



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 18, 2025 – 11:45 AM EST

PDB ID : 9MWO / pdb\_00009mwo  
Title : Structure of human endothelial nitric oxide synthase heme domain bound with N-(4-(2-((3-(thiophene-2-carboximidamido)benzyl)amino)ethyl)phenyl)thiophene-2-carboximidamide  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2025-01-17  
Resolution : 1.76 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](mailto: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)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

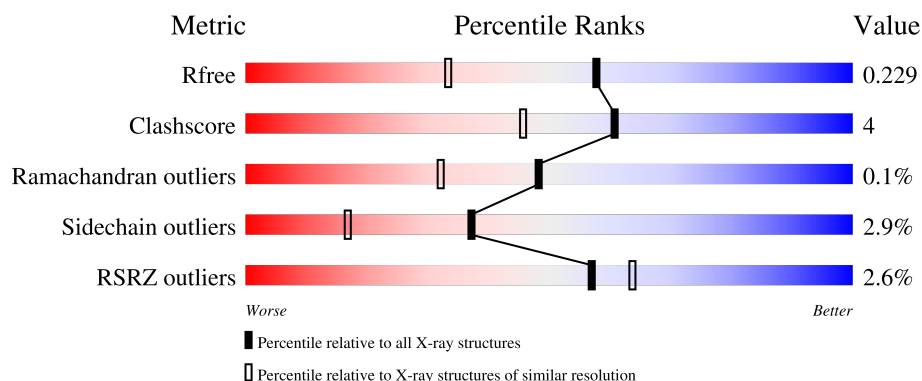
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

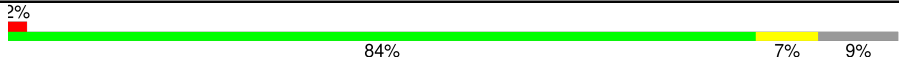



The reported resolution of this entry is 1.76 Å.

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))
$R_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	
1	B	440	
1	C	440	
1	D	440	

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	BTB	B	509	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14203 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.

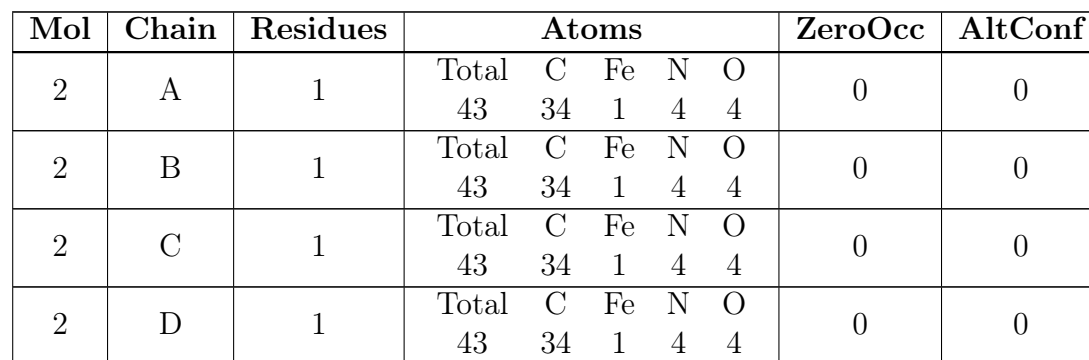
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	3	0
			3223	2052	567	588	16			
1	B	403	Total	C	N	O	S	0	4	0
			3238	2061	570	590	17			
1	C	402	Total	C	N	O	S	0	3	0
			3223	2052	567	588	16			
1	D	402	Total	C	N	O	S	0	5	0
			3230	2057	566	590	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

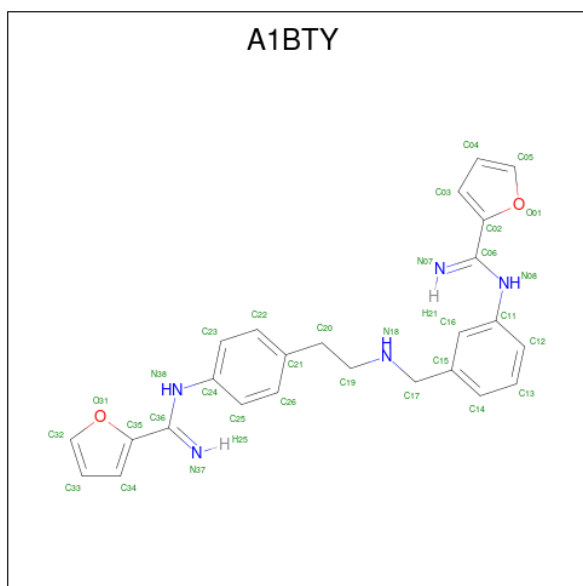
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



- 
- The chemical structure of H4B (Hydroxybenzoylserine) is shown with the following atom labels:
- Hydroxyl group:** O9 (oxygen), H (hydrogen).
  - Chiral center C9(R):** Carbon atom bonded to O9, C10(S), and C6(R).
  - Chiral center C10(S):** Carbon atom bonded to C9(R), C11, and O10 (hydroxyl group).
  - Amino group:** N5 (nitrogen), H (hydrogen).
  - Ring system:** A bicyclic system consisting of a benzene ring fused to a pyrimidine ring. Atoms include C4A, C6A, C7, C8A, C2, C4, and N1, N3, N8.
  - Carbonyl group:** C4 (carbon), O4 (oxygen).
  - Amino group:** N1 (nitrogen), N2 (nitrogen), H2 (hydrogen).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-[3-({[2-(4-{[(E)-(furan-2-yl)(imino)methyl]amino}phenyl)ethyl]amino}methyl)phenyl]furan-2-carboximidamide (CCD ID: A1BTY) (formula: C<sub>25</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	25	5	2		
4	B	1	Total	C	N	O	0	0
			32	25	5	2		
4	C	1	Total	C	N	O	0	0
			32	25	5	2		
4	D	1	Total	C	N	O	0	0
			32	25	5	2		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).



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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	Zn 1	0	0
9	C	1	Total 1	Zn 1	0	0

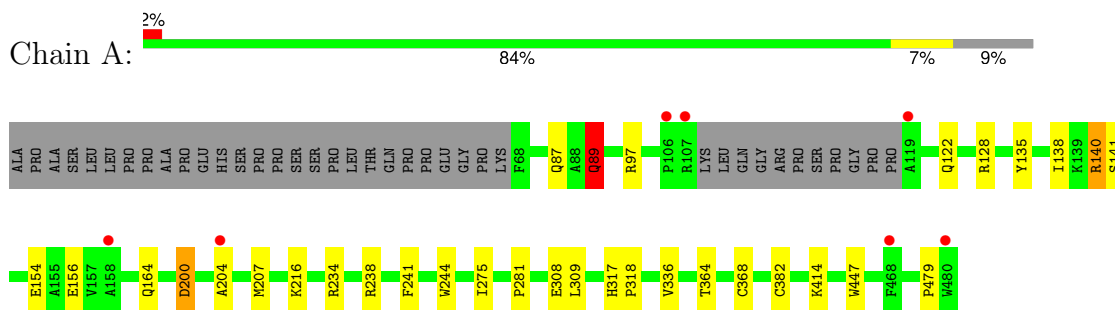
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	156	Total 156	O 156	0	0
10	B	230	Total 230	O 230	0	0
10	C	125	Total 125	O 125	0	0
10	D	217	Total 217	O 217	0	0

