



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 18, 2025 – 11:39 AM EST

PDB ID : 9MWN / pdb\_00009mwn  
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 : 2.00 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>.

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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 Phenix2.0
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

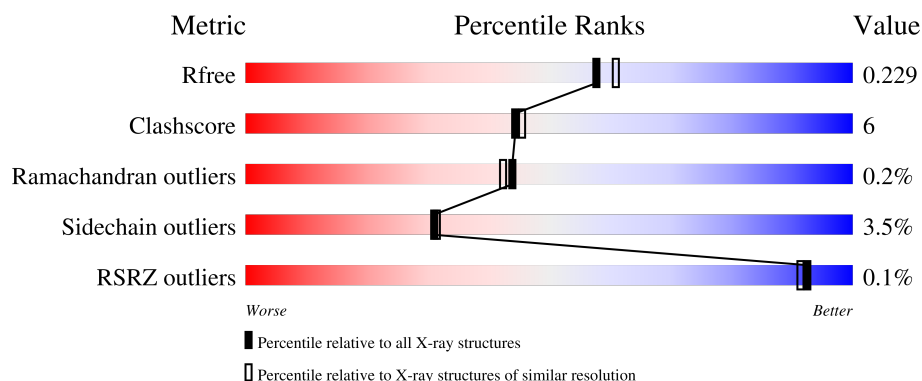
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	441	
1	B	441	
1	C	441	
1	D	441	

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14197 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	1	0
			3199	2038	563	582	16			
1	B	403	Total	C	N	O	S	0	2	0
			3224	2054	567	587	16			
1	C	400	Total	C	N	O	S	0	1	0
			3199	2038	563	582	16			
1	D	402	Total	C	N	O	S	0	2	0
			3214	2048	565	585	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:  $C_{34}H_{32}FeN_4O_4$ ).



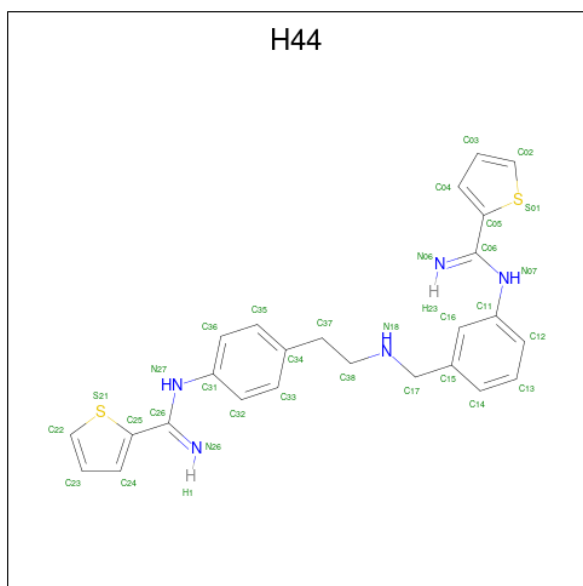
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



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

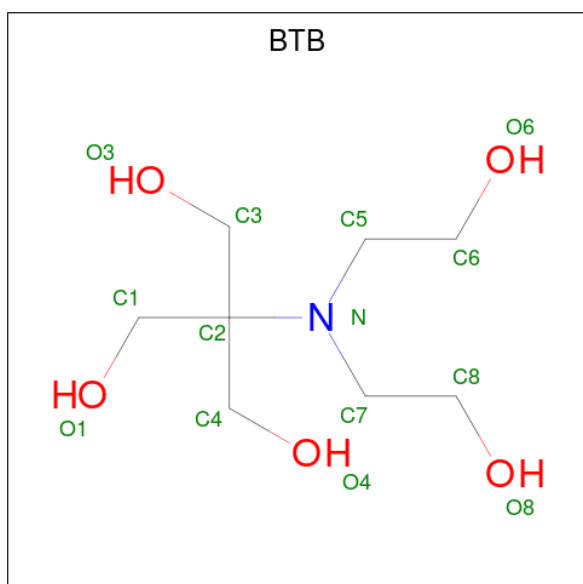
- Molecule 4 is N-(4-{2-[(3-{[(E)-imino(thiophen-2-yl)methyl]amino}benzyl)amino]ethyl}phenyl)thiophene-2-carboximidamide (CCD ID: H44) (formula: C<sub>25</sub>H<sub>25</sub>N<sub>5</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





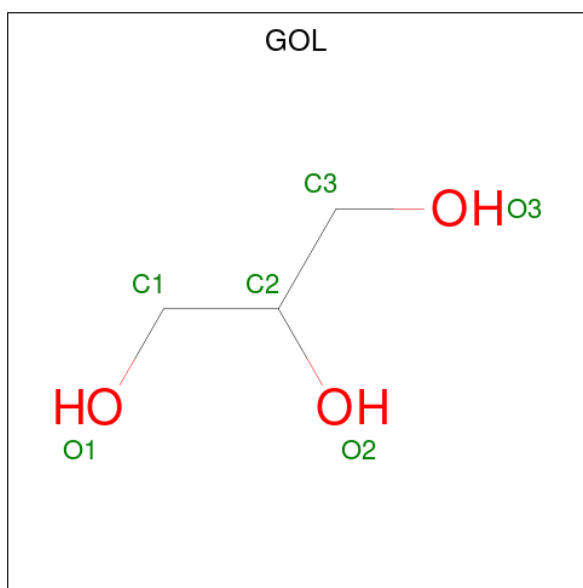
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula:  $C_8H_{19}NO_5$ ).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula:  $Cl$ ).

