



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 11:59 AM EDT

PDB ID : 7UMX / pdb_00007umx
Title : Crystal structure of Acinetobacter baumannii FabI in complex with NAD and (R,E)-3-(7-amino-8-oxo-6,7,8,9-tetrahydro-5H-pyrido[2,3-b]azepin-3-yl)-N-methyl-N-((3-methylbenzofuran-2-yl)methyl)acrylamide
Authors : Hajian, B.
Deposited on : 2022-04-08
Resolution : 2.39 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

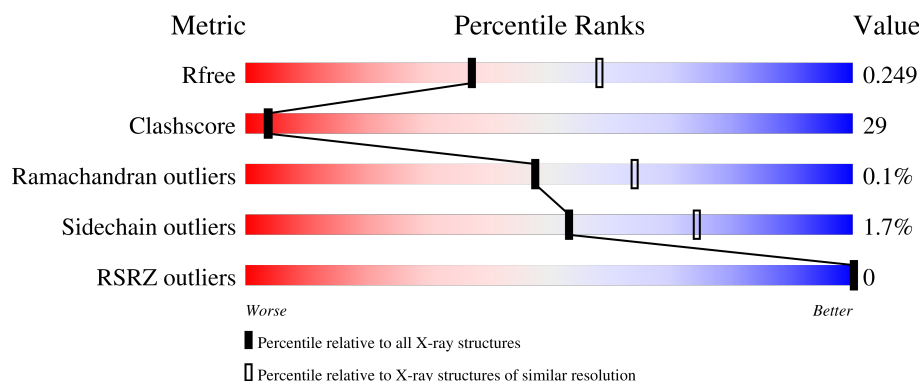
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

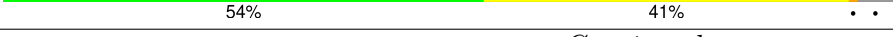
The reported resolution of this entry is 2.39 Å.

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))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	271	
1	B	271	
1	C	271	
1	D	271	

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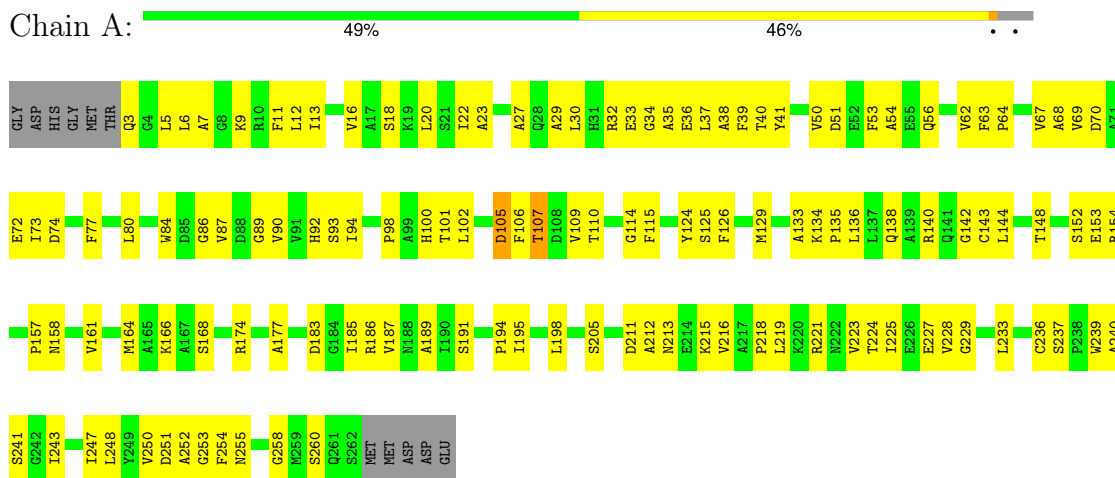
Mol	Chain	Length	Quality of chain
1	E	271	49% 45% • •
1	F	271	51% 44% • 5%

ENTRY-COMPOSITION INFOmissingINFO

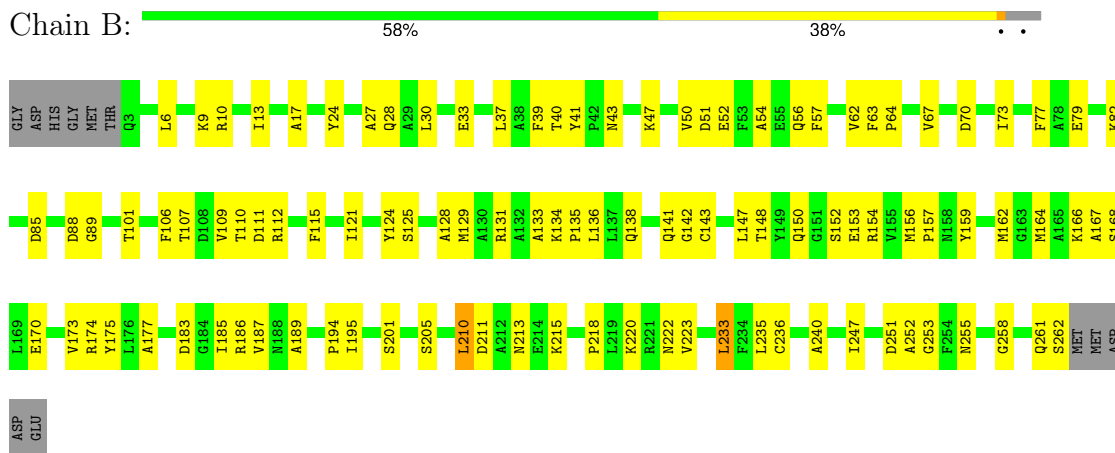
2 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

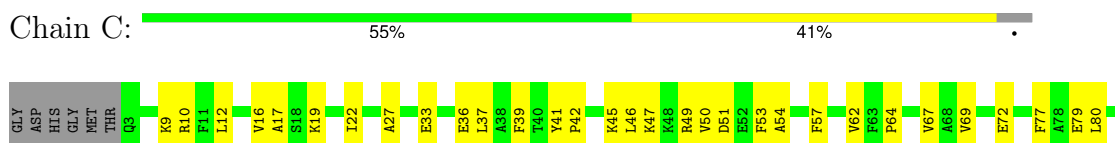
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

