



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 06:33 PM EDT

PDB ID : 1IQC / pdb_00001iqc
Title : Crystal structure of Di-Heme Peroxidase from Nitrosomonas europaea
Authors : Shimizu, H.
Deposited on : 2001-07-20
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

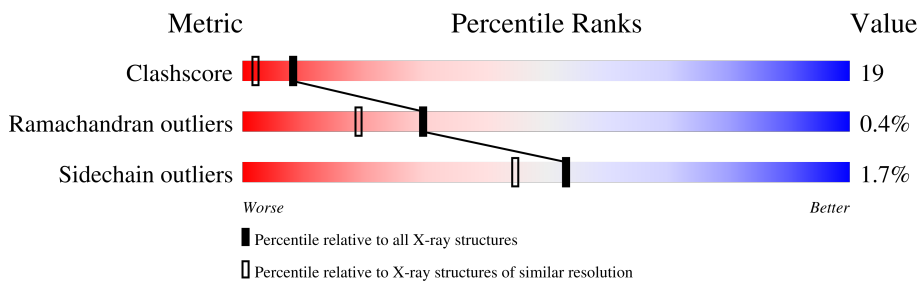
1 Overall quality at a glance

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	308	80% 19% .
1	B	308	72% 26% .
1	C	308	85% 14% .
1	D	308	50% 46% .

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	HEC	A	401	X	-	-	-
4	HEC	A	402	X	-	-	-
4	HEC	B	401	X	-	-	-
4	HEC	B	402	X	-	-	-
4	HEC	C	401	X	-	-	-
4	HEC	C	402	X	-	-	-
4	HEC	D	401	X	-	-	-
4	HEC	D	402	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10767 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 di-heme peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	B	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	C	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	D	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			

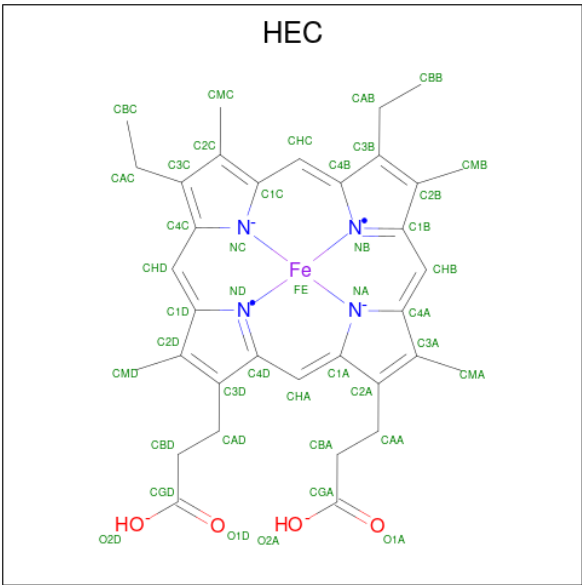
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

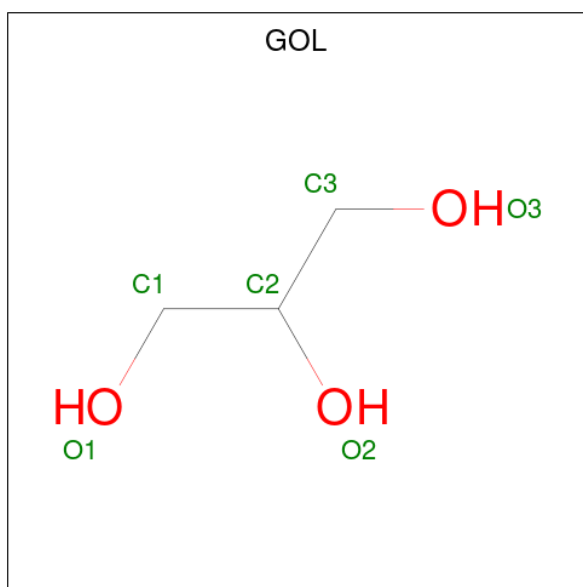
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	260	Total	O	0	0
			260	260		
6	B	199	Total	O	0	0
			199	199		
6	C	279	Total	O	0	0
			279	279		
6	D	120	Total	O	0	0
			120	120		

3 Residue-property plots

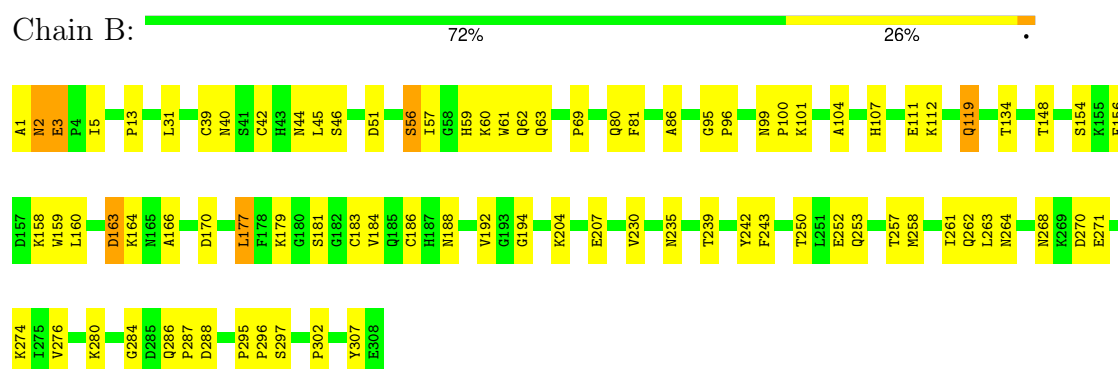
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

