



Full wwPDB Geometry-Only Validation Report ⓘ

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PDB ID : 7JOR
Title : Neutron structure of ferric Dehaloperoxidase B
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Deposited on : 2020-08-07
Resolution : 2.05 Å(reported)

This is a Full wwPDB Geometry-Only Validation 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)
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) : 2.23.1

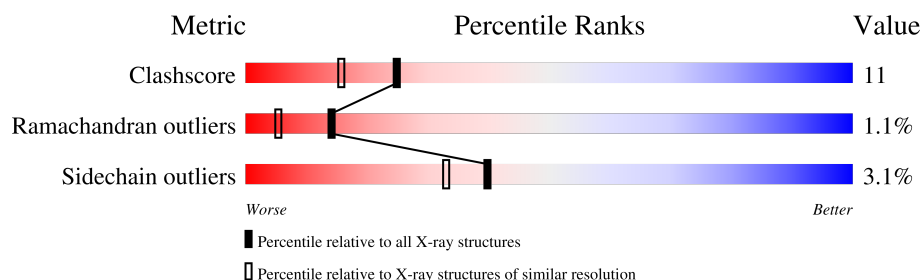
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

NEUTRON DIFFRACTION

The reported resolution of this entry is 2.05 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	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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	137	
1	B	137	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4930 atoms, of which 512 are hydrogens and 2112 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 Dehaloperoxidase B.

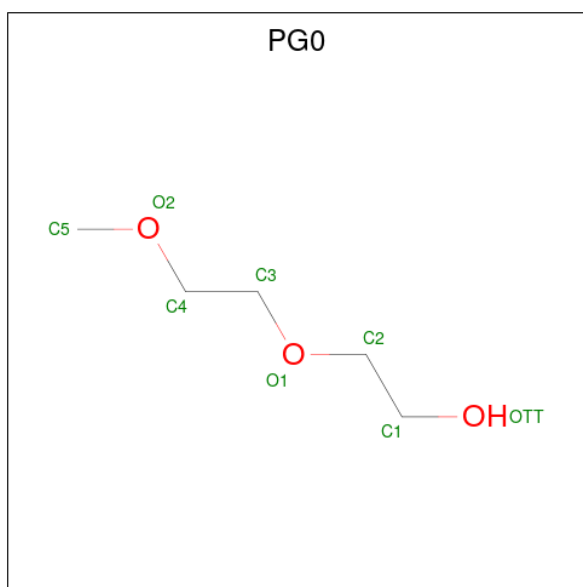
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	137	Total	C	D	H	N	O	S	1	134	0
			2330	683	1026	221	185	208	7			
1	B	137	Total	C	D	H	N	O	S	5	134	0
			2331	683	1029	219	187	206	7			

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	D	H	O	0	1
			21	5	1	12	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	22	Total	D	O	0	0
			51	29	22		
4	B	24	Total	D	O	0	0
			51	27	24		

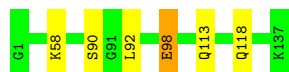
3 Residue-property plots [i](#)

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: Dehaloperoxidase B

Chain A:  96% . .



- Molecule 1: Dehaloperoxidase B

Chain B:  96% . .



4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PG0

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	2.04	2/1940 (0.1%)	0.85	6/2594 (0.2%)
1	B	0.45	0/1917	0.54	2/2562 (0.1%)
All	All	1.48	2/3857 (0.1%)	0.72	8/5156 (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	B	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98[A]	GLU	CG-CD	62.40	2.45	1.51
1	A	98[C]	GLU	CG-CD	62.40	2.45	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98[A]	GLU	CB-CG-CD	-18.32	64.74	114.20
1	A	98[C]	GLU	CB-CG-CD	-18.32	64.74	114.20
1	A	98[A]	GLU	CG-CD-OE2	-12.44	93.41	118.30
1	A	98[C]	GLU	CG-CD-OE2	-12.44	93.41	118.30
1	A	98[A]	GLU	CG-CD-OE1	-10.97	96.36	118.30
1	A	98[C]	GLU	CG-CD-OE1	-10.97	96.36	118.30
1	B	32[B]	LYS	O-C-N	-5.17	114.43	122.70
1	B	32[A]	LYS	O-C-N	-5.17	114.43	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	33[A]	ARG	Mainchain,Peptide
1	B	33[B]	ARG	Mainchain,Peptide

