



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 04:37 PM EDT

PDB ID : 9BDJ / pdb_00009bdj
EMDB ID : EMD-44453
Title : MicroED structure of bovine liver catalase with missing cone eliminated by suspended drop
Authors : Gillman, C.; Bu, G.; Gonen, T.
Deposited on : 2024-04-11
Resolution : 4.00 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis	: NOT EXECUTED
Mogul	: 2022.3.0, CSD as543be (2022)
MolProbity	: 4-5-2 with Phenix2.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	: NOT EXECUTED
MapQ	: NOT EXECUTED
CCP4	: 9.0.015 (Gargrove)
Density-Fitness	: 1.0.12
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.50

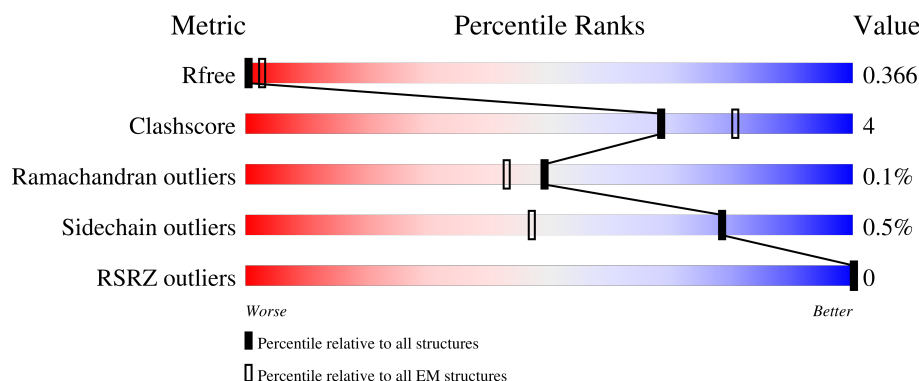
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 4.00 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)	EM structures (#Entries)
R_{free}	180332	208
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	527	
1	B	527	
1	C	527	
1	D	527	

2 Entry composition [i](#)

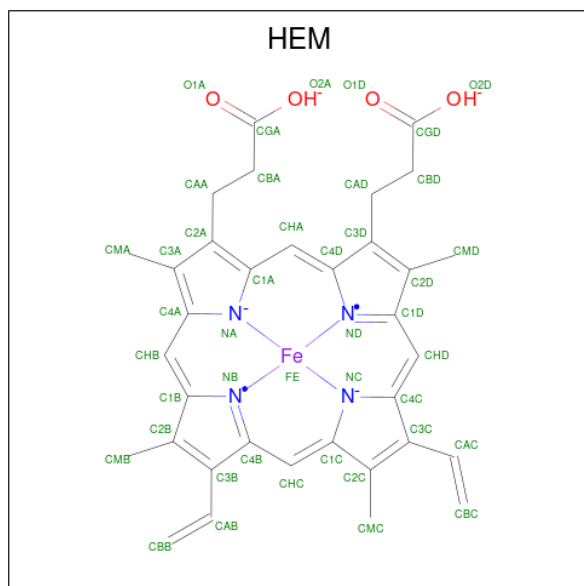
There are 3 unique types of molecules in this entry. The entry contains 16432 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Catalase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	B	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	C	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	D	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0

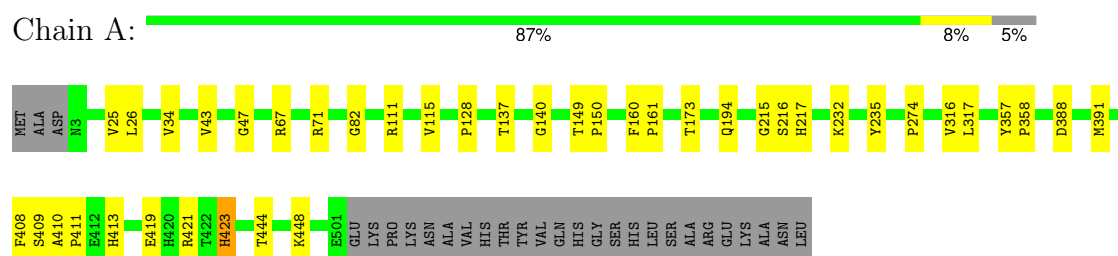
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- The chemical structure of NDP (Nucleoside Diphosphate) is shown. It consists of a ribose sugar (C1-C5) linked to a pyrimidine nucleobase (C6-C9) via a glycosidic bond. The sugar is also linked to a diphosphate group (P1, P2) via a pyrophosphate bridge. The phosphate groups are shown with their respective oxygen atoms (O1-O4) and hydrogen atoms (H1-H4). The nucleobase is a pyrimidine ring with an amino group (NH2) at the C4 position. The structure is labeled with atom names and numbers, and the overall molecule is identified as NDP.

Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0

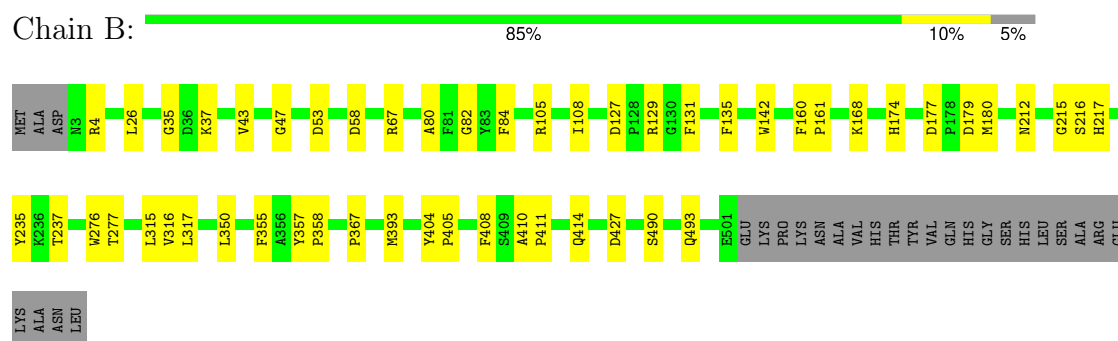
3 Residue-property plots [i](#)

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.

