



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 17, 2021 – 07:44 AM EDT

PDB ID : 1KSU
Title : Crystal Structure of His505Tyr Mutant Flavocytochrome c3 from *Shewanella frigidimarina*
Authors : Pankhurst, K.L.; Mowat, C.G.; Miles, C.S.; Leys, D.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on : 2002-01-14
Resolution : 2.00 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 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)
Xtriage (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) : 2.23.2

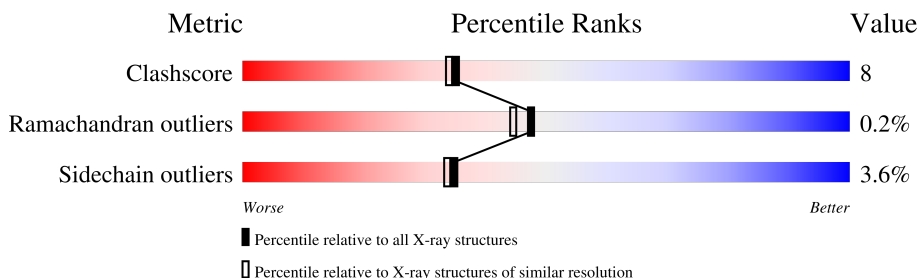
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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	
1	B	571	

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
4	FAD	A	2805	X	-	-	-
4	FAD	B	3805	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10753 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 c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4202	2608	738	831	25			
1	B	568	Total	C	N	O	S	0	0	0
			4216	2617	742	832	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	TYR	HIS	engineered mutation	UNP Q02469
B	505	TYR	HIS	engineered mutation	UNP Q02469

- Molecule 2 is SODIUM ION (three-letter code: 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 (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



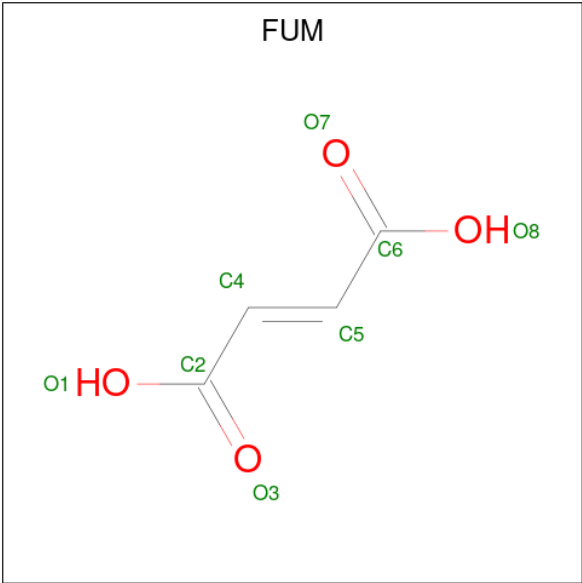
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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 (three-letter code: 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.

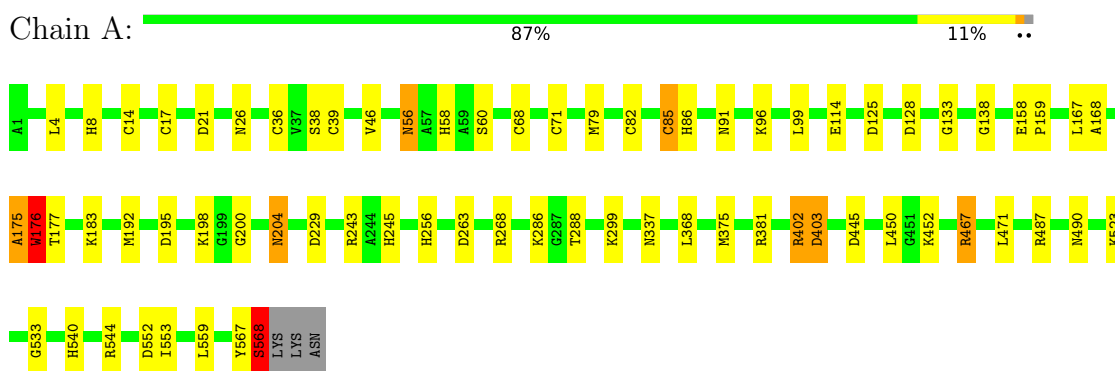
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	932	Total 932	O 932	0	0
6	B	935	Total 935	O 935	0	0

3 Residue-property plots [i](#)

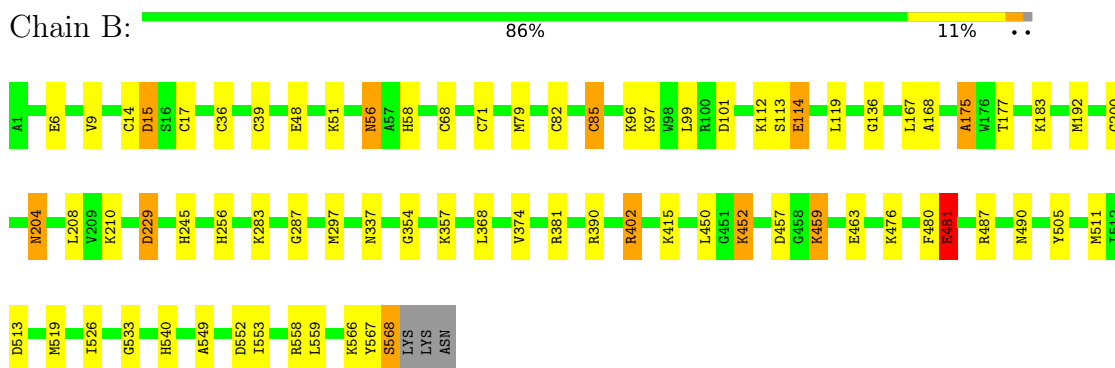
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: flavocytochrome c



- Molecule 1: flavocytochrome c



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	76.99Å 87.27Å 89.37Å 90.00° 104.43° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10753	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: HEM, FAD, NA, FUM

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	0.60	1/4272 (0.0%)	1.29	24/5779 (0.4%)
1	B	0.58	0/4286	1.26	21/5794 (0.4%)
All	All	0.59	1/8558 (0.0%)	1.28	45/11573 (0.4%)

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	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	TRP	N-CA	-5.74	1.34	1.46

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	C-N-CA	18.36	167.60	121.70
1	A	467	ARG	NE-CZ-NH2	12.80	126.70	120.30
1	B	175	ALA	O-C-N	-11.50	104.30	122.70
1	A	487	ARG	NE-CZ-NH2	11.50	126.05	120.30
1	A	381	ARG	NE-CZ-NH1	10.86	125.73	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ASP	Mainchain
1	A	175	ALA	Peptide
1	B	175	ALA	Mainchain,Peptide

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	4202	0	4124	61	0
1	B	4216	0	4160	80	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	172	0	120	28	0
3	B	172	0	120	32	0
4	A	53	0	30	5	0
4	B	53	0	30	6	0
5	A	8	0	2	3	0
5	B	8	0	2	1	0
6	A	932	0	0	8	0
6	B	935	0	0	18	0
All	All	10753	0	8588	143	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 8.