4.2 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	2109	221	39	2	0
1	B	2112	219	42	4	0
2	A	43	30	30	5	0
2	B	43	30	30	19	0
3	A	9	12	0	0	0
4	A	51	0	0	2	0
4	B	51	0	0	4	0
All	All	4418	512	141	36	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 11.

All (36) 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)
2:A:201:HEM:HMB2	2:A:201:HEM:HBB2	1.54	0.79
2:A:201:HEM:HBB2	2:A:201:HEM:CMB	2.11	0.75
2:B:201:HEM:HHA	2:B:201:HEM:HBA2	1.73	0.61
2:B:201:HEM:HHA	2:B:201:HEM:CBA	2.30	0.57
2:A:201:HEM:HMB2	2:A:201:HEM:CBB	2.28	0.56
2:A:201:HEM:CMB	2:A:201:HEM:CBB	2.85	0.55
2:B:201:HEM:HBA2	2:B:201:HEM:CHA	2.34	0.52
2:B:201:HEM:CBA	2:B:201:HEM:CHA	2.92	0.47

There are no symmetry-related clashes.

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	237/137 (173%)	231 (98%)	5 (2%)	1 (0%)	34	24
1	B	236/137 (172%)	225 (95%)	6 (2%)	5 (2%)	7	1
All	All	473/274 (173%)	456 (96%)	11 (2%)	6 (1%)	14	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34[A]	ASN
1	B	34[B]	ASN
1	B	34[C]	ASN
1	B	34[D]	ASN
1	B	36[B]	LYS
1	A	92[B]	LEU

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	204/116 (176%)	196 (96%)	8 (4%)	32	25
1	B	201/116 (173%)	195 (97%)	6 (3%)	41	34
All	All	405/232 (175%)	391 (96%)	14 (4%)	40	29

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58[A]	LYS
1	A	58[B]	LYS
1	A	90[A]	SER
1	A	90[B]	SER
1	A	113[A]	GLN
1	A	113[B]	GLN
1	A	118[B]	GLN
1	A	118[A]	GLN
1	B	33[A]	ARG
1	B	33[B]	ARG
1	B	85[A]	GLN
1	B	85[B]	GLN
1	B	88[A]	GLN
1	B	88[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

5 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
2	HEM	A	201	1	27,50,50	1.82	6 (22%)	17,82,82	1.05	2 (11%)
2	HEM	B	201	1	27,50,50	0.82	2 (7%)	17,82,82	1.25	0

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
2	HEM	A	201	1	-	2/6/54/54	-
2	HEM	B	201	1	-	4/6/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	HEM	C3C-C2C	-4.86	1.33	1.40
2	A	201	HEM	C3B-C2B	-4.63	1.34	1.40
2	A	201	HEM	C1D-ND	-2.77	1.30	1.36
2	B	201	HEM	C3B-C2B	-2.54	1.36	1.40
2	A	201	HEM	C3D-C2D	-2.18	1.31	1.37
2	A	201	HEM	C1A-CHA	-2.11	1.35	1.41
2	A	201	HEM	C4B-NB	-2.07	1.31	1.36
2	B	201	HEM	C4D-C3D	2.02	1.47	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	HEM	CBD-CAD-C3D	-2.18	108.47	112.48
2	A	201	HEM	C4A-C3A-C2A	2.13	108.48	107.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