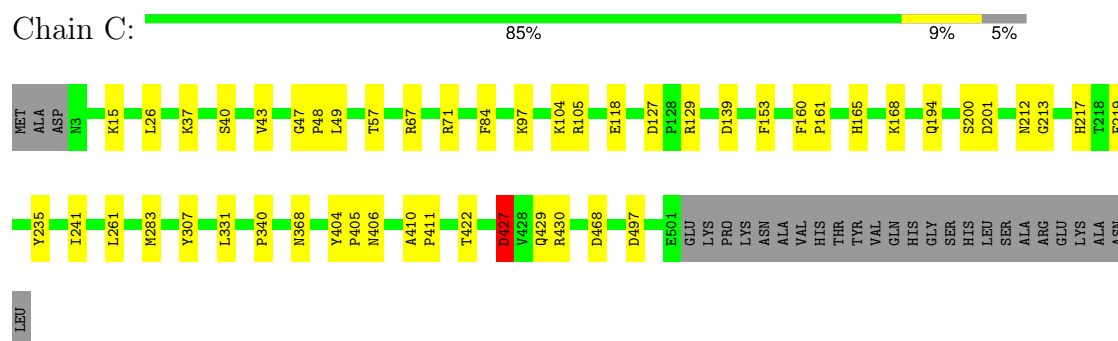
- Molecule 1: Catalase



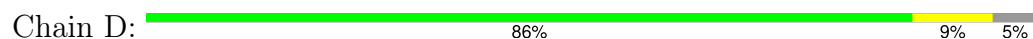
- Molecule 1: Catalase

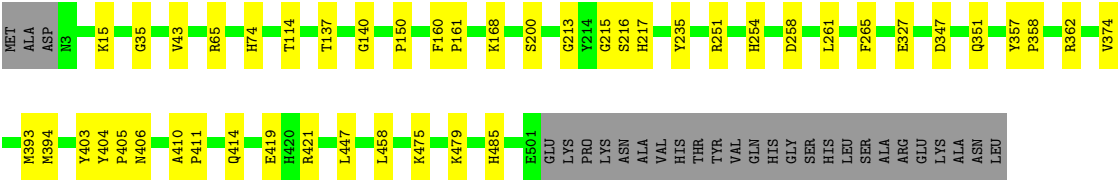


- Molecule 1: Catalase



- Molecule 1: Catalase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.65Å 173.30Å 182.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.11 – 4.00 44.11 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.9 (44.11-4.00) 82.0 (44.11-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 4.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.317 , 0.358 0.326 , 0.366	Depositor DCC
R_{free} test set	855 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	1.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 17.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16432	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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.

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: NDP, HEM

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	0.49	0/4137	0.86	0/5619
1	B	0.50	0/4137	0.84	0/5619
1	C	0.49	0/4137	0.85	0/5619
1	D	0.49	0/4137	0.85	0/5619
All	All	0.49	0/16548	0.85	0/22476

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	4017	0	3843	22	0
1	B	4017	0	3844	41	0
1	C	4017	0	3843	34	0
1	D	4017	0	3843	29	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	48	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	0	0
3	C	48	0	26	0	0
3	D	48	0	26	1	0
All	All	16432	0	15597	117	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 4.

The worst 5 of 117 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:235:TYR:CZ	1:B:276:TRP:HB2	2.15	0.82
1:B:235:TYR:CE1	1:B:315:LEU:HD12	2.23	0.73
2:B:601:HEM:HMD1	2:B:601:HEM:HBD2	1.69	0.73
2:A:601:HEM:HMB1	2:A:601:HEM:HBB2	1.72	0.71
2:D:601:HEM:HMB1	2:D:601:HEM:HBB2	1.74	0.69

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 PDB entries followed by that with respect to all EM entries.

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	497/527 (94%)	475 (96%)	21 (4%)	1 (0%)	43	75
1	B	497/527 (94%)	480 (97%)	17 (3%)	0	100	100
1	C	497/527 (94%)	475 (96%)	21 (4%)	1 (0%)	43	75
1	D	497/527 (94%)	475 (96%)	22 (4%)	0	100	100
All	All	1988/2108 (94%)	1905 (96%)	81 (4%)	2 (0%)	49	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASP
1	C	427	ASP

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 PDB entries followed by that with respect to all EM entries.