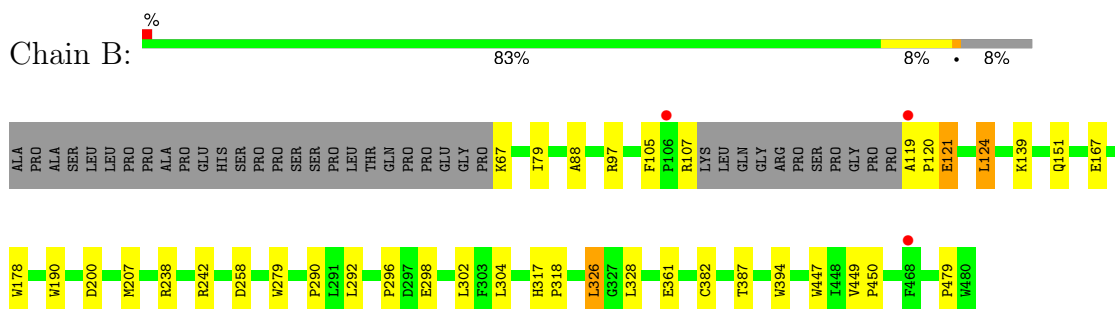
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

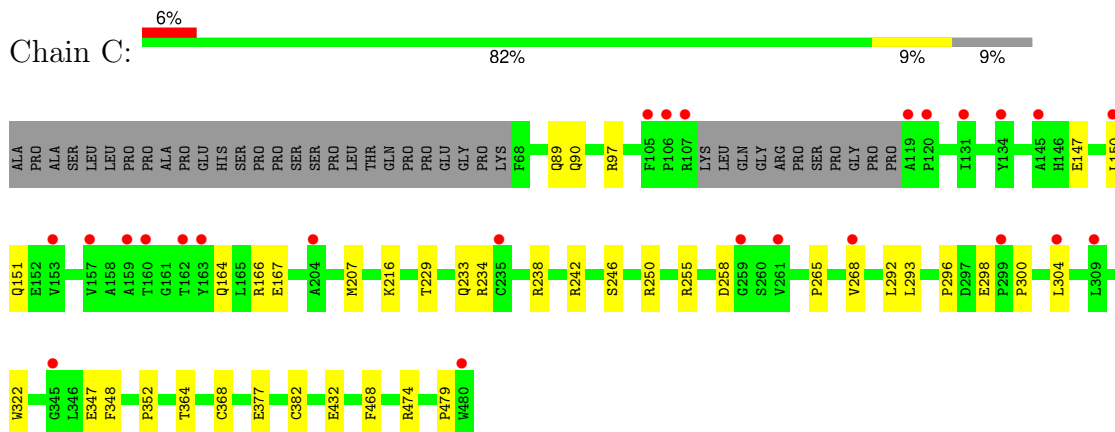
- Molecule 1: Nitric oxide synthase, endothelial



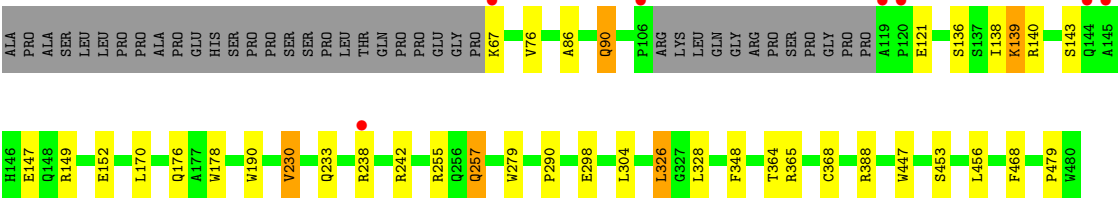
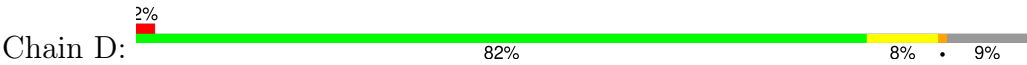
- Molecule 1: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.63Å 153.20Å 108.93Å 90.00° 90.86° 90.00°	Depositor
Resolution (Å)	39.91 – 1.76 39.91 – 1.76	Depositor EDS
% Data completeness (in resolution range)	96.8 (39.91-1.76) 97.3 (39.91-1.76)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.76Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.202 , 0.233 0.199 , 0.229	Depositor DCC
$R_{free}$ test set	9359 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, BTB, A1BTY, HEM, GD, H4B, CL

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	0.26	0/3324	0.45	0/4529
1	B	0.31	0/3339	0.48	0/4549
1	C	0.24	0/3324	0.43	0/4529
1	D	0.30	0/3334	0.47	0/4543
All	All	0.28	0/13321	0.46	0/18150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3223	0	3127	15	0
1	B	3238	0	3145	23	0
1	C	3223	0	3127	23	0
1	D	3230	0	3137	22	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	17	0	15	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	1	0
3	C	17	0	15	0	0
3	D	17	0	15	1	0
4	A	32	0	0	2	0
4	B	32	0	0	2	0
4	C	32	0	0	0	0
4	D	32	0	0	1	0
5	A	42	0	56	5	0
5	B	42	0	54	11	0
5	C	28	0	38	5	0
5	D	28	0	38	5	0
6	A	12	0	16	0	0
6	B	6	0	8	0	0
6	C	18	0	24	1	0
6	D	6	0	8	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	2	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	156	0	0	0	0
10	B	230	0	0	1	0
10	C	125	0	0	2	0
10	D	217	0	0	2	0
All	All	14203	0	12958	108	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 108 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:200:ASP:OD1	1:A:200:ASP:N	2.23	0.71
5:B:509:BTB:H61	1:C:322:TRP:CD1	2.26	0.70
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.77	0.67
1:C:377:GLU:OE1	5:C:504:BTB:O1	2.12	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.77	0.67

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	401/440 (91%)	387 (96%)	13 (3%)	1 (0%)	44	28
1	B	403/440 (92%)	395 (98%)	8 (2%)	0	100	100
1	C	401/440 (91%)	386 (96%)	15 (4%)	0	100	100
1	D	403/440 (92%)	394 (98%)	9 (2%)	0	100	100
All	All	1608/1760 (91%)	1562 (97%)	45 (3%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLN

### 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	344/373 (92%)	331 (96%)	13 (4%)	28	10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	346/373 (93%)	337 (97%)	9 (3%)	41	21
1	C	344/373 (92%)	338 (98%)	6 (2%)	56	39
1	D	346/373 (93%)	333 (96%)	13 (4%)	28	10
All	All	1380/1492 (92%)	1339 (97%)	41 (3%)	37	15

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	67	LYS
1	D	230	VAL
1	D	76	VAL
1	D	136[A]	SER
1	D	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	256	GLN
1	C	164	GLN
1	D	126	GLN
1	C	205	GLN
1	B	90	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