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

- Molecule 9 is GADOLINIUM ATOM (CCD ID: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Gd 1 1	0	0
9	B	1	Total Gd 1 1	0	0
9	D	1	Total Gd 1 1	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 11 is water.

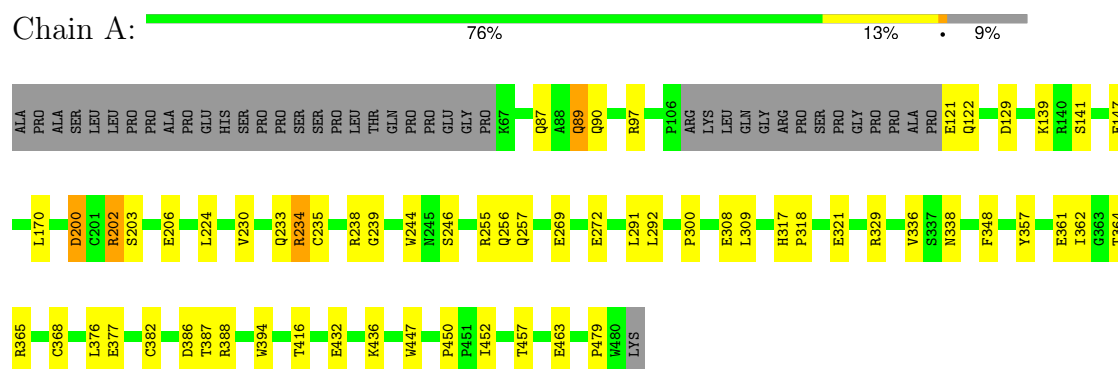
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	208	Total O 208 208	0	0
11	B	254	Total O 254 254	0	0
11	C	142	Total O 142 142	0	0
11	D	234	Total O 234 234	0	0



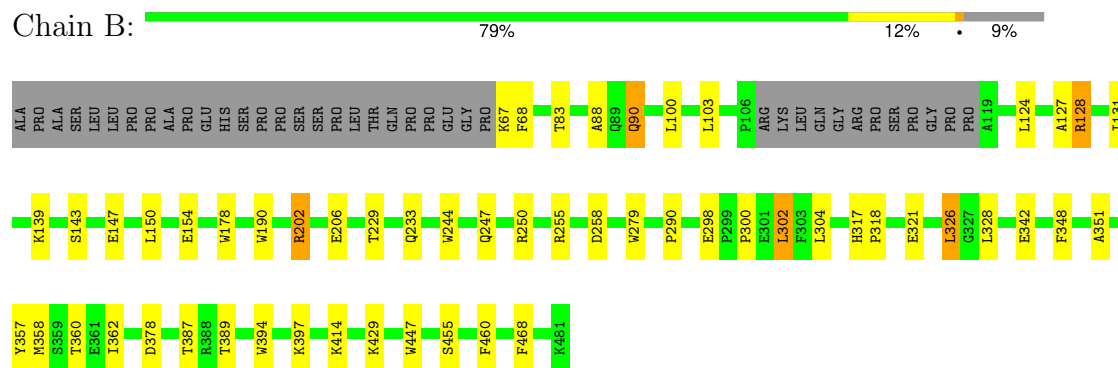
### 3 Residue-property plots

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

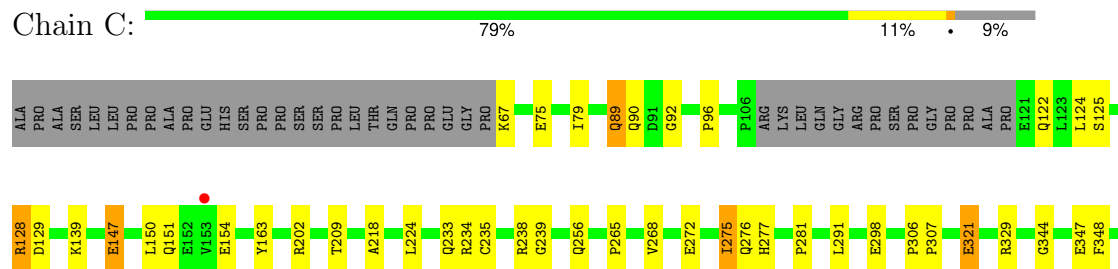
#### • Molecule 1: Nitric oxide synthase 3