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	431/454 (95%)	426 (99%)	5 (1%)	63	73
1	B	431/454 (95%)	431 (100%)	0	100	100
1	C	431/454 (95%)	429 (100%)	2 (0%)	81	82
1	D	431/454 (95%)	429 (100%)	2 (0%)	81	82
All	All	1724/1816 (95%)	1715 (100%)	9 (0%)	78	82

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	394	MET
1	D	419	GLU
1	A	419	GLU
1	A	423	HIS
1	C	422	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	101	HIS
1	C	485	HIS
1	D	432	ASN
1	D	351	GLN
1	D	371	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](#)

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$
3	NDP	C	602	-	51,52,52	0.60	1 (1%)	71,80,80	0.76	2 (2%)
2	HEM	D	601	1	50,50,50	1.62	7 (14%)	67,82,82	1.45	9 (13%)
3	NDP	A	602	-	51,52,52	0.56	1 (1%)	71,80,80	0.76	1 (1%)
2	HEM	B	601	1	50,50,50	1.64	8 (16%)	67,82,82	1.54	11 (16%)
2	HEM	A	601	1	50,50,50	1.60	7 (14%)	67,82,82	1.40	8 (11%)
3	NDP	D	602	-	51,52,52	0.60	1 (1%)	71,80,80	0.70	1 (1%)
2	HEM	C	601	1	50,50,50	1.61	7 (14%)	67,82,82	1.44	11 (16%)
3	NDP	B	602	-	51,52,52	0.59	1 (1%)	71,80,80	0.77	1 (1%)

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	NDP	C	602	-	-	11/34/77/77	0/5/5/5
2	HEM	D	601	1	-	4/14/54/54	-
3	NDP	A	602	-	-	9/34/77/77	0/5/5/5
2	HEM	B	601	1	-	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	1	-	5/14/54/54	-
3	NDP	D	602	-	-	9/34/77/77	0/5/5/5
2	HEM	C	601	1	-	2/14/54/54	-
3	NDP	B	602	-	-	9/34/77/77	0/5/5/5

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	HEM	FE-NB	6.23	2.14	1.94
2	B	601	HEM	FE-NB	5.94	2.13	1.94
2	C	601	HEM	FE-NB	5.82	2.12	1.94
2	A	601	HEM	FE-NB	5.66	2.12	1.94
2	C	601	HEM	FE-NC	4.67	2.10	1.95

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	HEM	CHC-C4B-NB	4.90	129.69	124.42
2	A	601	HEM	CHC-C4B-NB	4.63	129.41	124.42
2	B	601	HEM	CHC-C4B-NB	4.62	129.40	124.42
3	B	602	NDP	P2B-O2B-C2B	-3.76	113.40	123.43
2	D	601	HEM	CHD-C1D-ND	3.70	128.41	124.42

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	HEM	C2D-C3D-CAD-CBD
3	C	602	NDP	C5B-O5B-PA-O2A
3	C	602	NDP	C5B-O5B-PA-O3
3	C	602	NDP	O4B-C4B-C5B-O5B
3	D	602	NDP	C5B-O5B-PA-O2A

There are no ring outliers.

6 monomers are involved in 14 short contacts:

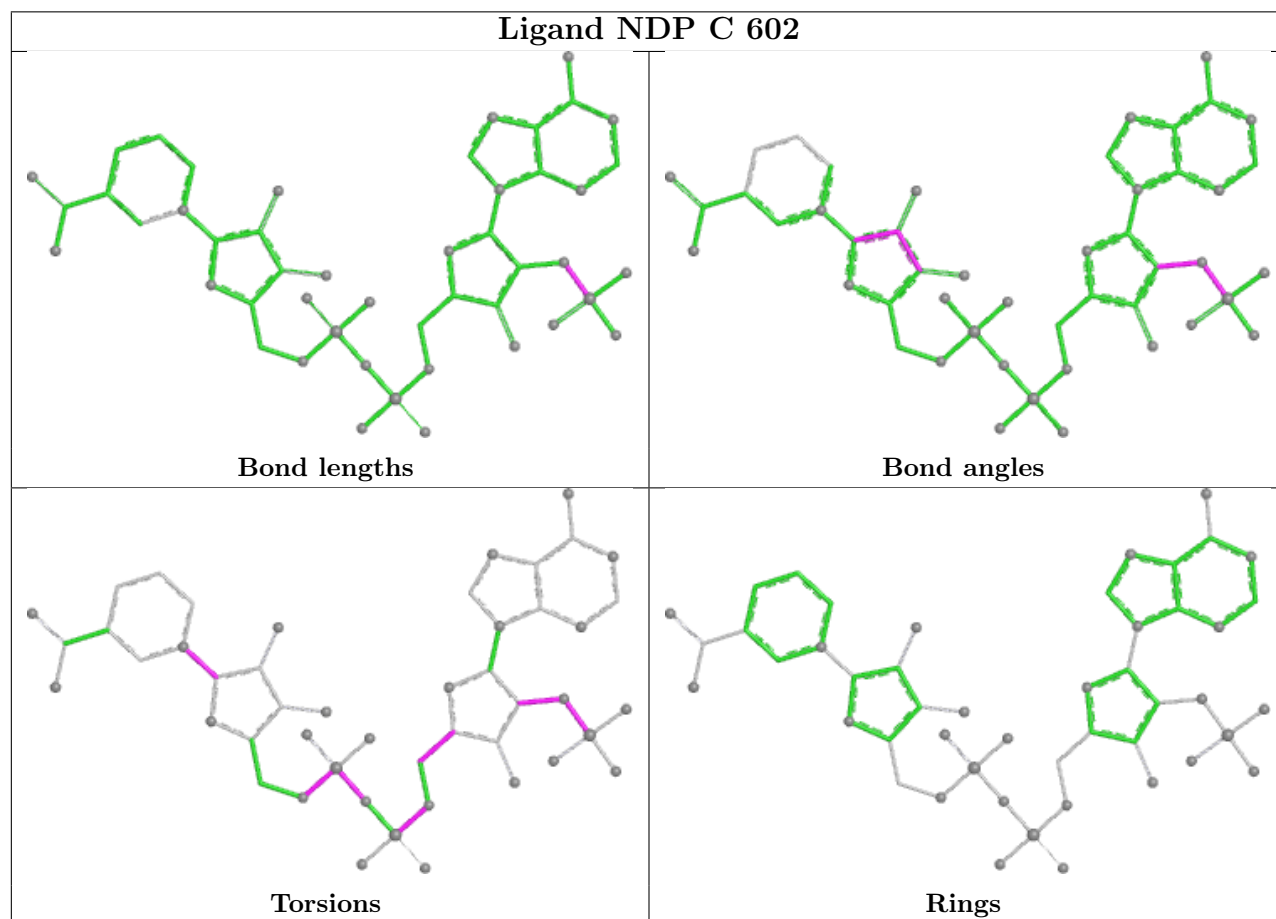
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	1	0
3	A	602	NDP	1	0
2	B	601	HEM	5	0