Of 40 ligands modelled in this entry, 11 are monoatomic - leaving 29 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	$\# Z  > 2$
6	GOL	D	506	-	5,5,5	0.42	0	5,5,5	0.37	0
3	H4B	D	502	-	16,18,18	0.90	0	14,26,26	2.41	5 (35%)
5	BTB	A	505	8	13,13,13	0.79	0	7,16,16	1.29	1 (14%)
5	BTB	D	504	8	13,13,13	0.42	0	7,16,16	0.54	0
4	A1BTY	C	503	-	27,35,35	0.92	3 (11%)	27,46,46	0.83	0
4	A1BTY	B	503	-	27,35,35	1.02	4 (14%)	27,46,46	1.25	3 (11%)
3	H4B	C	502	-	16,18,18	0.84	0	14,26,26	2.46	4 (28%)
5	BTB	A	506	-	13,13,13	0.40	0	7,16,16	0.38	0
6	GOL	B	506	-	5,5,5	0.36	0	5,5,5	0.29	0
2	HEM	B	501	1	42,50,50	1.64	8 (19%)	46,82,82	1.79	10 (21%)
5	BTB	B	505	-	13,13,13	0.53	0	7,16,16	0.75	0
6	GOL	C	508	-	5,5,5	0.39	0	5,5,5	0.42	0
6	GOL	C	509	-	5,5,5	0.35	0	5,5,5	0.36	0
5	BTB	C	507	-	13,13,13	0.35	0	7,16,16	0.25	0
5	BTB	D	505	-	13,13,13	0.42	0	7,16,16	0.58	0
6	GOL	A	508	-	5,5,5	0.46	0	5,5,5	1.04	0
3	H4B	A	502	-	16,18,18	0.91	0	14,26,26	2.47	4 (28%)
5	BTB	A	504	8	13,13,13	0.54	0	7,16,16	0.81	0
2	HEM	A	501	1	42,50,50	1.52	7 (16%)	46,82,82	1.82	9 (19%)
6	GOL	C	506	-	5,5,5	0.38	0	5,5,5	0.40	0
5	BTB	B	509	8	13,13,13	0.46	0	7,16,16	1.01	0
5	BTB	C	504	-	13,13,13	0.52	0	7,16,16	0.93	0
6	GOL	A	507	-	5,5,5	0.25	0	5,5,5	0.57	0
4	A1BTY	D	503	-	27,35,35	0.97	3 (11%)	27,46,46	1.41	5 (18%)
2	HEM	C	501	1	42,50,50	1.52	6 (14%)	46,82,82	1.65	11 (23%)
2	HEM	D	501	1	42,50,50	1.55	7 (16%)	46,82,82	1.63	9 (19%)
5	BTB	B	504	8	13,13,13	0.40	0	7,16,16	0.52	0
4	A1BTY	A	503	-	27,35,35	1.03	4 (14%)	27,46,46	1.14	2 (7%)
3	H4B	B	502	-	16,18,18	0.79	0	14,26,26	2.39	6 (42%)

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
6	GOL	D	506	-	-	2/4/4/4	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
5	BTB	A	505	8	-	7/21/21/21	-
5	BTB	D	504	8	-	0/21/21/21	-
4	A1BTY	C	503	-	-	4/15/23/23	0/4/4/4
4	A1BTY	B	503	-	-	5/15/23/23	0/4/4/4
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
5	BTB	A	506	-	-	4/21/21/21	-
6	GOL	B	506	-	-	2/4/4/4	-
2	HEM	B	501	1	-	0/12/54/54	-
5	BTB	B	505	-	-	13/21/21/21	-
6	GOL	C	508	-	-	2/4/4/4	-
6	GOL	C	509	-	-	2/4/4/4	-
5	BTB	C	507	-	-	2/21/21/21	-
5	BTB	D	505	-	-	15/21/21/21	-
6	GOL	A	508	-	-	4/4/4/4	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
5	BTB	A	504	8	-	6/21/21/21	-
2	HEM	A	501	1	-	0/12/54/54	-
6	GOL	C	506	-	-	4/4/4/4	-
5	BTB	B	509	8	-	3/21/21/21	-
5	BTB	C	504	-	-	11/21/21/21	-
6	GOL	A	507	-	-	0/4/4/4	-
4	A1BTY	D	503	-	-	4/15/23/23	0/4/4/4
2	HEM	C	501	1	-	2/12/54/54	-
2	HEM	D	501	1	-	0/12/54/54	-
5	BTB	B	504	8	-	4/21/21/21	-
4	A1BTY	A	503	-	-	6/15/23/23	0/4/4/4
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C4C	4.07	1.47	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3C-C2C	-3.71	1.35	1.40
2	B	501	HEM	C3C-CAC	3.66	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.64	1.35	1.40
2	D	501	HEM	C3C-C4C	3.54	1.46	1.41

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	H4B	C8A-C4A-C4	6.04	120.00	114.50
3	C	502	H4B	C8A-C4A-C4	5.67	119.66	114.50
3	B	502	H4B	C8A-C4A-C4	5.52	119.53	114.50
2	B	501	HEM	CBA-CAA-C2A	-5.51	103.27	112.54
2	A	501	HEM	C4B-CHC-C1C	5.49	129.80	122.56

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	A1BTY	N18-C19-C20-C21
4	B	503	A1BTY	N18-C19-C20-C21
4	C	503	A1BTY	N18-C19-C20-C21
4	D	503	A1BTY	C35-C36-N38-C24
4	D	503	A1BTY	N37-C36-N38-C24

There are no ring outliers.

21 monomers are involved in 46 short contacts:

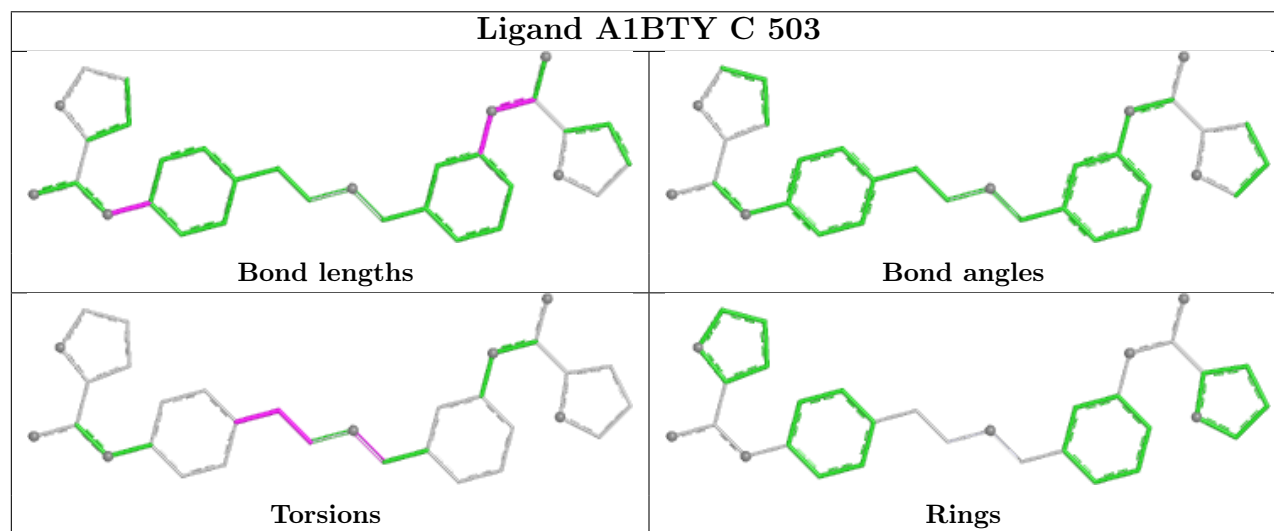
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	506	GOL	2	0
3	D	502	H4B	1	0
5	A	505	BTB	1	0
5	D	504	BTB	1	0
4	B	503	A1BTY	2	0
5	A	506	BTB	2	0
2	B	501	HEM	2	0
5	B	505	BTB	3	0
5	C	507	BTB	1	0
5	D	505	BTB	4	0
3	A	502	H4B	1	0
5	A	504	BTB	2	0
2	A	501	HEM	3	0