The worst 5 of 143 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:36:CYS:SG	3:A:802:HEM:CAB	2.44	1.04
1:B:36:CYS:SG	3:B:802:HEM:CAB	2.44	1.04
1:B:82:CYS:SG	3:B:804:HEM:CAB	2.48	1.02
1:B:68:CYS:SG	3:B:803:HEM:CAB	2.51	0.99
1:B:82:CYS:HG	3:B:804:HEM:CAB	1.77	0.97

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	566/571 (99%)	546 (96%)	19 (3%)	1 (0%)	47	44
1	B	566/571 (99%)	548 (97%)	17 (3%)	1 (0%)	47	44
All	All	1132/1142 (99%)	1094 (97%)	36 (3%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TRP
1	B	114	GLU

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	437/445 (98%)	422 (97%)	15 (3%)	37	36
1	B	441/445 (99%)	424 (96%)	17 (4%)	32	30
All	All	878/890 (99%)	846 (96%)	32 (4%)	35	34

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	476	LYS
1	B	481	GLU
1	A	523	LYS
1	A	490	ASN

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Mol	Chain	Res	Type
1	B	490	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	490	ASN
1	B	256	HIS
1	B	54	HIS
1	B	245	HIS
1	B	35	GLN

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 monosaccharides 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	801	1	27,50,50	2.14	7 (25%)	17,82,82	1.87	6 (35%)
4	FAD	A	2805	-	51,58,58	1.89	12 (23%)	60,89,89	2.95	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUM	A	2806	-	1,7,7	1.22	0	2,8,8	5.07	2 (100%)
3	HEM	B	802	1	27,50,50	1.97	4 (14%)	17,82,82	2.24	7 (41%)
3	HEM	B	804	1	27,50,50	2.16	6 (22%)	17,82,82	2.44	8 (47%)
3	HEM	A	803	1	27,50,50	2.08	6 (22%)	17,82,82	2.11	6 (35%)
3	HEM	B	803	1	27,50,50	2.01	5 (18%)	17,82,82	2.27	8 (47%)
3	HEM	A	802	1	27,50,50	2.09	7 (25%)	17,82,82	1.93	6 (35%)
3	HEM	B	801	1	27,50,50	2.09	7 (25%)	17,82,82	2.01	7 (41%)
3	HEM	A	804	1	27,50,50	2.14	7 (25%)	17,82,82	1.95	6 (35%)
5	FUM	B	3806	-	1,7,7	0.99	0	2,8,8	4.26	2 (100%)
4	FAD	B	3805	-	51,58,58	1.93	10 (19%)	60,89,89	3.07	20 (33%)

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	801	1	-	1/6/54/54	-
4	FAD	A	2805	-	1/1/9/9	10/30/50/50	0/6/6/6
5	FUM	A	2806	-	-	0/0/5/5	-
3	HEM	B	802	1	-	0/6/54/54	-
3	HEM	B	804	1	-	0/6/54/54	-
3	HEM	A	803	1	-	0/6/54/54	-
3	HEM	B	803	1	-	0/6/54/54	-
3	HEM	A	802	1	-	0/6/54/54	-
3	HEM	B	801	1	-	0/6/54/54	-
3	HEM	A	804	1	-	0/6/54/54	-
5	FUM	B	3806	-	-	0/0/5/5	-
4	FAD	B	3805	-	1/1/9/9	10/30/50/50	0/6/6/6

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	C3B-C2B	-5.74	1.32	1.40
4	B	3805	FAD	C4-C4X	5.62	1.51	1.41
4	A	2805	FAD	C4X-C10	5.52	1.44	1.38
3	B	804	HEM	C3C-C2C	-5.47	1.32	1.40
3	B	803	HEM	C3C-C2C	-5.34	1.33	1.40

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2805	FAD	C4-N3-C2	11.21	124.61	115.14
4	B	3805	FAD	C4-N3-C2	10.57	124.06	115.14
4	A	2805	FAD	C4X-C4-N3	-8.92	111.24	123.43
4	B	3805	FAD	C4X-C4-N3	-8.39	111.95	123.43
4	B	3805	FAD	C5A-C6A-N6A	7.60	131.90	120.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2805	FAD	C4'
4	B	3805	FAD	C4'

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2805	FAD	C2'-C3'-C4'-C5'
4	A	2805	FAD	O3'-C3'-C4'-O4'
4	A	2805	FAD	O3'-C3'-C4'-C5'
4	A	2805	FAD	PA-O3P-P-O5'
4	B	3805	FAD	C2'-C3'-C4'-C5'

