



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 18, 2025 – 11:45 AM EST

PDB ID : 9MWQ / pdb\_00009mwq  
Title : Structure of human endothelial nitric oxide synthase heme domain bound with N-(4-(2-((3-(isoxazole-3-carboximidamido)benzyl)amino)ethyl)phenyl)isoxazole-3-carboximidamide  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2025-01-17  
Resolution : 1.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

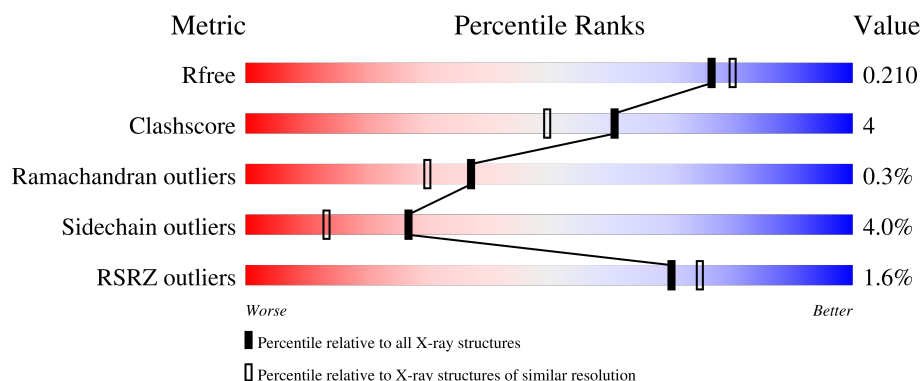
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>8%</div> </div> </div>
1	B	440	<div> <div>0%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	C	440	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>9%</div> </div> </div>
1	D	440	<div> <div>0%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>9%</div> </div> </div>

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	D	505	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14348 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.

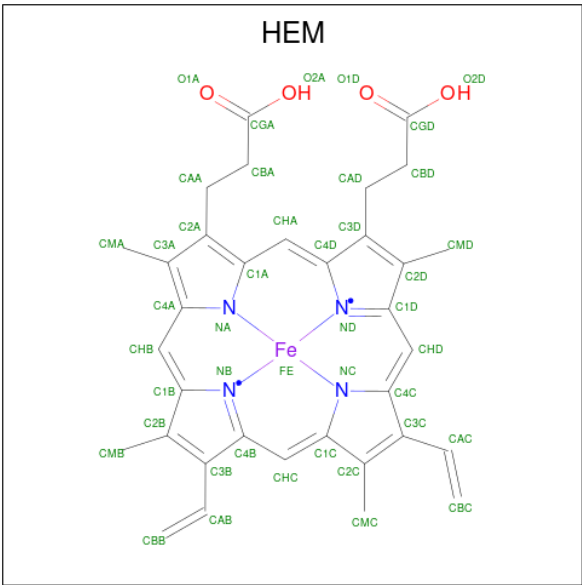
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	1	0
			3227	2055	570	586	16			
1	B	404	Total	C	N	O	S	0	4	0
			3245	2066	572	591	16			
1	C	401	Total	C	N	O	S	0	1	0
			3211	2044	567	584	16			
1	D	402	Total	C	N	O	S	0	4	0
			3227	2054	568	589	16			

There are 4 discrepancies between the modelled and reference sequences:

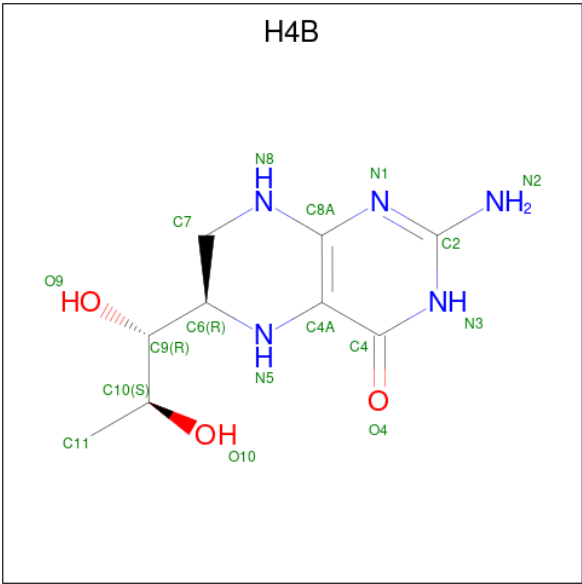
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



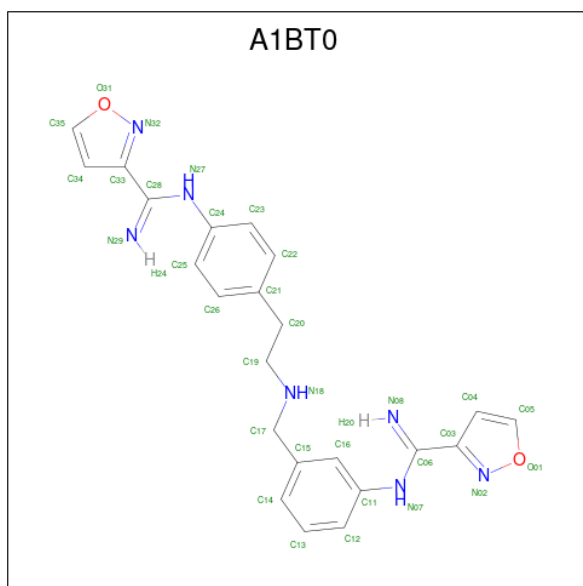
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>).



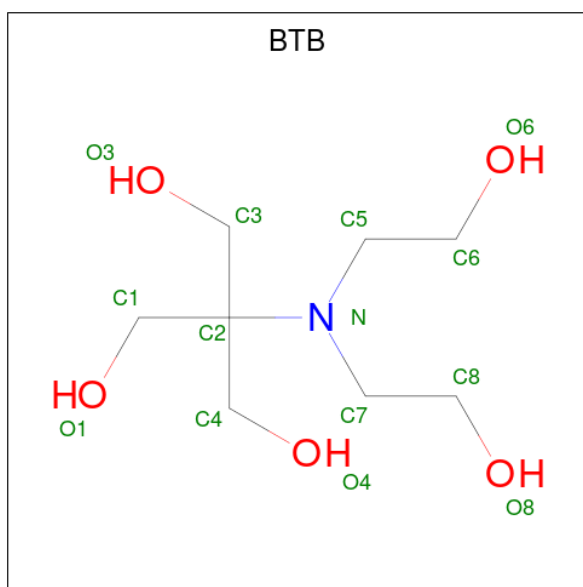
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-[3-({[2-(4-{[(E)-imino(1,2-oxazol-3-yl)methyl]amino}phenyl)ethyl]amino}methyl)phenyl]-1,2-oxazole-3-carboximidamide (CCD ID: A1BT0) (formula: C<sub>23</sub>H<sub>23</sub>N<sub>7</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



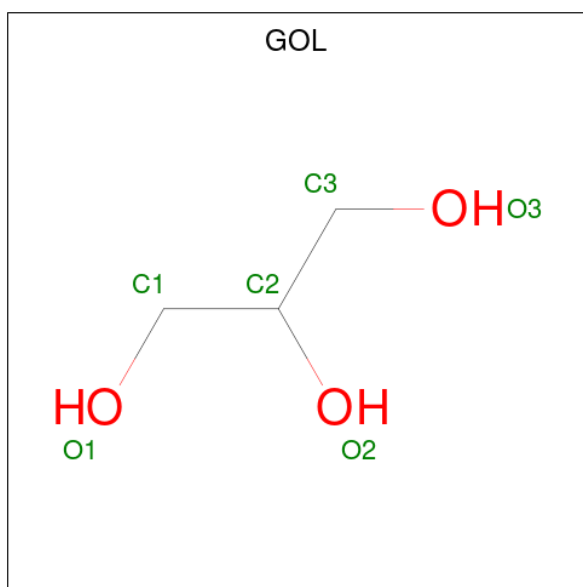
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	23	7	2		
4	B	1	Total	C	N	O	0	0
			32	23	7	2		
4	C	1	Total	C	N	O	0	0
			32	23	7	2		
4	D	1	Total	C	N	O	0	0
			32	23	7	2		

- 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	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	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	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	1	Total Gd 1 1	0	0
8	B	1	Total Gd 1 1	0	0
8	C	1	Total Gd 1 1	0	0
8	D	1	Total Gd 1 1	0	0

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

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

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

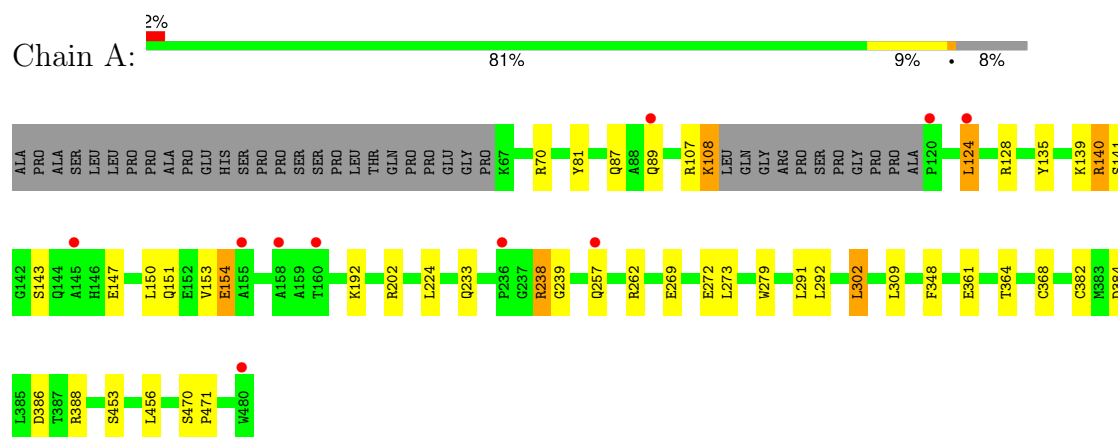
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	202	Total O 202 202	0	0
11	B	258	Total O 258 258	0	0
11	C	180	Total O 180 180	0	0
11	D	263	Total O 263 263	0	0

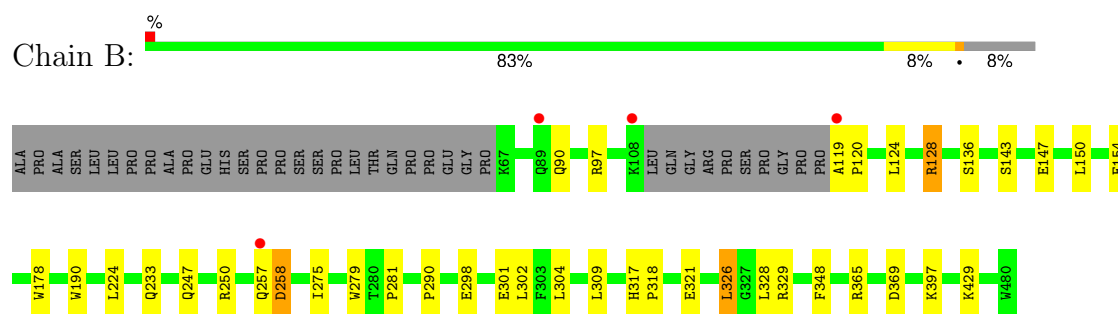
### 3 Residue-property plots [i](#)

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.