*Continued on next page...*

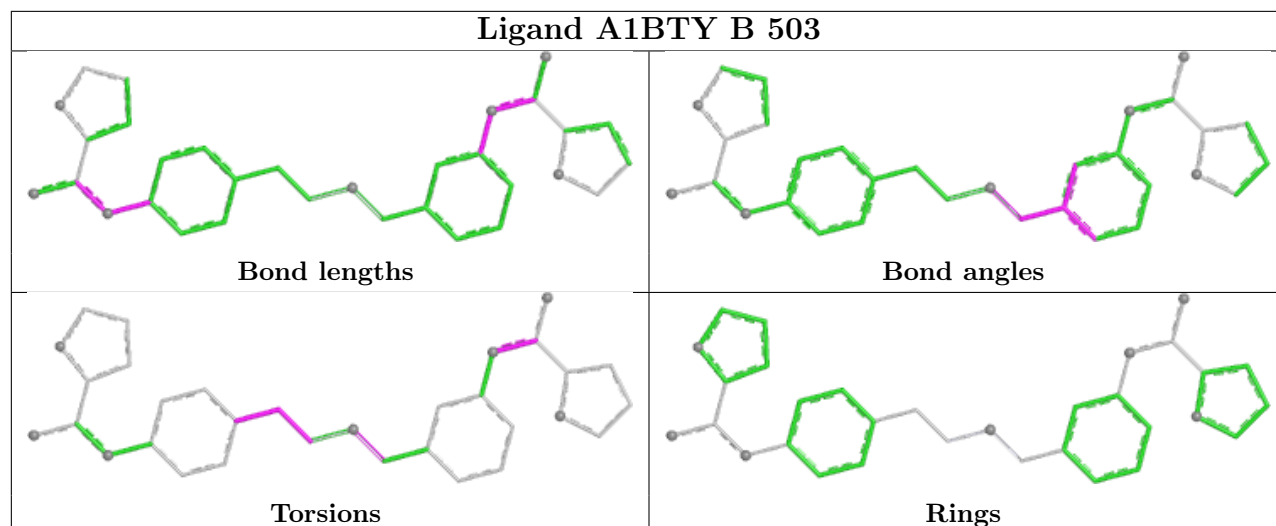
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	506	GOL	1	0
5	B	509	BTB	8	0
5	C	504	BTB	4	0
4	D	503	A1BTY	1	0
2	C	501	HEM	2	0
2	D	501	HEM	2	0
4	A	503	A1BTY	2	0
3	B	502	H4B	1	0

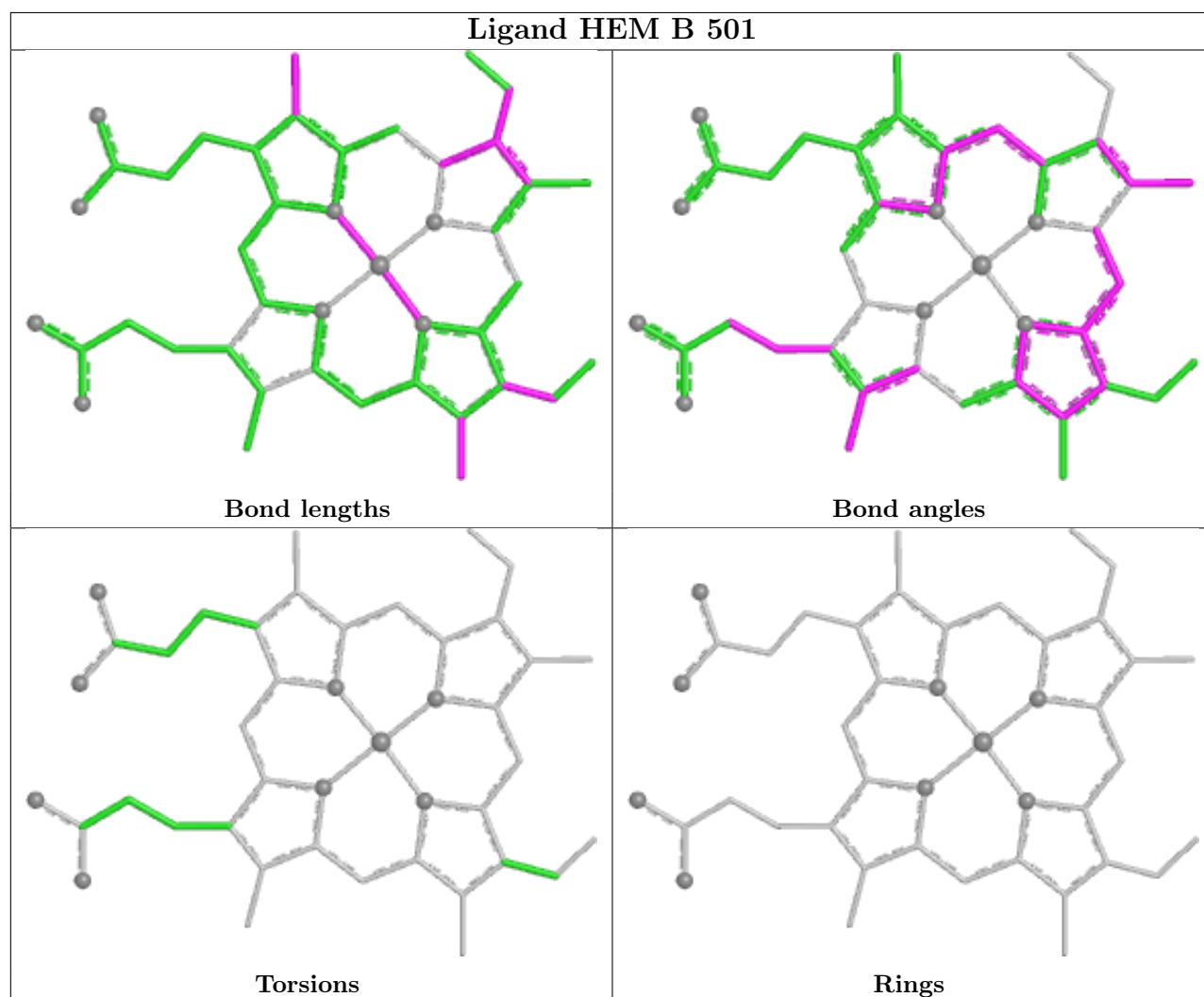
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