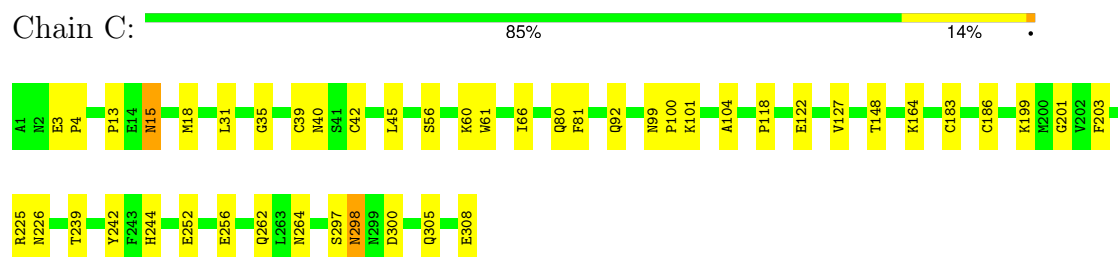
• Molecule 1: di-heme peroxidase



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• Molecule 1: di-heme peroxidase



A1	N2	E3	F4	I5	I8	V11	T12	M15	M18	A19	E20	L21	G22	K23	M24	L25	F26	F27	D28	P29	R30	L31	S32	K33	S34	G35	F36	I37	C39	N40	S41	C42	L45	D51	H59	K60	W61	Q62	Q63	I66	L72	N73	N77	L78	A79	Q80	F81	W82			
D83	G84	R85	A86	Q92	P96	N99	P100	K101	E102	M103	A104	E108	I109	A110	V113	V114	A115	Q119	Y120	R121	E122	R123	F124	K125	K126	V127	F128	G129	M130	D131	E132	V133	T134	I135	D136	R137	I138	T139	A140	A141	I142	A143	Q144	F145	E146	L149	V150	T151	P152	K155	F156
D157	E161	K164	N165	A166	L167	N168	Q169	D170	E171	L172	E173	L177	C183	V184	Q185	C186	H187	N188	G189	V192	G193	G194	S195	S196	Y197	Q198	K199	M200	G201	Y206	K209	N210	P211	R215	M216	D217	V218	T219	G220	N221	E222	K223	D224	R225	N226	V227	F228	K229	V230	N235	
I236	E237	L238	T239	Y240	P241	Y242	F243	H244	L251	E256	T257	M258	G259	R260	I261	Q262	L263	N264	N268	K269	D270	E271	K274	T281	K290	L291	P292	I293	L294	P295	P296	S297	N298	N299	D300	T301	P302	P306	Y307	E308											

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	88.13Å 55.11Å 144.00Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.9 (30.00-1.80)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10767	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: CA, HEC, MG, GOL

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	0.36	0/2441	0.91	8/3304 (0.2%)
1	B	0.33	0/2441	0.93	10/3304 (0.3%)
1	C	0.38	0/2441	0.92	8/3304 (0.2%)
1	D	0.32	0/2441	0.85	2/3304 (0.1%)
All	All	0.35	0/9764	0.90	28/13216 (0.2%)

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

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	SER	N-CA-C	7.22	120.97	110.28
1	C	56	SER	N-CA-C	6.88	120.45	110.28
1	C	127	VAL	N-CA-C	6.52	117.14	110.82
1	B	239	THR	N-CA-C	6.20	120.45	112.26
1	B	56	SER	N-CA-C	6.13	119.15	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	TYR	Sidechain

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	2388	0	2331	58	0
1	B	2388	0	2331	86	0
1	C	2388	0	2331	46	0
1	D	2388	0	2331	195	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	86	0	64	16	0
4	B	86	0	64	18	0
4	C	86	0	64	18	0
4	D	86	0	64	20	0
5	B	6	0	8	0	0
6	A	260	0	0	4	0
6	B	199	0	0	4	0
6	C	279	0	0	0	0
6	D	120	0	0	6	0
All	All	10767	0	9588	375	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 19.

The worst 5 of 375 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:186:CYS:SG	4:B:402:HEC:HAC	1.50	1.50
1:C:39:CYS:SG	4:C:401:HEC:CAB	2.08	1.41
1:A:39:CYS:SG	4:A:401:HEC:CAB	2.12	1.38
1:B:39:CYS:SG	4:B:401:HEC:CAB	2.13	1.37
1:A:42:CYS:SG	4:A:401:HEC:CAC	2.14	1.36

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	306/308 (99%)	296 (97%)	10 (3%)	0	100	100
1	B	306/308 (99%)	287 (94%)	16 (5%)	3 (1%)	12	4
1	C	306/308 (99%)	298 (97%)	8 (3%)	0	100	100
1	D	306/308 (99%)	285 (93%)	19 (6%)	2 (1%)	18	8
All	All	1224/1232 (99%)	1166 (95%)	53 (4%)	5 (0%)	30	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASN
1	D	2	ASN
1	B	163	ASP
1	D	215	ARG
1	B	3	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	260/260 (100%)	254 (98%)	6 (2%)	44	33
1	B	260/260 (100%)	258 (99%)	2 (1%)	73	70
1	C	260/260 (100%)	258 (99%)	2 (1%)	73	70
1	D	260/260 (100%)	252 (97%)	8 (3%)	35	23
All	All	1040/1040 (100%)	1022 (98%)	18 (2%)	53	45

