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	19	4	1		
3	B	1	Total	C	N	O	0	0
			24	19	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	146	Total	O	0	0
			146	146		

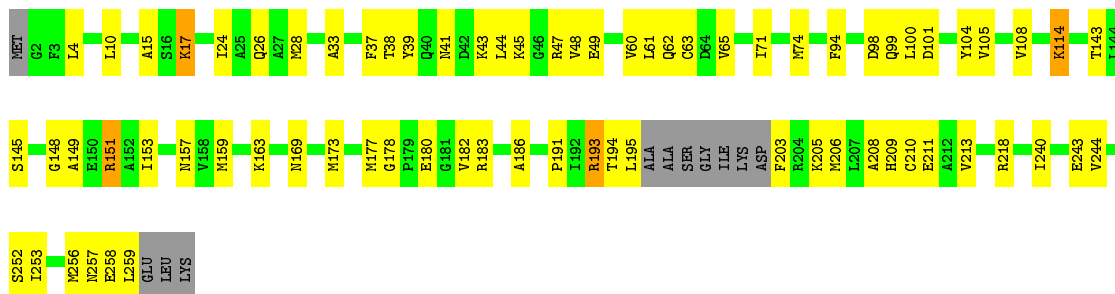
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

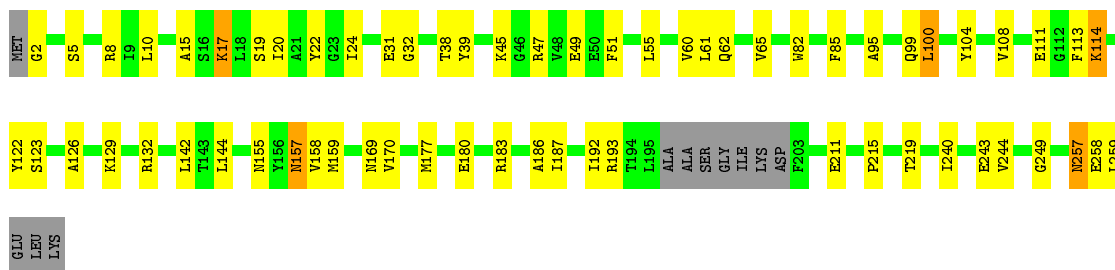
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

Chain A: 



- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

Chain B: 



4 Data and refinement statistics

Xtrriage (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	79.58Å 79.58Å 326.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	82.3 (20.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.199 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4165	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: AYM, 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	0.35	0/1897	0.59	0/2563
1	B	0.36	0/1894	0.60	0/2560
All	All	0.35	0/3791	0.60	0/5123

There are no bond length outliers.

There are no bond angle outliers.

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	1866	0	1842	67	0
1	B	1863	0	1840	46	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
3	A	24	0	20	3	0
3	B	24	0	20	3	0
4	A	154	0	0	5	0
4	B	146	0	0	3	0
All	All	4165	0	3774	112	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 15.