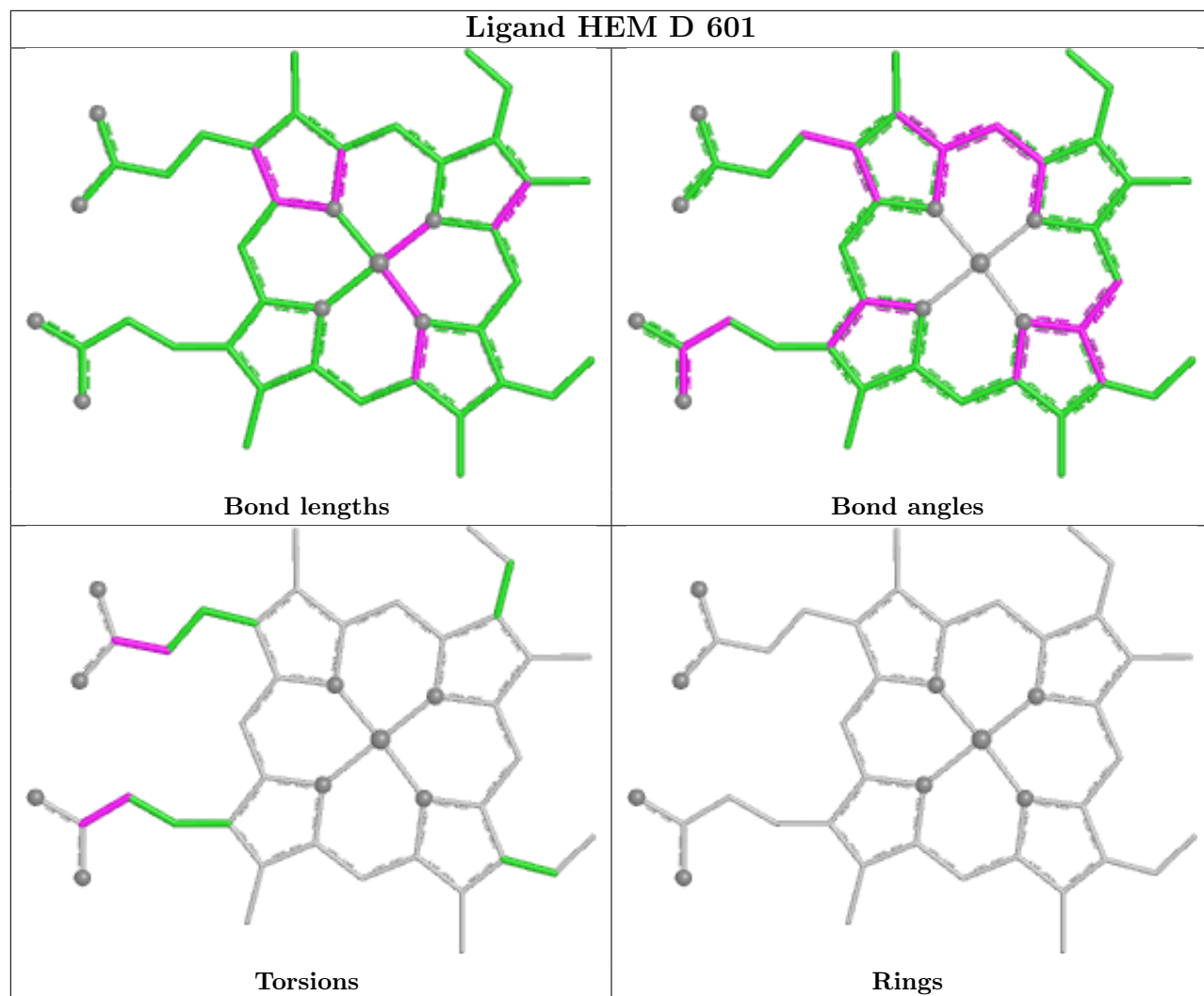
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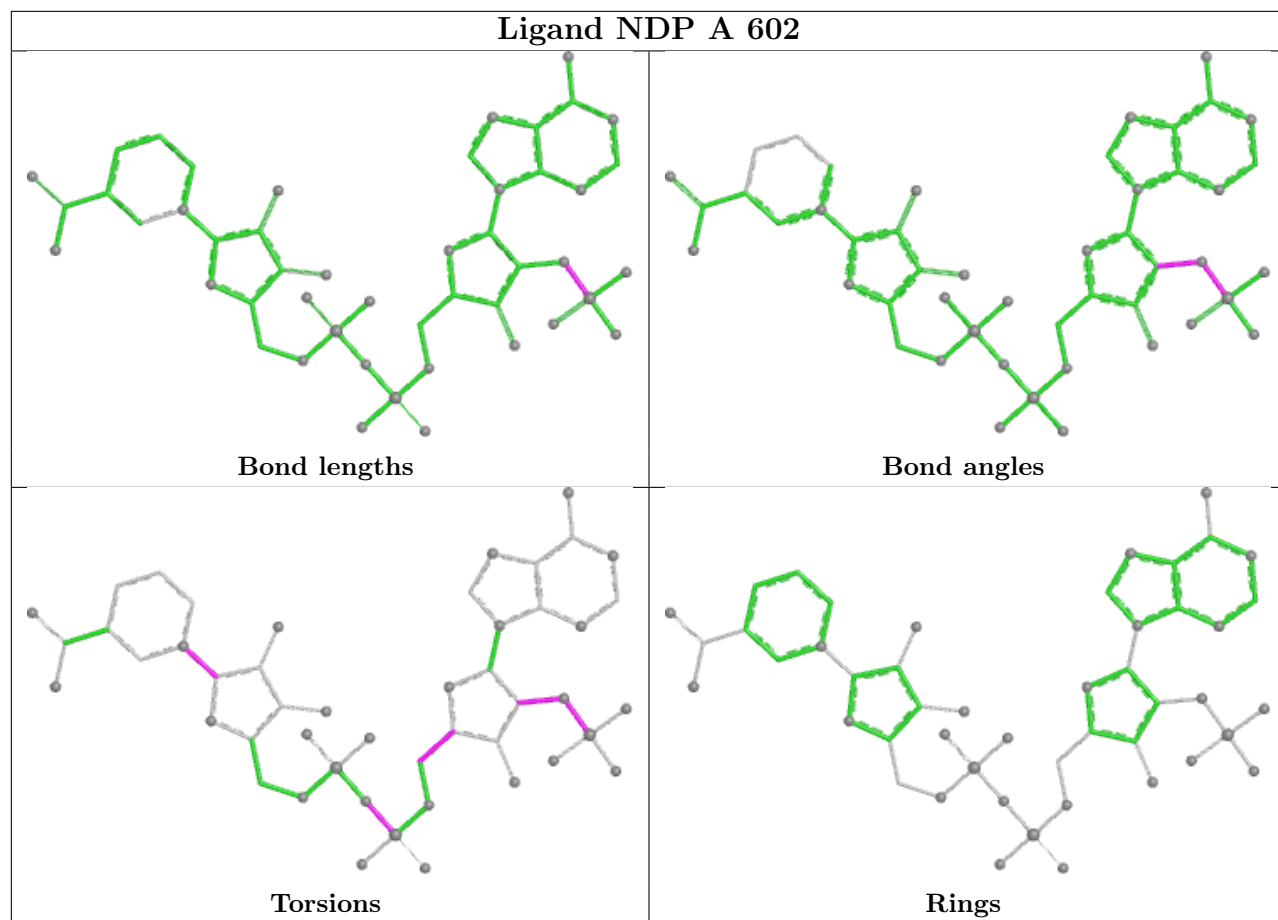