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	188	ASN
1	D	308	GLU
1	D	268	ASN
1	C	15	ASN
1	D	164	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	144	GLN
1	C	264	ASN
1	D	268	ASN
1	C	176	ASN
1	C	226	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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
4	HEC	C	402	1	50,50,50	1.19	2 (4%)	68,82,82	1.10	2 (2%)
5	GOL	B	1410	-	5,5,5	0.30	0	5,5,5	0.29	0
4	HEC	A	401	1,6	50,50,50	1.25	2 (4%)	68,82,82	1.18	2 (2%)
4	HEC	D	401	1,6	50,50,50	1.21	2 (4%)	68,82,82	0.95	2 (2%)
4	HEC	D	402	1	50,50,50	1.26	2 (4%)	68,82,82	1.33	7 (10%)
4	HEC	A	402	1	50,50,50	1.15	2 (4%)	68,82,82	1.08	2 (2%)
4	HEC	C	401	1,6	50,50,50	1.28	2 (4%)	68,82,82	1.17	2 (2%)
4	HEC	B	401	1,6	50,50,50	1.15	2 (4%)	68,82,82	1.15	2 (2%)
4	HEC	B	402	1	50,50,50	1.28	3 (6%)	68,82,82	1.10	2 (2%)

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
4	HEC	C	402	1	1/1/3/7	6/14/54/54	-
5	GOL	B	1410	-	-	0/4/4/4	-
4	HEC	A	401	1,6	1/1/3/7	5/14/54/54	-
4	HEC	D	401	1,6	1/1/3/7	10/14/54/54	-
4	HEC	D	402	1	1/1/3/7	8/14/54/54	-
4	HEC	A	402	1	1/1/3/7	6/14/54/54	-
4	HEC	C	401	1,6	1/1/3/7	6/14/54/54	-
4	HEC	B	401	1,6	1/1/3/7	6/14/54/54	-
4	HEC	B	402	1	1/1/3/7	5/14/54/54	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	HEC	CAC-C3C	-4.91	1.38	1.51
4	D	402	HEC	CAB-C3B	-4.67	1.39	1.51
4	C	401	HEC	CAB-C3B	-4.59	1.39	1.51
4	B	402	HEC	CAC-C3C	-4.57	1.39	1.51
4	A	402	HEC	CAC-C3C	-4.36	1.40	1.51

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	HEC	CBC-CAC-C3C	5.39	127.04	112.42
4	B	402	HEC	CBC-CAC-C3C	5.30	126.80	112.42
4	A	401	HEC	CBC-CAC-C3C	5.10	126.24	112.42
4	B	401	HEC	CBB-CAB-C3B	4.80	125.43	112.42
4	C	401	HEC	CBB-CAB-C3B	4.78	125.38	112.42

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	401	HEC	NA
4	A	402	HEC	NA
4	B	401	HEC	NA
4	B	402	HEC	NA
4	C	401	HEC	NA

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	HEC	C2C-C3C-CAC-CBC
4	B	401	HEC	C2C-C3C-CAC-CBC
4	D	402	HEC	C2C-C3C-CAC-CBC
4	A	402	HEC	C4C-C3C-CAC-CBC
4	B	401	HEC	C4C-C3C-CAC-CBC

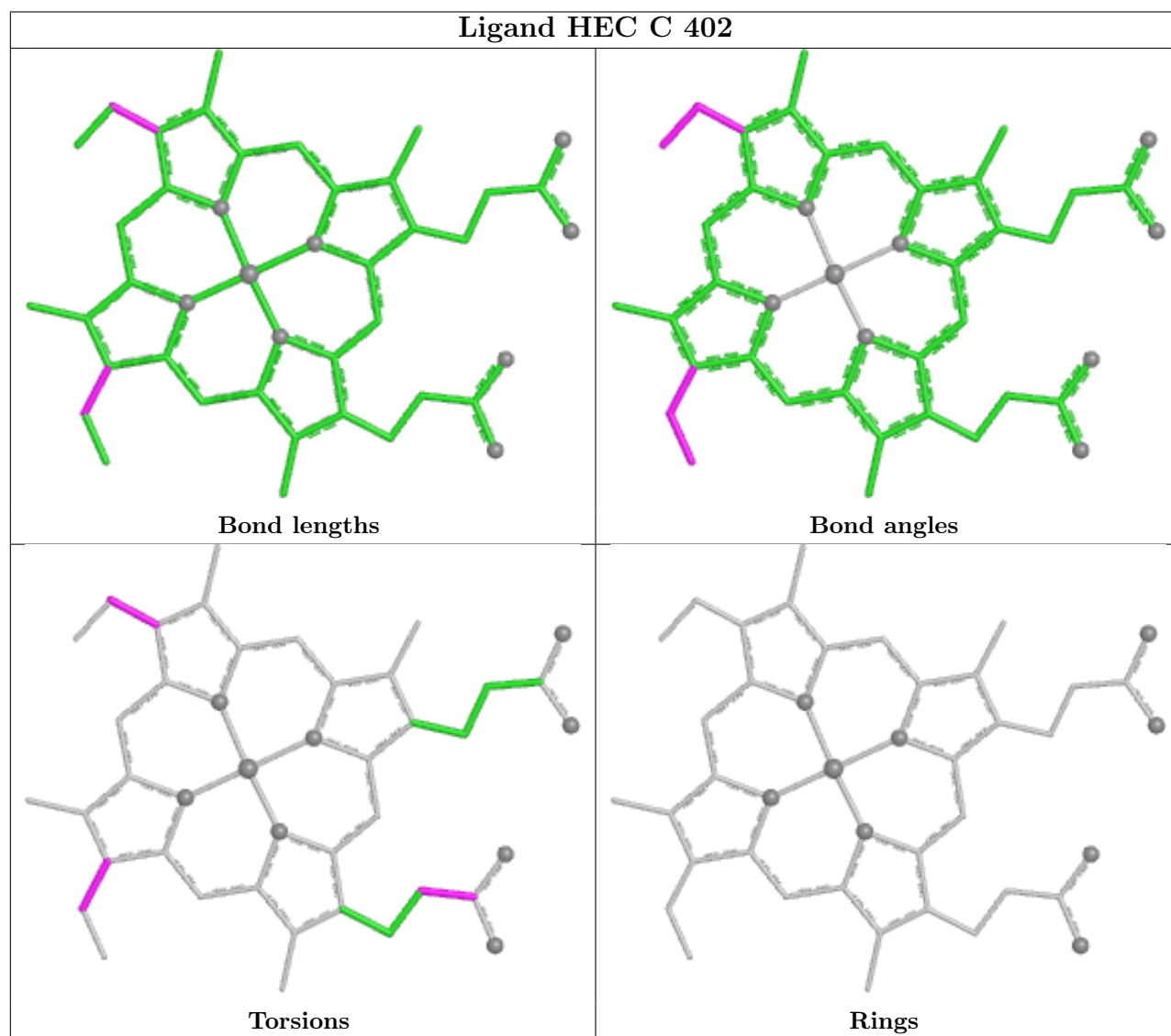
There are no ring outliers.