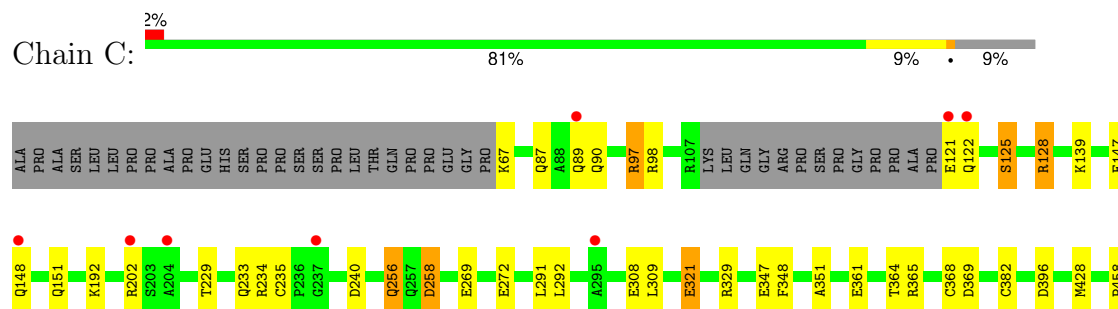
- Molecule 1: Nitric oxide synthase, endothelial

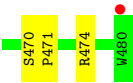


- Molecule 1: Nitric oxide synthase, endothelial

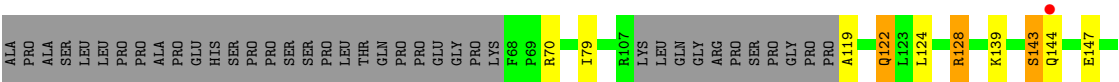
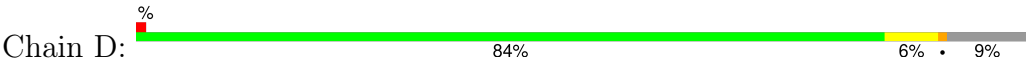


- Molecule 1: Nitric oxide synthase, endothelial





● 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, $\alpha$ , $\beta$ , $\gamma$	59.73Å 152.87Å 108.75Å 90.00° 90.76° 90.00°	Depositor
Resolution (Å)	38.77 – 1.94 38.77 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.77-1.94) 99.6 (38.77-1.94)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.172 , 0.211 0.172 , 0.210	Depositor DCC
$R_{free}$ test set	7246 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.073 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: H4B, GD, A1BT0, CA, GOL, ZN, HEM, CL, BTB

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	0.27	0/3322	0.46	0/4523
1	B	0.33	0/3349	0.52	0/4561
1	C	0.26	0/3305	0.46	0/4501
1	D	0.32	0/3331	0.50	0/4539
All	All	0.30	0/13307	0.48	0/18124

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	143	SER	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	3227	0	3138	22	0
1	B	3245	0	3157	22	0
1	C	3211	0	3117	19	0
1	D	3227	0	3131	25	0
2	A	43	0	30	2	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	0	0
3	B	17	0	15	0	0
3	C	17	0	15	0	0
3	D	17	0	15	1	0
4	A	32	0	0	1	0
4	B	32	0	0	0	0
4	C	32	0	0	1	0
4	D	32	0	0	1	0
5	A	28	0	37	3	0
5	B	28	0	36	6	0
5	C	28	0	38	4	0
5	D	28	0	36	11	0
6	A	18	0	24	0	0
6	B	6	0	8	0	0
6	C	12	0	16	0	0
6	D	6	0	8	0	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	1	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	2	0	0	0	0
10	B	1	0	0	0	0
11	A	202	0	0	4	0
11	B	258	0	0	1	0
11	C	180	0	0	1	0
11	D	263	0	0	2	0
All	All	14348	0	12926	109	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.

All (109) 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:279:TRP:HB2	1:A:302:LEU:HD11	1.60	0.83
5:A:504:BTB:O3	11:A:601:HOH:O	2.01	0.78
1:B:128:ARG:HG3	1:B:150:LEU:HD22	1.68	0.76
1:A:382:CYS:HA	5:A:504:BTB:H11	1.69	0.75
1:D:128:ARG:HG3	1:D:150:LEU:HD22	1.68	0.73
1:B:258:ASP:OD1	1:B:258:ASP:N	2.22	0.72
1:A:257:GLN:OE1	11:A:602:HOH:O	2.09	0.69
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.75	0.69
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.75	0.68
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.76	0.66
5:B:504:BTB:H82	5:B:504:BTB:O4	1.96	0.66
1:D:70:ARG:NH1	11:D:602:HOH:O	2.19	0.65
1:D:247:GLN:HB2	1:D:250:ARG:HD3	1.78	0.65
1:C:97:ARG:HG2	1:C:98:ARG:HG2	1.77	0.65
1:C:321:GLU:H	1:C:321:GLU:CD	2.05	0.63
5:D:504:BTB:O4	5:D:504:BTB:H82	1.99	0.62
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.82	0.62
1:D:258:ASP:OD1	1:D:258:ASP:N	2.29	0.61
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.17	0.61
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.81	0.61
1:C:382:CYS:HA	5:C:504:BTB:H31	1.83	0.60
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.85	0.58
1:B:298:GLU:OE2	5:B:505:BTB:O4	2.19	0.58
1:B:275:ILE:HG12	1:B:281:PRO:HG3	1.86	0.58
1:A:262:ARG:NH2	11:A:608:HOH:O	2.36	0.58
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.84	0.57
1:B:321:GLU:OE2	5:B:504:BTB:O4	2.22	0.57
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.86	0.57
1:A:386:ASP:OD2	1:A:388:ARG:HG2	2.05	0.55
1:B:97:ARG:HH11	1:B:97:ARG:HB3	1.71	0.55
5:C:505:BTB:O3	5:C:505:BTB:O4	2.12	0.55
1:B:143:SER:O	1:B:147:GLU:HG2	2.09	0.53
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.91	0.52
5:D:505:BTB:O8	5:D:505:BTB:O3	2.23	0.52
1:B:119:ALA:N	1:B:120:PRO:HD3	2.25	0.51
1:B:365:ARG:NH2	1:B:369:ASP:OD2	2.43	0.51
1:B:124:LEU:HD13	1:B:128:ARG:HH12	1.75	0.51
1:A:364:THR:O	1:A:368:CYS:HB2	2.11	0.50
1:B:397:LYS:NZ	11:B:605:HOH:O	2.43	0.50
1:A:192:LYS:NZ	11:A:609:HOH:O	2.42	0.50