All (112) 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:17:LYS:HD2	1:A:17:LYS:H	1.18	1.03
1:A:193:ARG:H	1:A:193:ARG:HD3	1.29	0.95
1:A:99:GLN:HE22	1:A:108:VAL:HA	1.39	0.86
1:A:101:ASP:HB2	4:A:446:HOH:O	1.77	0.85
1:A:193:ARG:H	1:A:193:ARG:CD	1.98	0.76
1:B:20:ILE:HG21	1:B:144:LEU:CD2	2.16	0.76
1:A:17:LYS:HD2	1:A:17:LYS:N	1.99	0.75
1:B:114:LYS:HE2	4:B:543:HOH:O	1.85	0.75
1:B:99:GLN:HE22	1:B:108:VAL:HA	1.53	0.74
1:A:38:THR:HA	1:A:61:LEU:O	1.90	0.72
1:A:4:LEU:HB3	1:A:33:ALA:HB2	1.73	0.68
1:A:258:GLU:HG2	1:A:259:LEU:HD12	1.76	0.67
1:A:39:TYR:CZ	1:A:62:GLN:HB2	2.31	0.65
1:A:49:GLU:HA	1:A:60:VAL:HG21	1.80	0.63
1:A:256:MET:HB3	1:A:259:LEU:HD13	1.79	0.63
1:A:99:GLN:NE2	1:A:108:VAL:HA	2.11	0.62
1:B:104:TYR:HD1	1:B:157:ASN:HB3	1.65	0.62
1:B:211:GLU:HG2	1:B:219:THR:HG23	1.82	0.62
1:B:38:THR:HA	1:B:61:LEU:O	2.01	0.61
1:B:8:ARG:HD3	1:B:82:TRP:CD1	2.36	0.61
1:A:104:TYR:HD1	1:A:157:ASN:HB3	1.66	0.60
1:B:20:ILE:HG21	1:B:144:LEU:HD21	1.84	0.60
1:A:94:PHE:HA	3:A:302:AYM:N03	2.17	0.60
1:B:193:ARG:HG3	1:B:193:ARG:O	2.01	0.59
1:A:209:HIS:O	1:A:213:VAL:HG22	2.03	0.59
1:A:211:GLU:HG2	1:A:218:ARG:HA	1.86	0.58
1:A:193:ARG:HB2	4:A:450:HOH:O	2.03	0.58
1:A:45:LYS:O	1:A:49:GLU:HG3	2.04	0.58
1:B:47:ARG:HD2	1:B:51:PHE:CE2	2.39	0.57
1:A:193:ARG:N	1:A:193:ARG:HD3	2.12	0.56
1:A:177:MET:O	1:A:180:GLU:HG2	2.05	0.55
1:B:142:LEU:HD11	1:B:187:ILE:HG13	1.88	0.55
1:B:122:TYR:CE2	1:B:126:ALA:HB2	2.42	0.54
1:A:108:VAL:HG13	1:B:129:LYS:HE2	1.90	0.54
1:B:49:GLU:HA	1:B:60:VAL:HG21	1.90	0.53
1:A:191:PRO:HG3	1:A:210:CYS:SG	2.49	0.53
1:B:192:ILE:HA	4:B:544:HOH:O	2.08	0.53
1:A:183:ARG:HD2	1:A:240:ILE:O	2.09	0.52
3:A:302:AYM:H131	3:A:302:AYM:H203	1.92	0.52
1:A:47:ARG:N	1:A:47:ARG:HD3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:PHE:O	1:A:206:MET:HB3	2.10	0.52
1:B:113:PHE:HA	1:B:158:VAL:HG21	1.92	0.52
1:B:20:ILE:HG21	1:B:144:LEU:HD22	1.89	0.52
3:B:402:AYM:H131	3:B:402:AYM:H203	1.91	0.52
1:A:114:LYS:HE2	4:A:345:HOH:O	2.08	0.51
1:A:205:LYS:O	1:A:208:ALA:HB3	2.11	0.51
1:A:259:LEU:HD12	1:A:259:LEU:H	1.76	0.51
1:A:108:VAL:O	1:B:129:LYS:CE	2.58	0.51
1:B:99:GLN:NE2	1:B:108:VAL:HA	2.24	0.50
1:B:211:GLU:CG	1:B:219:THR:HG23	2.41	0.50
1:B:215:PRO:HD2	1:B:249:GLY:O	2.11	0.49
1:A:62:GLN:HG2	1:A:63:CYS:N	2.27	0.49
1:B:177:MET:O	1:B:180:GLU:HG2	2.12	0.49
1:B:5:SER:HA	1:B:32:GLY:O	2.12	0.49
1:A:148:GLY:HA2	1:A:153:ILE:HD12	1.94	0.49