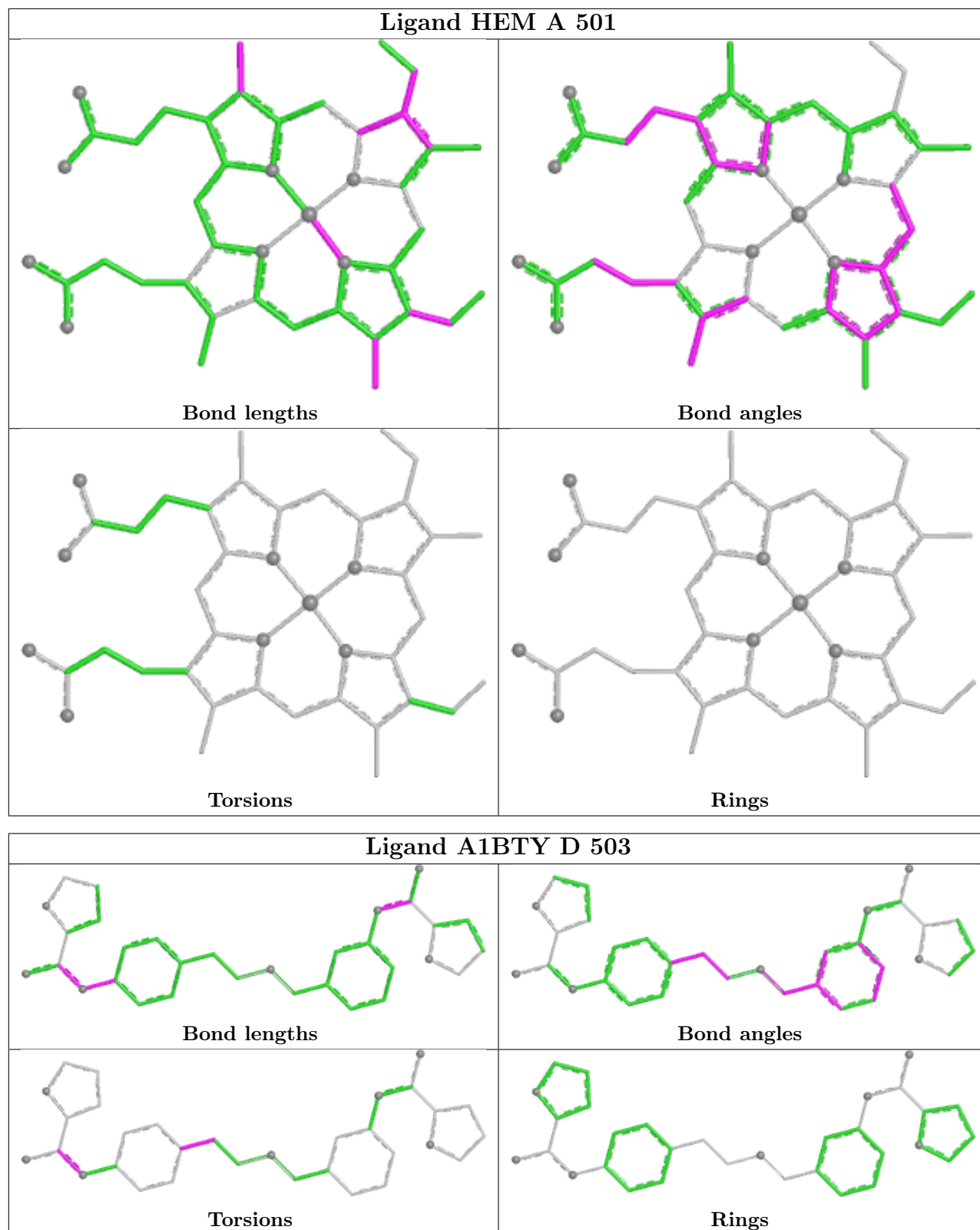


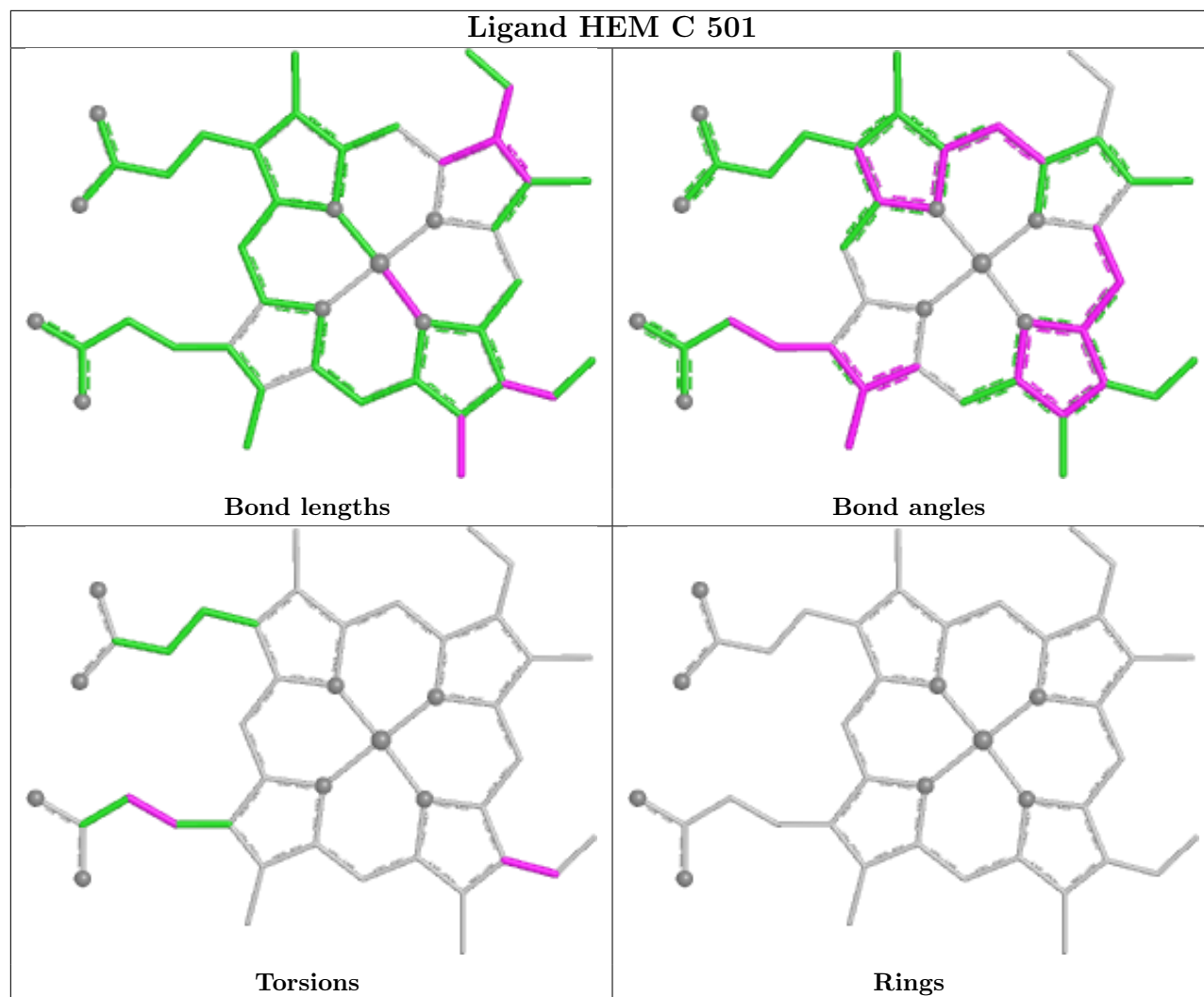
## Ligand A1BTY B 503

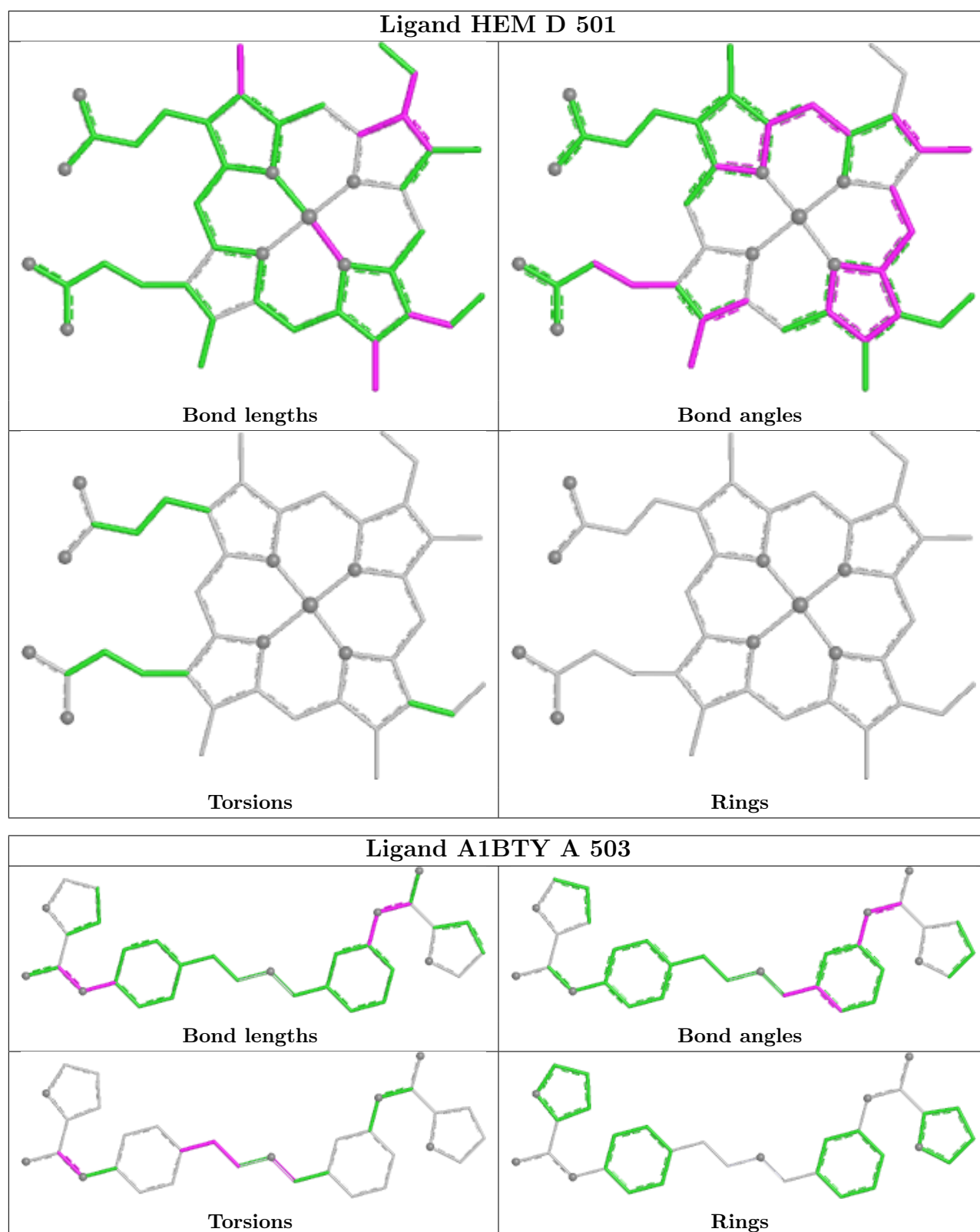


## Ligand HEM B 501









## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	402/440 (91%)	0.29	7 (1%) 69 74	24, 50, 81, 96	3 (0%)
1	B	403/440 (91%)	-0.06	3 (0%) 84 88	20, 38, 64, 85	4 (0%)
1	C	402/440 (91%)	0.64	25 (6%) 28 31	23, 57, 100, 117	3 (0%)
1	D	402/440 (91%)	0.07	7 (1%) 69 74	23, 39, 70, 91	5 (1%)
All	All	1609/1760 (91%)	0.23	42 (2%) 57 64	20, 45, 84, 117	15 (0%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	ALA	4.7
1	C	106	PRO	4.3
1	A	107	ARG	3.9
1	A	106	PRO	3.8
1	D	119	ALA	3.7

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

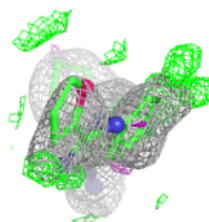
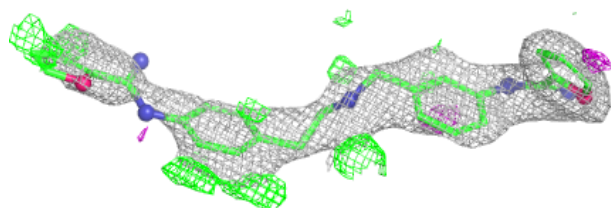
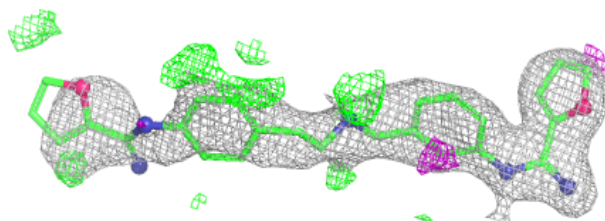
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	C	509	6/6	0.47	0.16	90,95,96,97	0
5	BTB	C	507	14/14	0.55	0.20	90,102,110,110	0
5	BTB	A	506	14/14	0.62	0.17	86,93,95,96	0
6	GOL	C	506	6/6	0.66	0.19	56,73,74,82	0
5	BTB	C	504	14/14	0.68	0.19	38,74,82,90	0
5	BTB	B	505	14/14	0.69	0.23	57,71,82,84	0
6	GOL	C	508	6/6	0.70	0.15	67,73,76,78	0
5	BTB	A	505	14/14	0.70	0.17	59,80,85,85	0
5	BTB	D	505	14/14	0.71	0.19	55,72,79,80	0
6	GOL	B	506	6/6	0.76	0.21	68,73,80,88	0