*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	1.93	0.50
1:C:365:ARG:NH2	1:C:369:ASP:OD2	2.46	0.49
1:A:70:ARG:HG3	1:A:81:TYR:CZ	2.47	0.49
1:B:97:ARG:HB3	1:B:97:ARG:NH1	2.27	0.49
1:C:240:ASP:OD1	11:C:602:HOH:O	2.19	0.48
1:D:298:GLU:OE2	5:D:505:BTB:O8	2.27	0.48
5:B:504:BTB:O4	5:B:504:BTB:C8	2.62	0.48
1:D:257:GLN:C	1:D:259:GLY:H	2.22	0.48
1:C:364:THR:O	1:C:368:CYS:HB2	2.13	0.48
1:C:269:GLU:O	1:C:272:GLU:HG2	2.13	0.48
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.45	0.48
1:C:308:GLU:H	1:C:308:GLU:CD	2.19	0.47
5:D:504:BTB:H11	5:D:504:BTB:H72	1.69	0.47
5:D:505:BTB:HO3	5:D:505:BTB:HO8	1.59	0.47
1:D:298:GLU:OE1	5:D:505:BTB:H72	2.15	0.46
1:D:298:GLU:OE1	5:D:505:BTB:H42	2.15	0.46
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.50	0.46
1:D:128:ARG:NH1	1:D:154:GLU:HG2	2.31	0.46
1:D:447:TRP:HA	3:D:502:H4B:N1	2.31	0.46
1:D:387:THR:HA	1:D:394:TRP:CD1	2.51	0.46
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.98	0.45
1:C:361:GLU:OE1	4:C:503:A1BT0:N07	2.50	0.45
1:A:150:LEU:O	1:A:153:VAL:HG22	2.17	0.45
1:D:361:GLU:OE1	4:D:503:A1BT0:N07	2.50	0.45
1:A:124:LEU:HD21	1:A:154:GLU:HG3	1.97	0.45
1:A:108:LYS:H	1:A:108:LYS:HG3	1.49	0.45
1:A:361:GLU:OE1	4:A:503:A1BT0:N07	2.50	0.45
1:D:321:GLU:CD	5:D:504:BTB:O4	2.60	0.45
5:B:505:BTB:H72	5:B:505:BTB:H41	1.54	0.45
1:A:135:TYR:HD1	1:A:140:ARG:HB2	1.82	0.44
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.79	0.44
5:B:504:BTB:H72	5:B:504:BTB:H11	1.61	0.44
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.91	0.44
1:C:256:GLN:C	1:C:258:ASP:H	2.25	0.44
1:D:388:ARG:HE	1:D:388:ARG:HB2	1.48	0.44
1:C:147:GLU:O	1:C:151:GLN:NE2	2.44	0.44
1:B:247:GLN:HB2	1:B:250:ARG:HD3	2.01	0.43
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.54	0.43
1:C:396:ASP:OD2	1:D:453:SER:OG	2.29	0.43
1:A:238:ARG:HG2	1:A:239:GLY:N	2.33	0.43
1:D:143:SER:O	1:D:147:GLU:HG2	2.19	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:SER:HB3	1:A:456:LEU:HD12	2.00	0.42
1:A:124:LEU:O	1:A:128:ARG:HG3	2.20	0.42
1:D:285:ARG:NH2	11:D:603:HOH:O	2.29	0.42
1:A:269:GLU:O	1:A:272:GLU:HG2	2.19	0.42
5:C:505:BTB:H11	5:C:505:BTB:H51	1.45	0.42
1:D:364:THR:O	1:D:368:CYS:HB2	2.19	0.42
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.93	0.42
5:C:504:BTB:H51	5:C:504:BTB:H32	1.60	0.42
5:D:505:BTB:H72	5:D:505:BTB:H42	1.49	0.42
1:C:428:MET:HG3	1:C:458:PRO:HB2	2.01	0.41
1:D:290:PRO:HB3	1:D:304:LEU:HD23	2.02	0.41
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.56	0.41
5:D:505:BTB:H51	5:D:505:BTB:H11	1.41	0.41
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.87	0.41
1:D:124:LEU:HB3	1:D:128:ARG:NH1	2.35	0.41
1:D:139:LYS:N	1:D:139:LYS:HD2	2.35	0.41
1:D:326:LEU:HB3	1:D:328:LEU:HG	2.03	0.41
1:C:125:SER:HA	1:C:128:ARG:NH1	2.36	0.41
1:C:229:THR:O	1:C:351:ALA:HA	2.21	0.41
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.94	0.41
1:D:70:ARG:HD2	1:D:79:ILE:HD13	2.03	0.41
1:A:384:ASP:OD1	5:A:504:BTB:O3	2.39	0.41
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.56	0.40
1:D:119:ALA:HB1	1:D:122:GLN:HG2	2.03	0.40
1:A:470:SER:HA	1:A:471:PRO:C	2.45	0.40
1:C:470:SER:HA	1:C:471:PRO:C	2.47	0.40
1:B:128:ARG:NH1	1:B:154:GLU:OE2	2.55	0.40
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.56	0.40

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	400/440 (91%)	392 (98%)	7 (2%)	1 (0%)	37	30
1	B	404/440 (92%)	397 (98%)	7 (2%)	0	100	100
1	C	398/440 (90%)	386 (97%)	11 (3%)	1 (0%)	37	30
1	D	402/440 (91%)	390 (97%)	10 (2%)	2 (0%)	25	15
All	All	1604/1760 (91%)	1565 (98%)	35 (2%)	4 (0%)	37	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	144	GLN
1	D	258	ASP
1	A	143	SER
1	C	258	ASP

### 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	344/373 (92%)	327 (95%)	17 (5%)	21	8
1	B	347/373 (93%)	336 (97%)	11 (3%)	34	22
1	C	342/373 (92%)	322 (94%)	20 (6%)	17	6
1	D	345/373 (92%)	337 (98%)	8 (2%)	45	33
All	All	1378/1492 (92%)	1322 (96%)	56 (4%)	27	12

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	89	GLN
1	A	107	ARG
1	A	108	LYS
1	A	124	LEU
1	A	139	LYS
1	A	140	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	141	SER
1	A	147	GLU
1	A	151	GLN
1	A	154	GLU
1	A	202	ARG
1	A	224	LEU
1	A	238	ARG
1	A	291	LEU
1	A	302	LEU
1	A	309	LEU
1	B	90	GLN
1	B	128	ARG
1	B	136	SER
1	B	224	LEU
1	B	257	GLN
1	B	258	ASP
1	B	301	GLU
1	B	309	LEU
1	B	326	LEU
1	B	329	ARG
1	B	429	LYS
1	C	67	LYS
1	C	87	GLN
1	C	89	GLN
1	C	90	GLN
1	C	97	ARG
1	C	121	GLU
1	C	122	GLN
1	C	125	SER
1	C	128	ARG
1	C	139	LYS
1	C	148	GLN
1	C	192	LYS
1	C	202	ARG
1	C	235	CYS
1	C	256	GLN
1	C	291	LEU
1	C	309	LEU
1	C	321	GLU
1	C	329	ARG
1	C	474	ARG
1	D	122	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	128	ARG
1	D	213[A]	ASN
1	D	213[B]	ASN
1	D	257	GLN
1	D	258	ASP
1	D	309	LEU
1	D	326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	B	403	ASN
1	D	122	GLN

### 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 40 ligands modelled in this entry, 13 are monoatomic - leaving 27 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
2	HEM	D	501	1	42,50,50	1.55	7 (16%)	46,82,82	1.82	9 (19%)
4	A1BT0	B	503	-	29,35,35	1.12	4 (13%)	29,46,46	1.54	4 (13%)
6	GOL	A	507	-	5,5,5	0.36	0	5,5,5	0.38	0
6	GOL	B	506	-	5,5,5	0.36	0	5,5,5	0.22	0
2	HEM	B	501	1	42,50,50	1.65	7 (16%)	46,82,82	1.51	6 (13%)
4	A1BT0	A	503	-	29,35,35	1.04	1 (3%)	29,46,46	1.16	1 (3%)
3	H4B	A	502	-	16,18,18	0.86	0	14,26,26	2.38	6 (42%)
2	HEM	C	501	1	42,50,50	1.50	4 (9%)	46,82,82	1.53	8 (17%)
5	BTB	C	505	-	13,13,13	0.43	0	7,16,16	0.51	0
2	HEM	A	501	1	42,50,50	1.55	5 (11%)	46,82,82	1.83	9 (19%)
3	H4B	B	502	-	16,18,18	0.83	0	14,26,26	2.52	5 (35%)
5	BTB	D	505	-	13,13,13	0.65	0	7,16,16	1.20	0
5	BTB	A	504	8	13,13,13	0.50	0	7,16,16	0.66	0
5	BTB	A	505	-	13,13,13	0.47	0	7,16,16	1.04	0
3	H4B	C	502	-	16,18,18	0.94	0	14,26,26	2.33	4 (28%)
6	GOL	C	507	-	5,5,5	0.39	0	5,5,5	0.21	0
4	A1BT0	D	503	-	29,35,35	1.16	2 (6%)	29,46,46	1.38	4 (13%)
5	BTB	C	504	8	13,13,13	0.48	0	7,16,16	1.00	0
5	BTB	B	505	-	13,13,13	0.47	0	7,16,16	0.85	1 (14%)
5	BTB	B	504	8	13,13,13	0.46	0	7,16,16	0.60	0
5	BTB	D	504	8	13,13,13	0.41	0	7,16,16	0.63	0
6	GOL	A	506	-	5,5,5	0.32	0	5,5,5	0.31	0
6	GOL	A	508	-	5,5,5	0.37	0	5,5,5	0.46	0
4	A1BT0	C	503	-	29,35,35	1.09	4 (13%)	29,46,46	1.06	2 (6%)
6	GOL	D	506	-	5,5,5	0.37	0	5,5,5	0.35	0
3	H4B	D	502	-	16,18,18	0.97	0	14,26,26	2.46	5 (35%)
6	GOL	C	506	-	5,5,5	0.36	0	5,5,5	0.55	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	D	501	1	-	0/12/54/54	-
4	A1BT0	B	503	-	-	5/15/23/23	0/4/4/4
6	GOL	A	507	-	-	4/4/4/4	-
6	GOL	B	506	-	-	2/4/4/4	-
2	HEM	B	501	1	-	1/12/54/54	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1BT0	A	503	-	-	4/15/23/23	0/4/4/4
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
2	HEM	C	501	1	-	3/12/54/54	-
5	BTB	C	505	-	-	9/21/21/21	-
2	HEM	A	501	1	-	2/12/54/54	-
3	H4B	B	502	-	-	1/8/17/17	0/2/2/2
5	BTB	D	505	-	-	14/21/21/21	-
5	BTB	A	504	8	-	4/21/21/21	-
5	BTB	A	505	-	-	10/21/21/21	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
6	GOL	C	507	-	-	0/4/4/4	-
4	A1BT0	D	503	-	-	5/15/23/23	0/4/4/4
5	BTB	C	504	8	-	8/21/21/21	-
5	BTB	B	505	-	-	12/21/21/21	-
5	BTB	B	504	8	-	7/21/21/21	-
5	BTB	D	504	8	-	7/21/21/21	-
6	GOL	A	506	-	-	2/4/4/4	-
6	GOL	A	508	-	-	2/4/4/4	-
4	A1BT0	C	503	-	-	6/15/23/23	0/4/4/4
6	GOL	D	506	-	-	2/4/4/4	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
6	GOL	C	506	-	-	2/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-4.44	1.34	1.40
2	A	501	HEM	C3C-C2C	-4.11	1.34	1.40
2	B	501	HEM	C3C-C4C	3.84	1.47	1.41
2	D	501	HEM	C3C-CAC	3.68	1.56	1.47
2	C	501	HEM	C3C-CAC	3.53	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.46	1.35	1.40
2	D	501	HEM	CAB-C3B	3.38	1.56	1.47
2	B	501	HEM	C3C-CAC	3.35	1.55	1.47
2	A	501	HEM	C3C-CAC	3.28	1.55	1.47
2	A	501	HEM	CAB-C3B	3.22	1.56	1.47
2	C	501	HEM	CAB-C3B	3.21	1.56	1.47
2	C	501	HEM	C3C-C4C	3.11	1.45	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-C2C	-3.00	1.36	1.40
2	A	501	HEM	C3C-C4C	2.95	1.45	1.41
2	B	501	HEM	CAB-C3B	2.92	1.55	1.47
4	B	503	A1BT0	C06-N07	-2.81	1.33	1.38
4	B	503	A1BT0	C28-N27	-2.70	1.33	1.38
2	D	501	HEM	CMB-C2B	2.65	1.56	1.50
2	D	501	HEM	C3C-C4C	2.57	1.45	1.41
2	A	501	HEM	FE-ND	2.56	2.12	1.98
4	B	503	A1BT0	C24-N27	-2.53	1.36	1.41
4	C	503	A1BT0	C24-N27	-2.52	1.36	1.41
4	D	503	A1BT0	C24-N27	-2.51	1.36	1.41
4	A	503	A1BT0	C11-N07	-2.46	1.36	1.41
4	C	503	A1BT0	C11-N07	-2.42	1.36	1.41
4	C	503	A1BT0	C28-N27	-2.39	1.34	1.38
4	B	503	A1BT0	C11-N07	-2.33	1.36	1.41
2	D	501	HEM	CMD-C2D	2.33	1.55	1.50
4	D	503	A1BT0	C28-N27	-2.26	1.34	1.38
2	B	501	HEM	FE-NB	2.25	2.10	1.98
2	B	501	HEM	CMA-C3A	2.21	1.56	1.51
4	C	503	A1BT0	C06-N07	-2.13	1.34	1.38
2	D	501	HEM	CMA-C3A	2.11	1.55	1.51
2	B	501	HEM	CMD-C2D	2.08	1.55	1.50