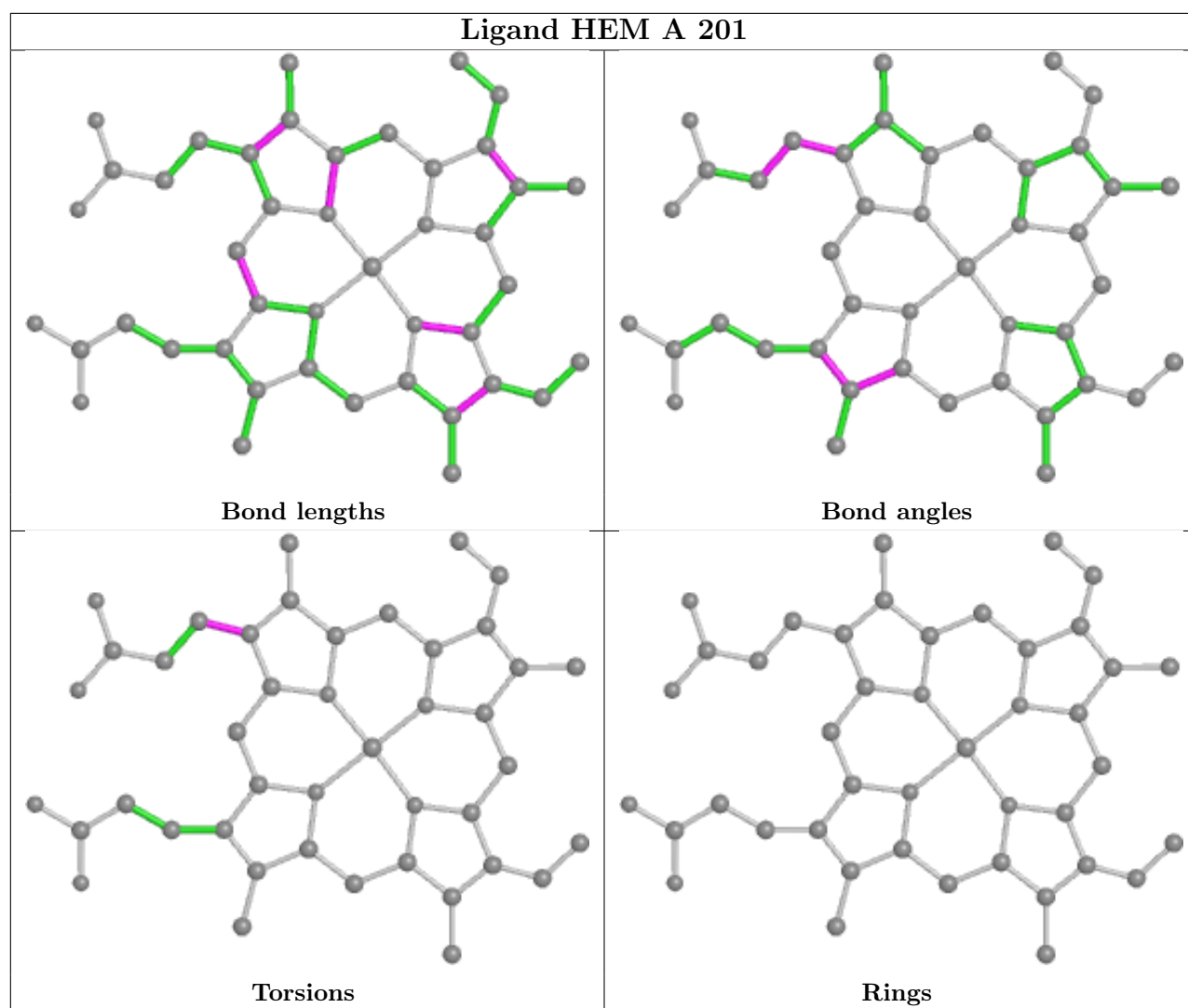
Mol	Chain	Res	Type	Atoms
2	A	201	HEM	C2D-C3D-CAD-CBD
2	A	201	HEM	C4D-C3D-CAD-CBD
2	B	201	HEM	C1A-C2A-CAA-CBA
2	B	201	HEM	C3A-C2A-CAA-CBA
2	B	201	HEM	C2A-CAA-CBA-CGA
2	B	201	HEM	C3D-CAD-CBD-CGD