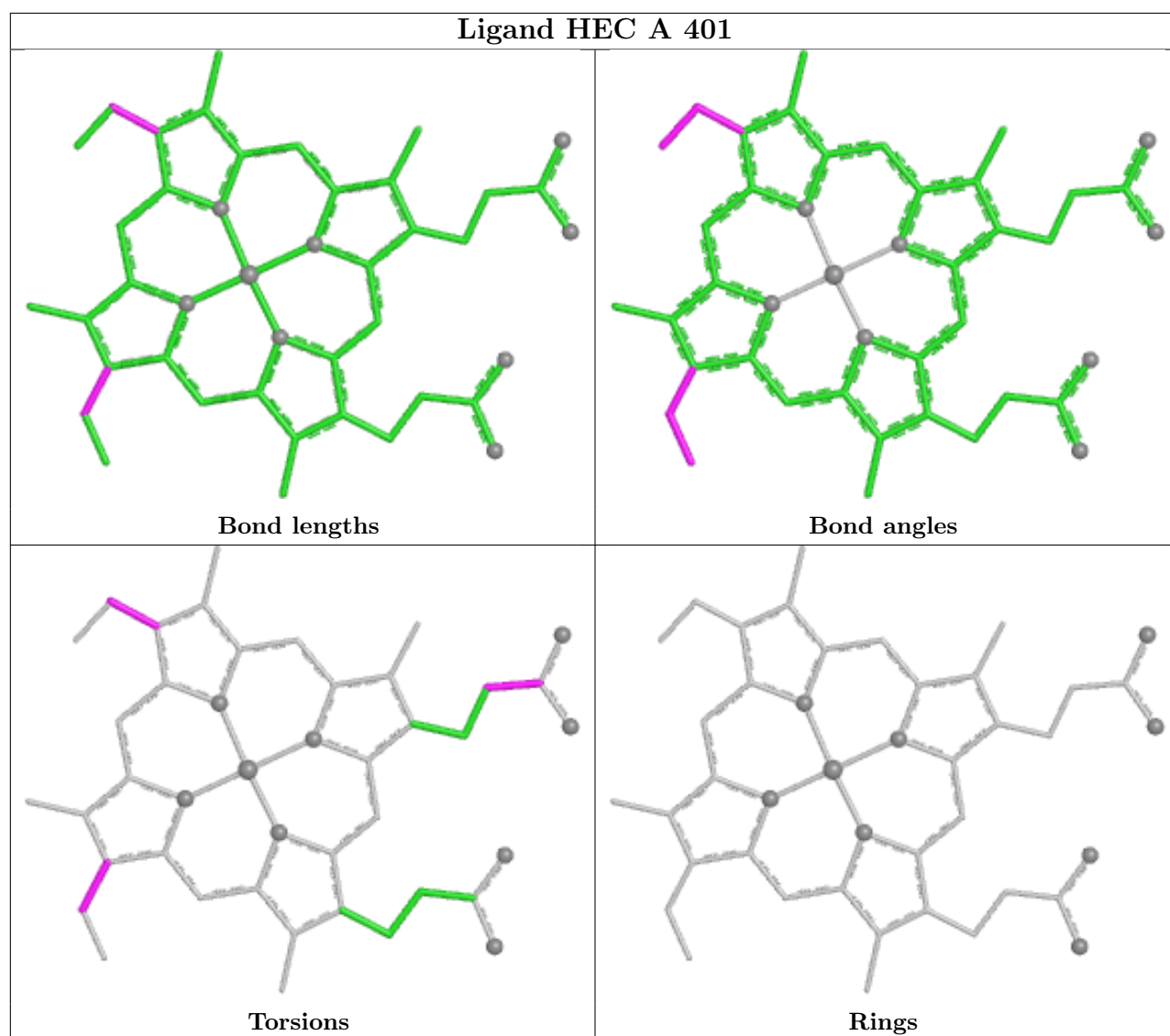
8 monomers are involved in 72 short contacts:

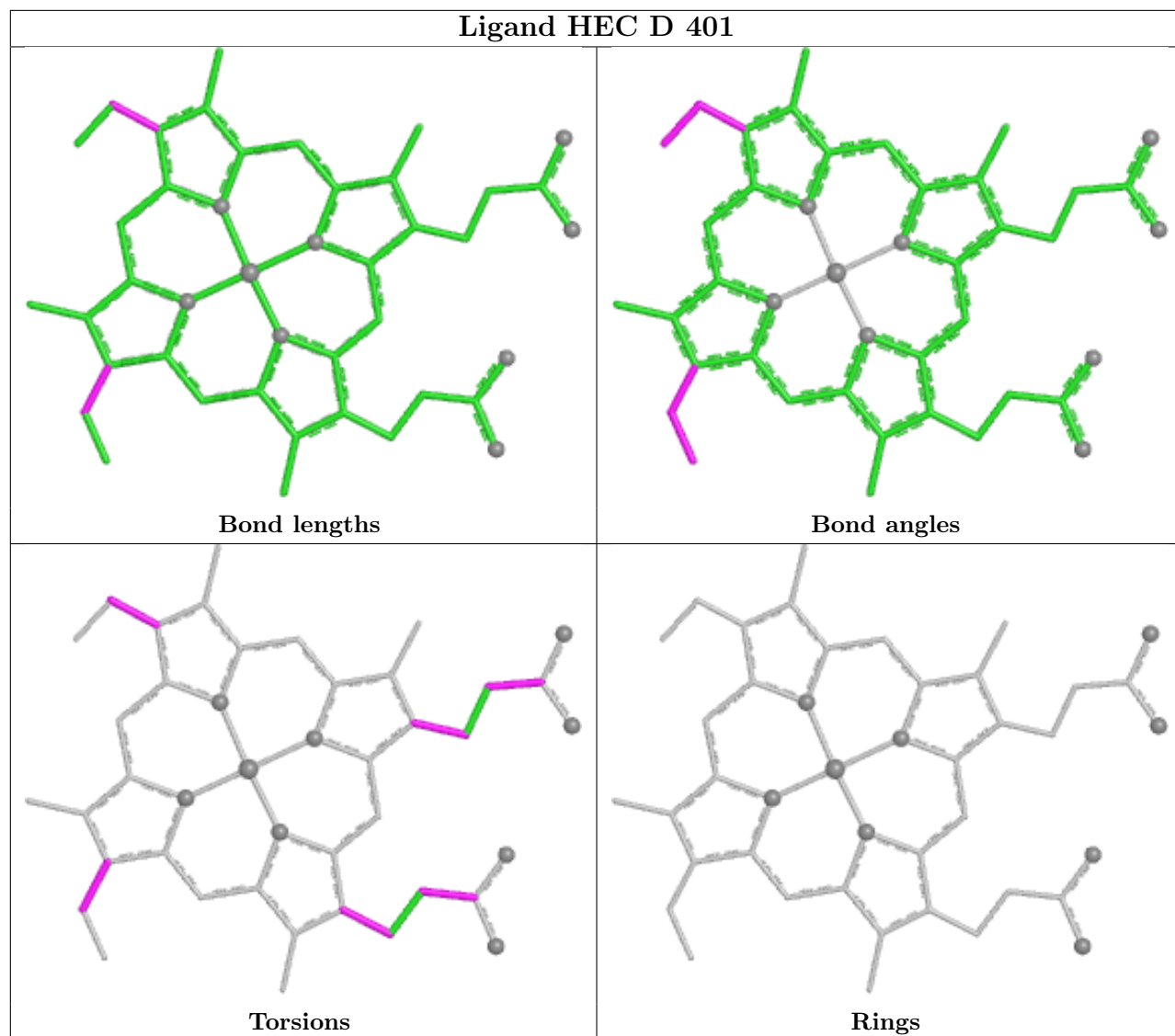
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	HEC	10	0
4	A	401	HEC	8	0
4	D	401	HEC	8	0
4	D	402	HEC	12	0
4	A	402	HEC	8	0
4	C	401	HEC	8	0
4	B	401	HEC	11	0
4	B	402	HEC	7	0

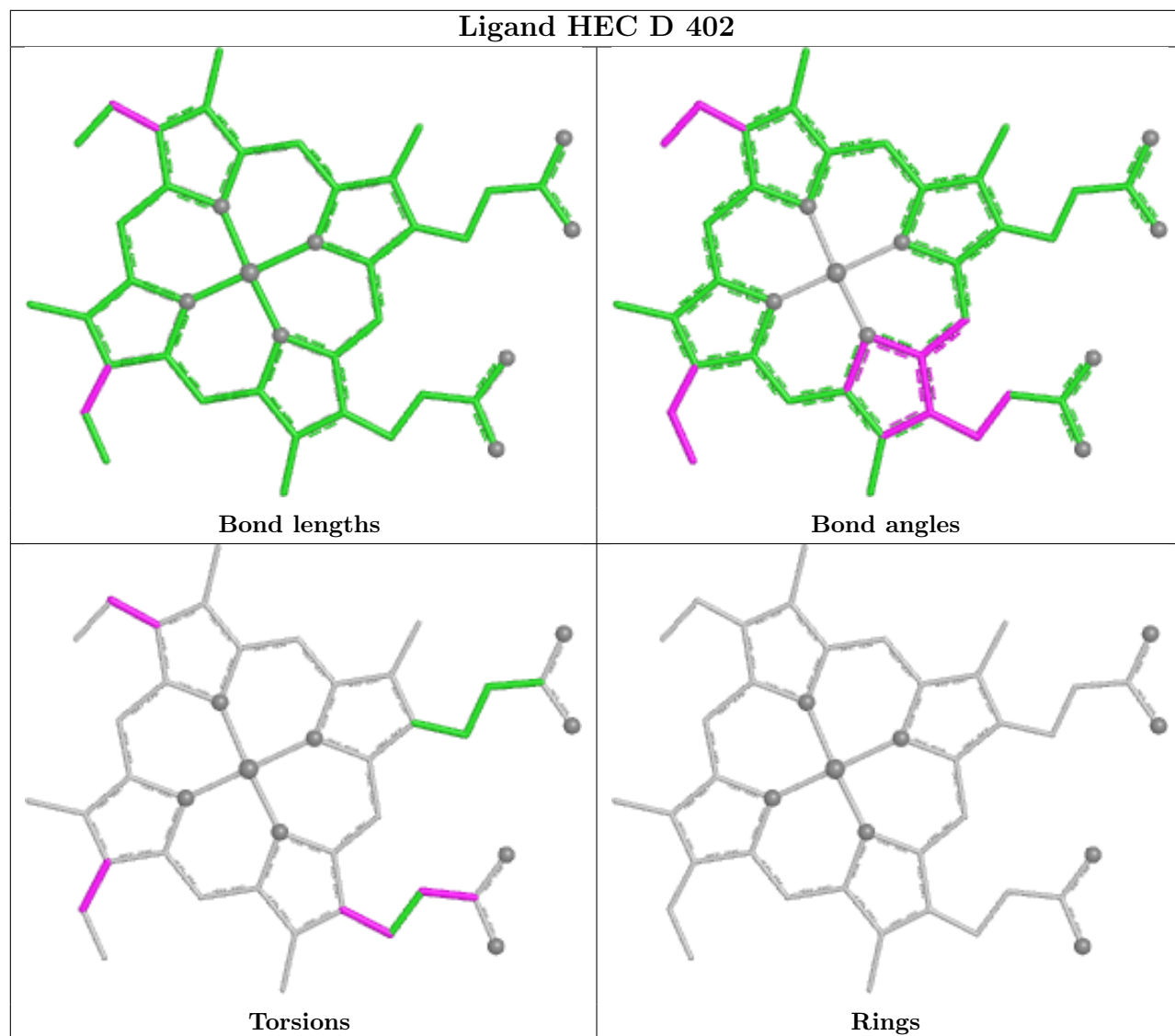
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