1:A:243:GLU:HG3	1:A:244:VAL:N	2.28	0.49
1:A:47:ARG:N	1:A:47:ARG:CD	2.75	0.48
1:B:258:GLU:H	1:B:258:GLU:CD	2.15	0.48
1:B:2:GLY:HA3	1:B:31:GLU:O	2.14	0.48
1:A:47:ARG:H	1:A:47:ARG:HD3	1.79	0.48
1:A:253:ILE:HD12	1:A:253:ILE:C	2.34	0.47
1:A:108:VAL:O	1:B:129:LYS:HE3	2.14	0.46
1:A:203:PHE:N	4:A:395:HOH:O	2.47	0.46
1:A:256:MET:CB	1:A:259:LEU:HD13	2.45	0.46
1:A:159:MET:HE2	1:A:163:LYS:HE2	1.98	0.46
1:B:100:LEU:HD11	1:B:159:MET:HG2	1.96	0.46
1:A:257:ASN:N	1:A:258:GLU:OE1	2.48	0.46
1:B:10:LEU:HD11	1:B:38:THR:HG23	1.98	0.46
1:B:95:ALA:HB3	1:B:100:LEU:HD21	1.97	0.46
1:A:173:MET:HB3	1:A:177:MET:CE	2.45	0.46
1:A:259:LEU:HD12	1:A:259:LEU:N	2.30	0.46
1:B:65:VAL:HB	1:B:123:SER:HB2	1.97	0.46
1:A:44:LEU:O	1:A:48:VAL:HG23	2.15	0.45
1:B:193:ARG:HE	1:B:193:ARG:HB2	1.55	0.45
1:A:65:VAL:HG22	2:A:301:NAD:N1A	2.31	0.45
1:B:15:ALA:HB2	2:B:401:NAD:O3B	2.17	0.45
1:B:183:ARG:HD2	1:B:240:ILE:O	2.16	0.45
1:B:257:ASN:HD22	1:B:257:ASN:HA	1.55	0.45
1:A:151:ARG:NH2	1:A:252:SER:O	2.50	0.45
1:B:39:TYR:CE2	1:B:45:LYS:HB2	2.52	0.45
1:A:194:THR:O	1:A:195:LEU:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ALA:HB2	2:A:301:NAD:O3B	2.17	0.44
1:B:155:ASN:HB2	3:B:402:AYM:H22	1.98	0.44
1:B:47:ARG:HD2	1:B:51:PHE:CZ	2.52	0.43
3:B:402:AYM:H141	4:B:545:HOH:O	2.17	0.43
1:A:101:ASP:HB3	4:A:445:HOH:O	2.17	0.43
1:A:63:CYS:HB2	1:A:74:MET:HG3	2.00	0.43
1:A:101:ASP:O	1:A:101:ASP:OD1	2.37	0.43
1:A:10:LEU:HD11	1:A:38:THR:HG23	2.00	0.42
1:A:149:ALA:HB2	1:A:163:LYS:HB3	1.99	0.42
1:A:17:LYS:CD	1:A:17:LYS:H	2.03	0.42
1:B:258:GLU:HG2	1:B:259:LEU:HD12	2.01	0.42
1:B:17:LYS:HA	1:B:22:TYR:CD2	2.55	0.42
1:A:41:ASN:OD1	1:A:43:LYS:HB3	2.19	0.42
1:B:20:ILE:O	1:B:24:ILE:HG13	2.19	0.42
1:A:159:MET:HG2	3:A:302:AYM:H08	2.02	0.42
1:B:243:GLU:HG3	1:B:244:VAL:N	2.35	0.42
1:A:105:VAL:HB	1:B:132:ARG:NH1	2.35	0.41
1:B:85:PHE:N	1:B:85:PHE:CD1	2.88	0.41
1:A:37:PHE:CD1	1:A:37:PHE:N	2.87	0.41
1:A:24:ILE:O	1:A:28:MET:HG3	2.21	0.41
1:B:170:VAL:HG21	1:B:186:ALA:HB2	2.01	0.41
1:A:149:ALA:HB2	1:A:163:LYS:CB	2.49	0.41
1:B:8:ARG:HD3	1:B:82:TRP:NE1	2.36	0.41
1:A:65:VAL:HA	1:A:71:ILE:HD11	2.02	0.41
1:A:143:THR:O	1:A:186:ALA:HA	2.21	0.41
1:B:19:SER:O	1:B:22:TYR:HB3	2.20	0.41
1:A:44:LEU:O	1:A:45:LYS:C	2.60	0.41
1:A:148:GLY:CA	1:A:153:ILE:HD12	2.51	0.41
1:A:145:SER:HA	1:A:163:LYS:HD2	2.02	0.40
1:A:193:ARG:N	1:A:193:ARG:CD	2.73	0.40
1:A:178:GLY:HA2	1:A:182:VAL:O	2.22	0.40

