



# Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 07:23 pm BST

PDB ID : 9FY7 / pdb\_00009fy7  
Title : Dye Type Peroxidase Aa from Streptomyces lividans with N3 ligand by serial electron diffraction (SerialED)  
Authors : Hofer, G.; Wang, L.; Pacoste, L.; Hager, P.; Finjallaz, A.; Williams, L.; Worral, J.; Steiner, R.; Xu, H.; Zou, X.  
Deposited on : 2024-07-03  
Resolution : 1.10 Å(reported)  
Based on initial model : 6I43

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

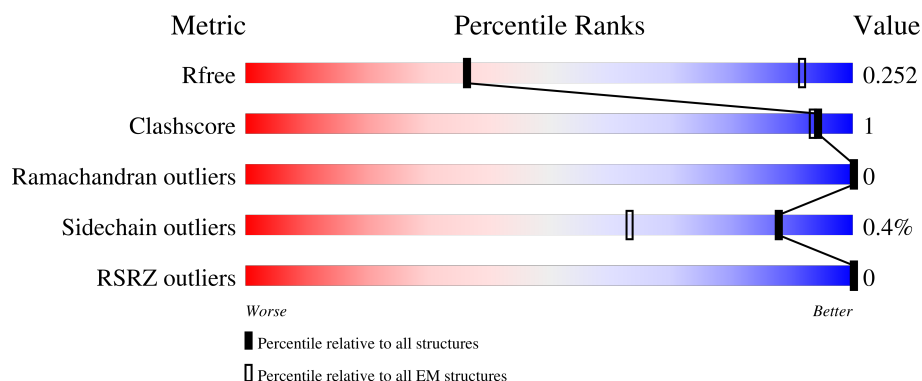
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

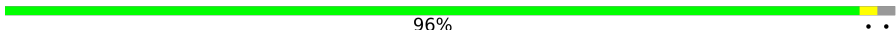
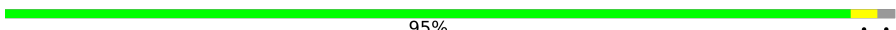
The reported resolution of this entry is 1.10 Å.

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)
$R_{free}$	164678	53
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RSRZ outliers	164674	54

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  $\geq 3$ , 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	371	 96%
1	B	371	 95%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12115 atoms, of which 5540 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.

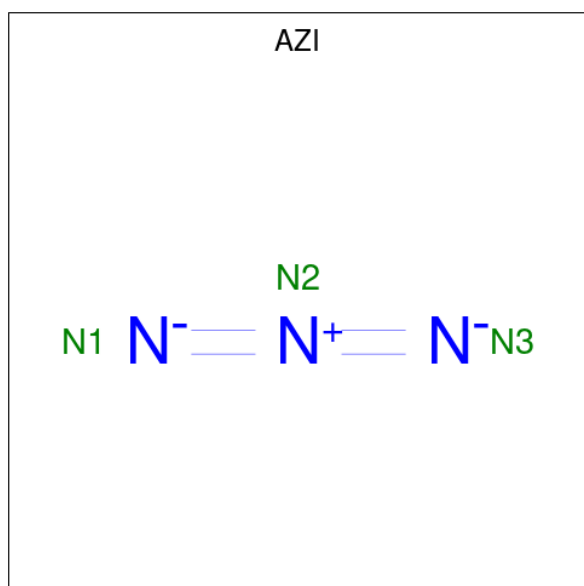
- Molecule 1 is a protein called Deferrochelataase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	365	Total	C	H	N	O	S	6	0
			5581	1773	2760	522	521	5		
1	B	364	Total	C	H	N	O	S	0	0
			5505	1753	2720	512	515	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	PHE	TYR	conflict	UNP A0A7U8YY09
B	389	PHE	TYR	conflict	UNP A0A7U8YY09

- Molecule 2 is AZIDE ION (CCD ID: AZI) (formula: N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