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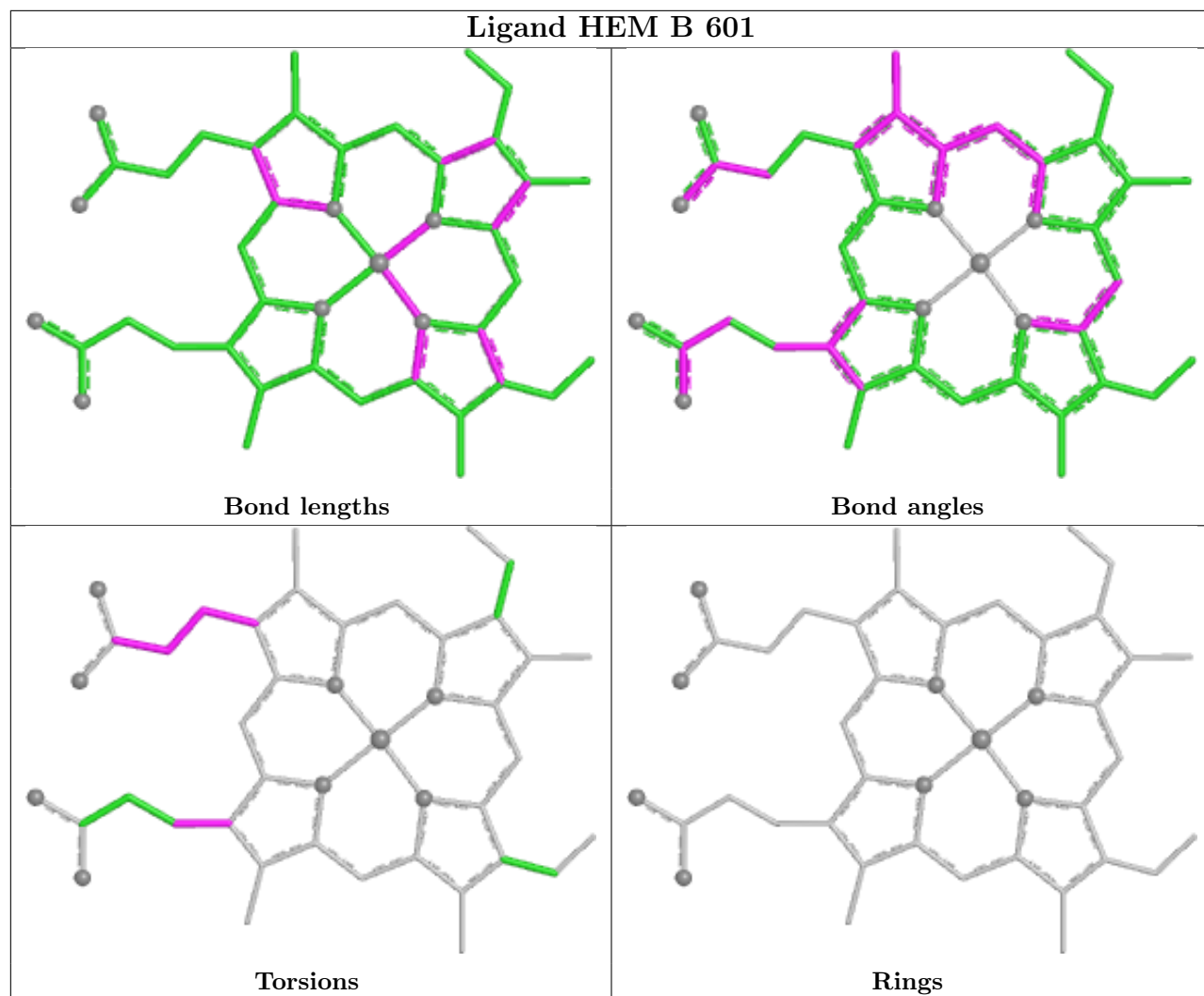
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	4	0
3	D	602	NDP	1	0
2	C	601	HEM	2	0