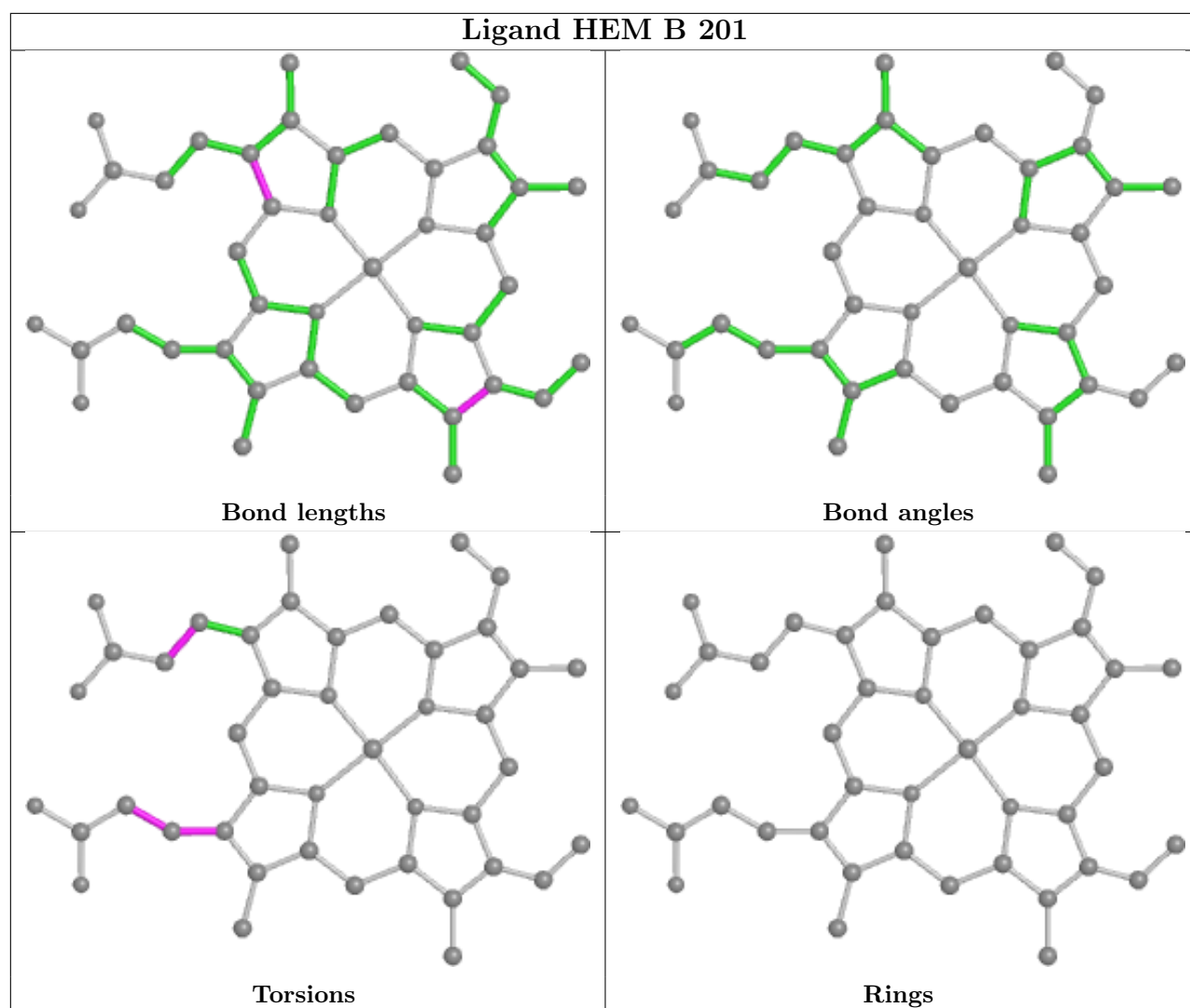
There are no ring outliers.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	HEM	5	0
2	B	201	HEM	19	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.





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.