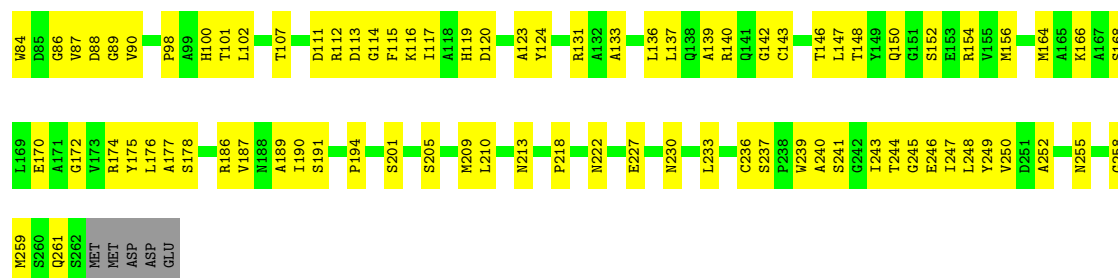


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

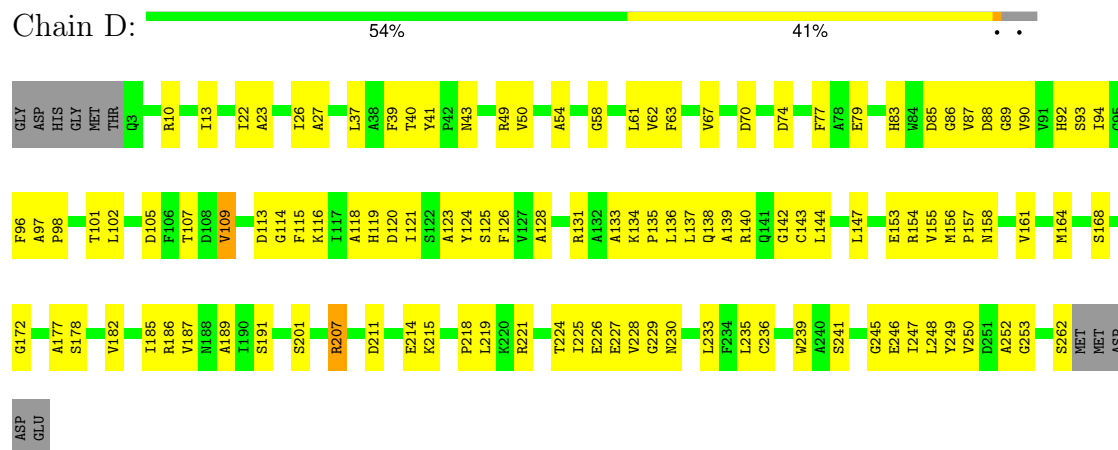


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

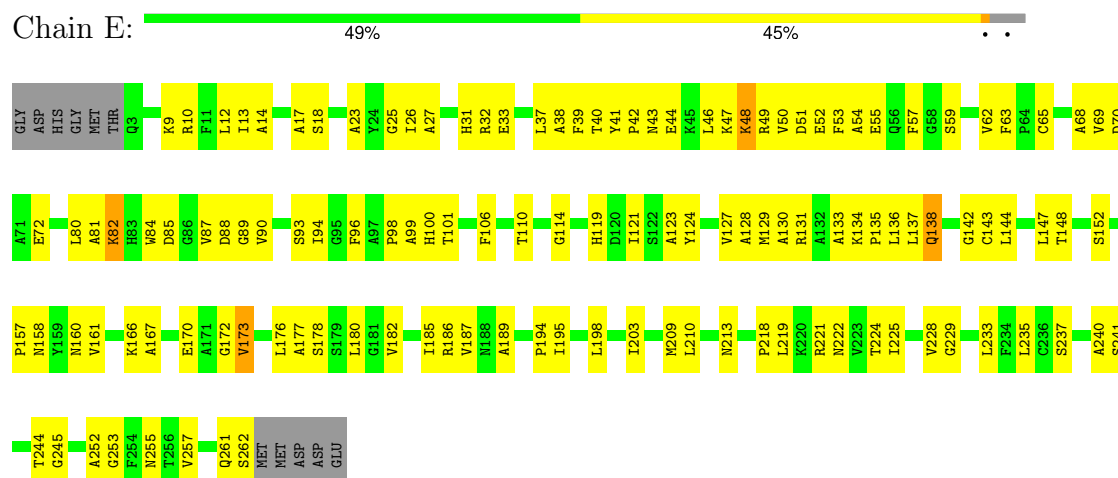




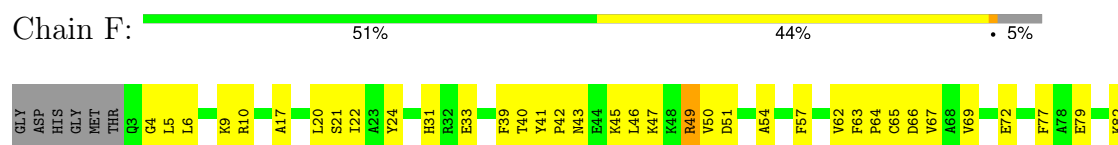
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



D251	D252	G253	F254	M255	V256	VAL	GLY	M259	S260	Q261	S262	MET	MET	ASP	ASP	GLU	K166	A167	E170	V173	A177	L180	I185	R186	I187	N188	A189	I190	S191	I195	R196	T197	A200	S201	G202	I203	F206	R207	K208	M209	L210	D211	A212	K215	V216	A217	P218	L219	K220	R221	N222	V223	E227	L233	F234	L235	C236	S237	A240	G245	E246	I247	L248	H83	M84	D85	G86	V87	D88	G89	V90	S93	A97	P98	A99	H100	T101	L102	D105	F106	V109	T110	D111	G114	F115	K116	I117	T121	S122	A133	K134	P135	L136	L137	Q138	A139	R140	Q141	G142	C143	L144	L147	T148	T149	Q150	G151	S152	F153	R154	Y159	N160	V161	M162	L168
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3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	255.12Å 79.25Å 89.90Å 90.00° 110.30° 90.00°	Depositor
Resolution (Å)	44.95 – 2.39 44.95 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.95-2.39) 96.4 (44.95-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.208 , 0.251 0.207 , 0.249	Depositor DCC
R_{free} test set	2004 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.447 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12368	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.93% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NQF, 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	0.11	0/1962	0.29	0/2660
1	B	0.10	0/1977	0.31	0/2677
1	C	0.11	0/1971	0.29	0/2670
1	D	0.13	0/1974	0.31	1/2673 (0.0%)
1	E	0.20	0/1977	0.45	1/2677 (0.0%)
1	F	0.12	0/1965	0.30	0/2659
All	All	0.13	0/11826	0.33	2/16016 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	82	LYS	CD-CE-NZ	-12.12	73.11	111.90
1	D	207	ARG	CG-CD-NE	-6.10	98.57	112.00

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1926	0	1890	132	0
1	B	1941	0	1924	120	1
1	C	1935	0	1913	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1938	0	1915	120	1
1	E	1941	0	1924	136	1
1	F	1930	0	1911	121	1
2	A	30	24	0	0	0
2	B	30	24	0	0	0
2	C	30	24	0	1	0
2	D	30	24	0	1	0
2	E	30	24	0	1	0
2	F	30	24	0	0	0
3	A	44	0	25	4	0
3	B	44	0	25	5	0
3	C	44	0	25	8	0
3	D	44	0	25	8	0
3	E	44	0	25	7	0
3	F	44	0	25	4	0
4	A	23	0	0	11	0
4	B	44	0	0	29	0
4	C	28	0	0	13	0
4	D	27	0	0	16	0
4	E	22	0	0	19	0
4	F	25	0	0	19	0
All	All	12224	144	11627	688	2

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 29.