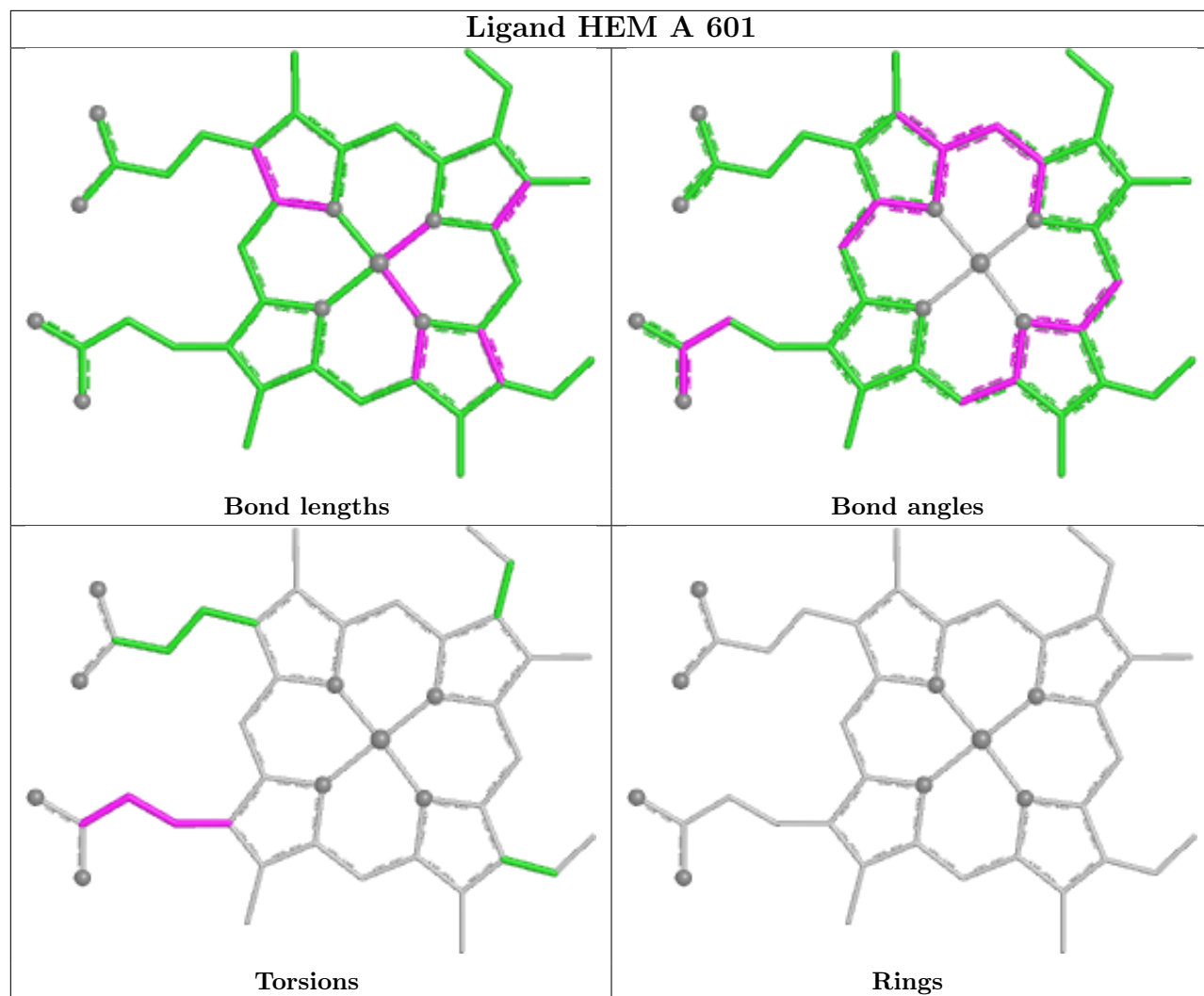
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