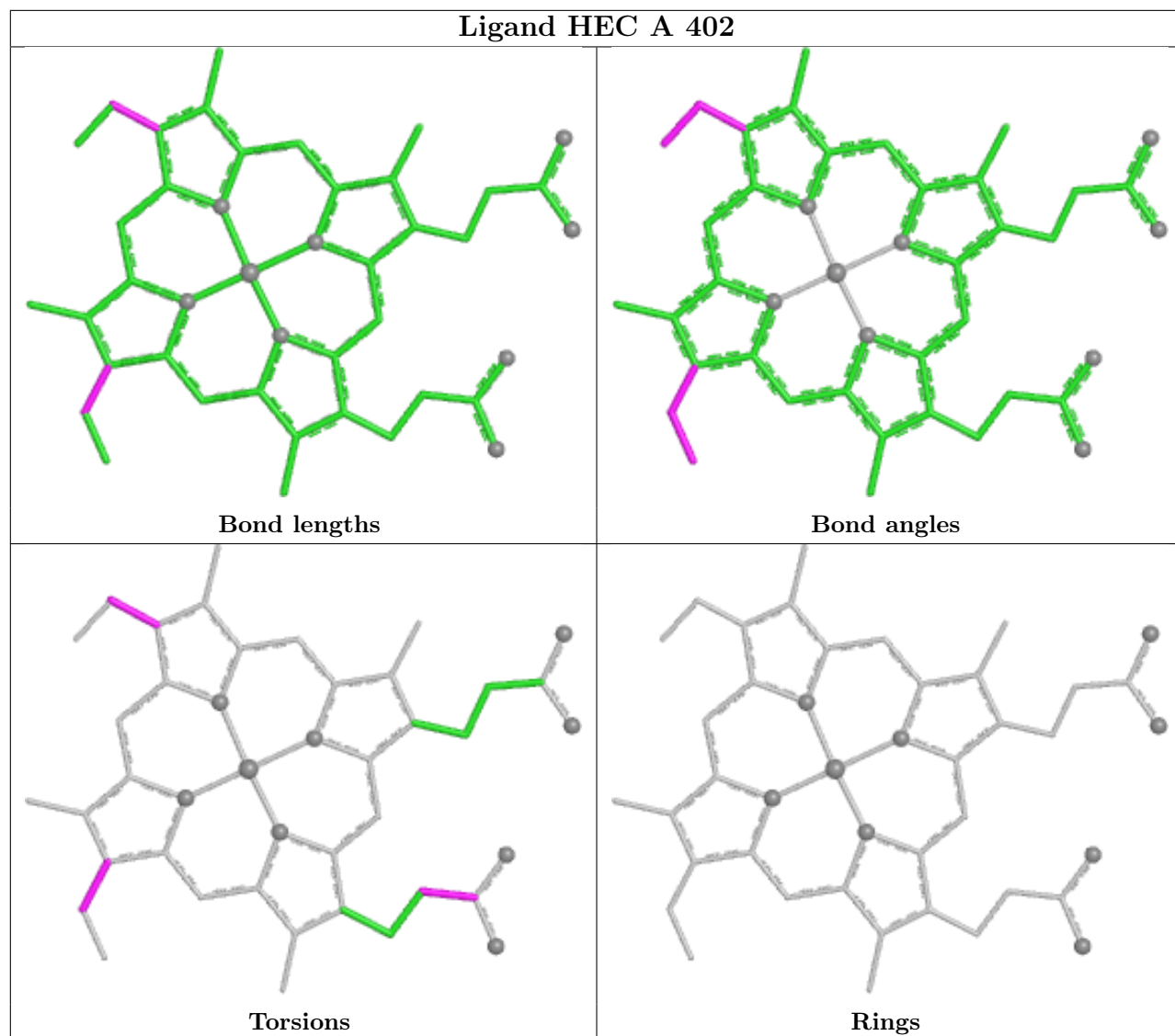
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