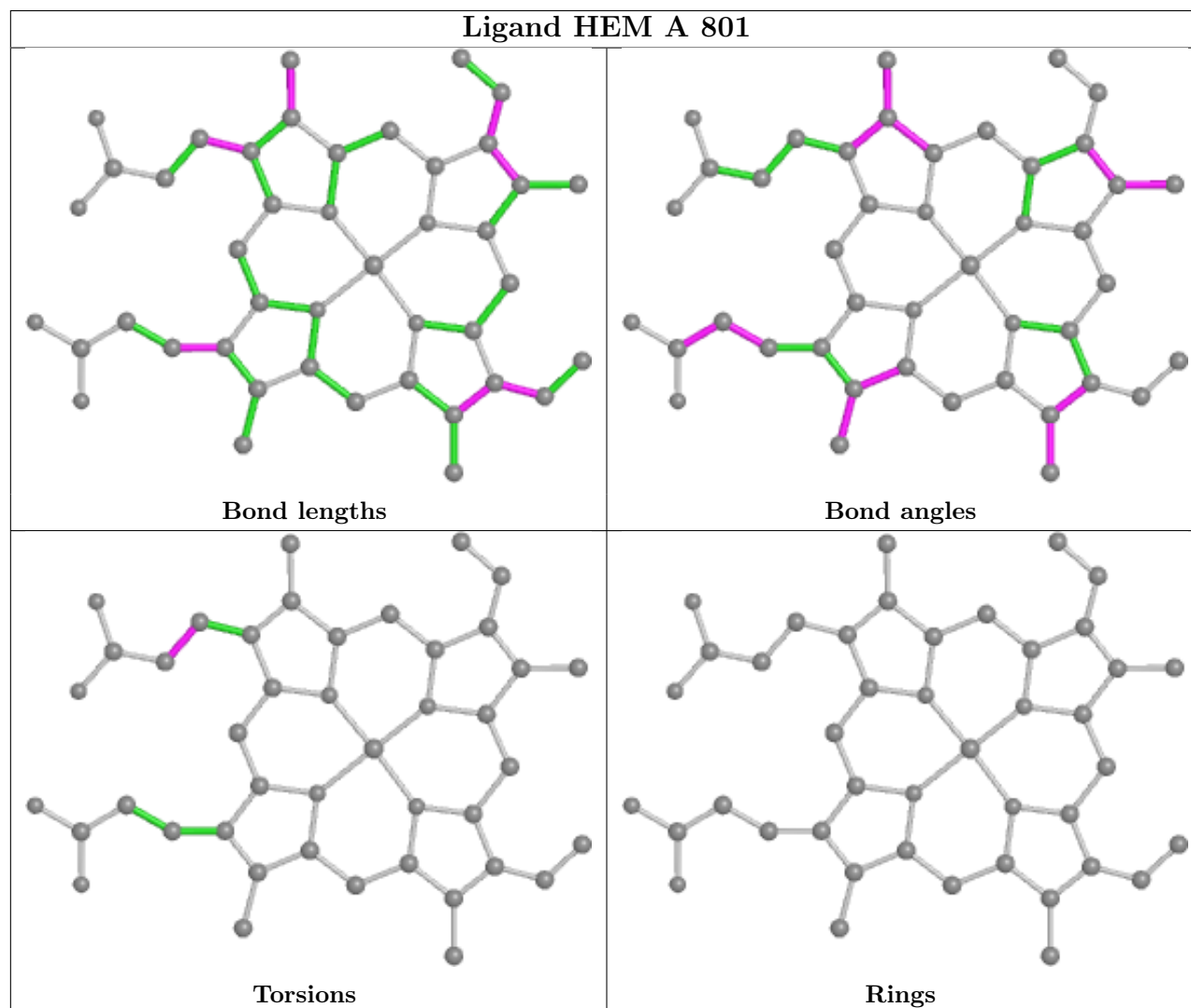
There are no ring outliers.

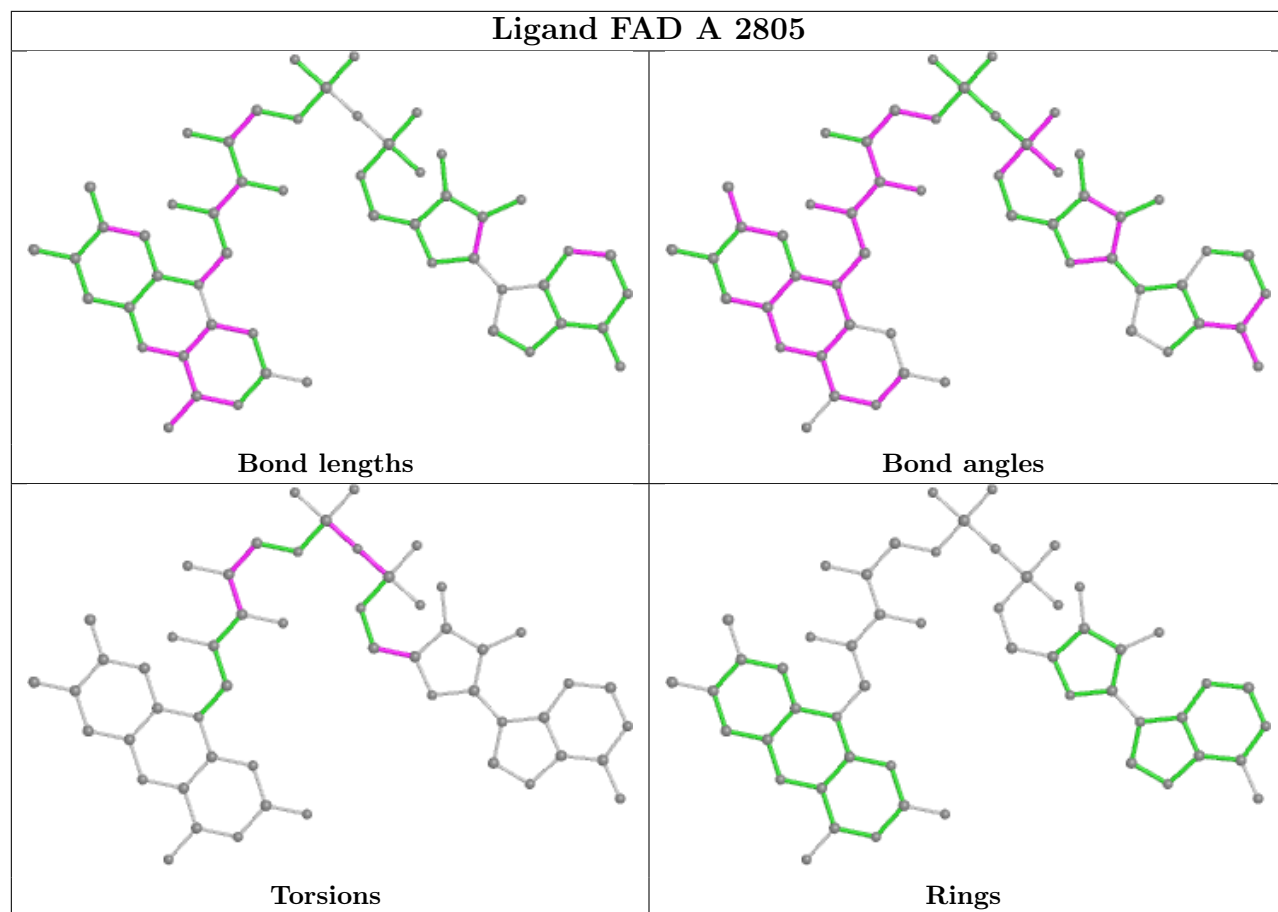
12 monomers are involved in 75 short contacts:

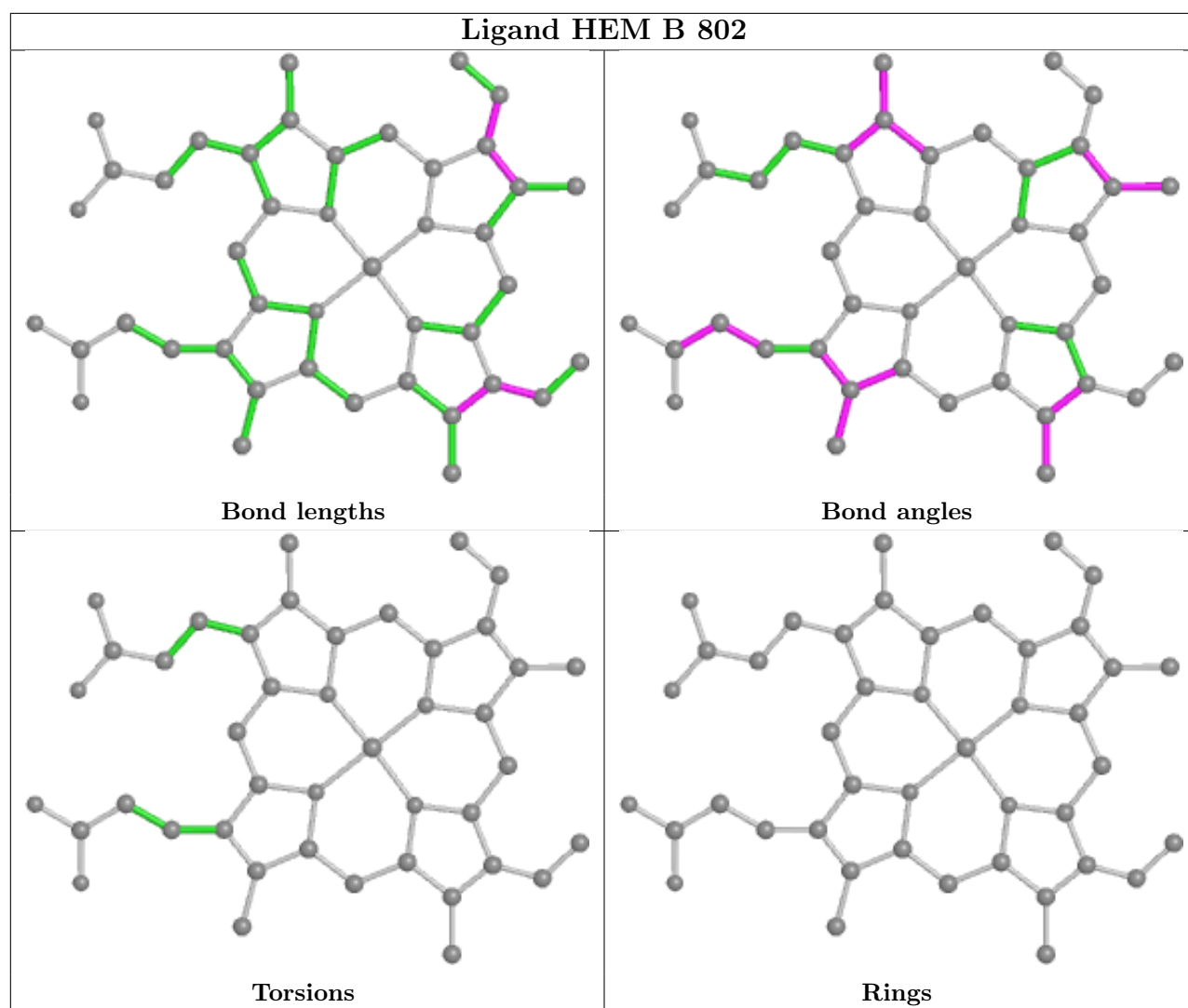
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	HEM	4	0
4	A	2805	FAD	5	0
5	A	2806	FUM	3	0
3	B	802	HEM	6	0
3	B	804	HEM	8	0
3	A	803	HEM	6	0
3	B	803	HEM	11	0
3	A	802	HEM	7	0
3	B	801	HEM	7	0
3	A	804	HEM	11	0
5	B	3806	FUM	1	0
4	B	3805	FAD	6	0