6	GOL	A	508	6/6	0.77	0.23	58,64,74,77	0
4	A1BTY	C	503	32/32	0.81	0.18	43,77,93,94	0
6	GOL	D	506	6/6	0.83	0.27	76,79,83,85	0
4	A1BTY	A	503	32/32	0.86	0.16	32,65,103,105	0
5	BTB	D	504	14/14	0.86	0.17	50,59,78,84	0
5	BTB	B	504	14/14	0.86	0.15	41,61,71,74	0
4	A1BTY	D	503	32/32	0.88	0.17	26,54,116,119	0
4	A1BTY	B	503	32/32	0.89	0.16	25,57,98,102	0
8	GD	C	511	1/1	0.91	0.09	113,113,113,113	0
5	BTB	B	509	14/14	0.92	0.11	32,74,85,88	0
6	GOL	A	507	6/6	0.92	0.09	37,53,66,71	0
5	BTB	A	504	14/14	0.92	0.14	19,69,76,77	0
3	H4B	C	502	17/17	0.93	0.08	40,47,54,58	0
3	H4B	A	502	17/17	0.94	0.09	30,40,50,51	0
3	H4B	D	502	17/17	0.94	0.08	26,36,43,44	0
8	GD	A	510	1/1	0.95	0.09	85,85,85,85	0
7	CL	C	510	1/1	0.95	0.08	60,60,60,60	0
8	GD	A	511	1/1	0.96	0.07	102,102,102,102	0
3	H4B	B	502	17/17	0.96	0.06	27,35,42,43	0
2	HEM	A	501	43/43	0.97	0.08	28,37,48,57	0
7	CL	A	509	1/1	0.97	0.07	50,50,50,50	0
8	GD	B	508	1/1	0.97	0.05	45,45,45,45	0
2	HEM	C	501	43/43	0.97	0.09	30,43,57,59	0
2	HEM	D	501	43/43	0.98	0.06	20,27,41,46	0
7	CL	B	507	1/1	0.98	0.06	44,44,44,44	0
2	HEM	B	501	43/43	0.98	0.06	20,27,38,43	0
7	CL	D	507	1/1	0.98	0.07	40,40,40,40	0
8	GD	D	508	1/1	0.98	0.04	41,41,41,41	0
9	ZN	C	505	1/1	0.98	0.03	38,38,38,38	0
9	ZN	A	512	1/1	1.00	0.04	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