The worst 5 of 688 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:3:GLN:HA	1:A:34:GLY:HA3	1.26	1.16
1:F:46:LEU:HD13	1:F:49:ARG:HD2	1.20	1.11
1:B:255:ASN:O	1:C:154:ARG:NH1	1.84	1.11
1:B:51:ASP:HA	1:B:62:VAL:HG21	1.38	1.05
1:B:156:MET:HE1	1:C:259:MET:HG2	1.39	1.02

All (2) 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:D:207:ARG:NH2	1:E:81:ALA:O[1_565]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LYS:O	1:F:207:ARG:NH1[1_565]	1.94	0.26

4.3 Torsion angles [i](#)

4.3.1 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	258/271 (95%)	248 (96%)	9 (4%)	1 (0%)	30	43
1	B	258/271 (95%)	250 (97%)	8 (3%)	0	100	100
1	C	258/271 (95%)	249 (96%)	9 (4%)	0	100	100
1	D	258/271 (95%)	249 (96%)	9 (4%)	0	100	100
1	E	258/271 (95%)	248 (96%)	10 (4%)	0	100	100
1	F	254/271 (94%)	244 (96%)	10 (4%)	0	100	100
All	All	1544/1626 (95%)	1488 (96%)	55 (4%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	THR

4.3.2 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	190/208 (91%)	187 (98%)	3 (2%)	55	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	195/208 (94%)	193 (99%)	2 (1%)	68	84
1	C	194/208 (93%)	191 (98%)	3 (2%)	57	77
1	D	194/208 (93%)	190 (98%)	4 (2%)	47	69
1	E	195/208 (94%)	190 (97%)	5 (3%)	40	63
1	F	194/208 (93%)	191 (98%)	3 (2%)	57	77
All	All	1162/1248 (93%)	1142 (98%)	20 (2%)	53	74

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	138	GLN
1	F	49	ARG
1	F	201	SER
1	F	122	SER
1	C	201	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	150	GLN
1	F	31	HIS
1	E	31	HIS
1	F	75	ASN
1	E	213	ASN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

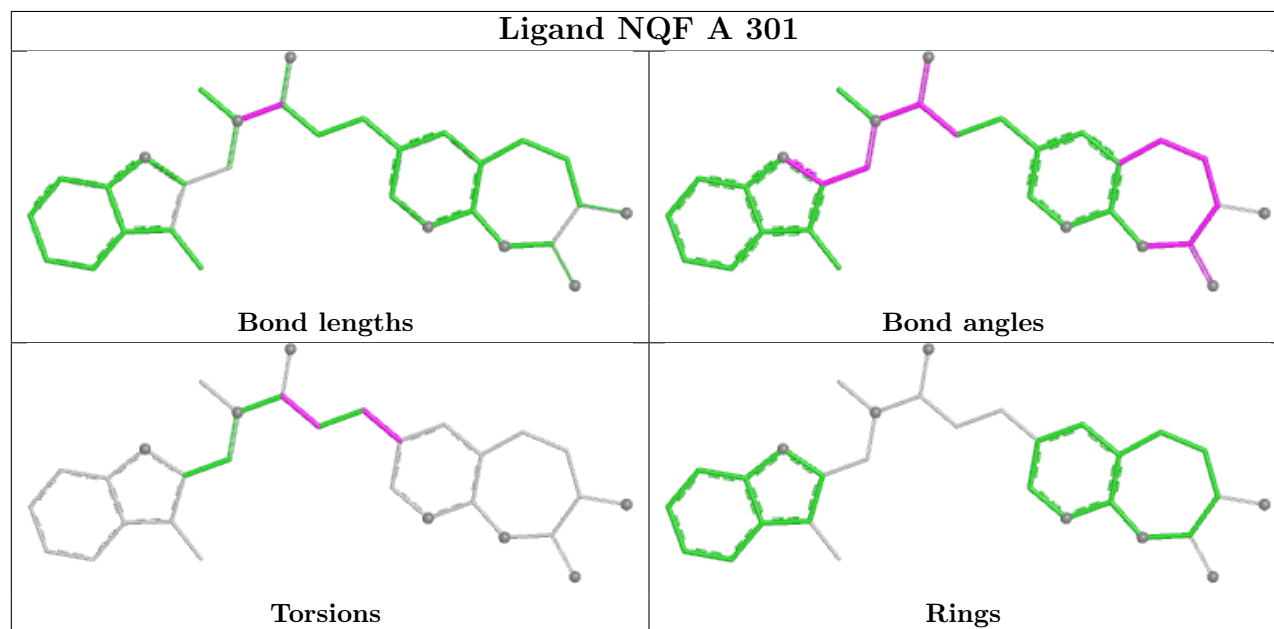
There are no chirality outliers.