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBA-CAA-C2A	-6.92	100.91	112.54
3	C	502	H4B	C8A-C4A-C4	5.70	119.69	114.50
2	B	501	HEM	CBA-CAA-C2A	-5.45	103.38	112.54
3	B	502	H4B	C8A-C4A-C4	5.32	119.34	114.50
3	D	502	H4B	C8A-C4A-C4	5.26	119.28	114.50
3	A	502	H4B	C8A-C4A-C4	4.84	118.91	114.50
2	A	501	HEM	C4B-CHC-C1C	4.63	128.66	122.56
2	A	501	HEM	CBA-CAA-C2A	-4.39	105.15	112.54
3	D	502	H4B	N1-C2-N3	-4.05	119.27	125.48
3	D	502	H4B	C2-N3-C4	4.00	121.52	115.96
3	A	502	H4B	N1-C2-N3	-3.88	119.53	125.48
3	A	502	H4B	C2-N3-C4	3.81	121.26	115.96
2	C	501	HEM	C4B-CHC-C1C	3.81	127.58	122.56
3	B	502	H4B	C2-N3-C4	3.72	121.14	115.96
3	B	502	H4B	N1-C2-N3	-3.55	120.04	125.48
4	B	503	A1BT0	C15-C17-N18	-3.45	101.94	112.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	H4B	N1-C2-N3	-3.42	120.25	125.48
2	C	501	HEM	C3B-C2B-C1B	3.28	108.88	106.41
2	A	501	HEM	C3B-C4B-NB	-3.28	107.11	109.47
2	A	501	HEM	C3B-C2B-C1B	3.25	108.85	106.41
4	B	503	A1BT0	C19-C20-C21	-3.23	105.56	112.83
2	C	501	HEM	CBA-CAA-C2A	-3.19	107.17	112.54
2	D	501	HEM	C3B-C2B-C1B	3.16	108.78	106.41
3	C	502	H4B	C2-N3-C4	3.13	120.32	115.96
2	A	501	HEM	C4D-ND-C1D	3.12	108.90	105.21
2	A	501	HEM	C3D-C4D-ND	-3.06	106.81	110.17
3	B	502	H4B	O10-C10-C9	-3.01	104.79	109.77
2	A	501	HEM	CMA-C3A-C4A	-2.99	124.08	128.46
2	B	501	HEM	C4C-CHD-C1D	2.98	126.49	122.56
2	D	501	HEM	C4B-CHC-C1C	2.95	126.45	122.56
4	D	503	A1BT0	C17-C15-C14	-2.92	114.97	120.94
2	A	501	HEM	C1B-NB-C4B	2.87	108.60	105.21
2	B	501	HEM	C4B-CHC-C1C	2.82	126.28	122.56
3	D	502	H4B	N2-C2-N1	2.79	121.41	117.22
2	D	501	HEM	CMA-C3A-C4A	-2.79	124.37	128.46
4	B	503	A1BT0	C17-C15-C14	-2.79	115.25	120.94
3	A	502	H4B	C2-N1-C8A	2.77	121.17	114.59
3	C	502	H4B	C2-N1-C8A	2.75	121.13	114.59
2	D	501	HEM	C4D-ND-C1D	2.74	108.45	105.21
3	D	502	H4B	C2-N1-C8A	2.67	120.93	114.59
3	B	502	H4B	C2-N1-C8A	2.60	120.78	114.59
2	D	501	HEM	C3D-C4D-ND	-2.59	107.34	110.17
2	D	501	HEM	C3B-C4B-NB	-2.54	107.65	109.47
4	D	503	A1BT0	C24-N27-C28	-2.49	122.69	128.41
2	B	501	HEM	CMC-C2C-C3C	2.47	129.61	124.68
2	B	501	HEM	C4D-ND-C1D	2.42	108.07	105.21
4	A	503	A1BT0	C17-C15-C14	-2.39	116.05	120.94
2	C	501	HEM	C4A-C3A-C2A	2.32	108.61	107.00
4	C	503	A1BT0	C15-C17-N18	-2.31	105.53	112.79
2	C	501	HEM	CMA-C3A-C4A	-2.25	125.16	128.46
2	C	501	HEM	C4D-ND-C1D	2.24	107.86	105.21
4	D	503	A1BT0	C15-C17-N18	-2.19	105.88	112.79
4	D	503	A1BT0	C13-C12-C11	2.18	122.25	119.73
2	C	501	HEM	C1B-NB-C4B	2.16	107.77	105.21
2	B	501	HEM	C3B-C2B-C1B	2.13	108.01	106.41
4	C	503	A1BT0	C17-C15-C14	-2.11	116.64	120.94
2	A	501	HEM	CHB-C1B-NB	2.09	126.96	124.37
3	A	502	H4B	N2-C2-N1	2.08	120.35	117.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C1B-NB-C4B	2.08	107.67	105.21
2	C	501	HEM	C4C-CHD-C1D	2.08	125.30	122.56
4	B	503	A1BT0	C05-C04-C03	2.06	108.94	105.41
2	D	501	HEM	CMA-C3A-C2A	2.04	128.78	124.94
3	A	502	H4B	C4-C4A-N5	2.03	121.47	118.57
5	B	505	BTB	O1-C1-C2	-2.01	106.68	111.40

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	A1BT0	N18-C19-C20-C21
4	B	503	A1BT0	C33-C28-N27-C24
4	B	503	A1BT0	N29-C28-N27-C24
4	C	503	A1BT0	N18-C19-C20-C21
4	C	503	A1BT0	C33-C28-N27-C24
4	C	503	A1BT0	N29-C28-N27-C24
4	D	503	A1BT0	N29-C28-N27-C24
5	A	504	BTB	O1-C1-C2-C3
5	A	504	BTB	O1-C1-C2-C4
5	A	504	BTB	O1-C1-C2-N
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C1-C2-N-C7
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C3-C2-N-C7
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	B	504	BTB	C1-C2-C4-O4
5	B	504	BTB	C4-C2-N-C5
5	B	505	BTB	O1-C1-C2-N
5	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	C	504	BTB	O1-C1-C2-C3
5	C	504	BTB	O1-C1-C2-C4
5	C	504	BTB	O1-C1-C2-N
5	C	504	BTB	C1-C2-C3-O3
5	C	504	BTB	C1-C2-C4-O4
5	C	504	BTB	C3-C2-C4-O4
5	C	504	BTB	N-C2-C4-O4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-C2-C4-O4
5	C	505	BTB	N-C2-C4-O4
5	D	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	O1-C1-C2-C3
5	D	505	BTB	O1-C1-C2-C4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-N-C5
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C5
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C5
5	D	505	BTB	C4-C2-N-C7
6	A	506	GOL	C1-C2-C3-O3
6	A	507	GOL	O1-C1-C2-C3
6	A	507	GOL	C1-C2-C3-O3
6	A	508	GOL	O1-C1-C2-C3
6	B	506	GOL	O1-C1-C2-C3
6	C	506	GOL	O1-C1-C2-C3
6	D	506	GOL	O1-C1-C2-C3
5	A	505	BTB	N-C7-C8-O8
2	C	501	HEM	C2A-CAA-CBA-CGA
6	A	507	GOL	O2-C2-C3-O3
4	A	503	A1BT0	C15-C17-N18-C19
4	C	503	A1BT0	C15-C17-N18-C19
4	D	503	A1BT0	N18-C19-C20-C21
5	B	505	BTB	C4-C2-C3-O3
6	A	506	GOL	O2-C2-C3-O3
6	A	507	GOL	O1-C1-C2-O2
6	A	508	GOL	O1-C1-C2-O2
6	C	506	GOL	O1-C1-C2-O2
6	D	506	GOL	O1-C1-C2-O2
5	B	505	BTB	N-C7-C8-O8
4	B	503	A1BT0	N18-C19-C20-C21
2	C	501	HEM	C1A-C2A-CAA-CBA
6	B	506	GOL	O1-C1-C2-O2
5	D	505	BTB	N-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