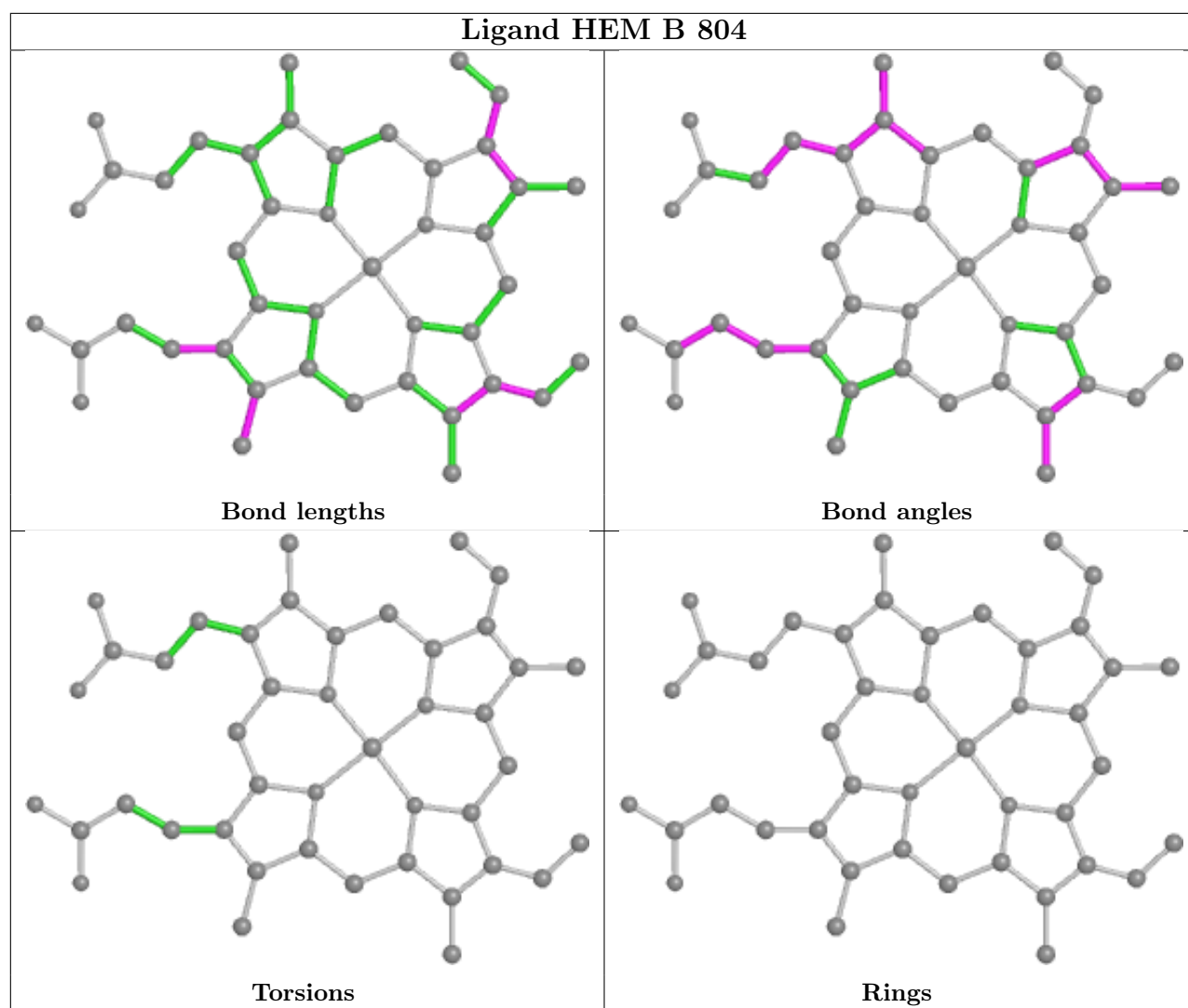
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

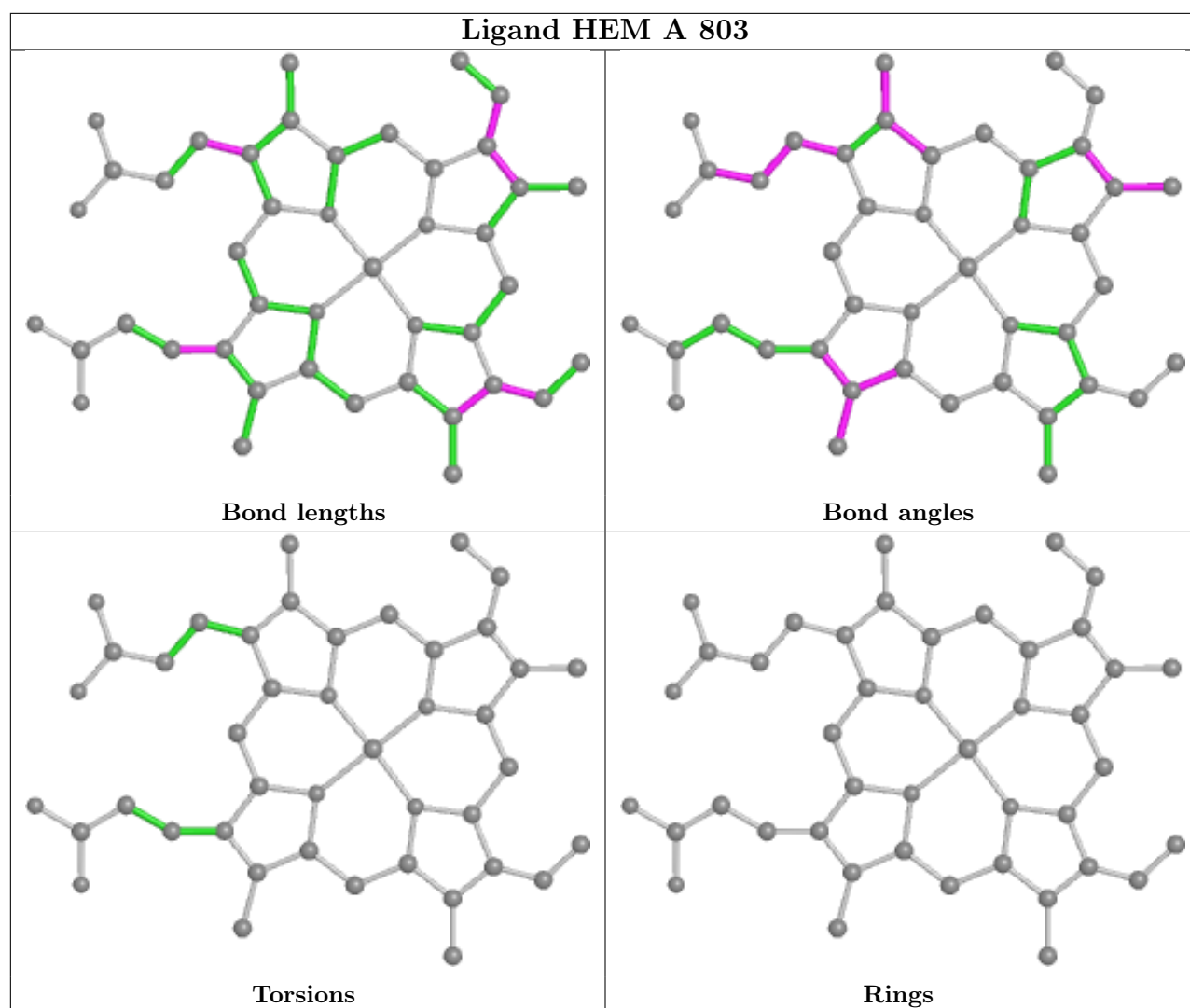
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