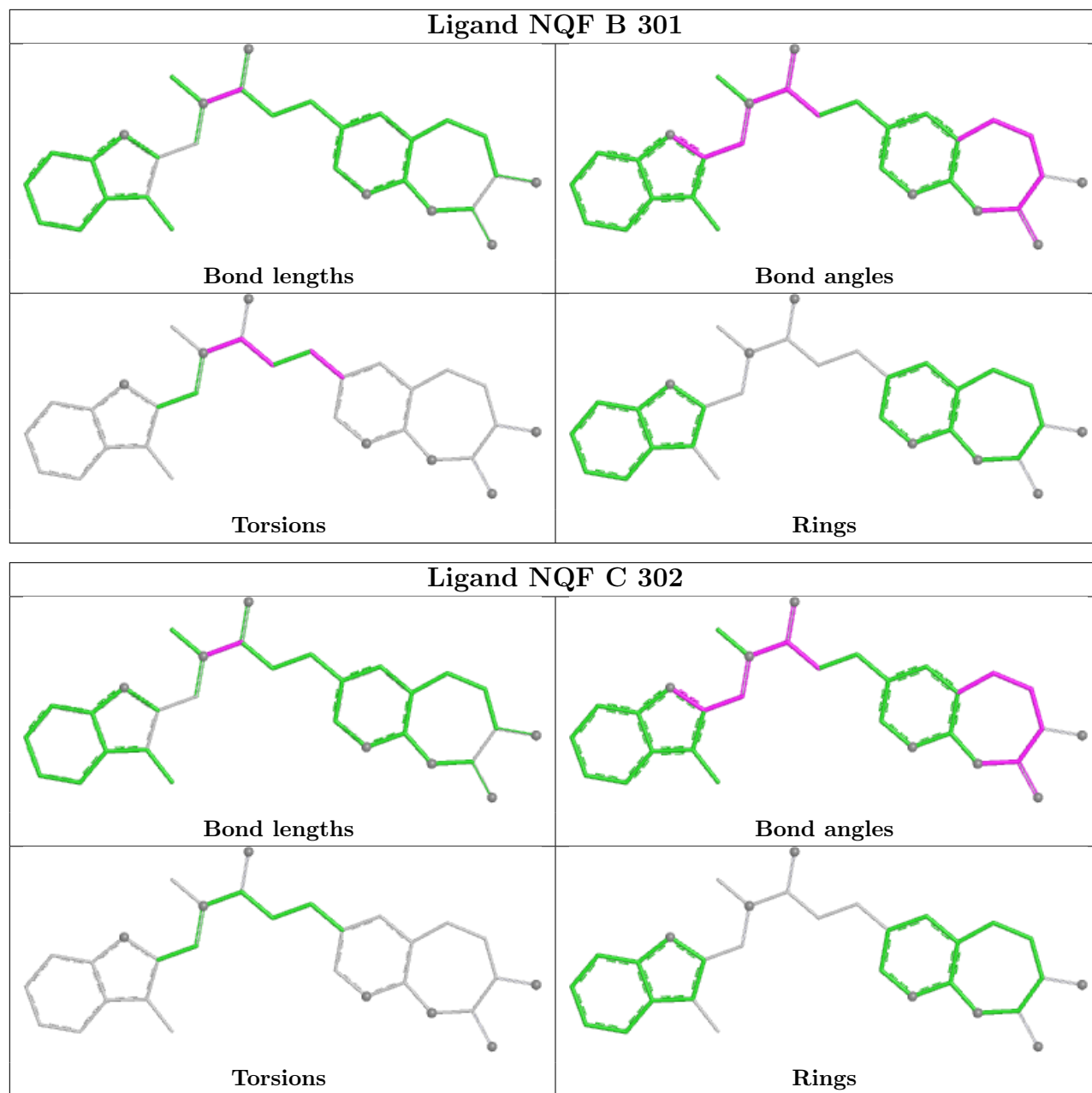
There are no torsion outliers.

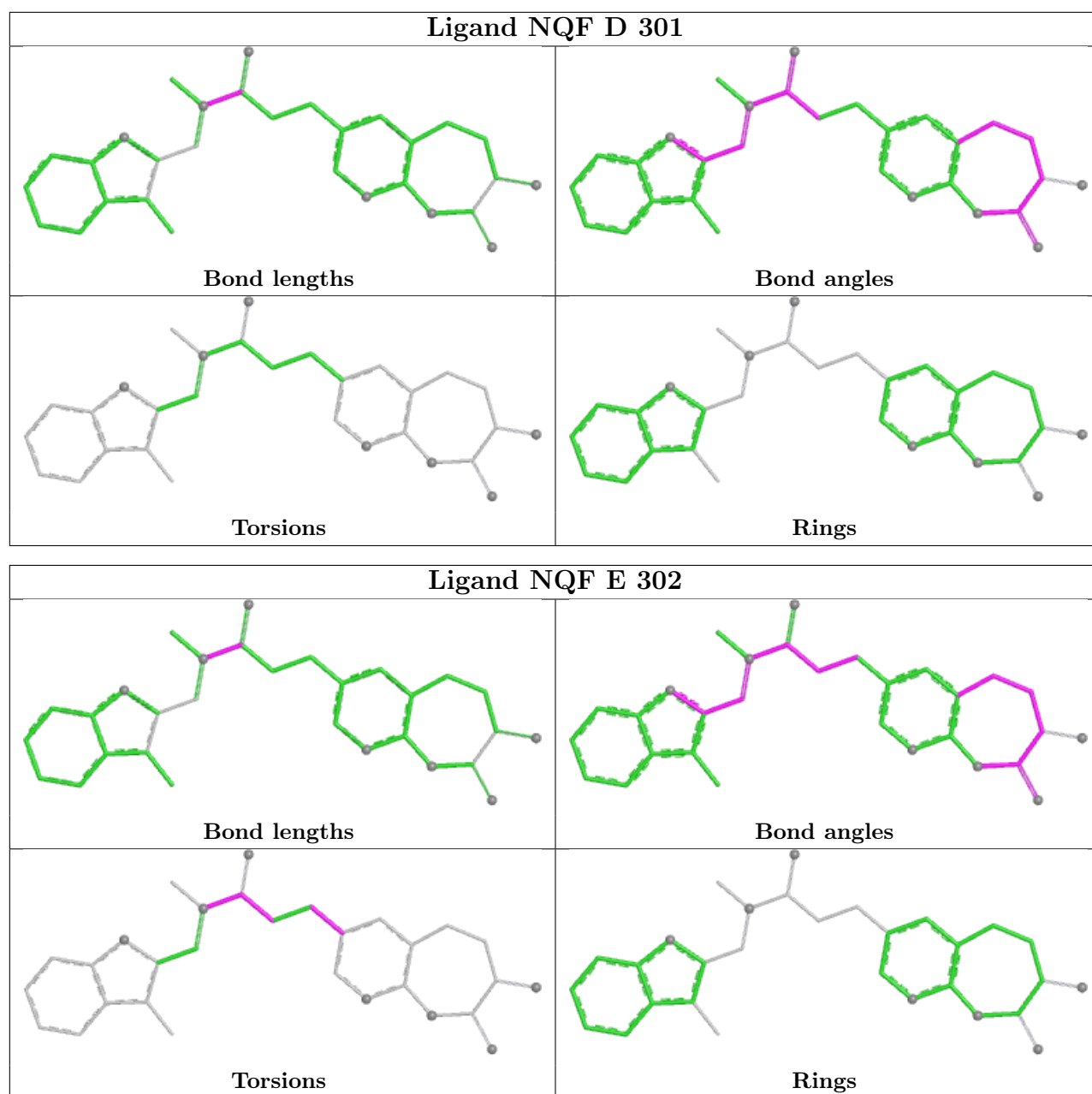
There are no ring outliers.