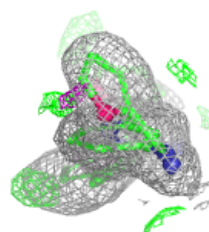
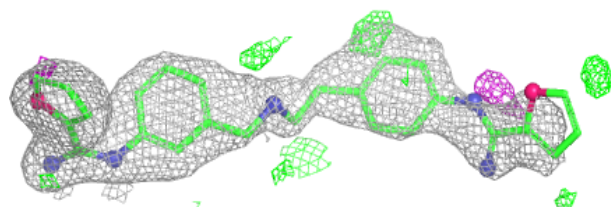
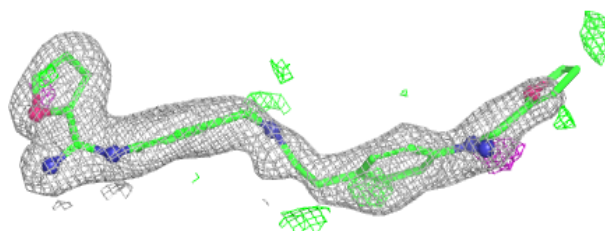
**Electron density around A1BTY C 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



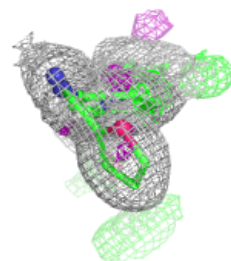
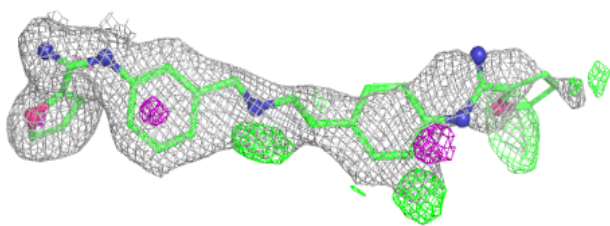
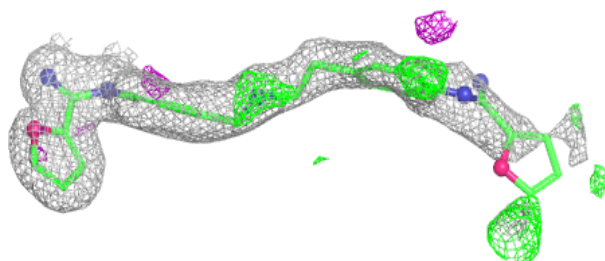
**Electron density around A1BTY A 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

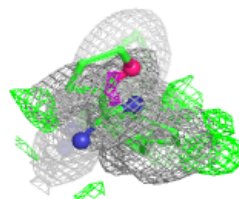
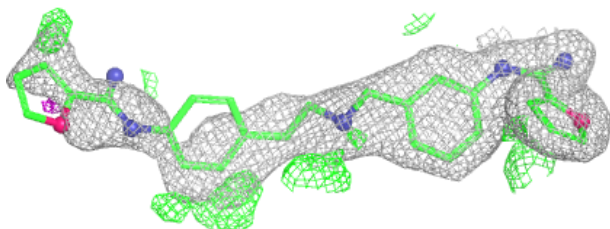
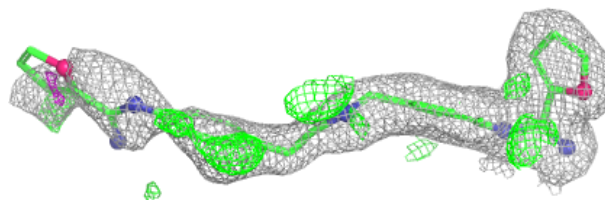


**Electron density around A1BTY D 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

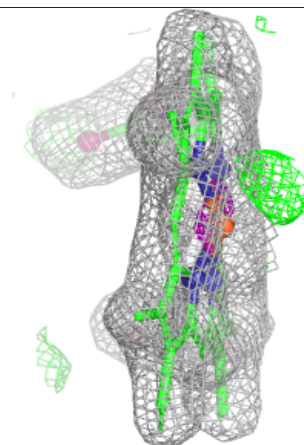
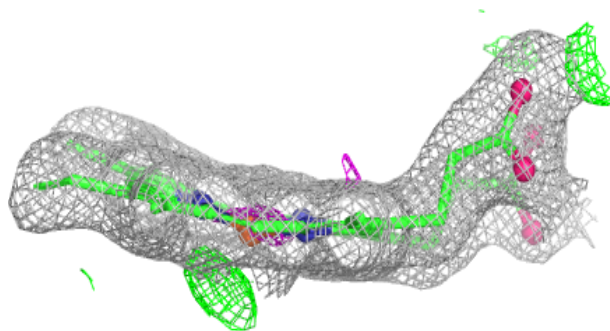
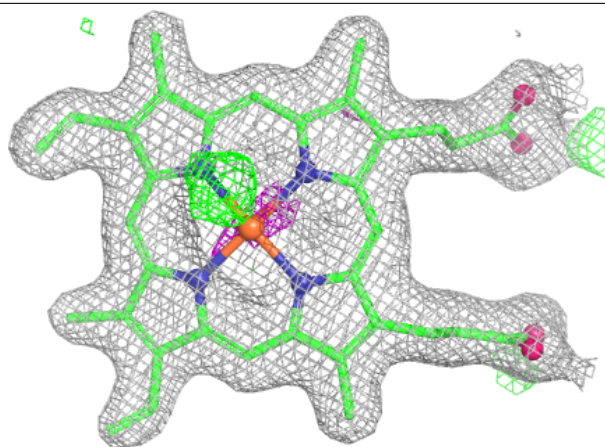
**Electron density around A1BTY B 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