There are no symmetry-related clashes.

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	247/262 (94%)	231 (94%)	16 (6%)	0	100	100
1	B	247/262 (94%)	232 (94%)	14 (6%)	1 (0%)	34	48
All	All	494/524 (94%)	463 (94%)	30 (6%)	1 (0%)	47	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	ASN

5.3.2 Protein sidechains [i](#)

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	191/201 (95%)	183 (96%)	8 (4%)	30	47
1	B	191/201 (95%)	183 (96%)	8 (4%)	30	47
All	All	382/402 (95%)	366 (96%)	16 (4%)	30	47

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	26	GLN
1	A	98	ASP
1	A	100	LEU
1	A	114	LYS
1	A	151	ARG
1	A	169	ASN
1	A	193	ARG
1	B	17	LYS
1	B	55	LEU
1	B	62	GLN
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	111	GLU
1	B	114	LYS
1	B	169	ASN
1	B	257	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	40	GLN
1	A	99	GLN
1	A	169	ASN
1	A	175	ASN
1	A	257	ASN
1	B	26	GLN
1	B	29	HIS
1	B	40	GLN
1	B	54	GLN
1	B	62	GLN
1	B	99	GLN
1	B	169	ASN
1	B	175	ASN
1	B	257	ASN

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 carbohydrates 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
2	NAD	B	401	-	42,48,48	1.97	8 (19%)	50,73,73	1.35	4 (8%)
3	AYM	A	302	-	23,26,26	2.93	10 (43%)	32,36,36	2.46	11 (34%)
2	NAD	A	301	-	42,48,48	2.07	8 (19%)	50,73,73	1.37	3 (6%)
3	AYM	B	402	-	23,26,26	2.91	10 (43%)	32,36,36	2.60	11 (34%)

