



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 08:05 PM EDT

PDB ID : 1M64 / pdb_00001m64
Title : Crystal structure of Q363F mutant flavocytochrome c3
Authors : Mowat, C.G.; Pankhurst, K.L.; Miles, C.S.; Leys, D.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on : 2002-07-12
Resolution : 1.80 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) : **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) : 2.50

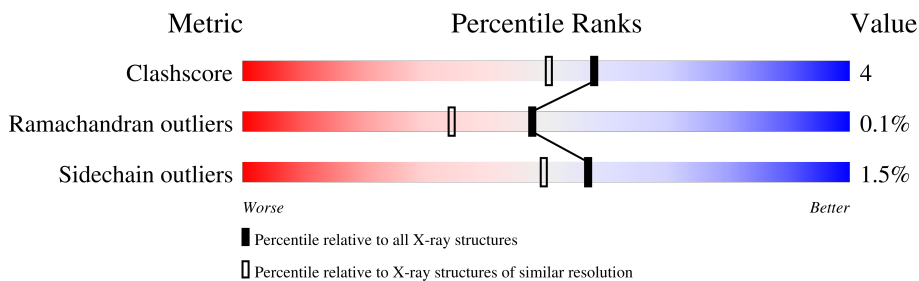
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	571	91% 8% ..
1	B	571	88% 10% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FUM	A	3001	-	X	-	-
5	FUM	B	4001	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10932 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 flavocytochrome c3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4183	2599	733	826	25			
1	B	568	Total	C	N	O	S	0	0	0
			4178	2593	732	828	25			

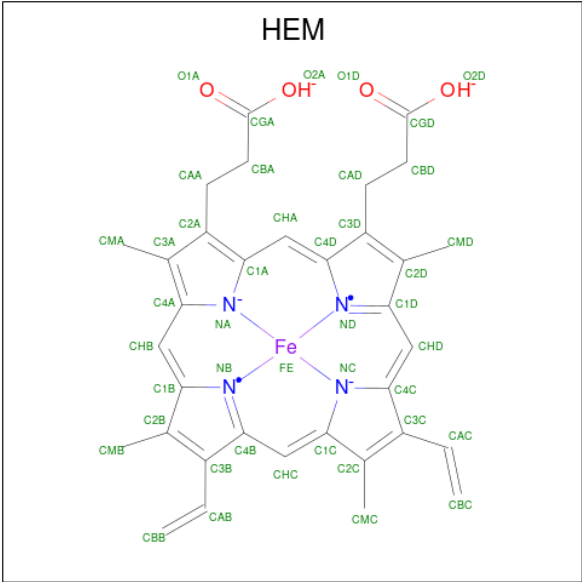
There are 2 discrepancies between the modelled and reference sequences:

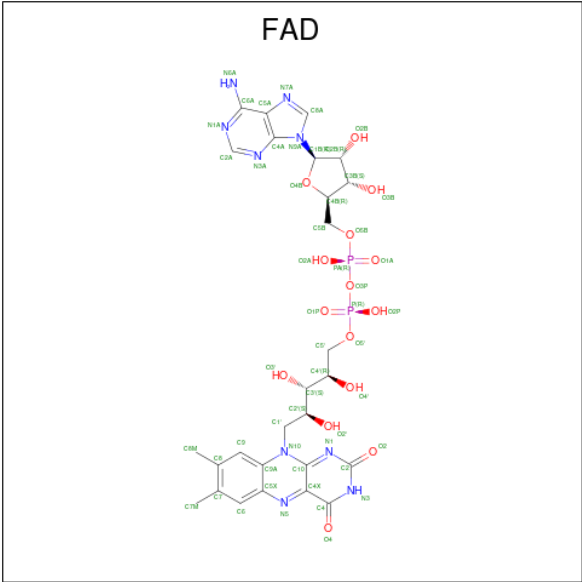
Chain	Residue	Modelled	Actual	Comment	Reference
A	363	PHE	GLN	engineered mutation	UNP Q02469
B	363	PHE	GLN	engineered mutation	UNP Q02469

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

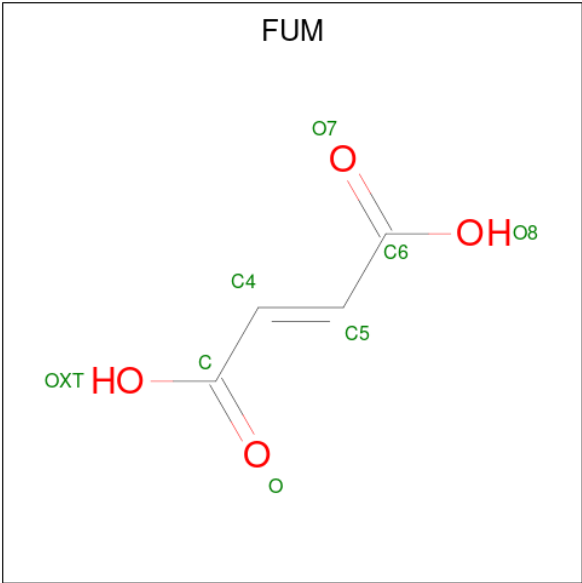
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1072	Total 1072	O 1072	0	0
6	B	1031	Total 1031	O 1031	0	0

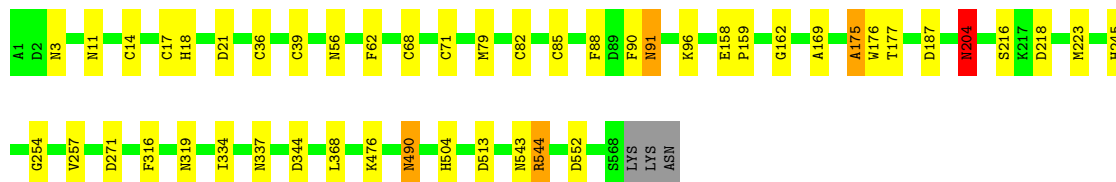
3 Residue-property plots

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. 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.