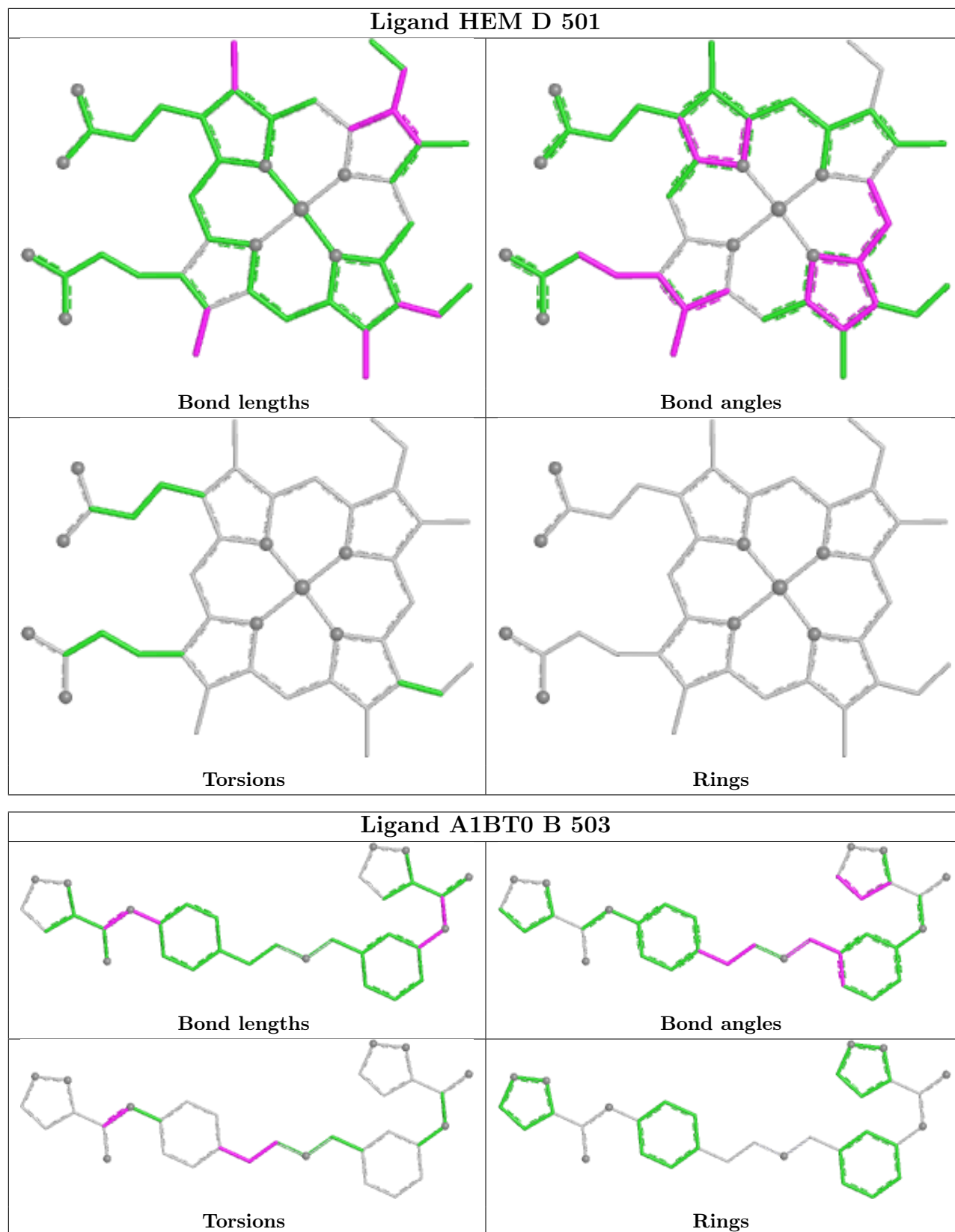
Mol	Chain	Res	Type	Atoms
5	D	505	BTB	N-C7-C8-O8
5	A	504	BTB	C4-C2-C3-O3
5	B	505	BTB	O1-C1-C2-C4
4	A	503	A1BT0	C19-C20-C21-C22
4	A	503	A1BT0	C19-C20-C21-C26
4	C	503	A1BT0	C19-C20-C21-C22
5	D	504	BTB	C6-C5-N-C7
4	B	503	A1BT0	C19-C20-C21-C22
4	C	503	A1BT0	C19-C20-C21-C26
4	B	503	A1BT0	C19-C20-C21-C26
2	C	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
4	D	503	A1BT0	C19-C20-C21-C22
4	D	503	A1BT0	C19-C20-C21-C26
5	B	504	BTB	C1-C2-N-C5
5	B	504	BTB	C3-C2-N-C5
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C1-C2-N-C7
5	B	505	BTB	C3-C2-N-C5
5	B	505	BTB	C4-C2-N-C7
5	C	504	BTB	N-C2-C3-O3
5	C	505	BTB	C1-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
5	C	505	BTB	C4-C2-N-C7
5	D	504	BTB	C1-C2-N-C5
5	D	504	BTB	C3-C2-N-C5
4	D	503	A1BT0	C33-C28-N27-C24
2	A	501	HEM	C2A-CAA-CBA-CGA
3	B	502	H4B	N5-C6-C9-O9
5	B	504	BTB	N-C2-C4-O4
5	B	504	BTB	C1-C2-N-C7
5	B	504	BTB	C4-C2-N-C7
5	B	505	BTB	C3-C2-N-C7
5	B	505	BTB	C4-C2-N-C5
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5
5	D	504	BTB	C4-C2-N-C5

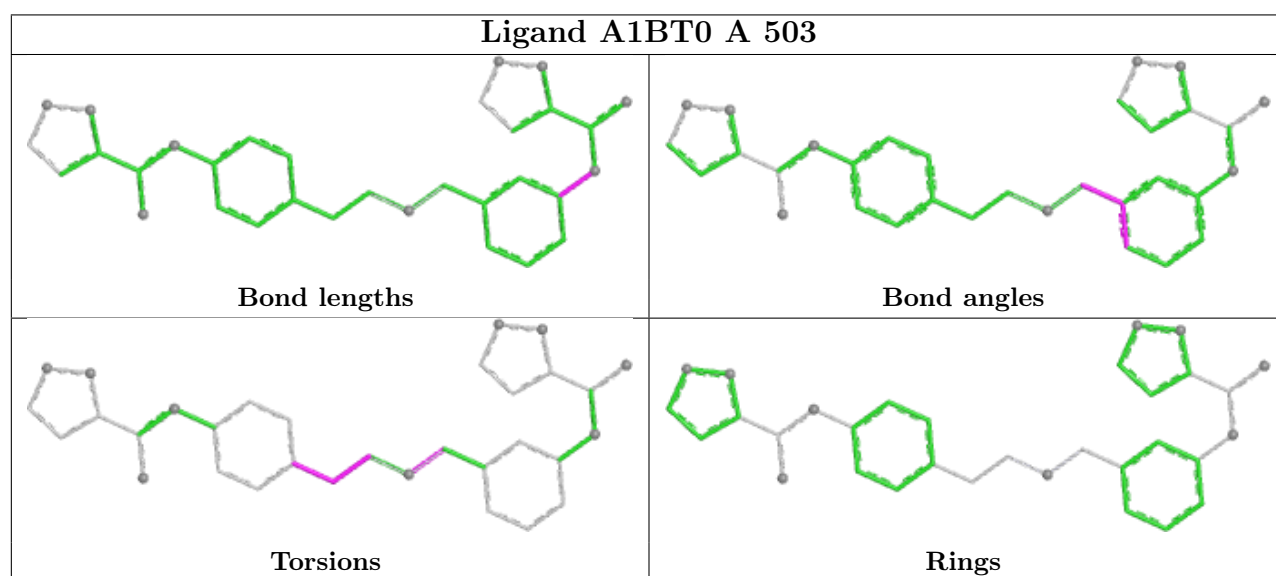
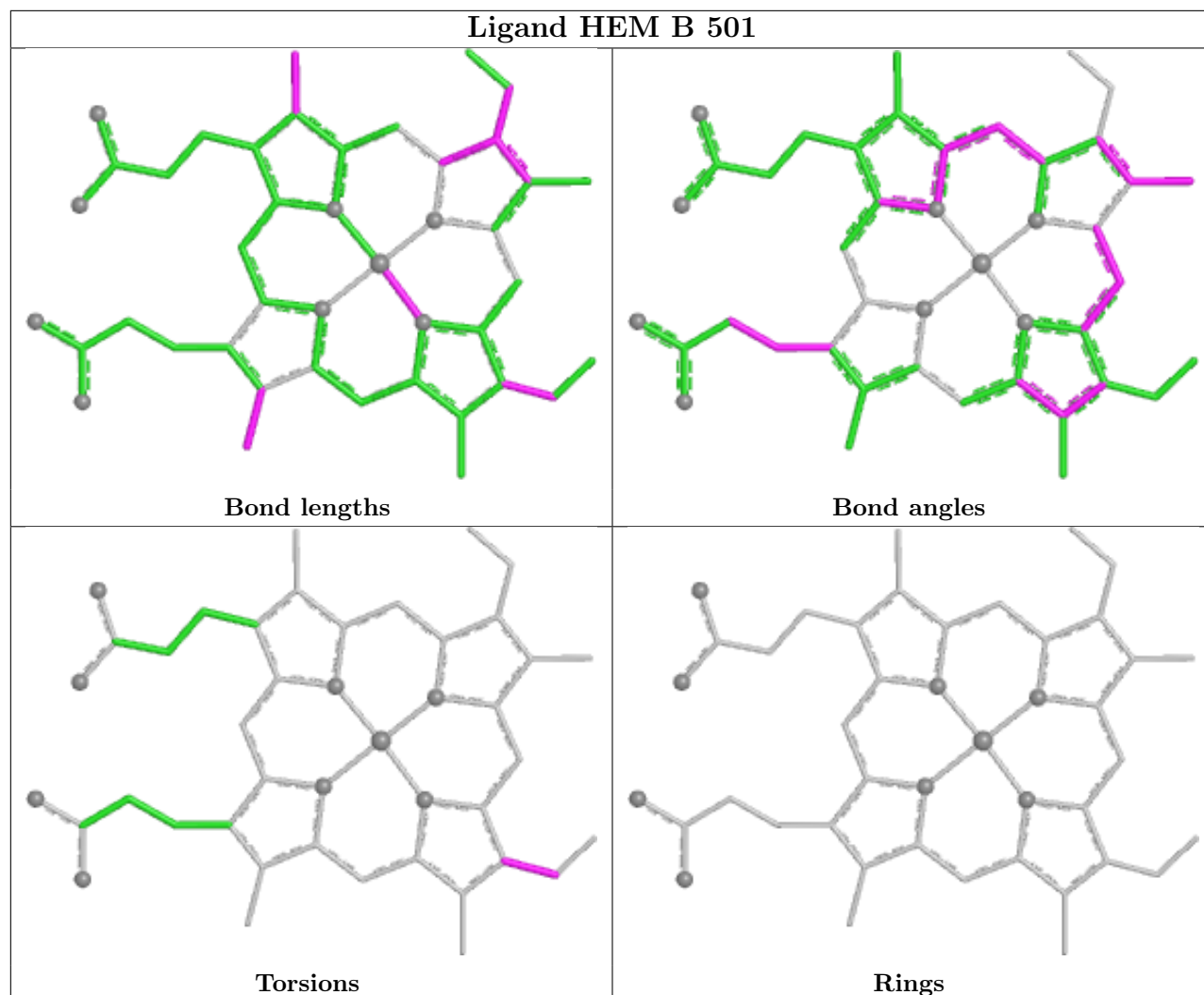
There are no ring outliers.