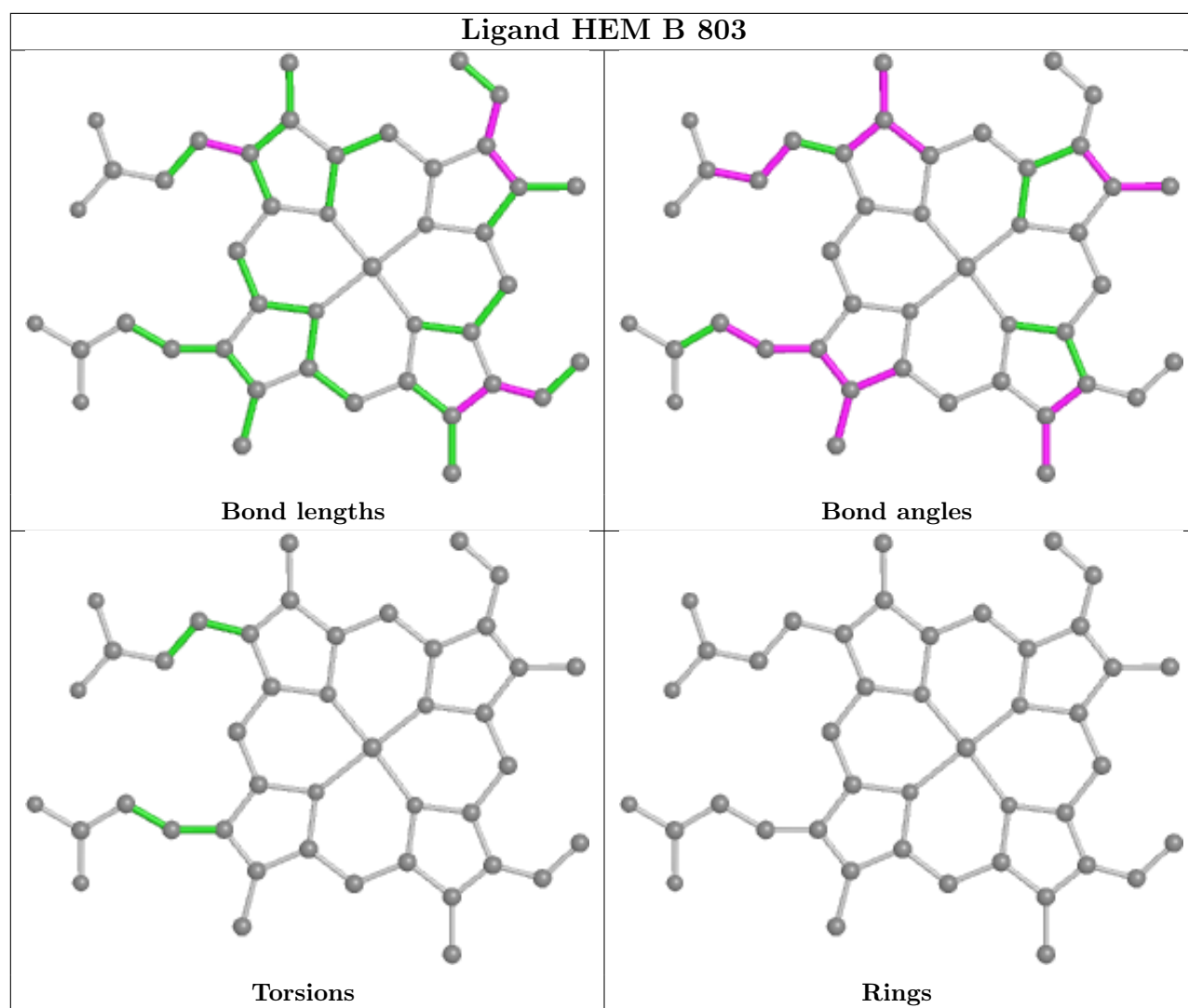


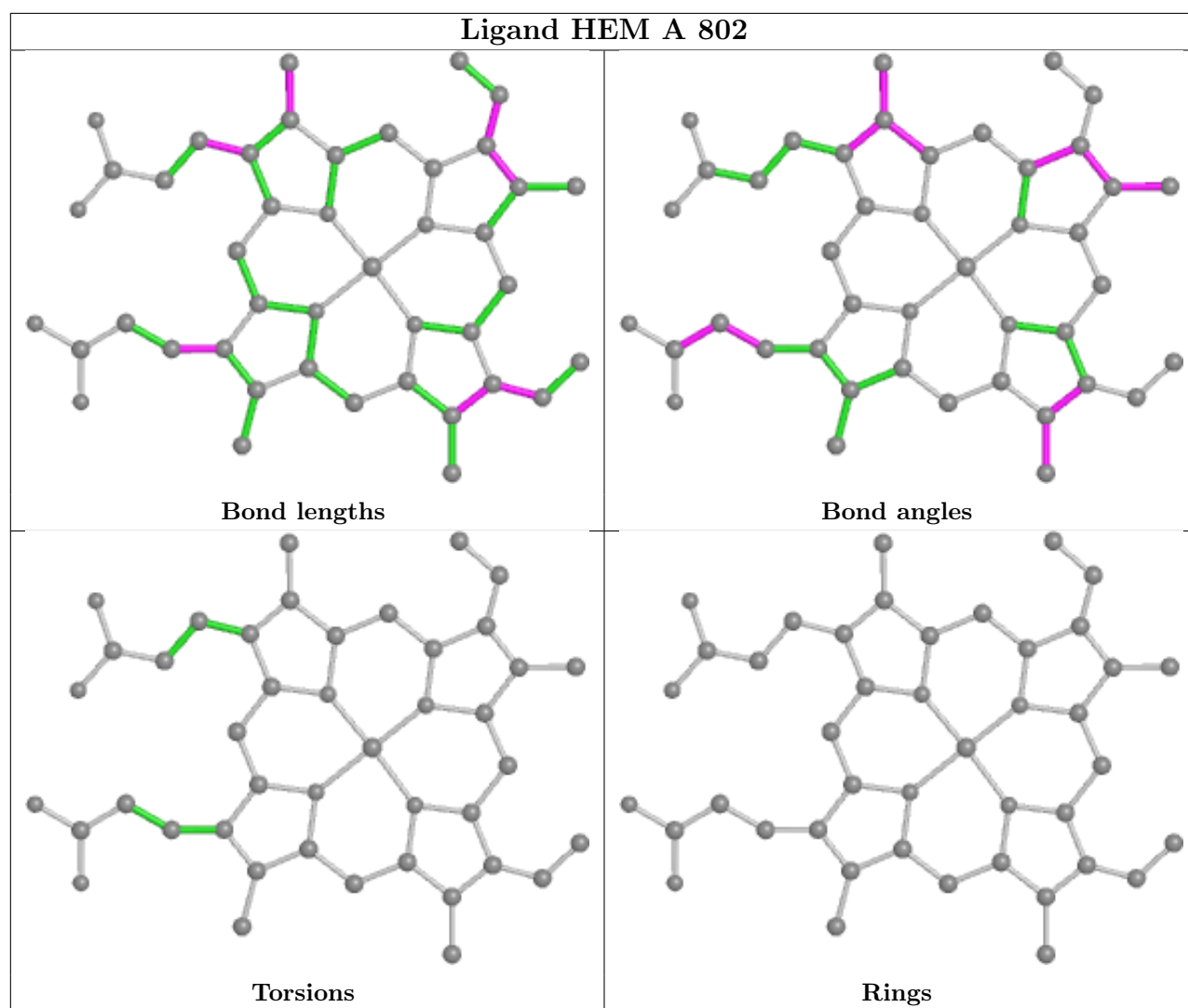