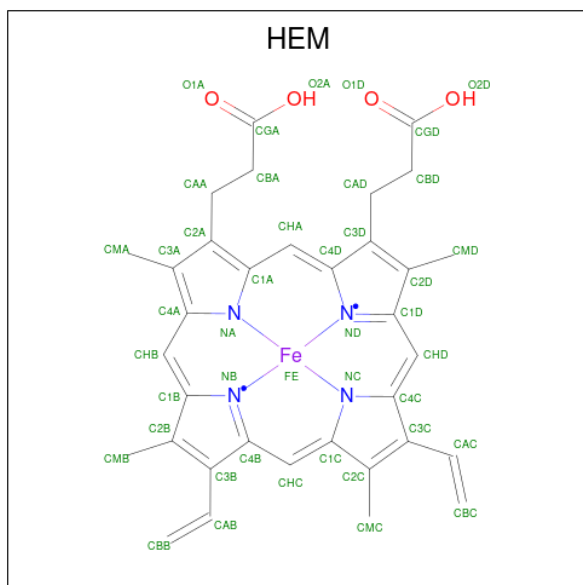
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	N	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	N	0
			3	3	

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



### 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: Deferrochelataase

Chain A:  96% ..



- Molecule 1: Deferrochelataase

Chain B:  95% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.77Å 67.40Å 73.63Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	21.47 – 1.10 21.47 – 1.10	Depositor EDS
% Data completeness (in resolution range)	79.6 (21.47-1.10) 79.6 (21.47-1.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 1.10Å)	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	0.216 , 0.239 0.236 , 0.252	Depositor DCC
$R_{free}$ test set	209285 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.039 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.55	0/2914	0.57	0/3950
1	B	0.54	0/2853	0.59	0/3869
All	All	0.54	0/5767	0.58	0/7819

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	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	ARG	Sidechain
1	A	277[A]	ARG	Sidechain
1	A	75[A]	ARG	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	2821	2760	2727	2	0
1	B	2785	2720	2720	7	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	43	30	30	2	0
3	B	43	30	30	1	0
4	A	457	0	0	0	2
4	B	420	0	0	2	1
All	All	6575	5540	5507	12	2

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 1.

All (12) 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:167:LYS:NZ	4:B:601:HOH:O	2.06	0.88
1:B:55:GLY:N	4:B:602:HOH:O	2.23	0.70
3:A:502:HEM:HBB2	3:A:502:HEM:HMB2	1.92	0.51
3:A:502:HEM:HBB2	3:A:502:HEM:CMB	2.45	0.46
1:B:341:LEU:HD23	1:B:341:LEU:C	2.41	0.46
1:B:220:LYS:HG3	1:B:231:PRO:HB3	1.98	0.45
1:B:138:LEU:HA	1:B:187:CYS:O	2.16	0.45
1:A:215:GLN:OE1	1:A:277[B]:ARG:HD3	2.18	0.43
1:B:147:SER:OG	1:B:181:ASP:OD1	2.29	0.41
1:A:92:VAL:HG21	1:A:418:LYS:HE3	2.02	0.41
3:B:502:HEM:HBB2	3:B:502:HEM:HMB2	2.03	0.41
1:B:324:ASP:OD2	1:B:385:ALA:HB2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:913:HOH:O	4:B:643:HOH:O[1_554]	2.03	0.17
4:A:917:HOH:O	4:A:947:HOH:O[2_545]	2.15	0.05



## 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 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	369/371 (100%)	362 (98%)	7 (2%)	0	100	100
1	B	362/371 (98%)	358 (99%)	4 (1%)	0	100	100
All	All	731/742 (98%)	720 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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 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	284/281 (101%)	283 (100%)	1 (0%)	89	72
1	B	278/281 (99%)	277 (100%)	1 (0%)	89	72
All	All	562/562 (100%)	560 (100%)	2 (0%)	88	72

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	GLN
1	B	367	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	AZI	B	501	3	0,2,2	-	-	0,1,1	-	-
2	AZI	A	501	3	0,2,2	-	-	0,1,1	-	-
3	HEM	B	502	1,2	41,50,50	1.18	2 (4%)	45,82,82	1.50	8 (17%)
3	HEM	A	502	1,2	41,50,50	1.36	5 (12%)	45,82,82	1.52	7 (15%)