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	B	401	-	-	8/26/62/62	0/5/5/5
3	AYM	A	302	-	-	4/13/13/13	0/3/3/3
2	NAD	A	301	-	-	11/26/62/62	0/5/5/5
3	AYM	B	402	-	-	4/13/13/13	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAD	C2N-N1N	9.11	1.46	1.35
2	B	401	NAD	C2N-N1N	8.66	1.45	1.35
3	B	402	AYM	C06-C05	7.40	1.53	1.39
3	A	302	AYM	C06-C05	7.31	1.53	1.39
3	B	402	AYM	C10-N12	6.24	1.43	1.35
3	A	302	AYM	C10-N12	6.16	1.43	1.35
3	A	302	AYM	C04-N03	5.12	1.45	1.34
3	B	402	AYM	C04-N03	4.95	1.44	1.34
3	A	302	AYM	C02-N03	4.54	1.48	1.35
2	A	301	NAD	O4D-C1D	4.51	1.47	1.41
3	B	402	AYM	C02-N03	4.28	1.47	1.35
2	B	401	NAD	O4D-C1D	4.22	1.47	1.41
2	A	301	NAD	C2A-N3A	3.61	1.37	1.32
2	B	401	NAD	C2A-N3A	3.40	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	AYM	C09-C08	3.21	1.41	1.33
2	A	301	NAD	C2N-C3N	3.17	1.43	1.39
3	A	302	AYM	C09-C08	3.09	1.41	1.33
3	A	302	AYM	C23-C24	3.04	1.43	1.36
2	B	401	NAD	C2N-C3N	2.98	1.43	1.39
2	A	301	NAD	C4A-N3A	2.95	1.39	1.35
2	A	301	NAD	C6N-N1N	2.87	1.42	1.35
2	B	401	NAD	C6N-N1N	2.82	1.42	1.35
2	B	401	NAD	C4A-N3A	2.78	1.39	1.35
3	B	402	AYM	C23-C24	2.77	1.43	1.36
3	B	402	AYM	C22-C21	2.76	1.43	1.36
3	A	302	AYM	C22-C21	2.68	1.42	1.36
2	B	401	NAD	O4B-C1B	2.61	1.44	1.41
2	A	301	NAD	C4N-C3N	2.51	1.43	1.39
3	A	302	AYM	C23-C22	2.47	1.44	1.38
2	B	401	NAD	C4N-C3N	2.47	1.43	1.39
3	B	402	AYM	C23-C22	2.44	1.44	1.38
3	B	402	AYM	C07-C06	2.37	1.43	1.38
2	A	301	NAD	O4B-C1B	2.32	1.44	1.41
3	A	302	AYM	C21-C17	2.31	1.47	1.41
3	B	402	AYM	C02-N01	2.18	1.41	1.35
3	A	302	AYM	C02-N01	2.17	1.41	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	AYM	C09-C10-N12	8.92	124.69	118.00
3	A	302	AYM	C09-C10-N12	7.62	123.72	118.00
3	B	402	AYM	C24-C18-N19	-5.16	126.05	132.29
3	A	302	AYM	C24-C18-N19	-4.95	126.30	132.29
2	B	401	NAD	N3A-C2A-N1A	-4.82	121.14	128.68
2	A	301	NAD	N3A-C2A-N1A	-4.80	121.17	128.68
3	B	402	AYM	C20-N19-C15	4.25	128.26	124.09
3	A	302	AYM	C20-N19-C15	4.04	128.05	124.09
2	B	401	NAD	C4A-C5A-N7A	3.70	113.25	109.40
2	A	301	NAD	C4A-C5A-N7A	3.70	113.25	109.40
3	B	402	AYM	C16-C17-C18	3.64	109.45	106.27
3	B	402	AYM	O11-C10-C09	-3.64	114.49	122.06
3	A	302	AYM	C14-C15-C16	-3.57	124.61	129.24
3	A	302	AYM	C05-C04-N03	-3.51	120.33	124.21
3	A	302	AYM	C16-C17-C18	3.46	109.29	106.27
3	B	402	AYM	C14-C15-C16	-3.40	124.84	129.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	AYM	O11-C10-C09	-3.35	115.08	122.06
3	B	402	AYM	C21-C17-C18	-3.22	115.30	119.87
2	A	301	NAD	C1B-N9A-C4A	-3.14	121.12	126.64
3	B	402	AYM	C05-C04-N03	-3.11	120.77	124.21
3	A	302	AYM	C21-C17-C18	-3.09	115.48	119.87
2	B	401	NAD	C1B-N9A-C4A	-2.99	121.38	126.64
3	B	402	AYM	C24-C18-C17	2.83	125.31	121.37
3	A	302	AYM	C24-C18-C17	2.72	125.15	121.37
3	A	302	AYM	C07-C02-N01	-2.63	116.57	121.14
3	B	402	AYM	C14-N12-C10	2.56	126.34	119.96
3	A	302	AYM	C14-N12-C10	2.48	126.13	119.96
3	B	402	AYM	C07-C02-N01	-2.34	117.08	121.14
2	B	401	NAD	O4B-C1B-C2B	-2.10	103.86	106.93

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	C5D-O5D-PN-O2N
2	B	401	NAD	O4D-C1D-N1N-C2N
3	A	302	AYM	C04-C05-C08-C09
2	A	301	NAD	O4B-C4B-C5B-O5B
2	A	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	C5D-O5D-PN-O2N
2	A	301	NAD	O4D-C1D-N1N-C2N
2	A	301	NAD	O4D-C1D-N1N-C6N
2	A	301	NAD	C2D-C1D-N1N-C2N
2	A	301	NAD	C2D-C1D-N1N-C6N
3	A	302	AYM	C06-C05-C08-C09
3	A	302	AYM	C08-C09-C10-O11
3	B	402	AYM	C06-C05-C08-C09
3	A	302	AYM	C08-C09-C10-N12
3	B	402	AYM	C04-C05-C08-C09
3	B	402	AYM	C08-C09-C10-N12
3	B	402	AYM	C08-C09-C10-O11
2	B	401	NAD	PA-O3-PN-O1N
2	A	301	NAD	PA-O3-PN-O1N
2	B	401	NAD	PN-O3-PA-O5B
2	B	401	NAD	PA-O3-PN-O2N
2	A	301	NAD	PN-O3-PA-O5B