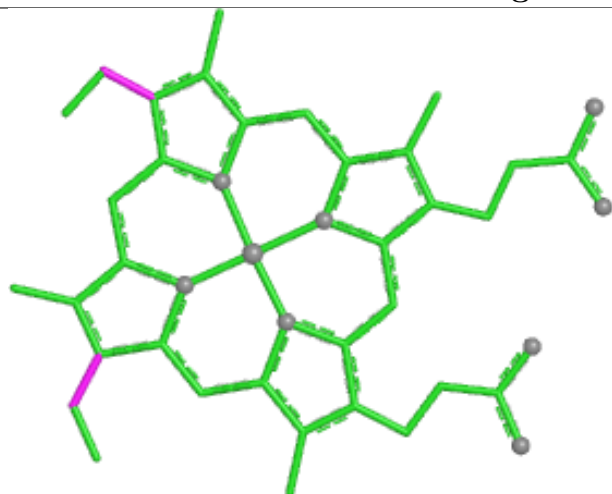




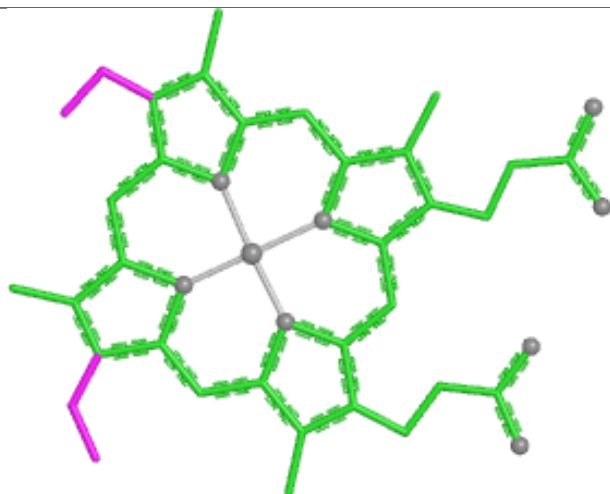




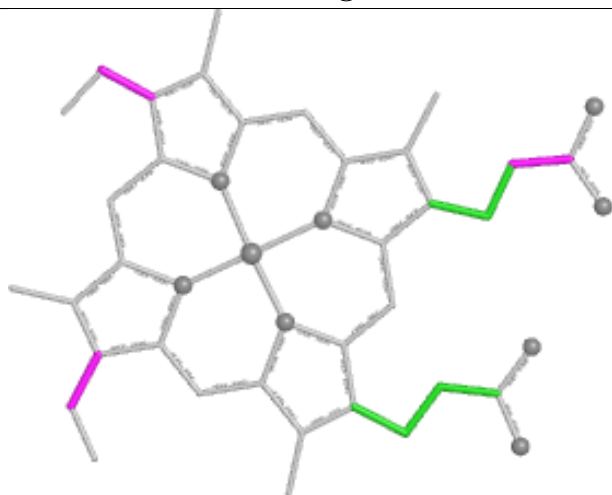
Ligand HEC C 401



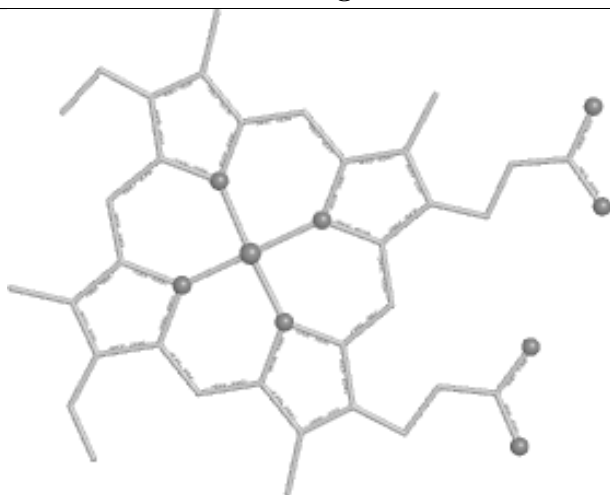
Bond lengths



Bond angles

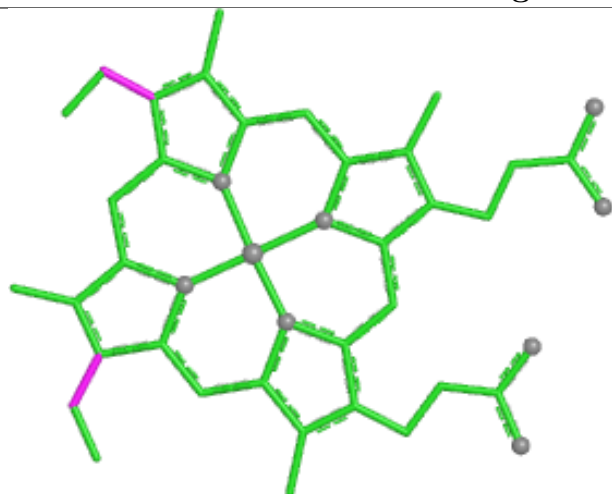


Torsions