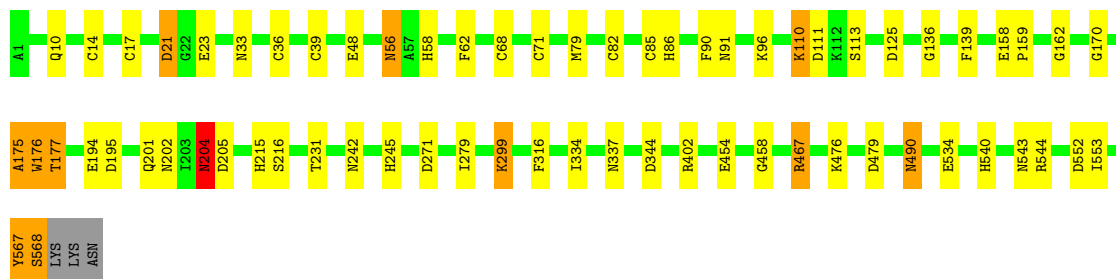
• Molecule 1: flavocytochrome c3

Chain A:  91% 8% ..



• Molecule 1: flavocytochrome c3

Chain B:  88% 10% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.52Å 88.89Å 91.19Å 90.00° 104.42° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-1.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.163 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10932	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: NA, FAD, FUM, 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	0.77	1/4254 (0.0%)	1.54	33/5760 (0.6%)
1	B	0.78	1/4249 (0.0%)	1.55	43/5756 (0.7%)
All	All	0.77	2/8503 (0.0%)	1.54	76/11516 (0.7%)

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	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	TRP	N-CA	-6.50	1.35	1.46
1	B	176	TRP	N-CA	-6.44	1.37	1.46

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ALA	CA-C-N	24.30	167.96	121.54
1	B	175	ALA	C-N-CA	24.30	167.96	121.54
1	A	175	ALA	CA-C-N	23.62	177.00	122.20
1	A	175	ALA	C-N-CA	23.62	177.00	122.20
1	B	204	ASN	CA-CB-CG	10.18	122.78	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ALA	Peptide
1	B	175	ALA	Peptide

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	4183	0	4070	31	0
1	B	4178	0	4053	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	172	0	120	23	0
3	B	172	0	120	23	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
5	A	8	0	1	0	0
5	B	8	0	1	0	0
6	A	1072	0	0	2	0
6	B	1031	0	0	5	0
All	All	10932	0	8427	77	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 77 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:36:CYS:SG	3:B:802:HEM:CAB	2.50	1.00
1:B:82:CYS:SG	3:B:804:HEM:CAB	2.51	0.98
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.52	0.98
1:A:36:CYS:SG	3:A:802:HEM:CAB	2.52	0.97
1:B:68:CYS:SG	3:B:803:HEM:CAB	2.52	0.97

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	566/571 (99%)	546 (96%)	20 (4%)	0	100	100
1	B	566/571 (99%)	544 (96%)	21 (4%)	1 (0%)	43	31
All	All	1132/1142 (99%)	1090 (96%)	41 (4%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	176	TRP

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	429/445 (96%)	424 (99%)	5 (1%)	63	57
1	B	429/445 (96%)	421 (98%)	8 (2%)	50	41
All	All	858/890 (96%)	845 (98%)	13 (2%)	57	49

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	110	LYS
1	B	204	ASN
1	B	544	ARG
1	B	467	ARG
1	B	490	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	202	ASN
1	B	275	ASN
1	B	245	HIS
1	B	389	ASN
1	A	389	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	HEM	A	804	1	50,50,50	1.33	8 (16%)	67,82,82	1.09	4 (5%)
3	HEM	B	802	1	50,50,50	1.27	6 (12%)	67,82,82	1.22	6 (8%)
5	FUM	A	3001	-	7,7,7	2.61	4 (57%)	8,8,8	1.94	4 (50%)
3	HEM	A	801	1	50,50,50	1.36	7 (14%)	67,82,82	1.10	4 (5%)
3	HEM	A	803	1	50,50,50	1.43	9 (18%)	67,82,82	1.18	5 (7%)
3	HEM	A	802	1	50,50,50	1.36	9 (18%)	67,82,82	1.43	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	B	804	1	50,50,50	1.34	7 (14%)	67,82,82	1.19	9 (13%)
3	HEM	B	803	1	50,50,50	1.29	5 (10%)	67,82,82	1.10	3 (4%)
4	FAD	B	4000	-	58,58,58	1.37	4 (6%)	85,89,89	1.16	6 (7%)
3	HEM	B	801	1	50,50,50	1.39	9 (18%)	67,82,82	1.16	5 (7%)
4	FAD	A	3000	-	58,58,58	1.39	8 (13%)	85,89,89	1.22	8 (9%)
5	FUM	B	4001	-	7,7,7	2.84	4 (57%)	8,8,8	2.04	4 (50%)

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	HEM	A	804	1	-	5/14/54/54	-
3	HEM	B	802	1	-	2/14/54/54	-
5	FUM	A	3001	-	-	2/5/5/5	-
3	HEM	A	801	1	-	4/14/54/54	-
3	HEM	A	803	1	-	2/14/54/54	-
3	HEM	A	802	1	-	3/14/54/54	-
3	HEM	B	804	1	-	3/14/54/54	-
3	HEM	B	803	1	-	2/14/54/54	-
4	FAD	B	4000	-	-	10/34/50/50	0/6/6/6
3	HEM	B	801	1	-	3/14/54/54	-
4	FAD	A	3000	-	-	10/34/50/50	0/6/6/6
5	FUM	B	4001	-	-	2/5/5/5	-

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4001	FUM	O-C	4.42	1.33	1.23
5	B	4001	FUM	O7-C6	4.16	1.33	1.23
5	A	3001	FUM	O-C	4.16	1.33	1.23
4	B	4000	FAD	C6-C5X	4.16	1.46	1.40
4	B	4000	FAD	C2'-C3'	3.89	1.60	1.53

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3000	FAD	O5'-C5'-C4'	-4.80	96.56	109.36
3	B	803	HEM	CAD-CBD-CGD	4.77	126.32	113.67
4	B	4000	FAD	O5'-C5'-C4'	-4.59	97.10	109.36
3	A	802	HEM	C3B-C4B-NB	-3.84	106.71	109.47
3	A	802	HEM	CAA-CBA-CGA	3.55	123.08	113.67

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	4000	FAD	N10-C1'-C2'-O2'
4	A	3000	FAD	C2'-C3'-C4'-O4'
4	B	4000	FAD	C2'-C3'-C4'-O4'
5	B	4001	FUM	O-C-C4-C5
4	A	3000	FAD	O3'-C3'-C4'-O4'

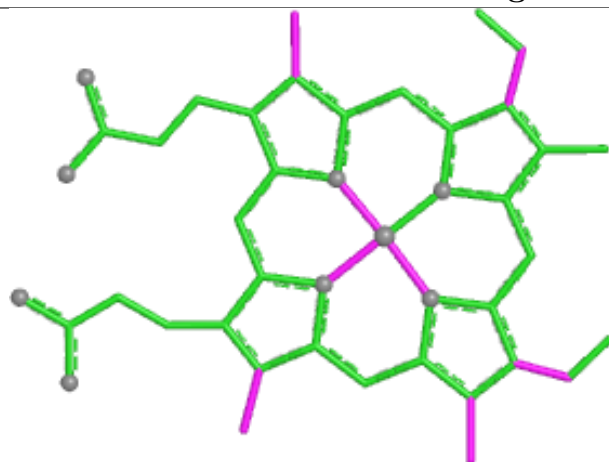
There are no ring outliers.