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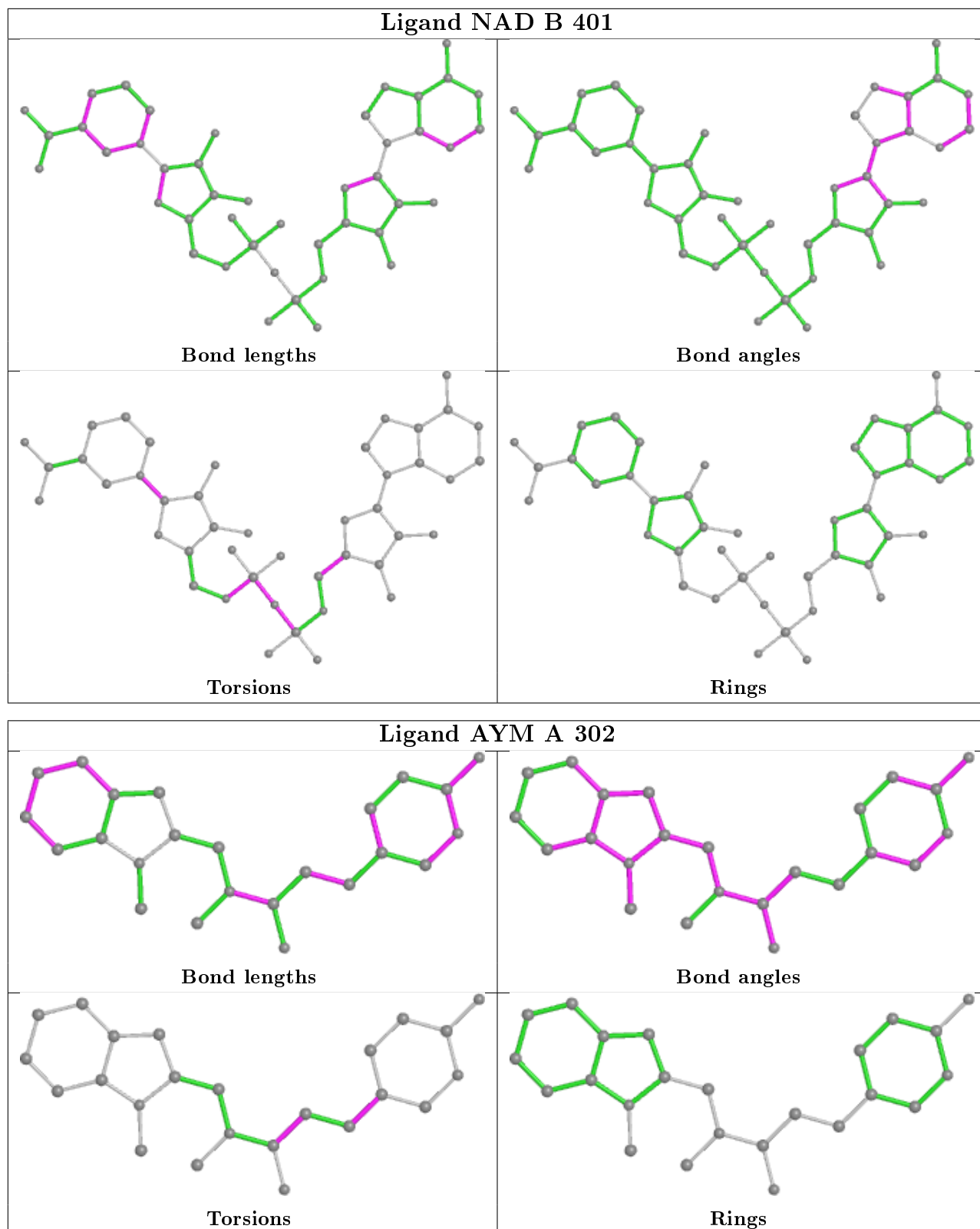
Mol	Chain	Res	Type	Atoms
2	B	401	NAD	C5D-O5D-PN-O3
2	A	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	PA-O3-PN-O2N