No monomer is involved in short contacts.

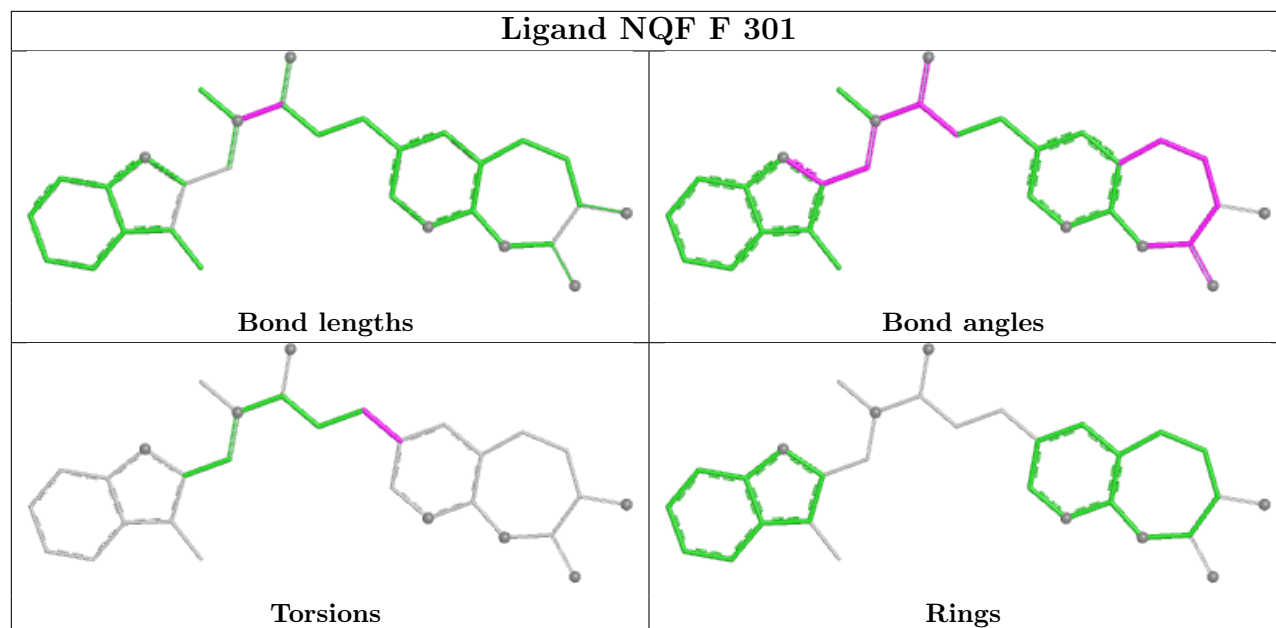
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