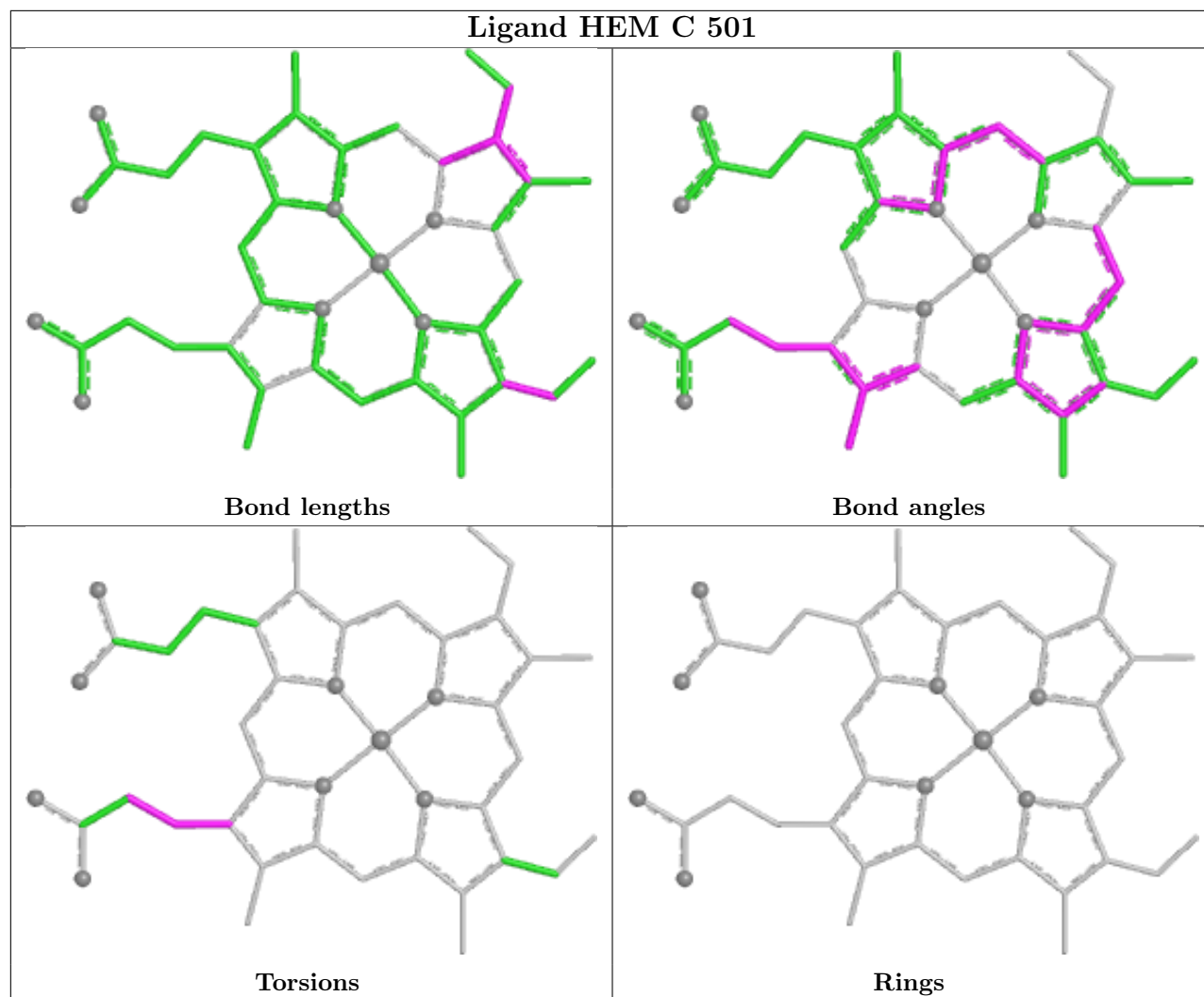
15 monomers are involved in 36 short contacts:

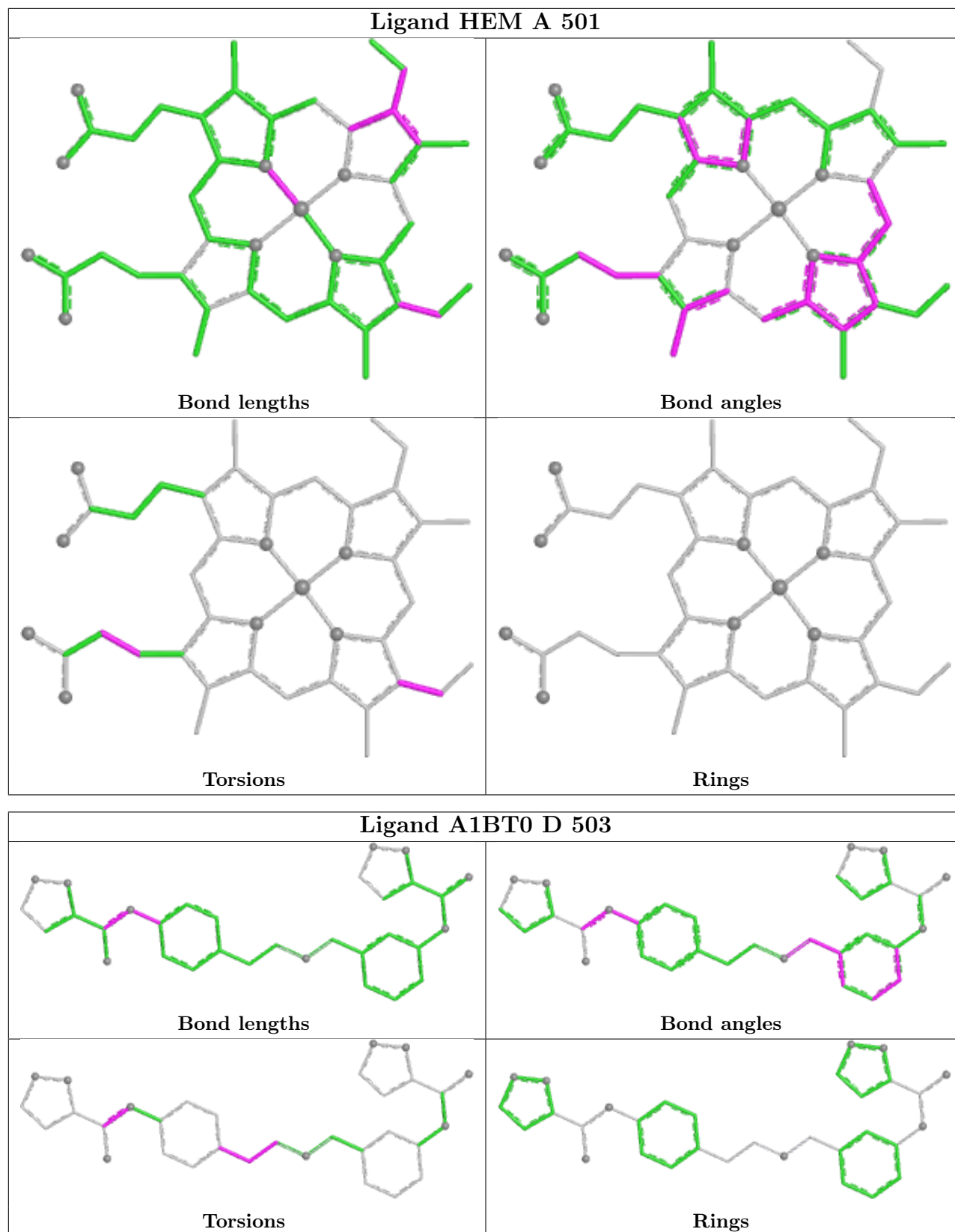
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	HEM	2	0
2	B	501	HEM	2	0
4	A	503	A1BT0	1	0
2	C	501	HEM	2	0
5	C	505	BTB	2	0
2	A	501	HEM	2	0
5	D	505	BTB	7	0
5	A	504	BTB	3	0
4	D	503	A1BT0	1	0
5	C	504	BTB	2	0
5	B	505	BTB	2	0
5	B	504	BTB	4	0
5	D	504	BTB	4	0
4	C	503	A1BT0	1	0
3	D	502	H4B	1	0