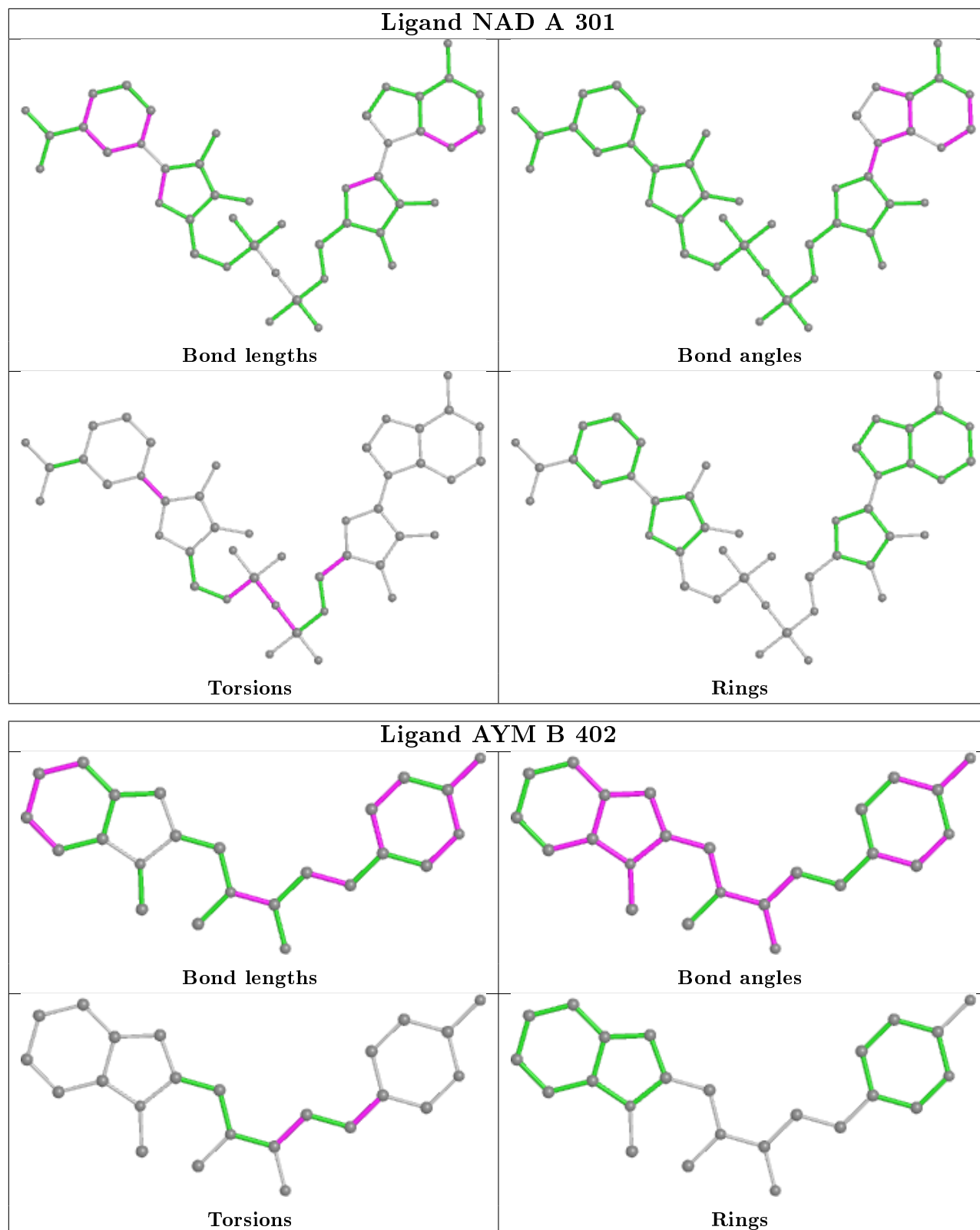
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAD	1	0
3	A	302	AYM	3	0
2	A	301	NAD	2	0
3	B	402	AYM	3	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

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.