8 monomers are involved in 46 short contacts:

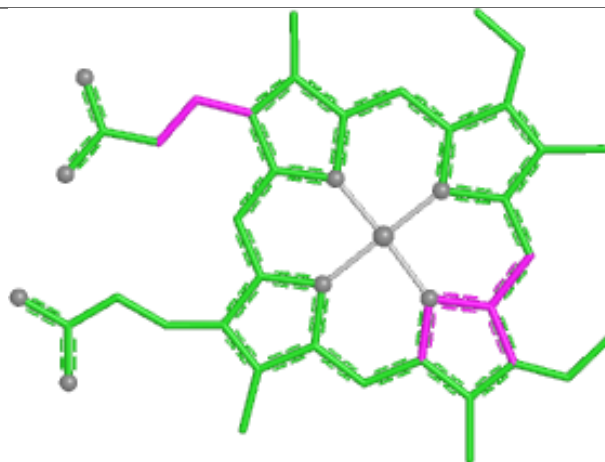
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	HEM	6	0
3	B	802	HEM	6	0
3	A	801	HEM	7	0
3	A	803	HEM	6	0
3	A	802	HEM	4	0
3	B	804	HEM	7	0
3	B	803	HEM	6	0
3	B	801	HEM	4	0

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.

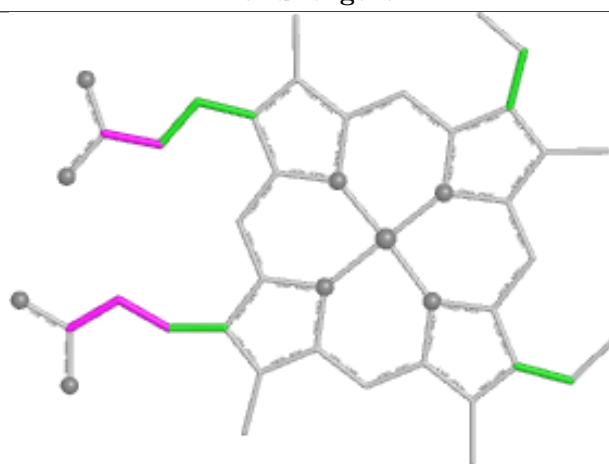
Ligand HEM A 804



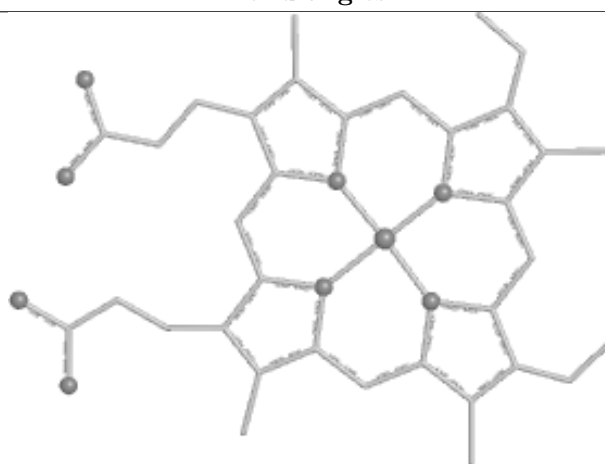
Bond lengths