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	B	502	1,2	-	4/12/54/54	-
3	HEM	A	502	1,2	-	4/12/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	HEM	C3C-C2C	-4.40	1.34	1.40
3	B	502	HEM	C3C-C2C	-3.58	1.35	1.40
3	A	502	HEM	C3C-CAC	2.67	1.53	1.47
3	A	502	HEM	C3B-C2B	-2.38	1.32	1.37
3	B	502	HEM	C1B-NB	-2.23	1.36	1.40
3	A	502	HEM	C1B-NB	-2.20	1.36	1.40
3	A	502	HEM	CAB-C3B	2.03	1.53	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	HEM	C4D-ND-C1D	3.78	108.98	105.07
3	A	502	HEM	C4A-C3A-C2A	-3.63	104.47	107.00
3	B	502	HEM	C1B-NB-C4B	3.61	108.80	105.07
3	A	502	HEM	C1B-NB-C4B	3.59	108.78	105.07
3	B	502	HEM	C4B-CHC-C1C	3.41	127.06	122.56
3	B	502	HEM	CHD-C1D-ND	3.32	128.04	124.43
3	A	502	HEM	C4B-CHC-C1C	3.27	126.87	122.56
3	A	502	HEM	C4C-CHD-C1D	2.66	126.07	122.56
3	B	502	HEM	CHA-C4D-ND	2.56	127.55	124.38
3	B	502	HEM	CMC-C2C-C3C	2.47	129.29	124.68
3	A	502	HEM	C4D-ND-C1D	2.46	107.61	105.07
3	B	502	HEM	CHB-C1B-NB	2.38	127.32	124.38
3	A	502	HEM	O1D-CGD-CBD	-2.13	116.23	123.08
3	A	502	HEM	CMC-C2C-C3C	2.12	128.64	124.68
3	B	502	HEM	C3D-C4D-ND	-2.10	107.82	110.17

There are no chirality outliers.

All (8) torsion outliers are listed below:

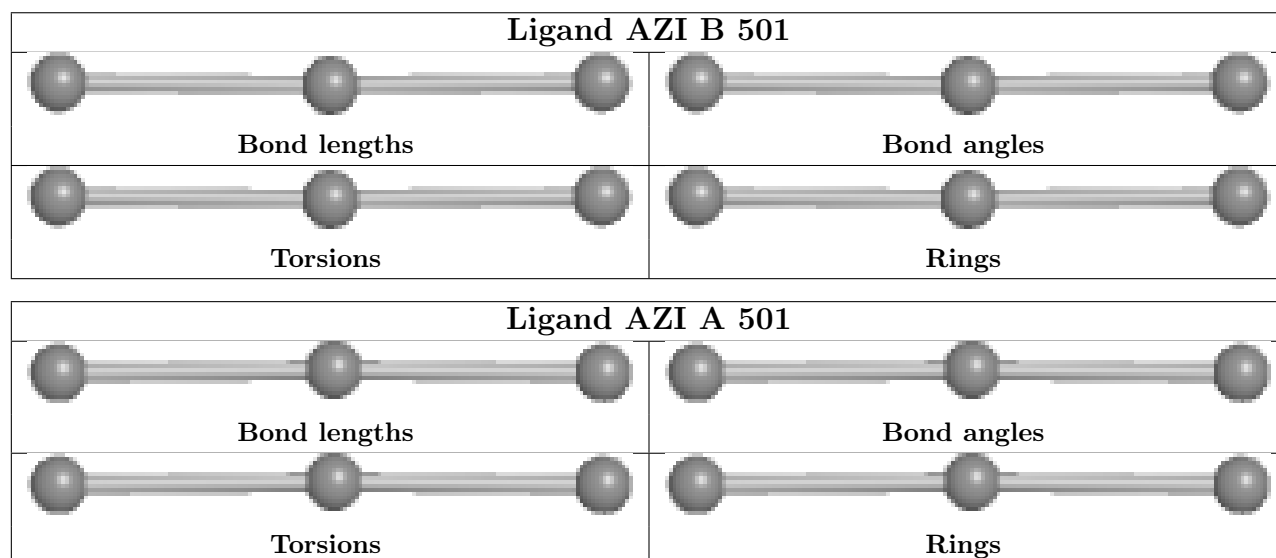
Mol	Chain	Res	Type	Atoms
3	B	502	HEM	CAA-CBA-CGA-O2A
3	A	502	HEM	CAD-CBD-CGD-O1D
3	A	502	HEM	CAD-CBD-CGD-O2D
3	B	502	HEM	CAD-CBD-CGD-O1D
3	B	502	HEM	CAD-CBD-CGD-O2D
3	B	502	HEM	CAA-CBA-CGA-O1A
3	A	502	HEM	CAA-CBA-CGA-O2A
3	A	502	HEM	CAA-CBA-CGA-O1A