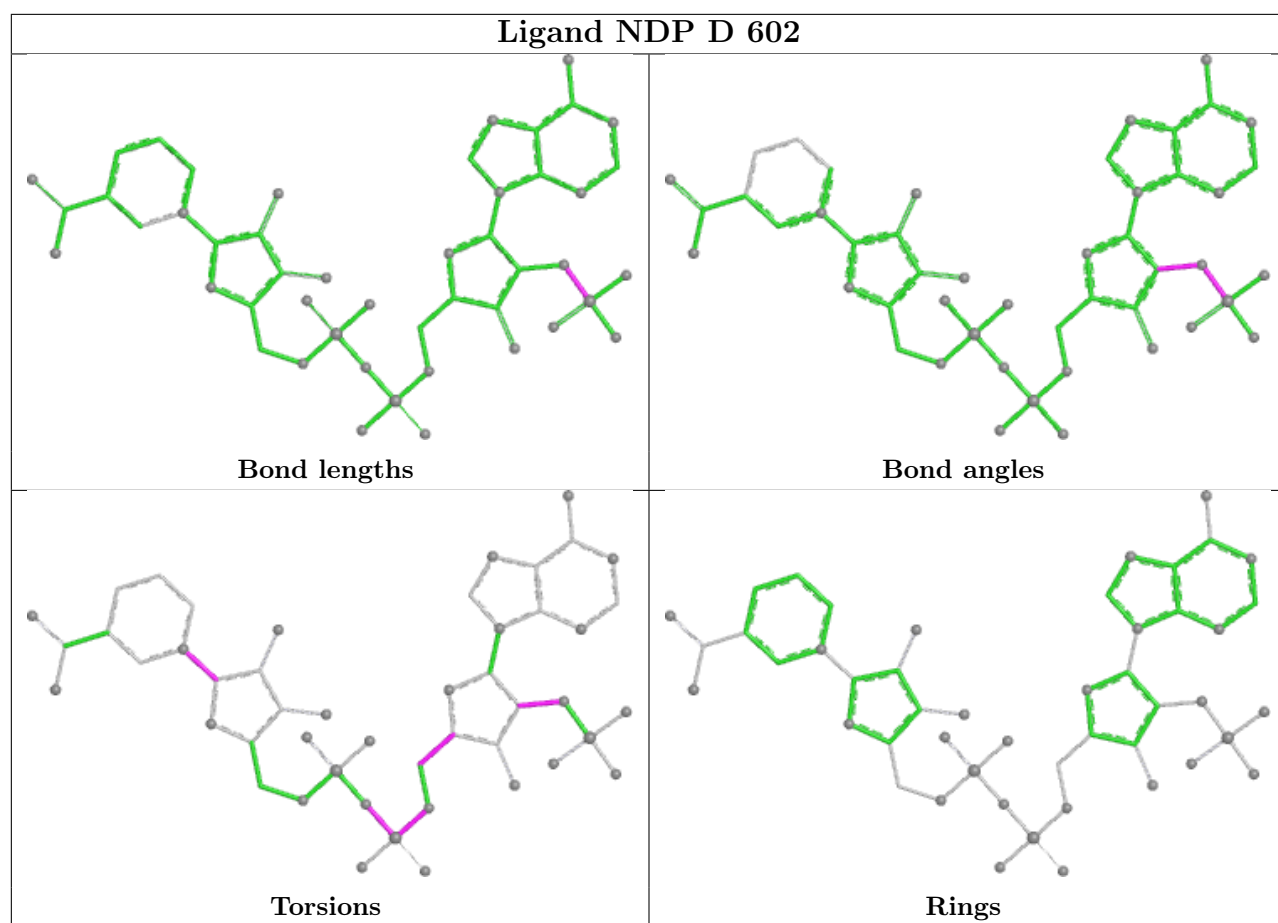


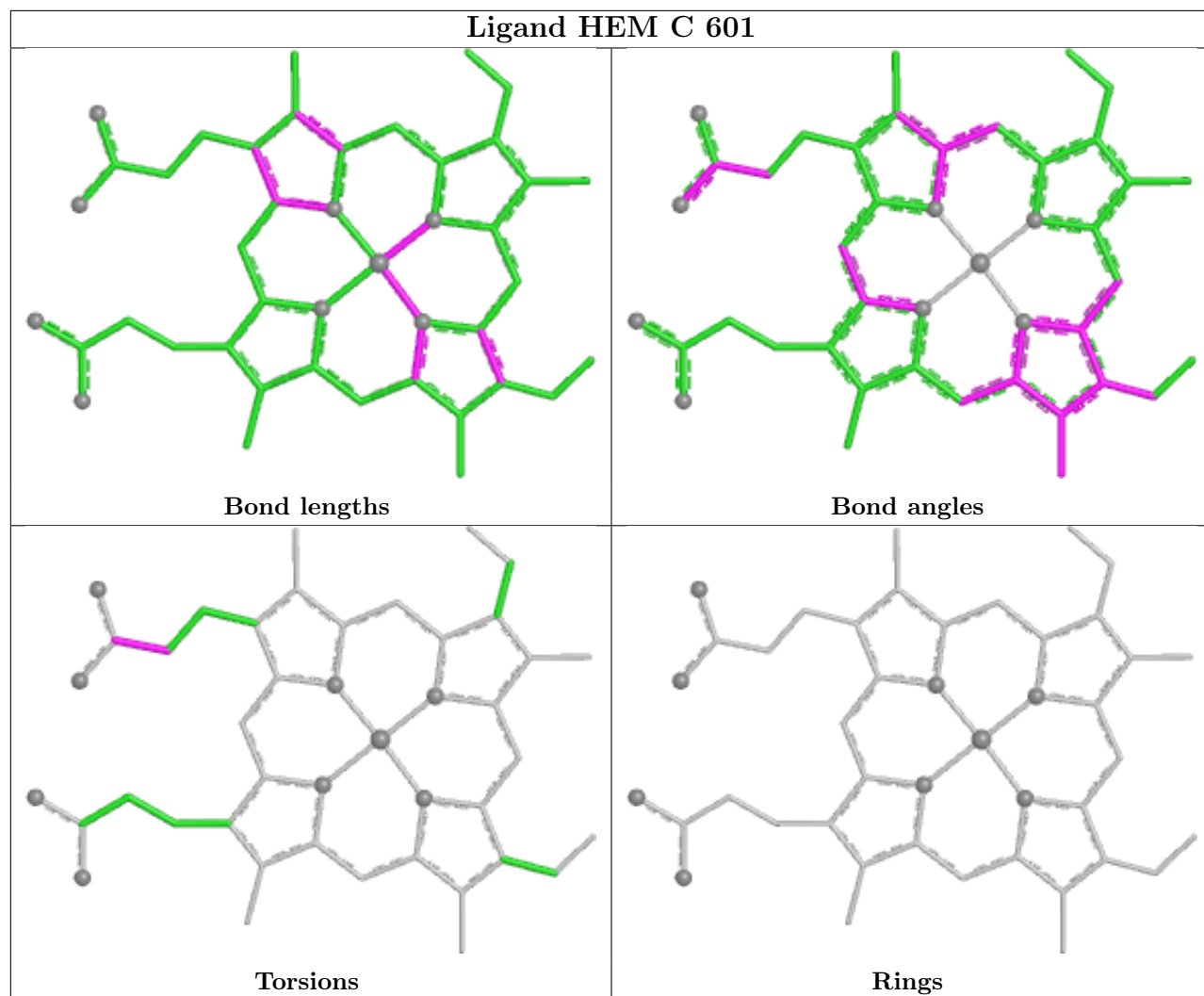