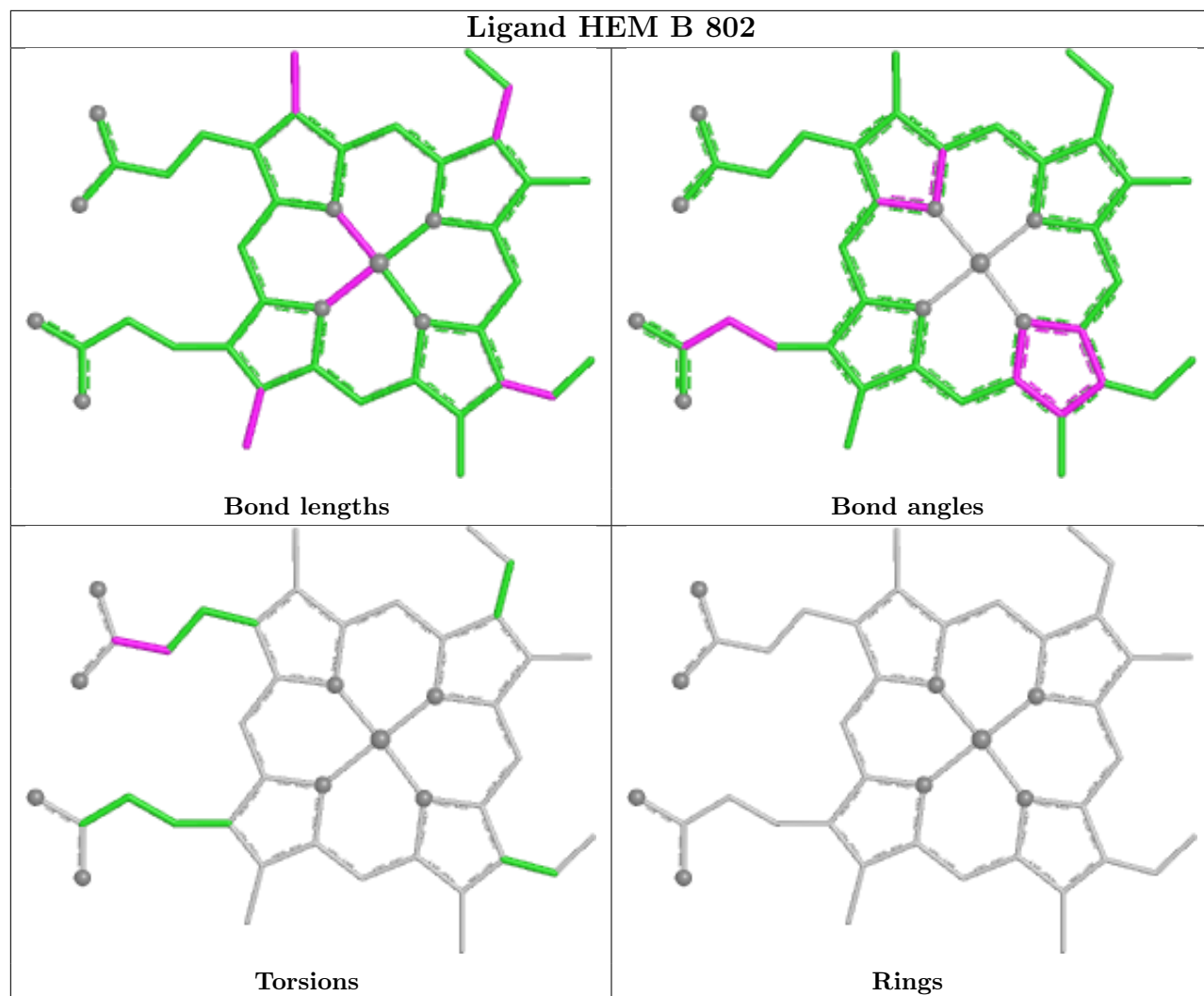
Bond angles

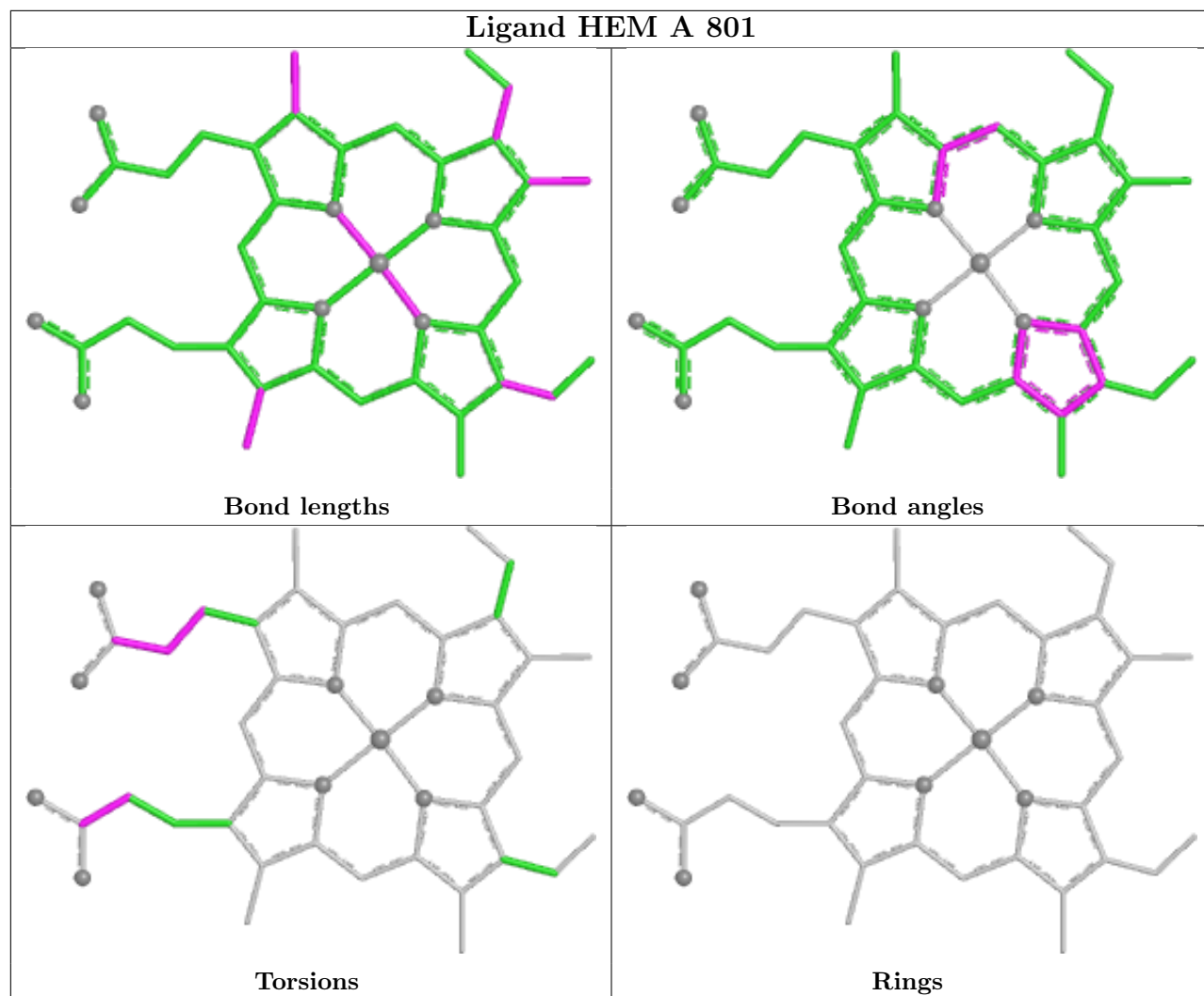


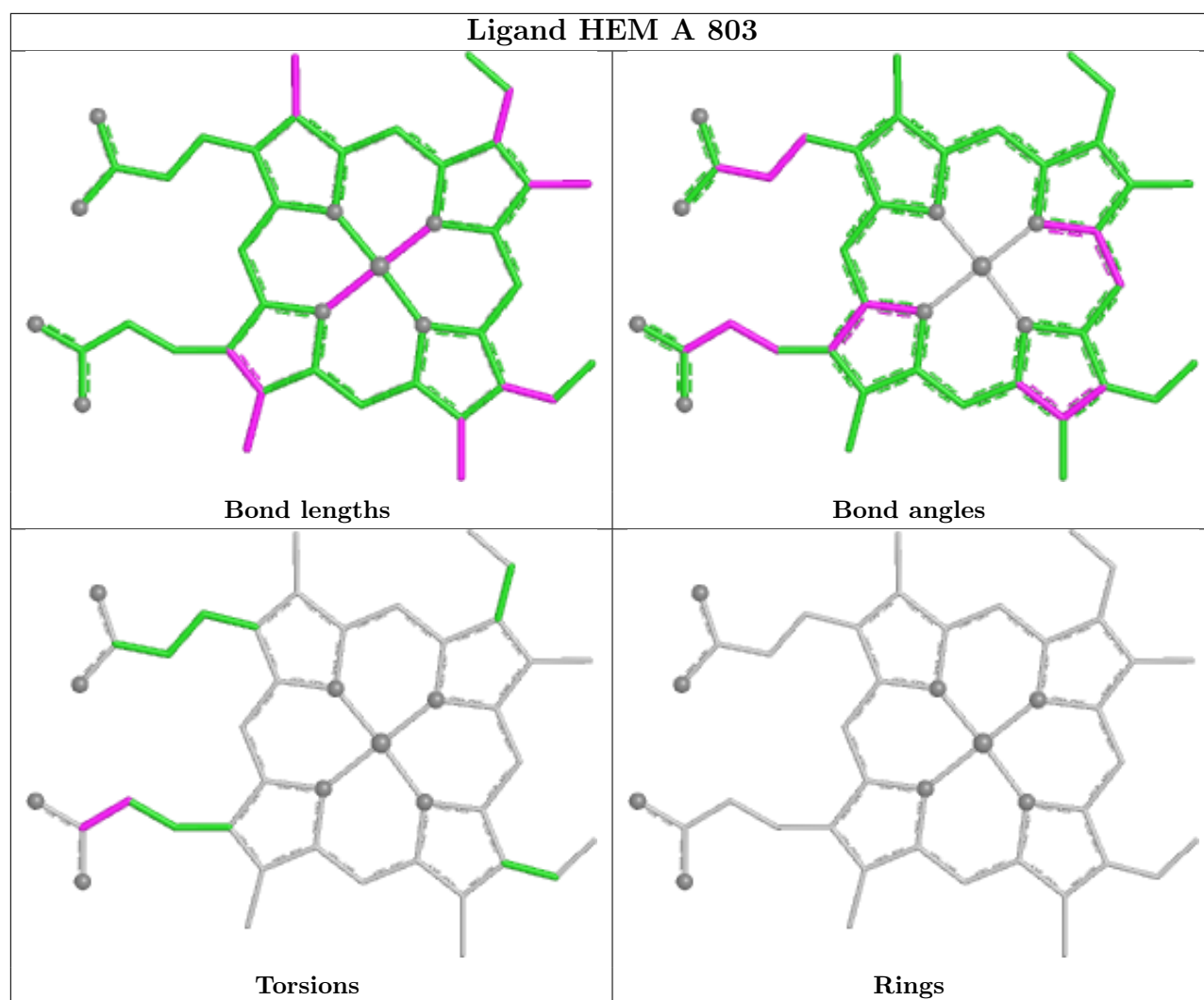
Torsions

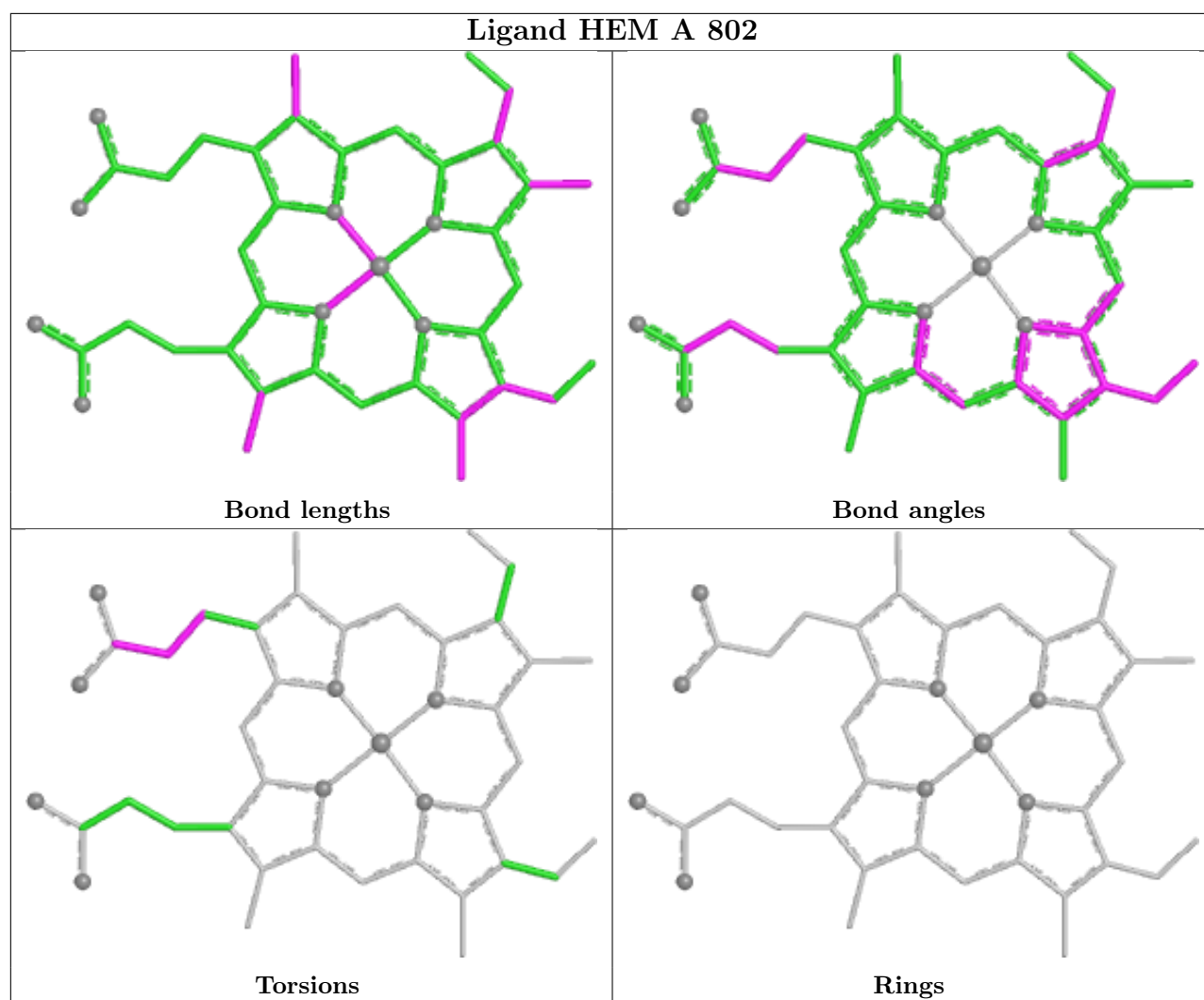