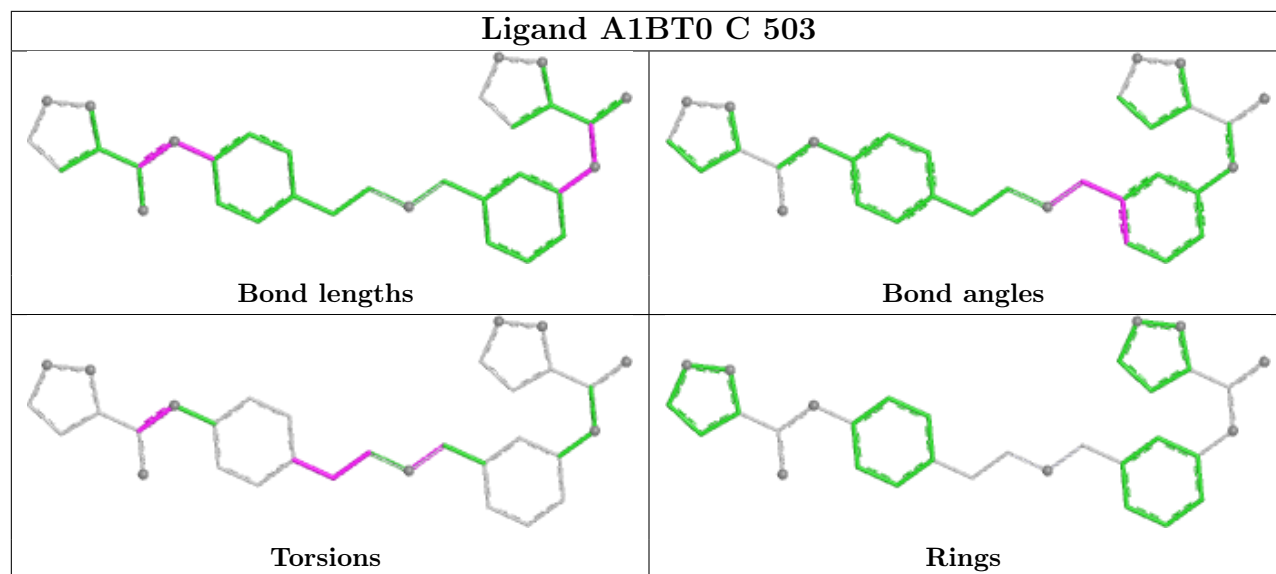
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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 ⓘ

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	403/440 (91%)	0.14	10 (2%) 58 64	19, 42, 81, 113	1 (0%)
1	B	404/440 (91%)	-0.28	4 (0%) 79 83	19, 32, 56, 107	4 (0%)
1	C	401/440 (91%)	0.22	9 (2%) 62 68	21, 45, 84, 119	1 (0%)
1	D	402/440 (91%)	-0.21	3 (0%) 84 88	19, 33, 61, 123	4 (0%)
All	All	1610/1760 (91%)	-0.03	26 (1%) 70 75	19, 37, 76, 123	10 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	GLN	4.6
1	A	120	PRO	4.3
1	D	144	GLN	4.2
1	B	119	ALA	3.5
1	C	204	ALA	3.4
1	D	257	GLN	3.0
1	D	259	GLY	2.8
1	C	480	TRP	2.8
1	A	158	ALA	2.6
1	C	237	GLY	2.5
1	A	89	GLN	2.4
1	A	124	LEU	2.4
1	A	155	ALA	2.3
1	C	121	GLU	2.3
1	B	257	GLN	2.3
1	C	295	ALA	2.2
1	C	148	GLN	2.2
1	B	89	GLN	2.2
1	C	89	GLN	2.2
1	A	145	ALA	2.2
1	C	202	ARG	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	236	PRO	2.1
1	B	108	LYS	2.1
1	C	122	GLN	2.1
1	A	160	THR	2.0
1	A	480	TRP	2.0

## 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(Å <sup>2</sup> )	Q<0.9
6	GOL	C	507	6/6	0.54	0.15	74,78,80,81	0
6	GOL	A	507	6/6	0.63	0.15	76,78,80,81	0
5	BTB	B	505	14/14	0.63	0.20	74,82,89,91	0
5	BTB	A	505	14/14	0.70	0.20	58,73,85,93	0
6	GOL	B	506	6/6	0.74	0.23	72,77,81,82	0
5	BTB	C	504	14/14	0.74	0.19	77,83,104,105	0
6	GOL	C	506	6/6	0.76	0.15	48,69,79,79	0
5	BTB	C	505	14/14	0.79	0.15	71,79,92,92	0
5	BTB	D	505	14/14	0.80	0.15	38,62,75,78	0
6	GOL	A	506	6/6	0.80	0.11	60,69,72,72	0
6	GOL	A	508	6/6	0.83	0.20	66,72,74,74	0
4	A1BT0	C	503	32/32	0.83	0.18	29,71,125,126	0
5	BTB	D	504	14/14	0.85	0.17	41,52,69,74	0
4	A1BT0	A	503	32/32	0.85	0.16	27,56,110,111	0
5	BTB	B	504	14/14	0.87	0.16	55,64,81,83	0
3	H4B	C	502	17/17	0.88	0.10	43,52,60,61	0
6	GOL	D	506	6/6	0.88	0.17	69,70,73,77	0
3	H4B	A	502	17/17	0.89	0.11	38,52,57,59	0

*Continued on next page...*

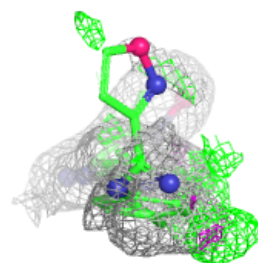
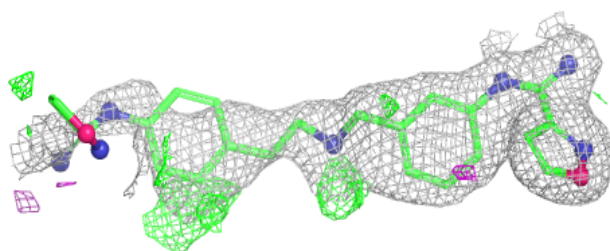
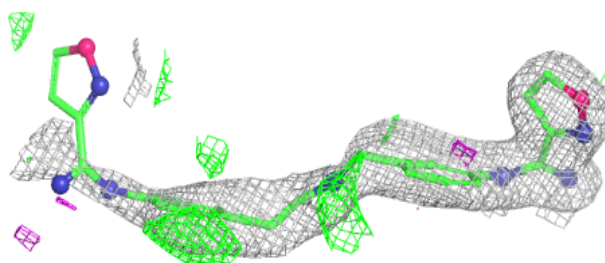
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BTB	A	504	14/14	0.89	0.15	20,70,76,78	0
3	H4B	D	502	17/17	0.90	0.10	27,41,49,53	0
4	A1BT0	B	503	32/32	0.92	0.13	21,45,113,117	0
3	H4B	B	502	17/17	0.92	0.08	35,40,49,49	0
4	A1BT0	D	503	32/32	0.92	0.14	21,49,114,116	0
8	GD	A	510	1/1	0.96	0.12	96,96,96,96	0
8	GD	C	509	1/1	0.96	0.12	109,109,109,109	0
2	HEM	C	501	43/43	0.97	0.07	23,36,56,61	0
7	CL	B	507	1/1	0.98	0.06	36,36,36,36	0
7	CL	C	508	1/1	0.98	0.06	46,46,46,46	0
7	CL	D	507	1/1	0.98	0.07	35,35,35,35	0
2	HEM	A	501	43/43	0.98	0.07	22,32,49,57	0
8	GD	B	508	1/1	0.98	0.04	39,39,39,39	0
7	CL	A	509	1/1	0.98	0.05	45,45,45,45	0
8	GD	D	508	1/1	0.98	0.03	37,37,37,37	0
10	CA	A	513	1/1	0.98	0.18	74,74,74,74	0
10	CA	B	509	1/1	0.98	0.10	36,36,36,36	0
9	ZN	C	510	1/1	0.99	0.03	33,33,33,33	0
10	CA	A	512	1/1	0.99	0.05	25,25,25,25	0
2	HEM	D	501	43/43	0.99	0.05	16,23,37,43	0
2	HEM	B	501	43/43	0.99	0.05	16,21,35,41	0
9	ZN	A	511	1/1	1.00	0.01	30,30,30,30	0

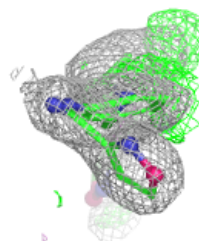
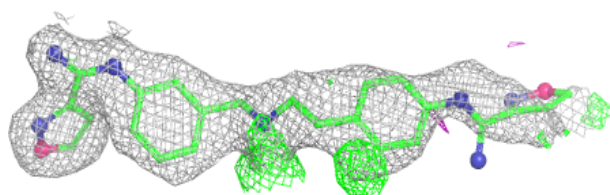
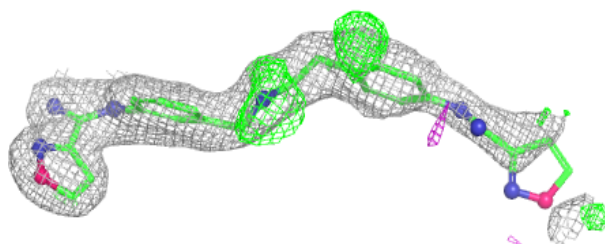
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1BT0 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)

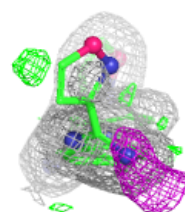
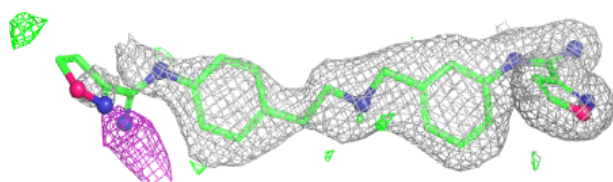
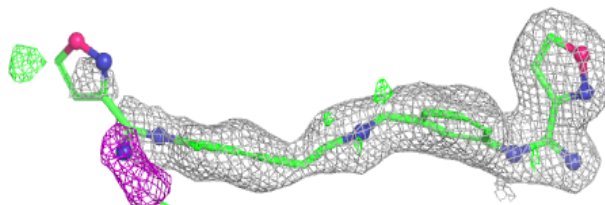
**Electron density around A1BT0 A 503:**