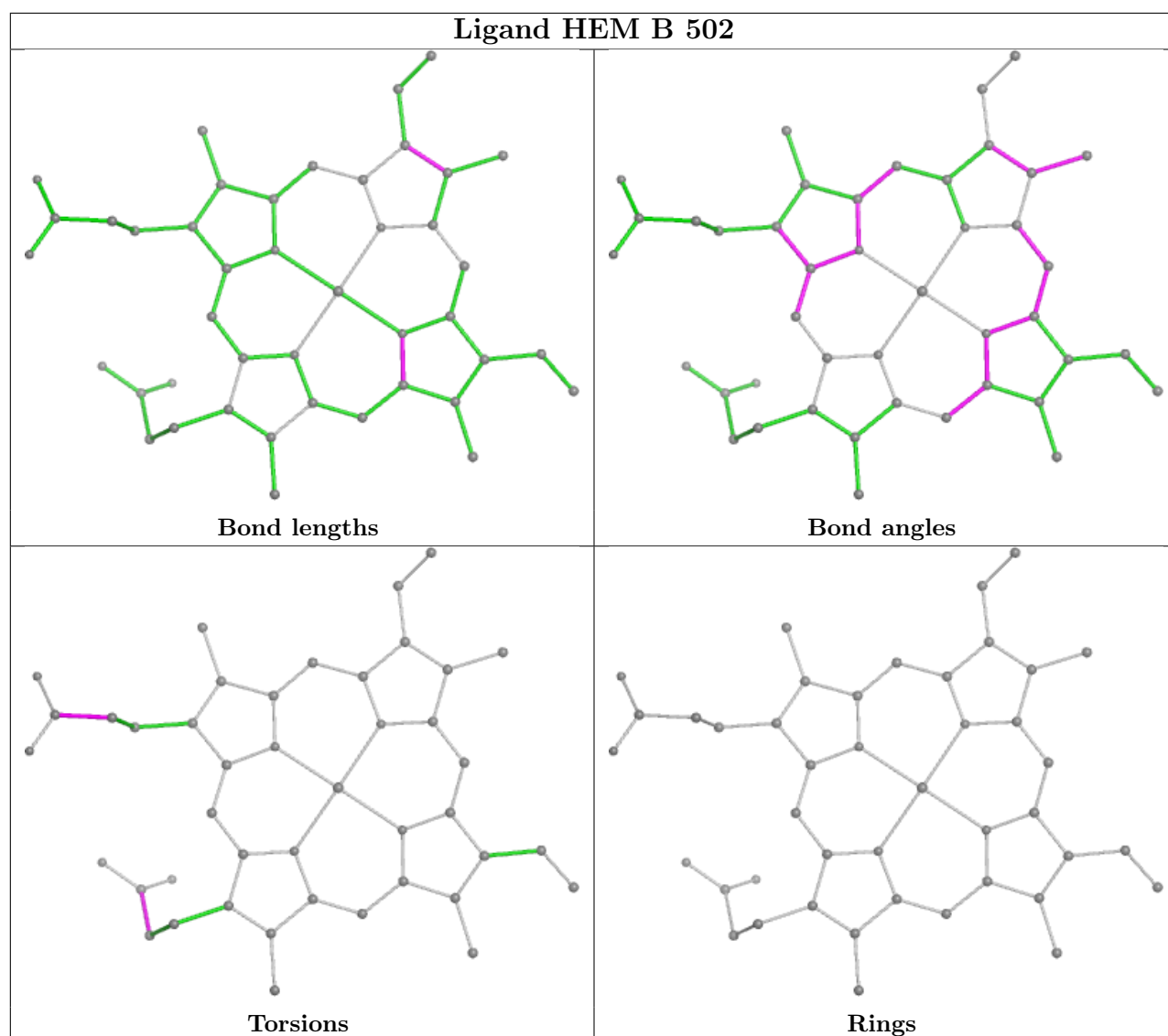
There are no ring outliers.