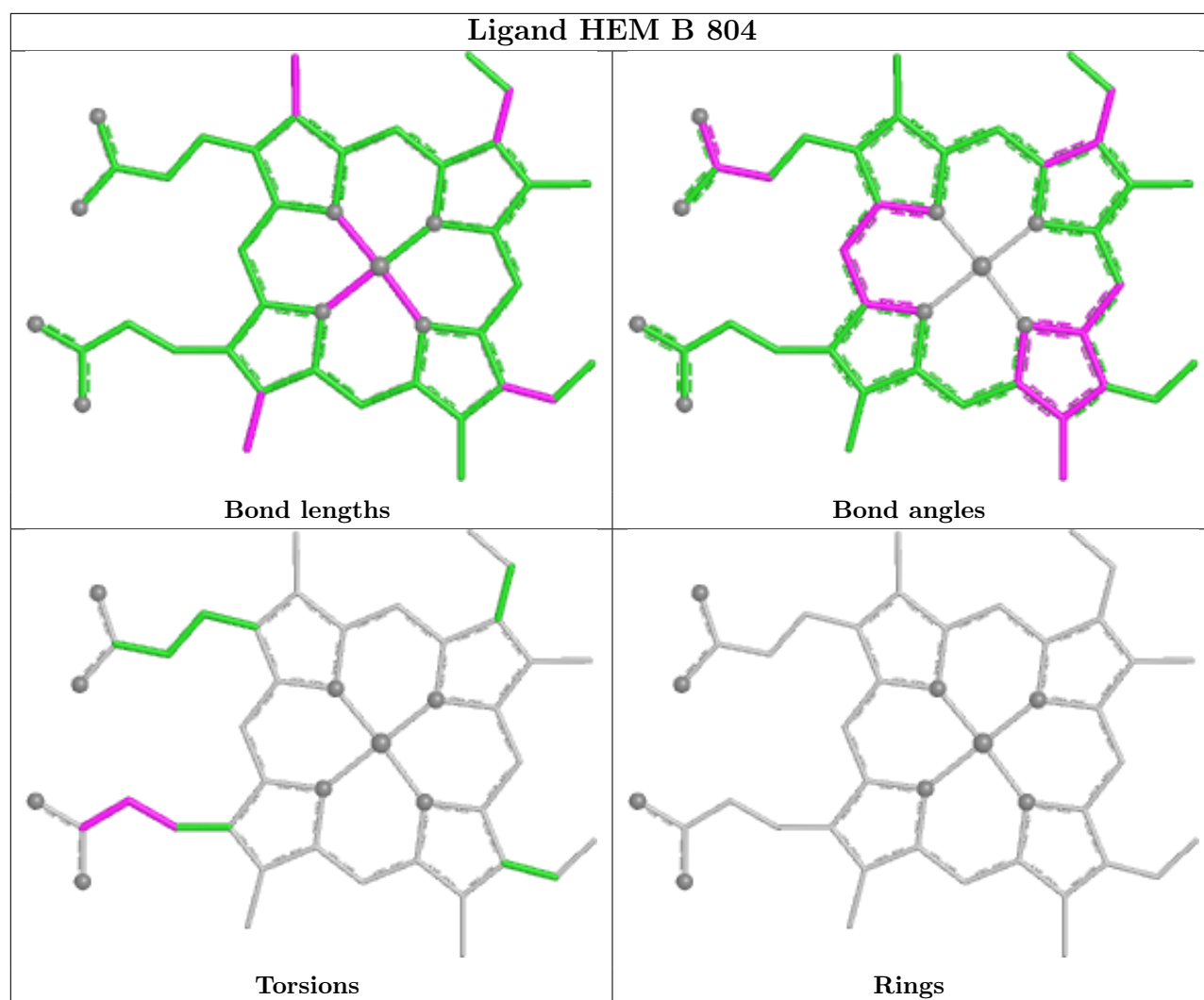
Rings

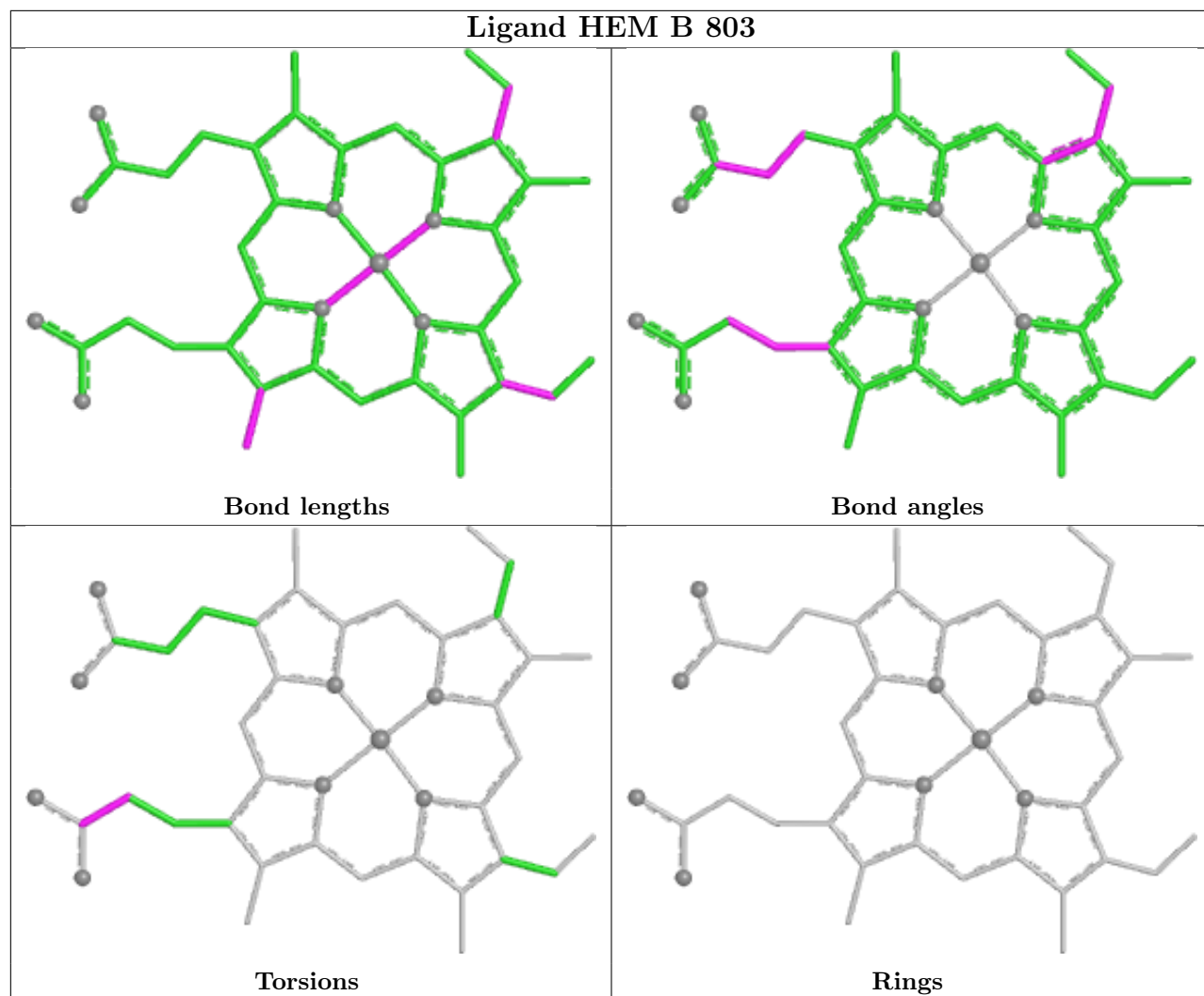


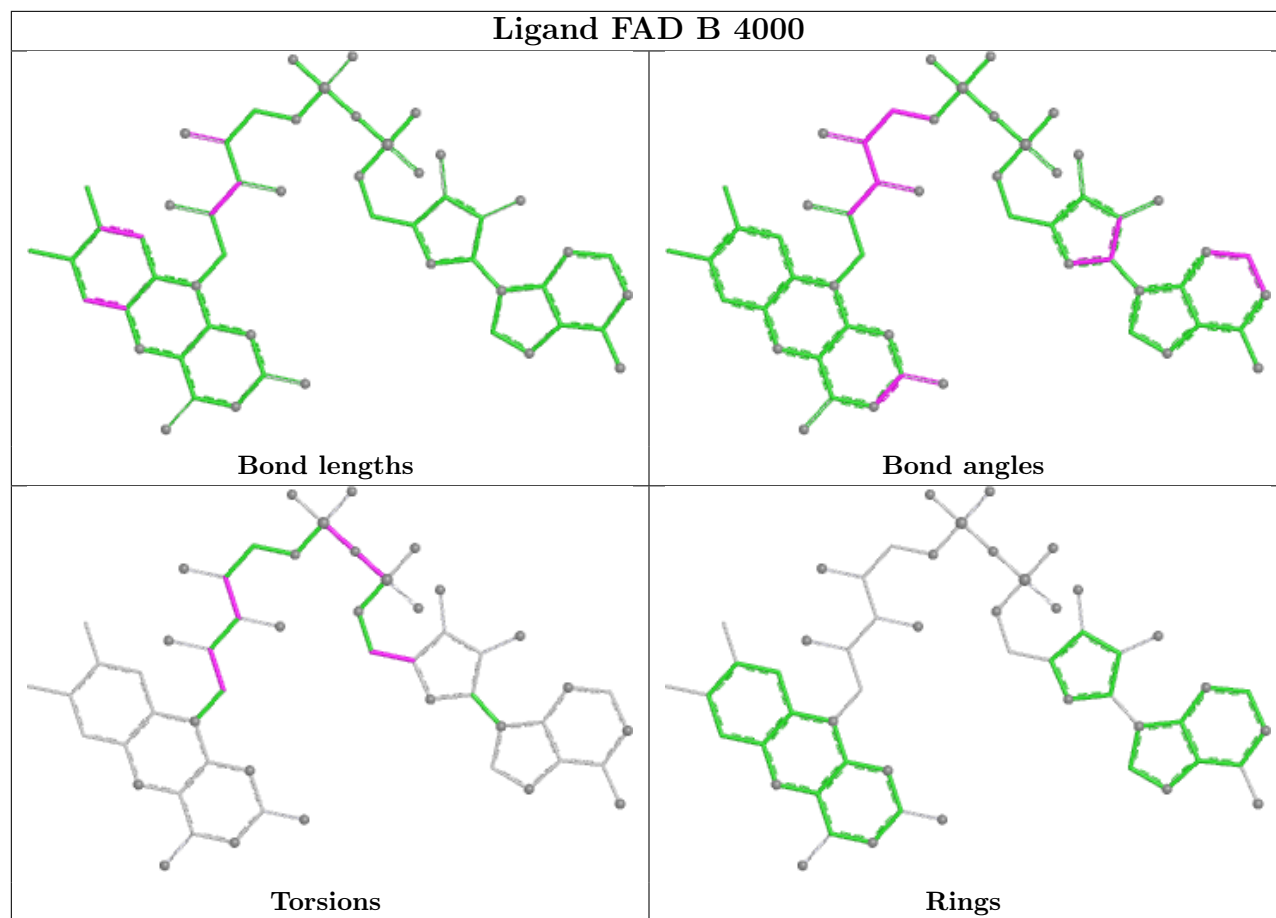