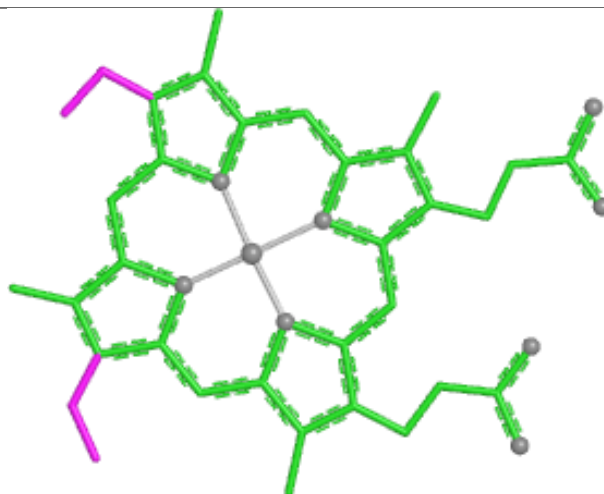


Rings

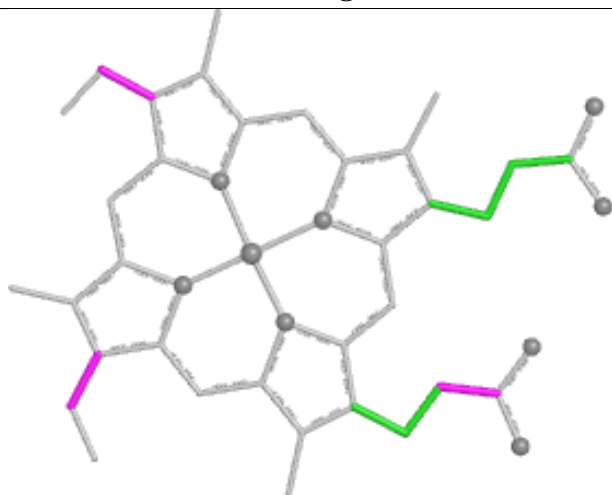
Ligand HEC B 401



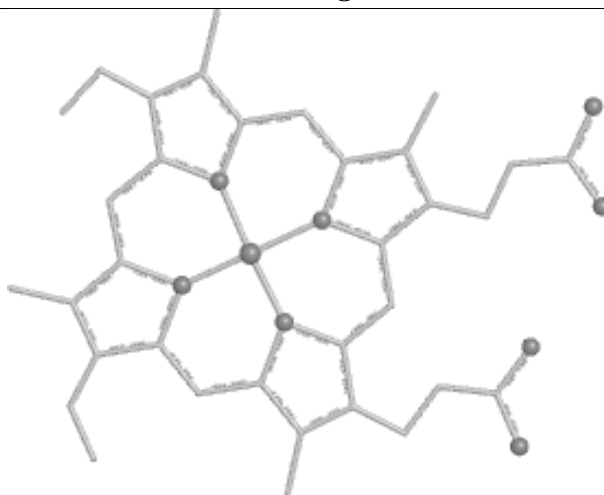
Bond lengths



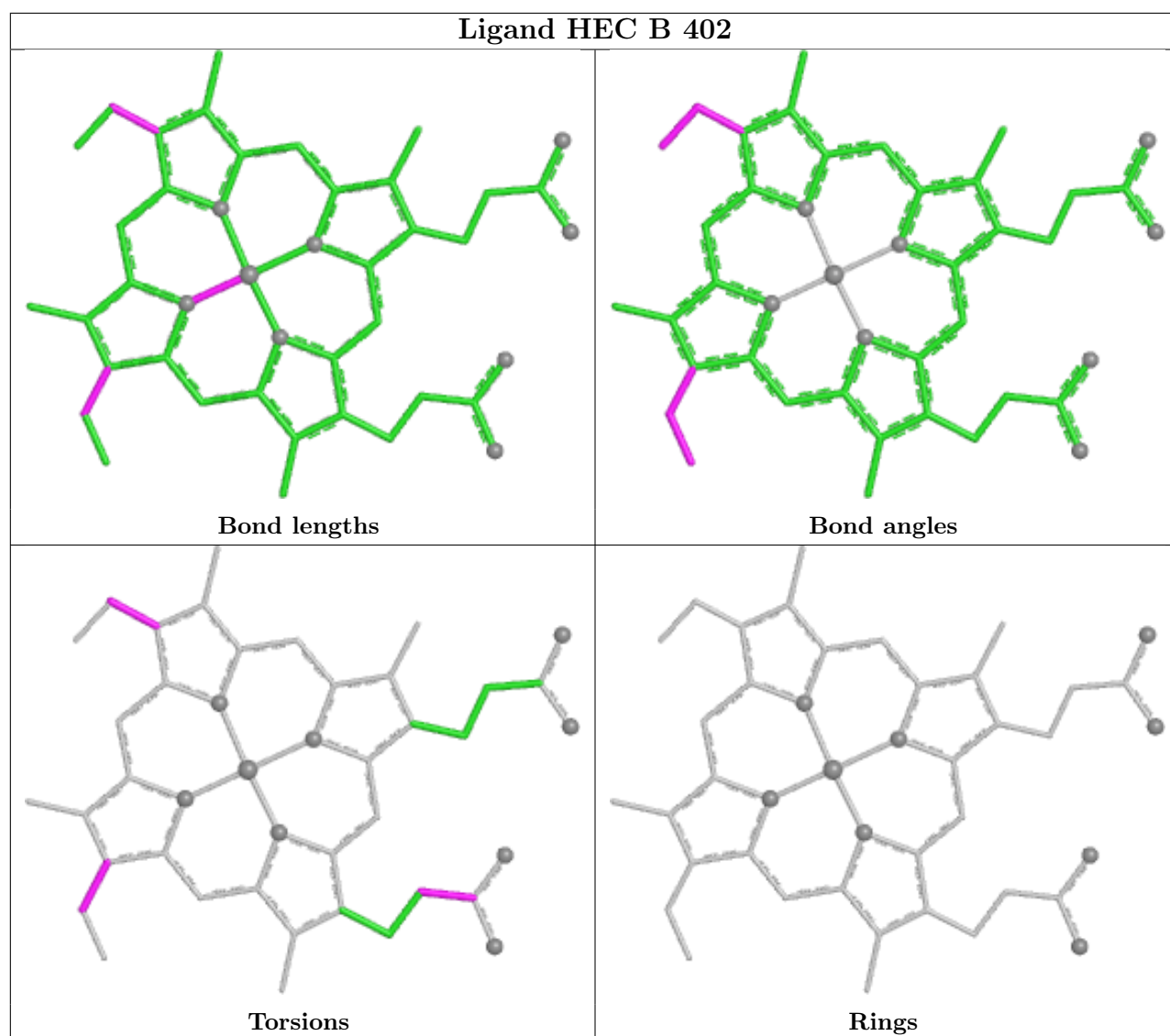
Bond angles



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.