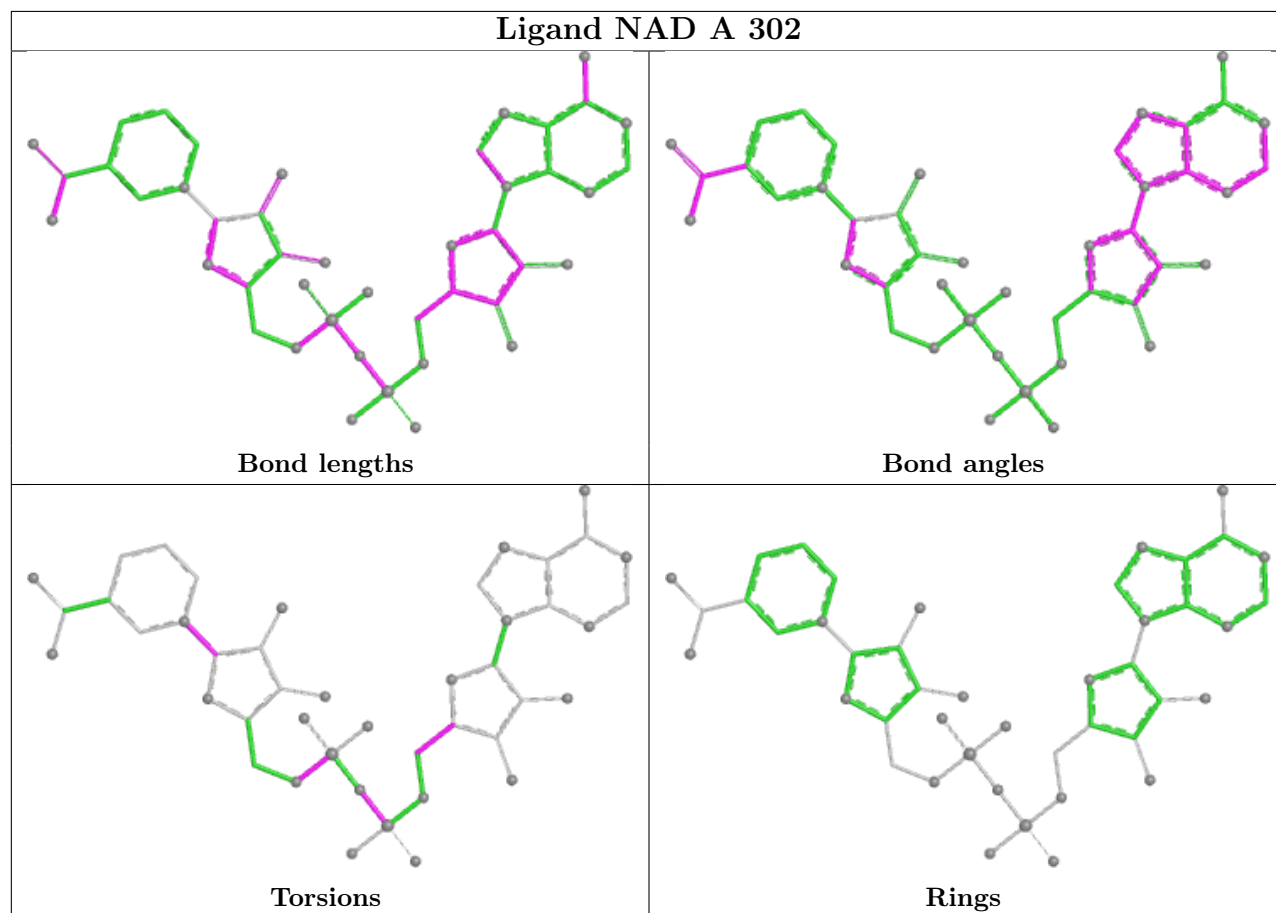


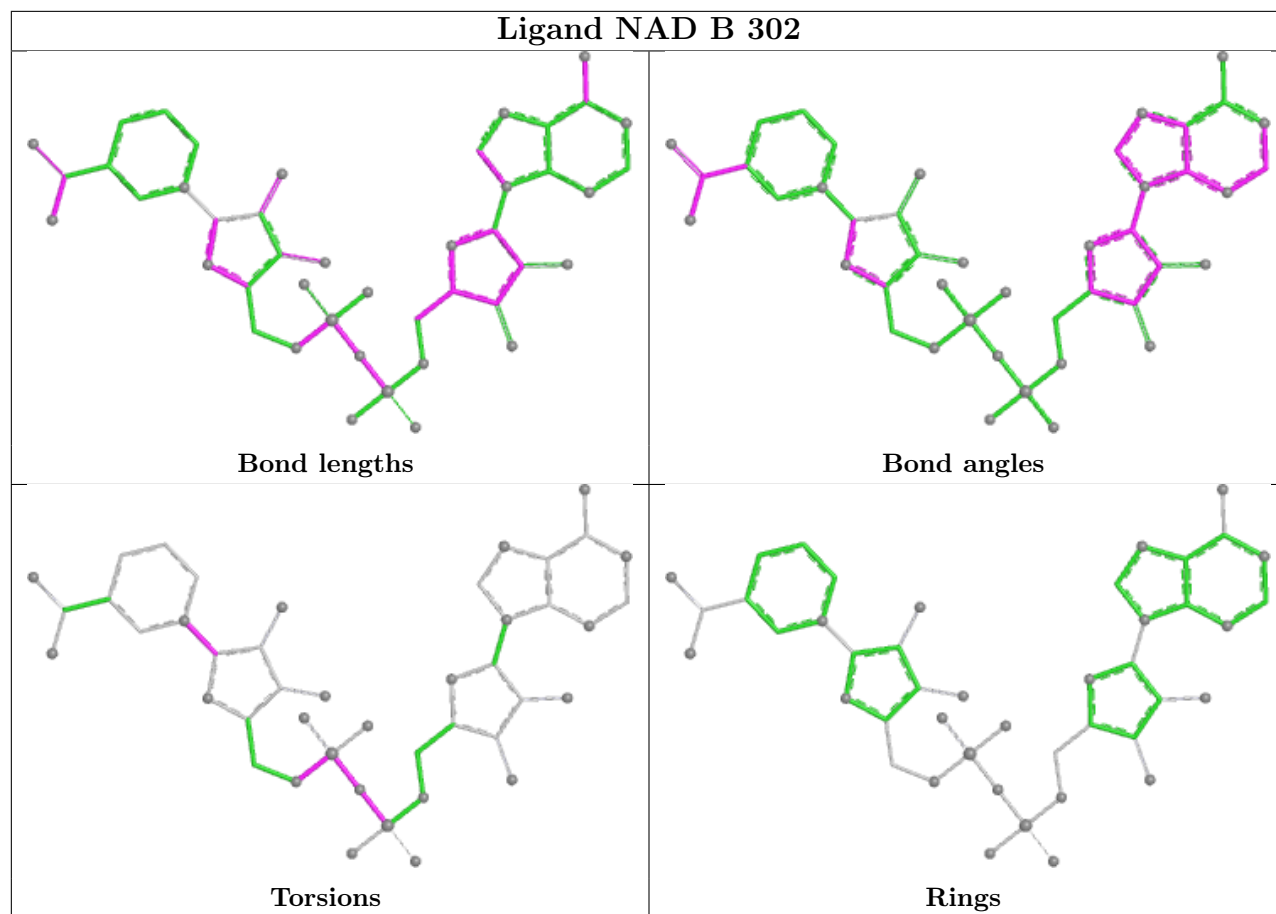


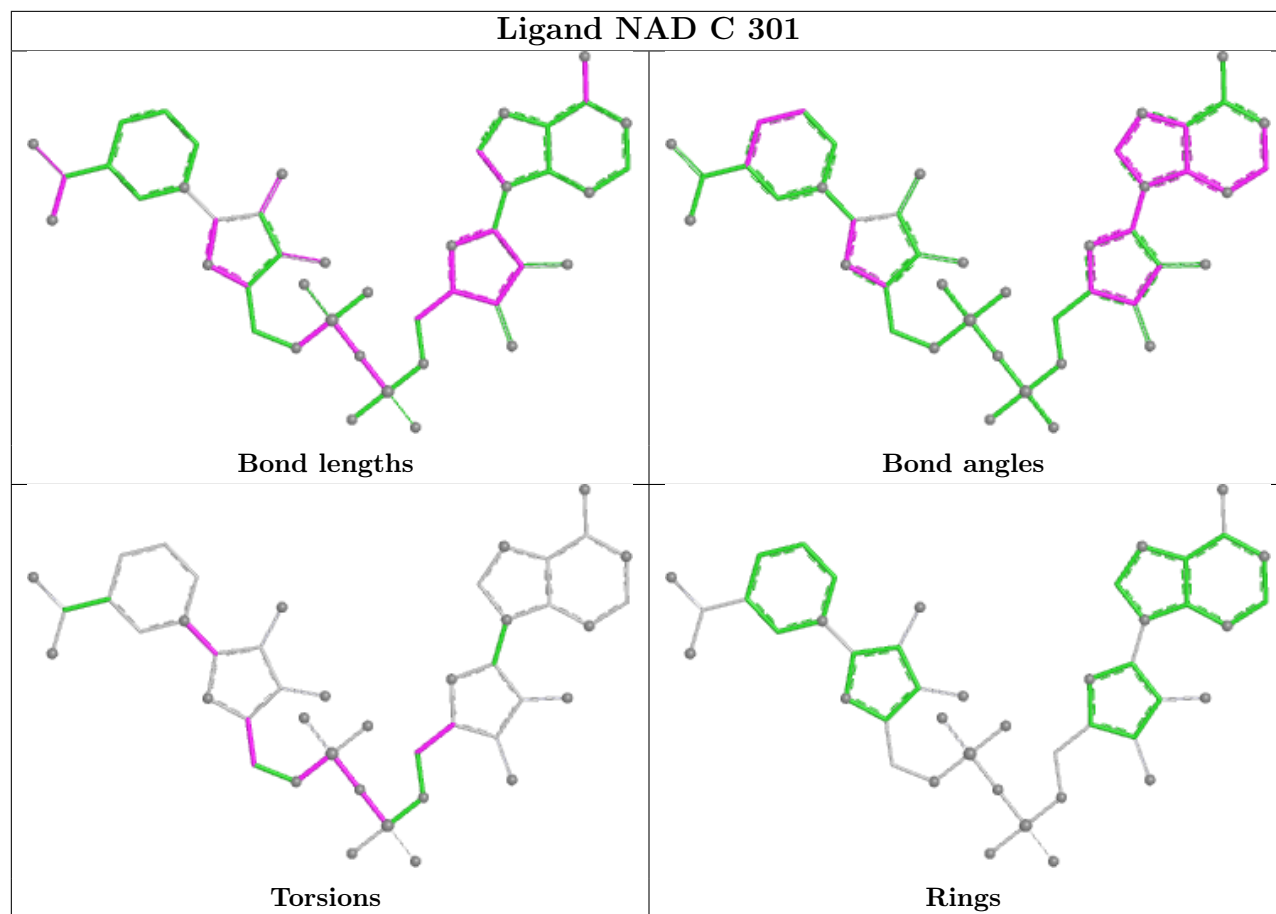
Ligand NQF F 301

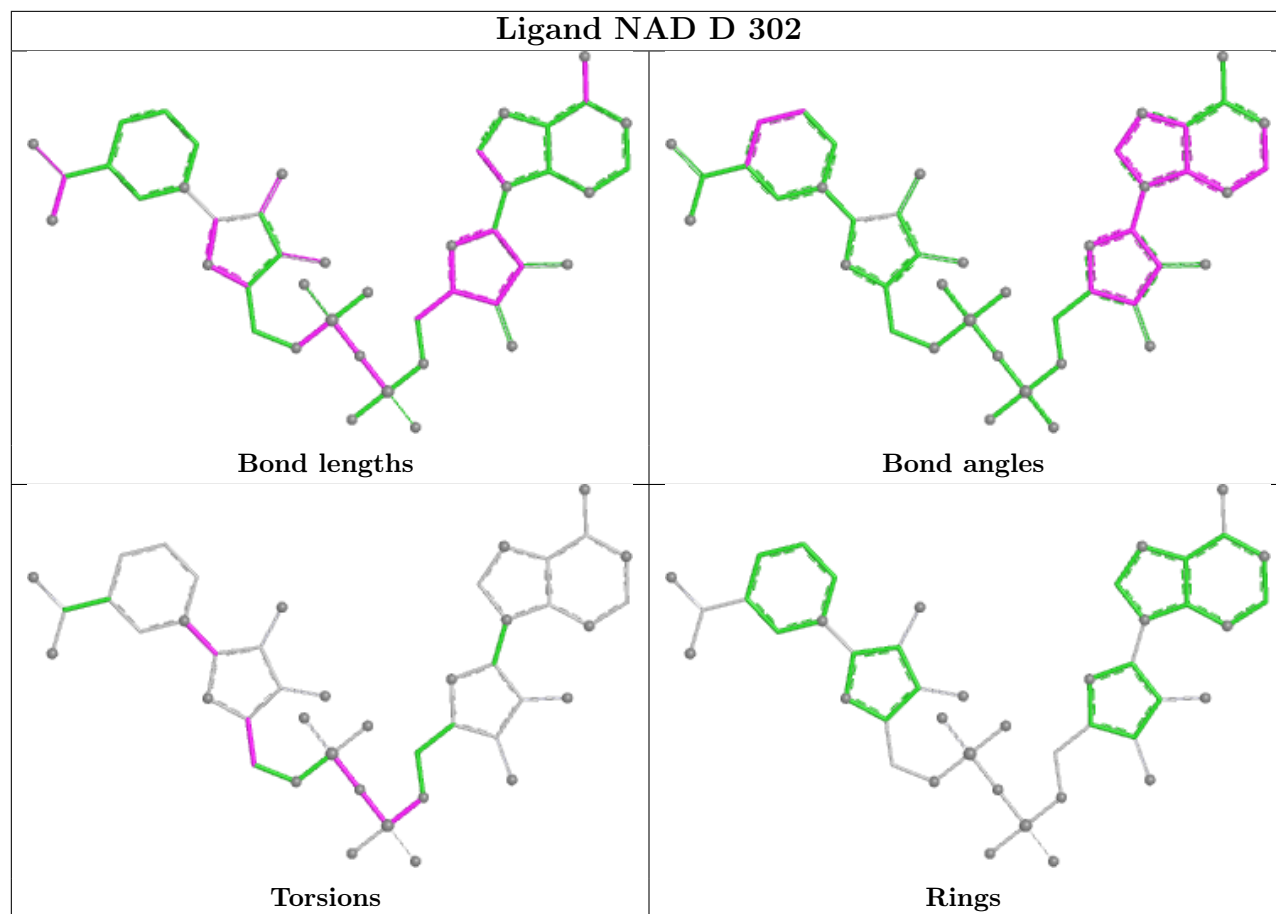


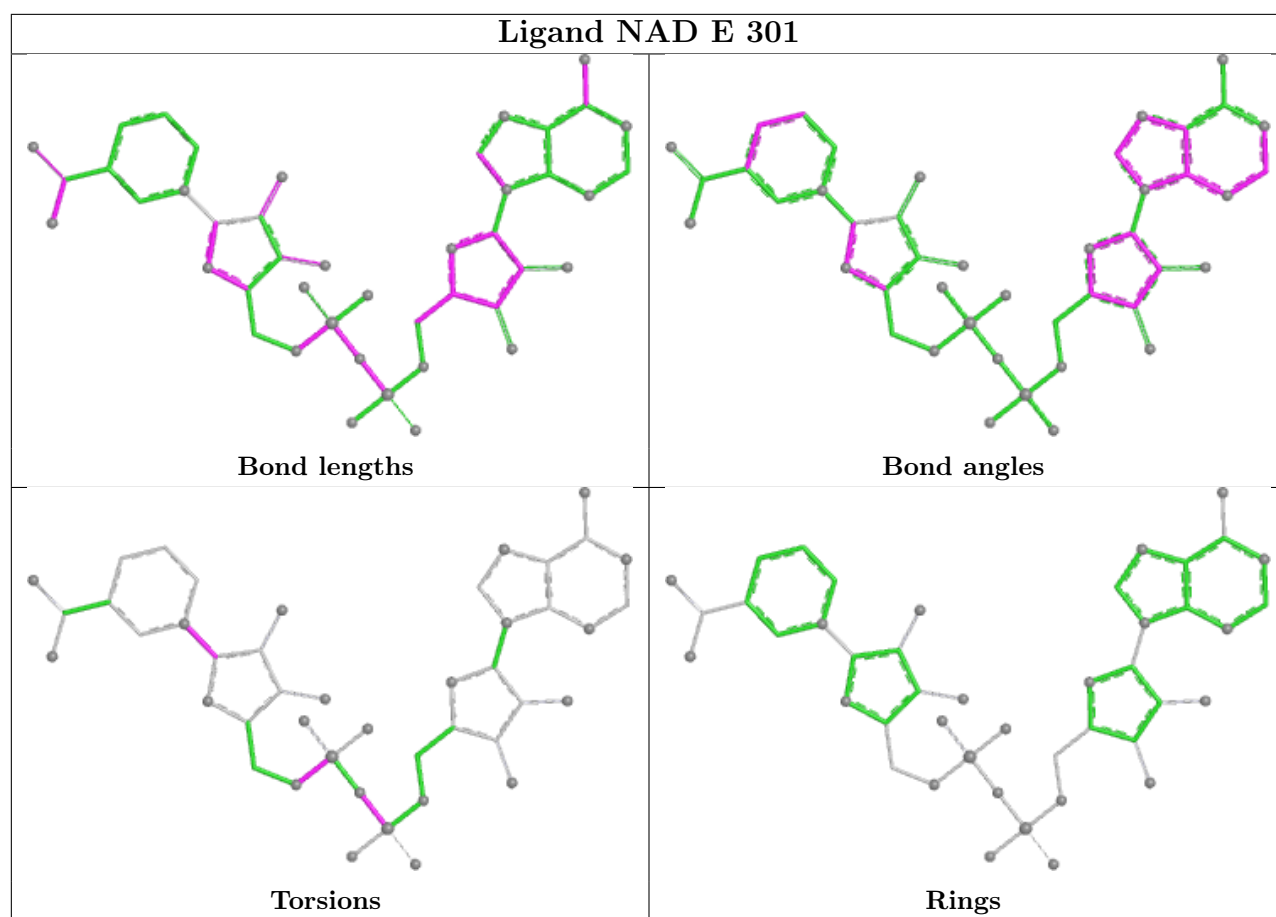
Ligand NAD A 302

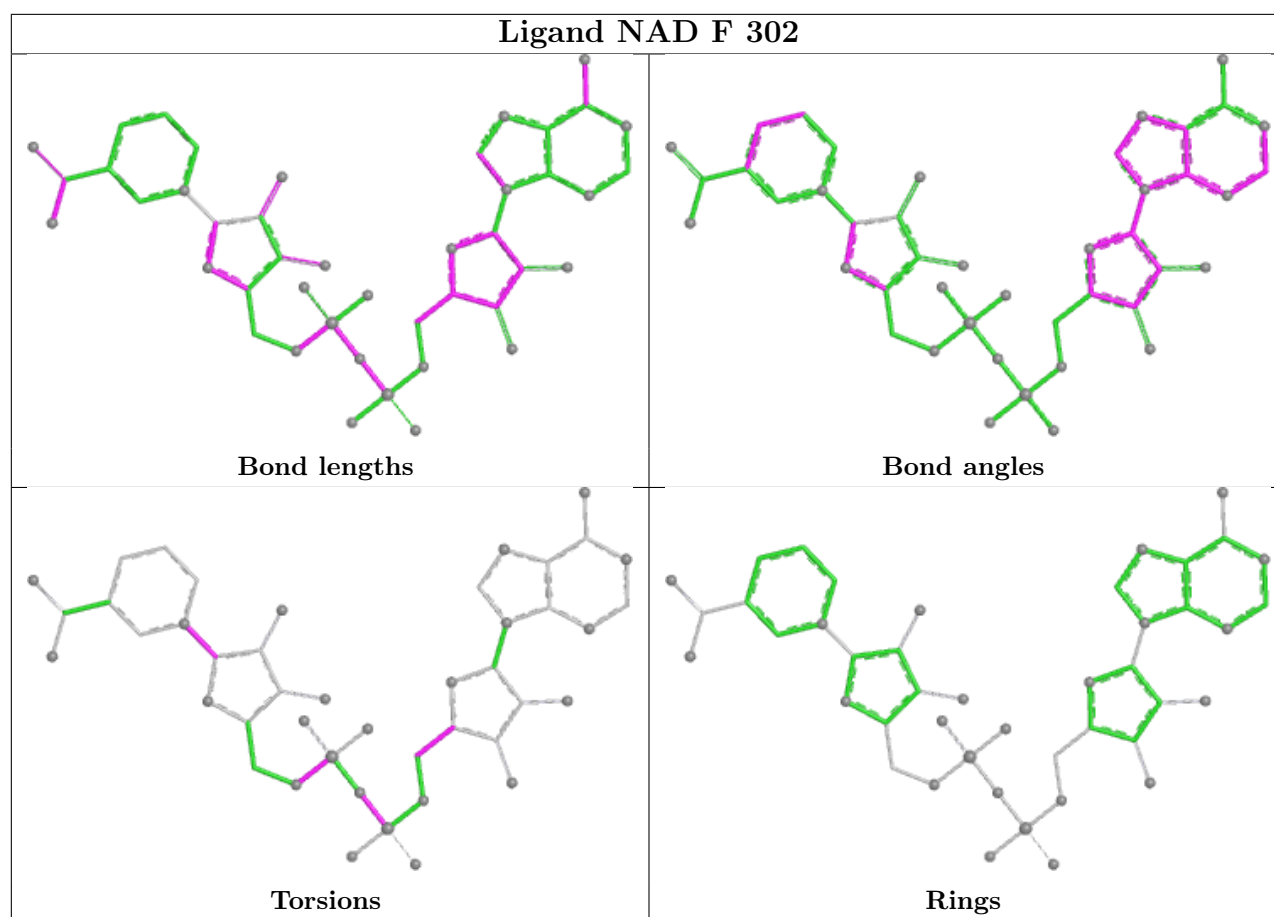












4.7 Other polymers [i](#)

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	260/271 (95%)	-1.21	0 100 100	27, 40, 55, 92	0
1	B	260/271 (95%)	-1.25	0 100 100	27, 38, 54, 70	0
1	C	260/271 (95%)	-1.24	0 100 100	28, 41, 58, 68	0
1	D	260/271 (95%)	-1.19	0 100 100	30, 44, 61, 85	0
1	E	260/271 (95%)	-1.12	0 100 100	33, 52, 69, 87	0
1	F	258/271 (95%)	-1.11	0 100 100	34, 49, 68, 82	0
All	All	1558/1626 (95%)	-1.19	0 100 100	27, 44, 63, 92	0

There are no RSRZ outliers to report.

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

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

5.4 Other polymers ⓘ

There are no such residues in this entry.