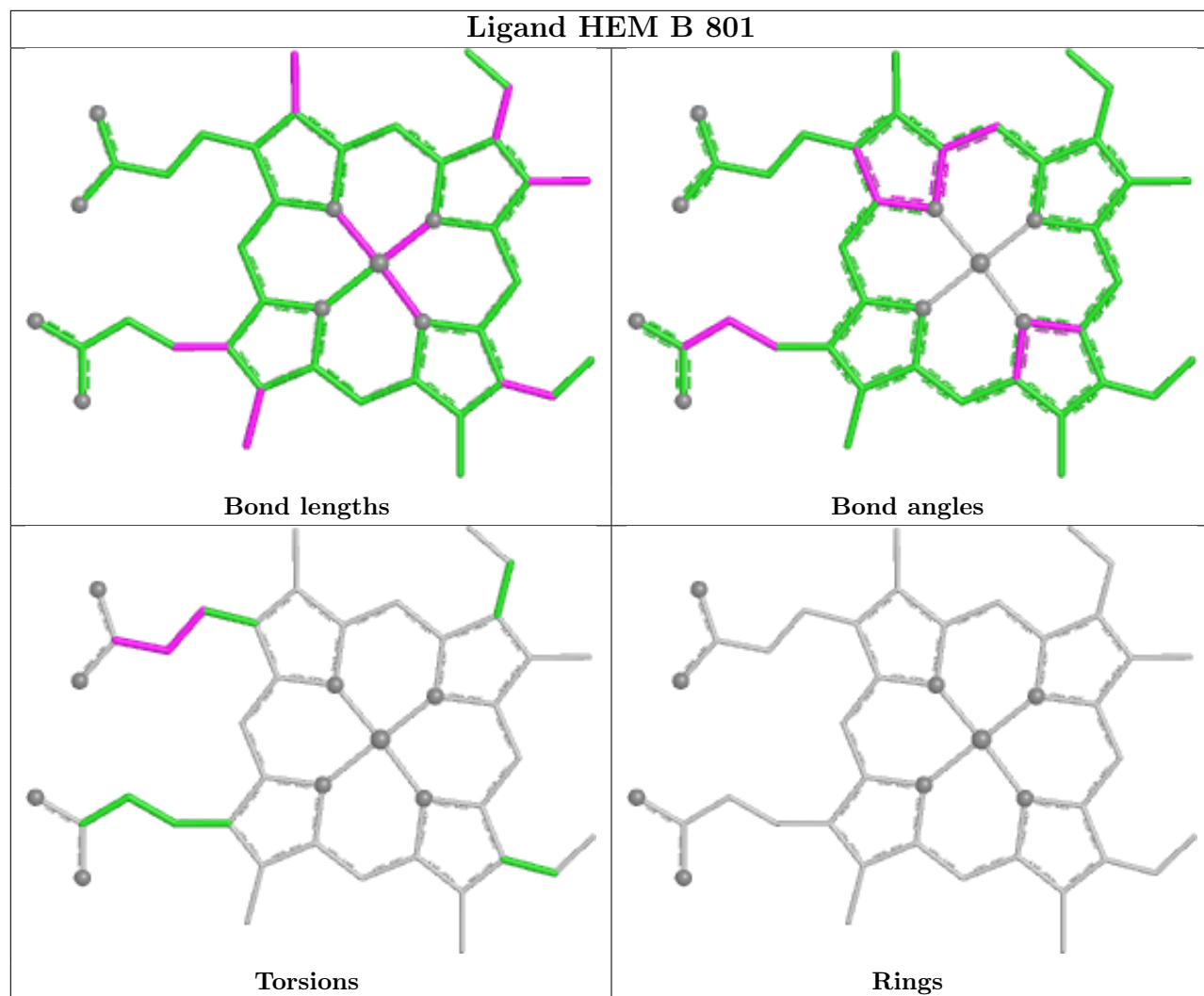


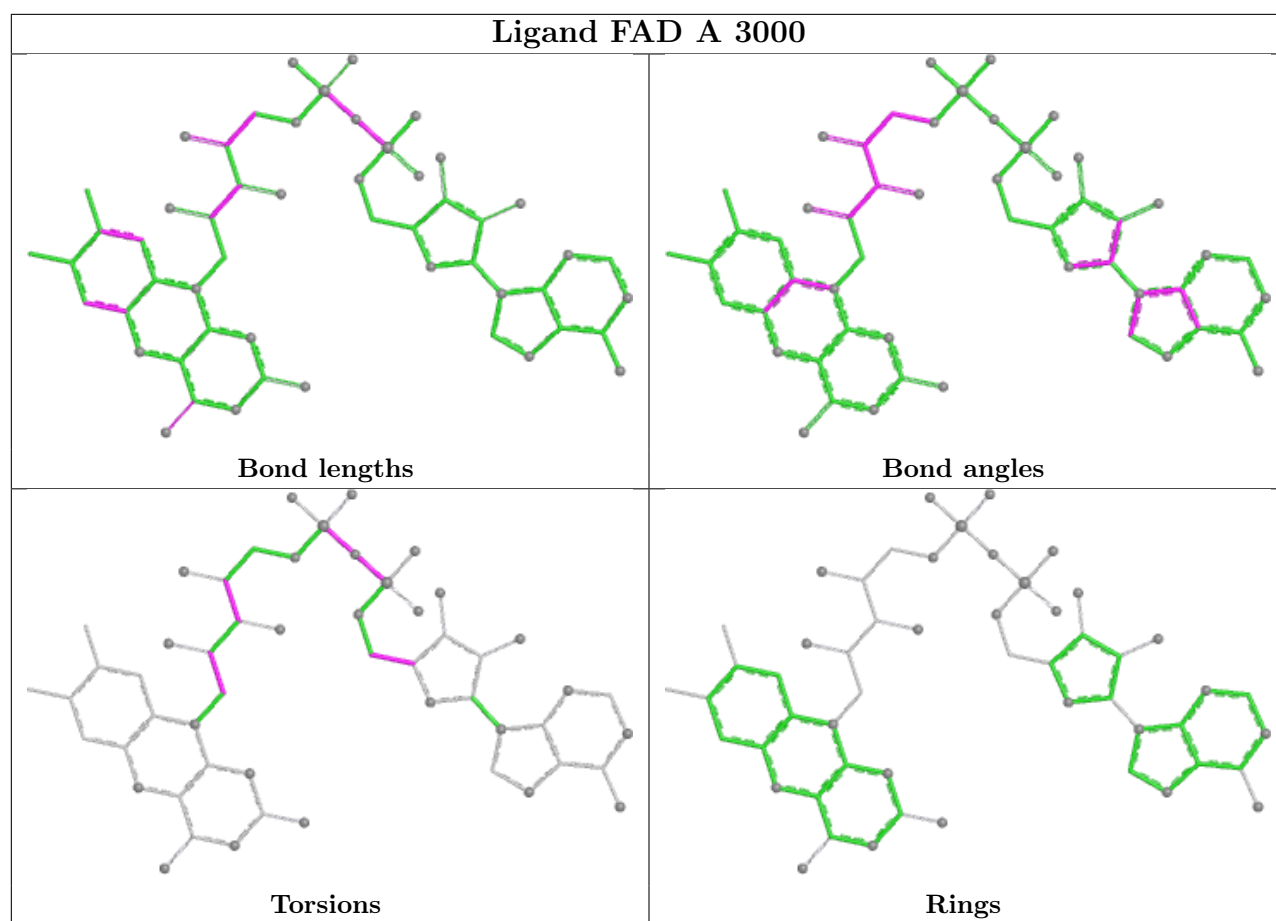












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.