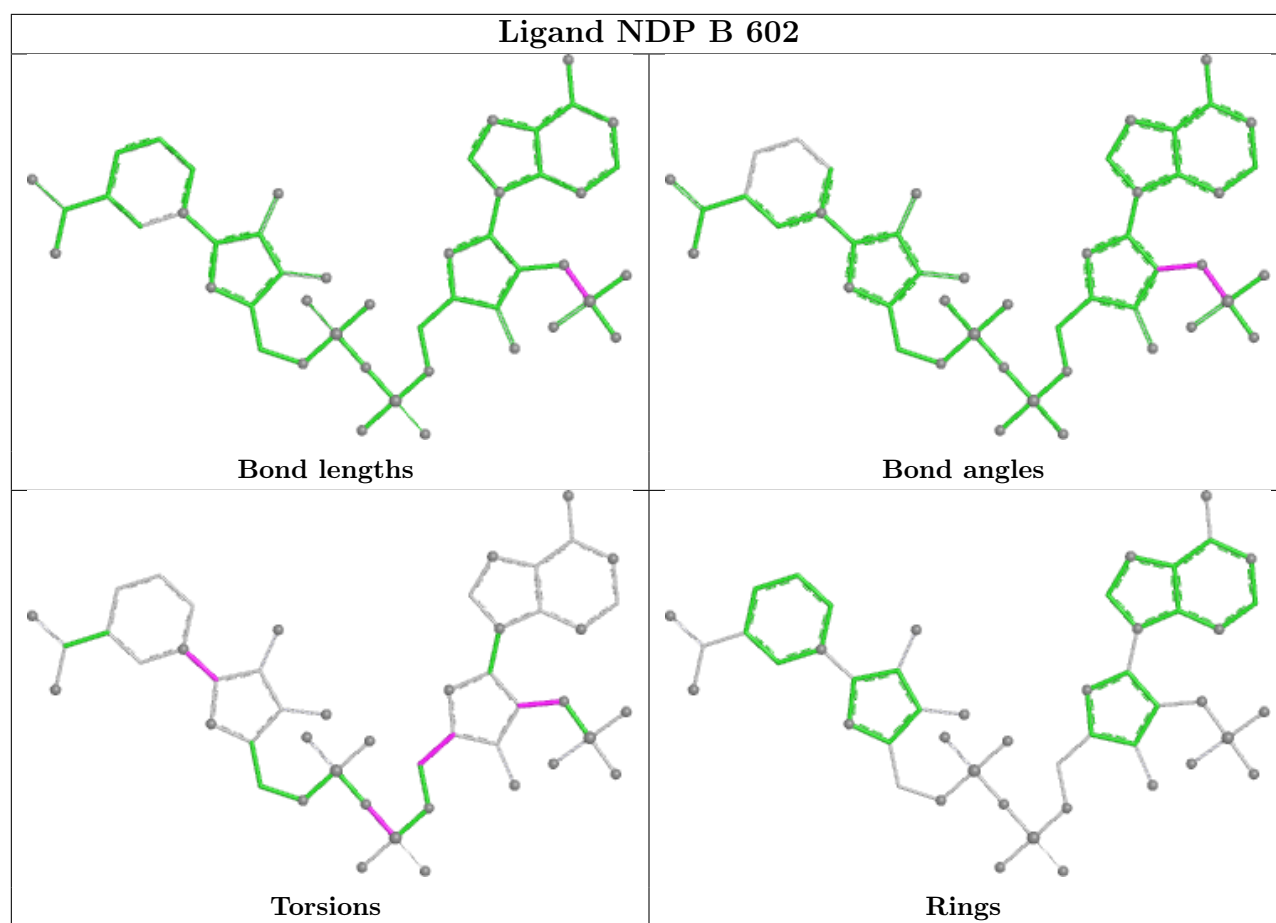












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.