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

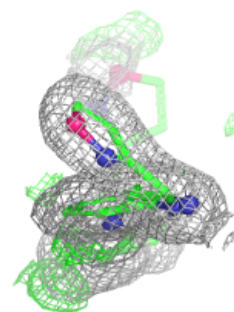
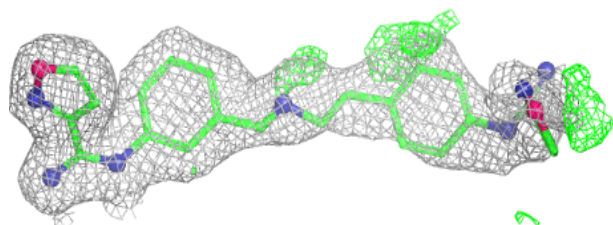
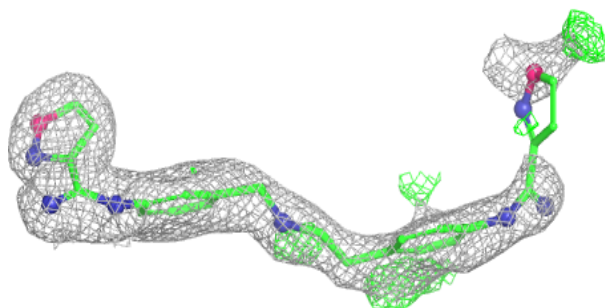


**Electron density around A1BT0 B 503:**

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

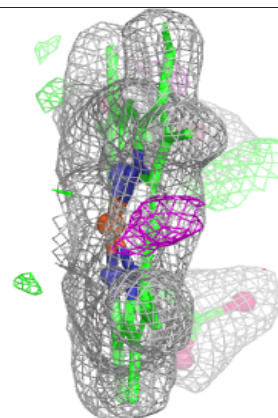
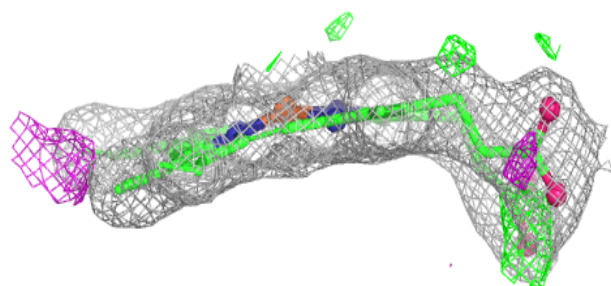
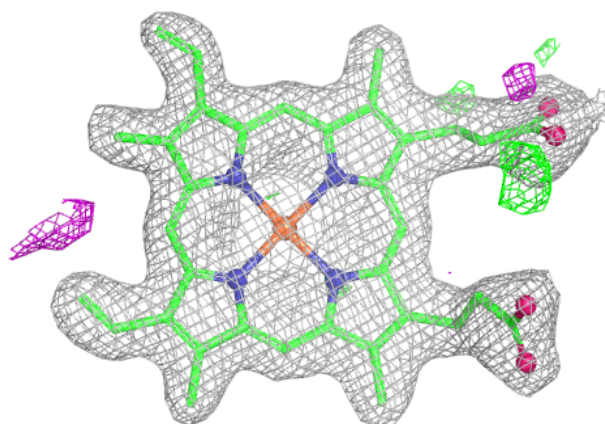
**Electron density around A1BT0 D 503:**

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



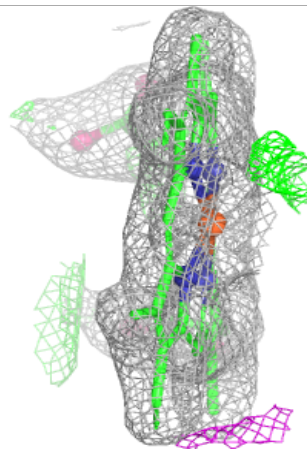
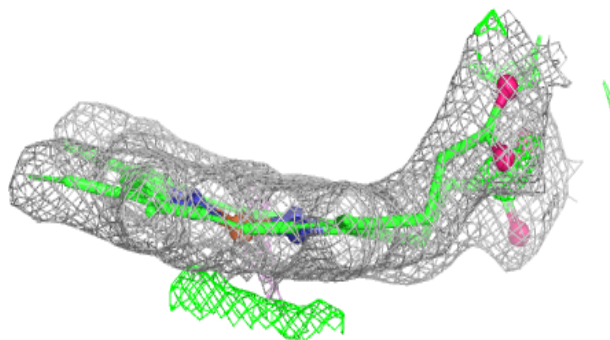
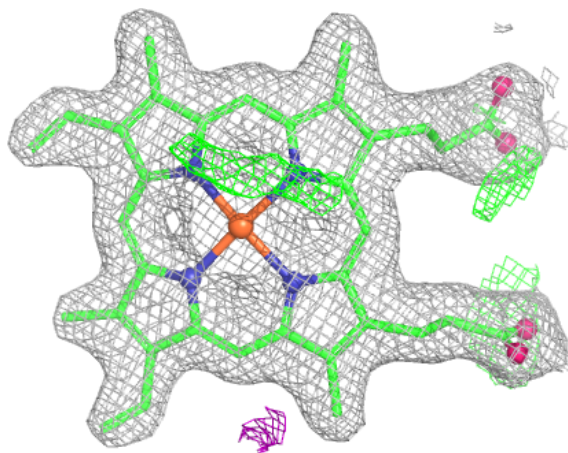
**Electron density around HEM C 501:**

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



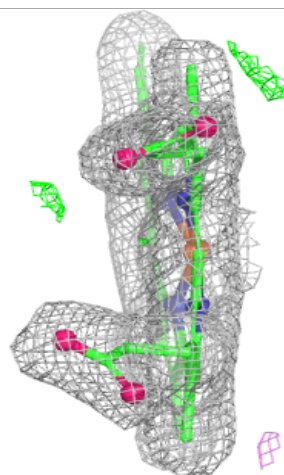
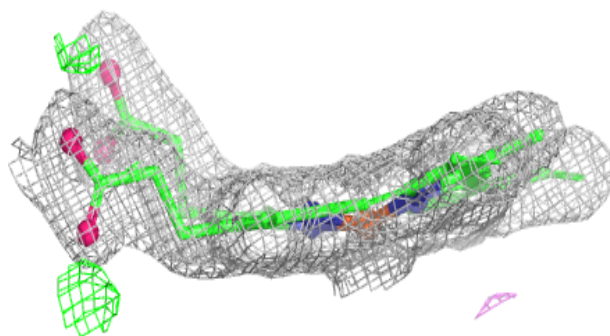
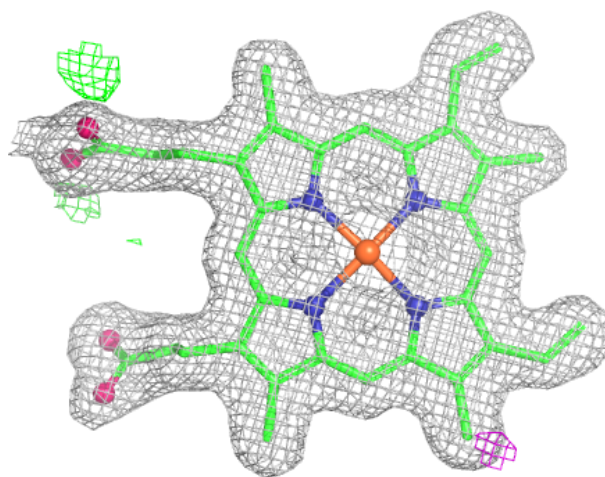
**Electron density around HEM A 501:**

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



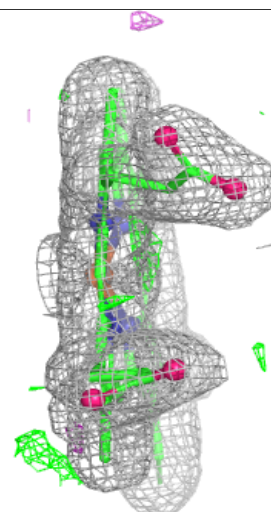
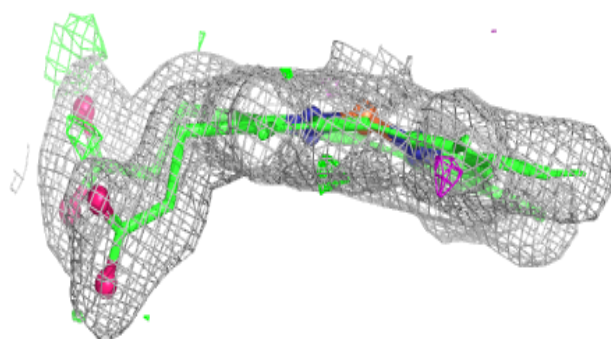
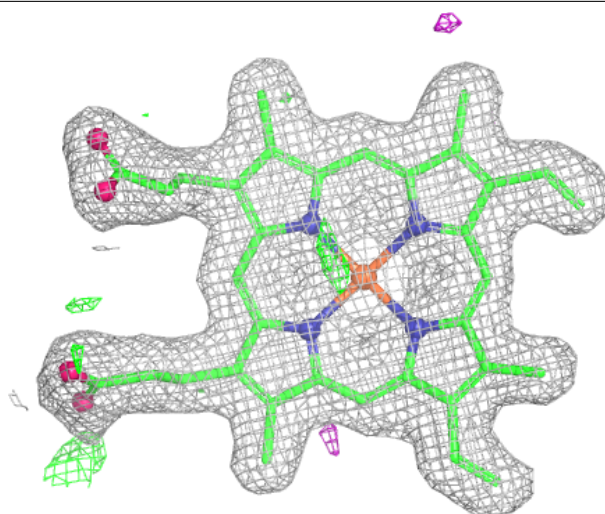
**Electron density around HEM D 501:**

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



**Electron density around HEM B 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 [i](#)

There are no such residues in this entry.