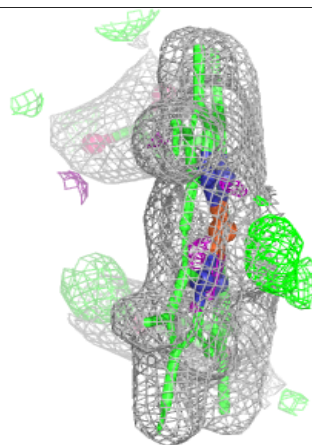
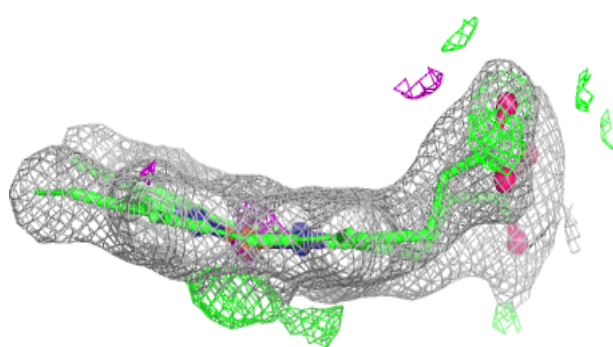
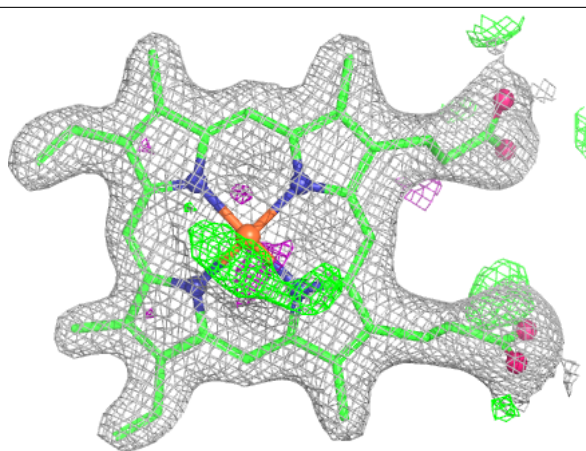
**Electron density around HEM A 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 501:**

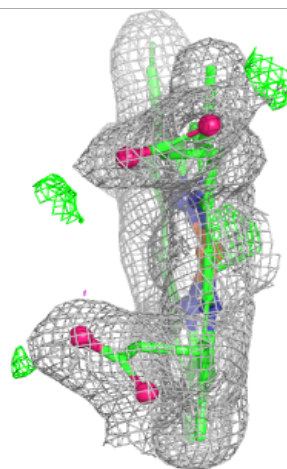
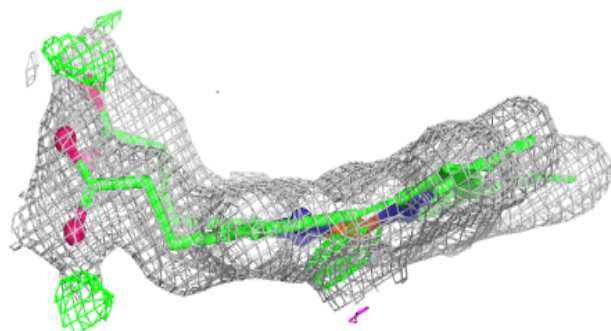
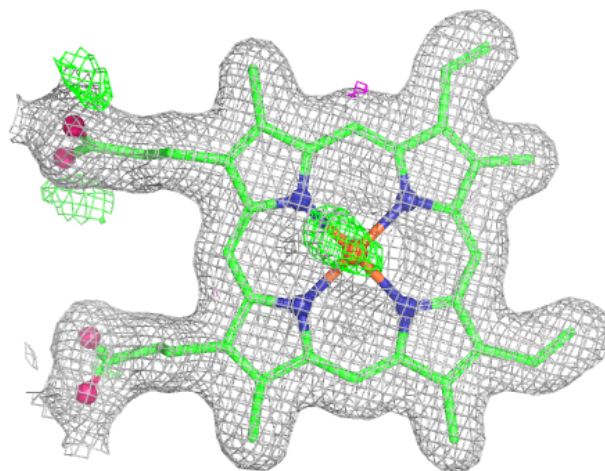
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



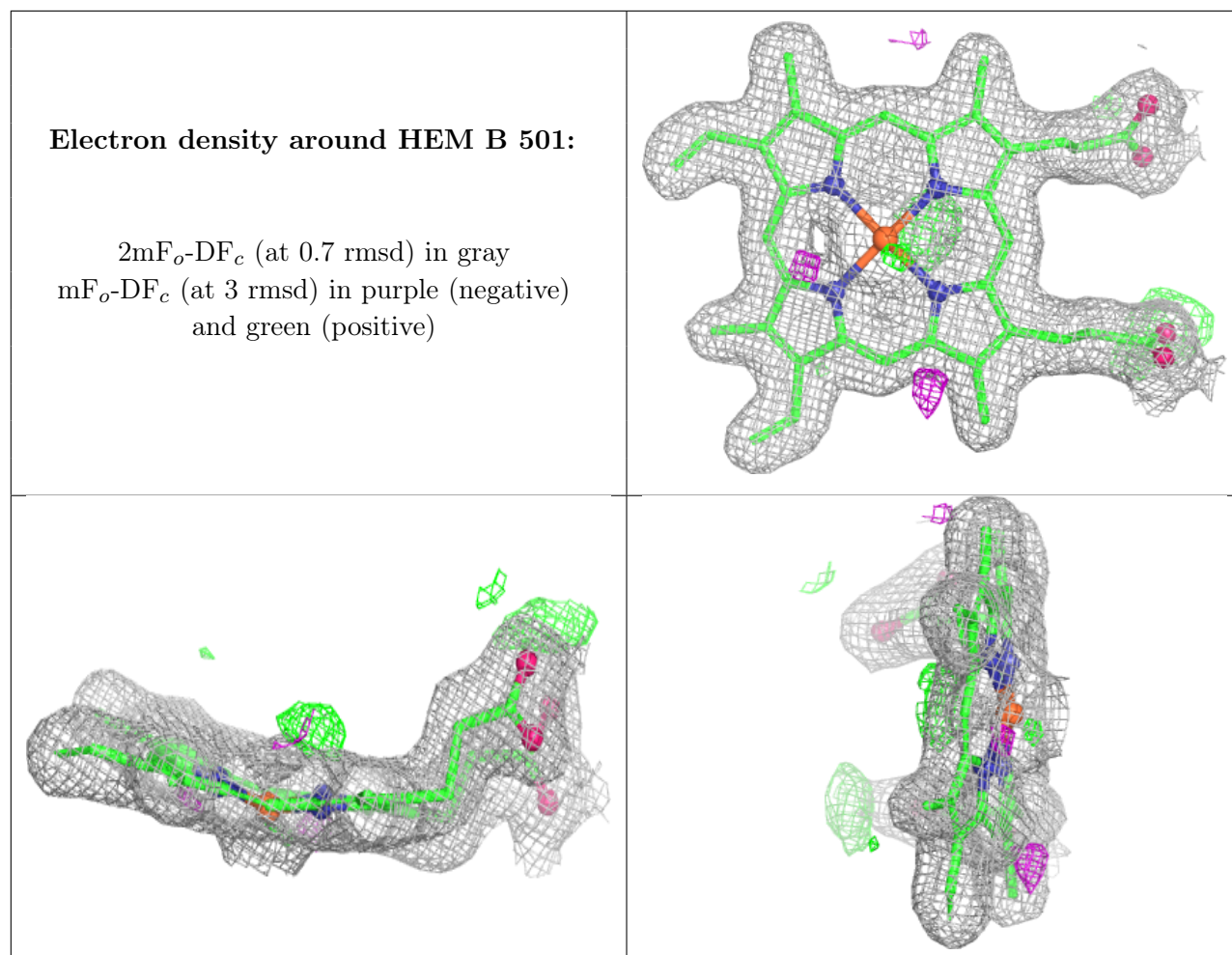


**Electron density around HEM D 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers ⓘ

There are no such residues in this entry.