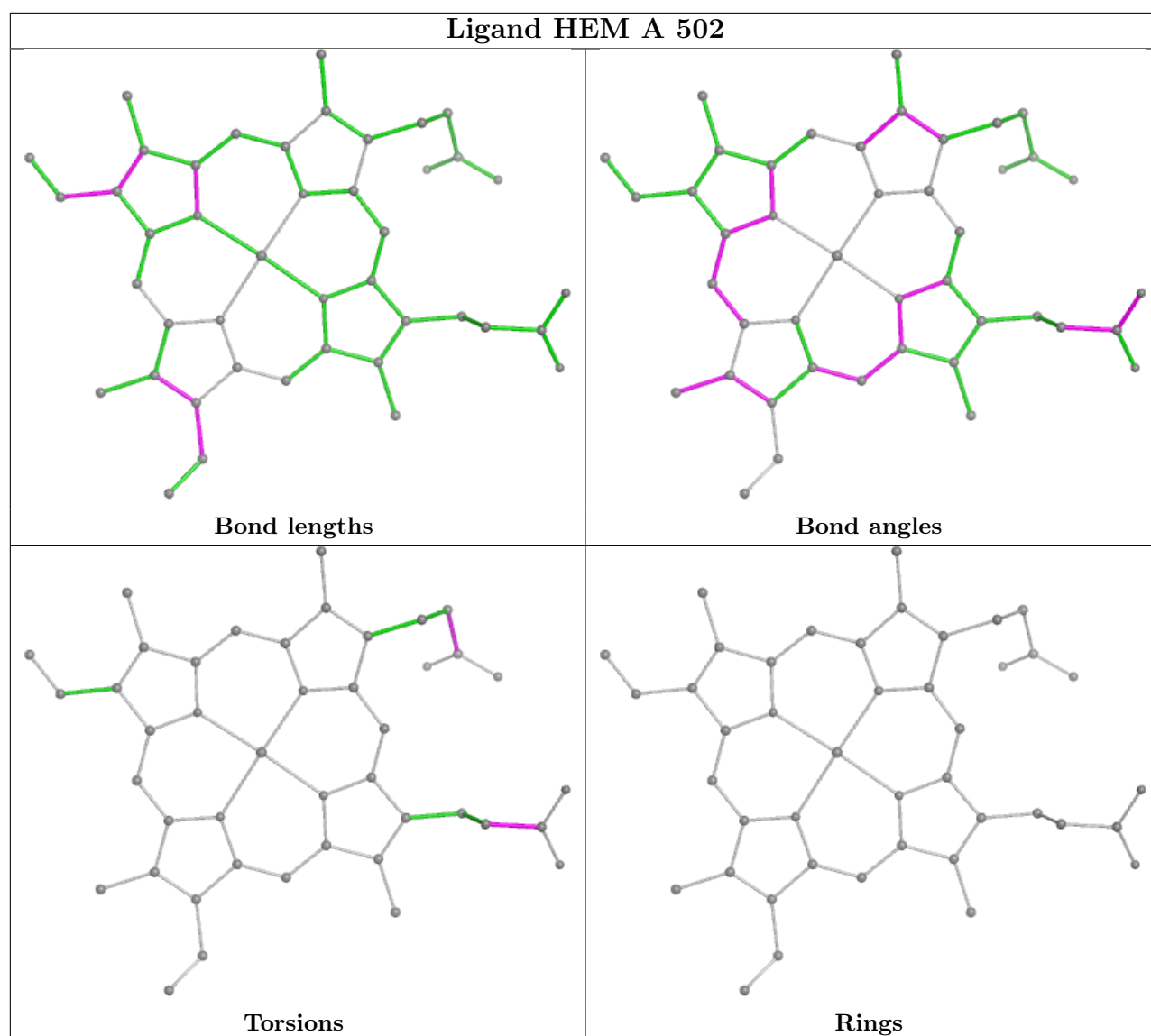
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	HEM	1	0
3	A	502	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.