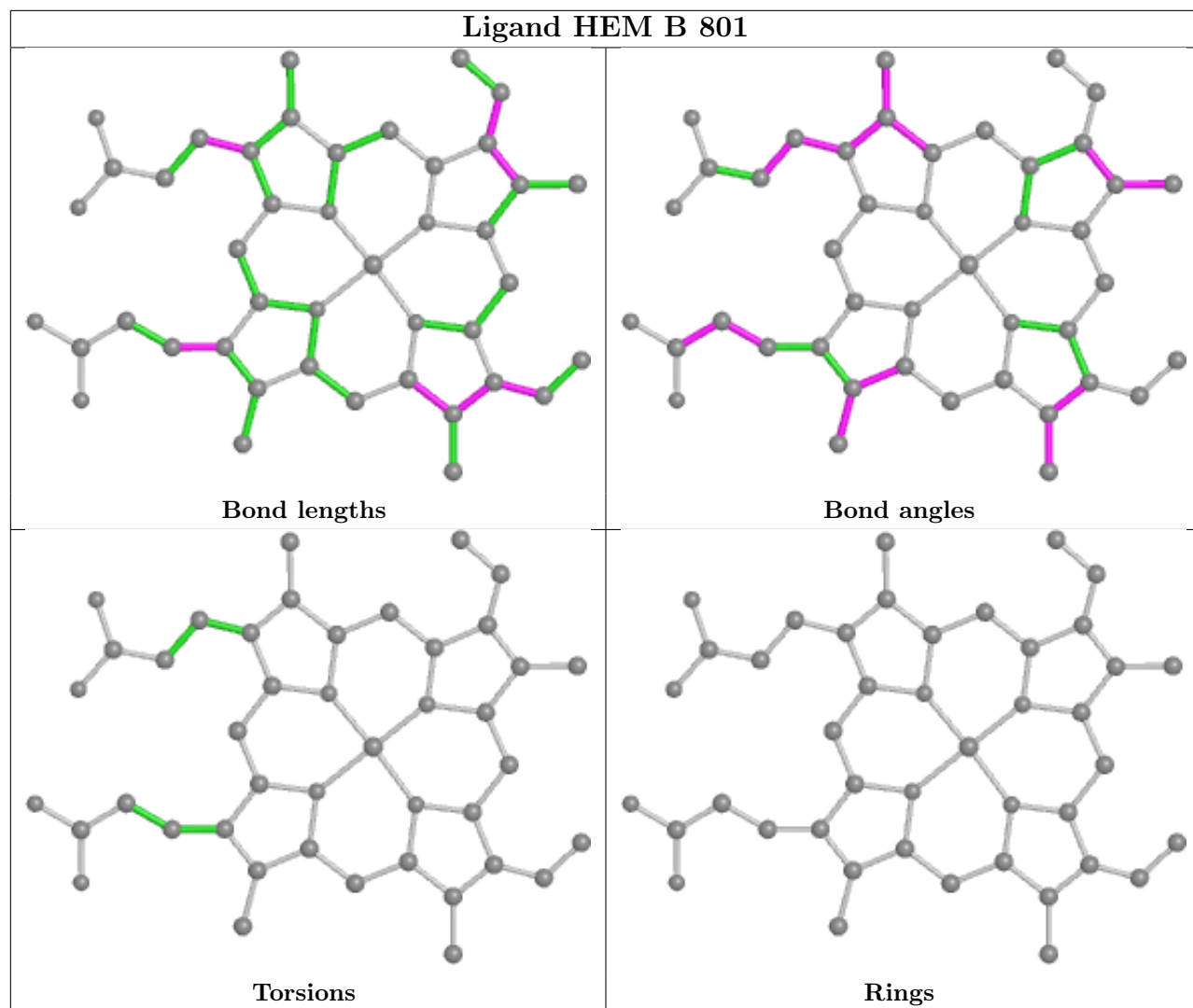


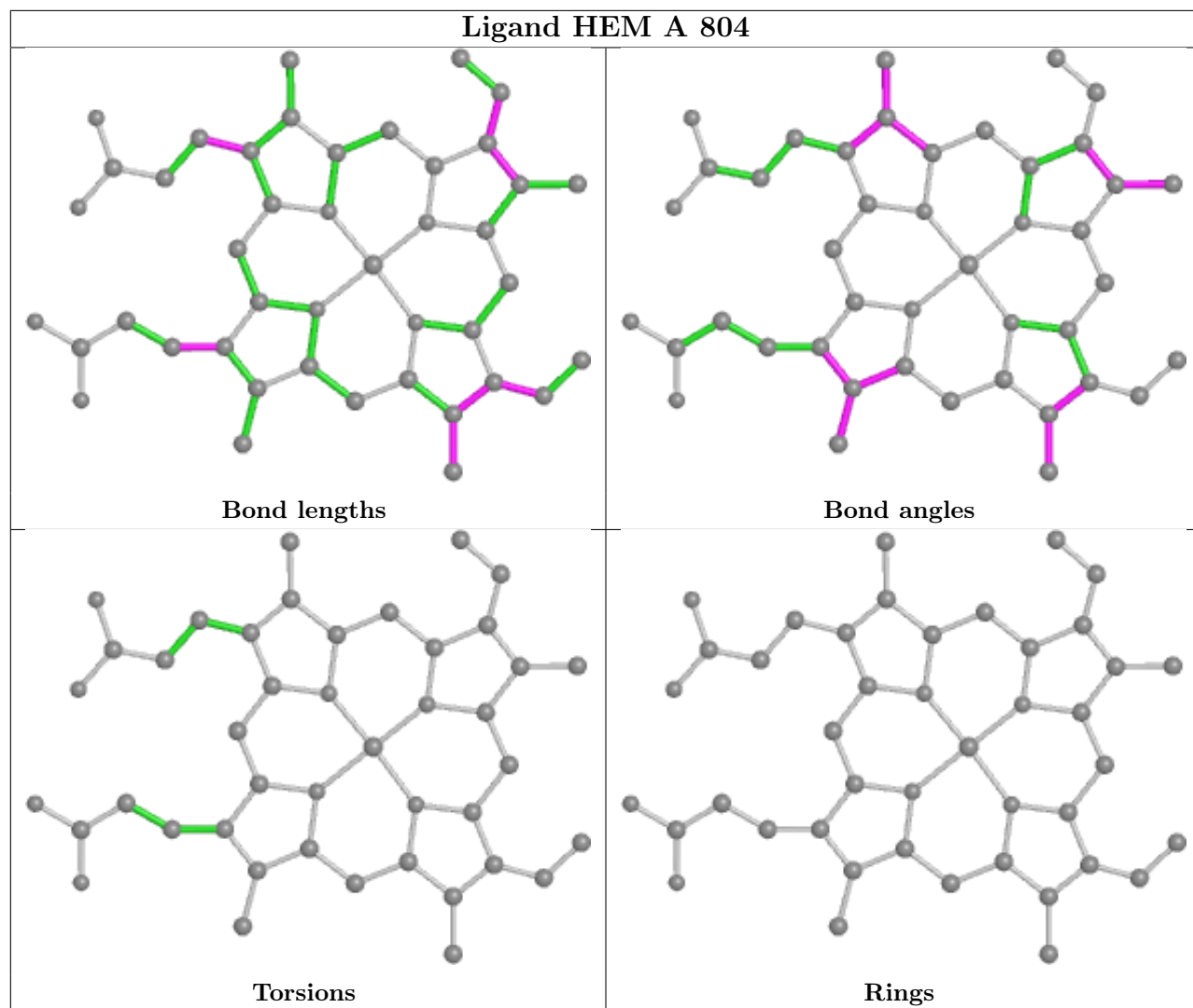


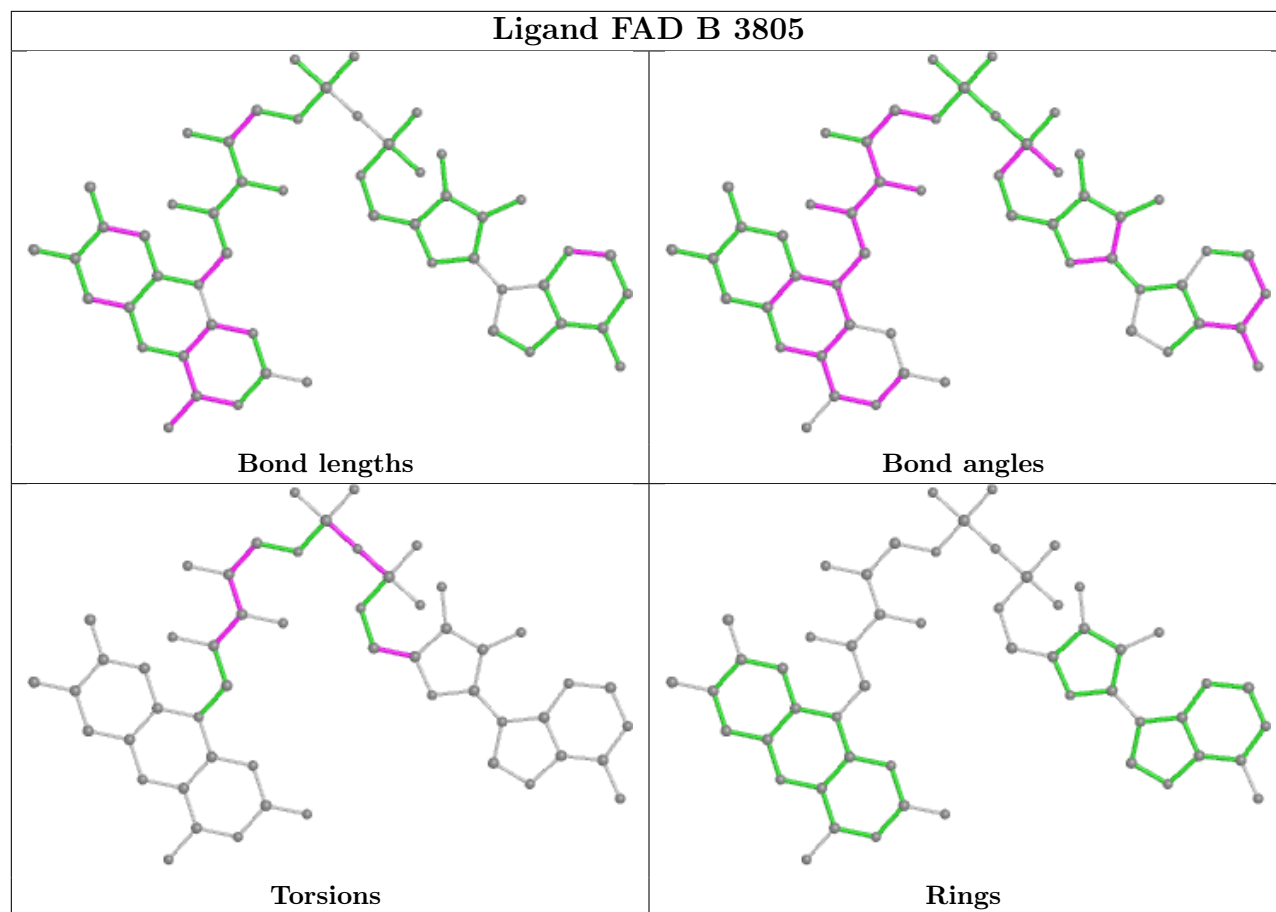












5.7 Other polymers [i](#)

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.