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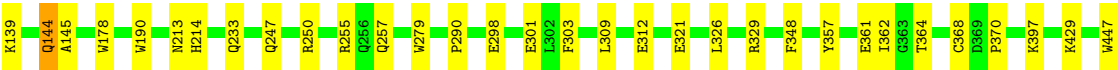
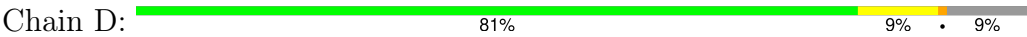


#### • Molecule 1: Nitric oxide synthase 3





● Molecule 1: Nitric oxide synthase 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.64Å 151.73Å 108.31Å 90.00° 90.88° 90.00°	Depositor
Resolution (Å)	29.38 – 2.00 29.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.38-2.00) 99.9 (29.38-2.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.192 , 0.234 0.187 , 0.229	Depositor DCC
$R_{free}$ test set	6544 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.118 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14197	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 3.23% 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, CL, H44, ACT, BTB, GOL, HEM, ZN, GD

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	0.29	0/3293	0.48	0/4487
1	B	0.36	0/3322	0.55	0/4525
1	C	0.26	0/3293	0.45	0/4487
1	D	0.34	0/3312	0.51	0/4514
All	All	0.31	0/13220	0.50	0/18013

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	3199	0	3104	35	0
1	B	3224	0	3134	33	0
1	C	3199	0	3104	29	0
1	D	3214	0	3121	31	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	17	0	15	2	0

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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	23	5	0
4	B	32	0	23	2	0
4	C	32	0	23	1	0
4	D	32	0	23	3	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	1	0
5	D	4	0	3	0	0
6	A	28	0	37	7	0
6	B	28	0	37	9	0
6	C	28	0	38	3	0
6	D	28	0	37	6	0
7	A	6	0	8	0	0
7	C	6	0	8	0	0
7	D	6	0	8	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	B	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	208	0	0	1	0
11	B	254	0	0	4	0
11	C	142	0	0	2	0
11	D	234	0	0	4	0
All	All	14197	0	12920	156	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 6.

All (156) 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:C:275:ILE:HD11	1:C:281:PRO:HB3	1.59	0.83
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.74	0.70
1:B:128:ARG:HG3	1:B:150:LEU:HD22	1.72	0.70
1:D:144:GLN:HG2	1:D:145:ALA:H	1.56	0.69
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.78	0.65
1:D:298:GLU:CD	6:D:506:BTB:H42	2.23	0.64
1:C:298:GLU:OE2	11:C:601:HOH:O	2.15	0.64
4:A:503:H44:H18	4:A:503:H44:H12	1.80	0.64
1:B:397:LYS:NZ	11:B:603:HOH:O	2.31	0.63
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.81	0.63
6:C:505:BTB:O4	6:C:505:BTB:O1	2.15	0.63
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.81	0.63
1:B:298:GLU:CD	6:B:506:BTB:H42	2.24	0.62
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.32	0.62
1:C:147:GLU:HA	1:C:150:LEU:HD12	1.82	0.61
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.83	0.61
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.81	0.60
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.82	0.60
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.85	0.59
1:A:321:GLU:H	1:A:321:GLU:CD	2.09	0.59
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.85	0.59
1:B:397:LYS:NZ	11:B:605:HOH:O	2.35	0.58
1:A:200:ASP:OD1	1:A:200:ASP:N	2.28	0.57
1:D:144:GLN:HG2	1:D:145:ALA:N	2.20	0.57
1:A:97:ARG:HG3	1:B:88:ALA:HB3	1.88	0.56
1:D:213:ASN:HB2	11:D:773:HOH:O	2.06	0.55
1:A:382:CYS:HA	6:A:505:BTB:H32	1.89	0.54
6:A:505:BTB:H41	1:D:326:LEU:HD12	1.88	0.54
1:C:321:GLU:H	1:C:321:GLU:CD	2.16	0.54
1:A:235:CYS:SG	1:A:238:ARG:HD2	2.48	0.54
1:A:386:ASP:OD2	1:A:388:ARG:HG2	2.08	0.54
1:D:364:THR:O	1:D:368:CYS:HB2	2.07	0.53
1:C:96:PRO:O	1:D:92:GLY:N	2.34	0.53
1:A:234:ARG:HA	1:A:238:ARG:NH1	2.25	0.52
1:B:321:GLU:OE2	6:B:505:BTB:O4	2.27	0.52
1:B:414:LYS:NZ	11:B:609:HOH:O	2.42	0.52
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.45	0.51
1:C:364:THR:O	1:C:368:CYS:HB2	2.10	0.51
1:D:357:TYR:CD2	1:D:362:ILE:HD11	2.45	0.51
1:D:447:TRP:HA	3:D:502:H4B:N1	2.25	0.51
1:B:387:THR:HA	1:B:394:TRP:CD1	2.46	0.51
1:A:447:TRP:HA	3:A:502:H4B:N1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:PHE:CD2	1:B:83:THR:HA	2.45	0.50
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.92	0.50
1:A:246:SER:HA	1:A:338:ASN:HB3	1.93	0.50
1:A:269:GLU:O	1:A:272:GLU:HG2	2.12	0.50
1:B:447:TRP:HA	3:B:502:H4B:N1	2.27	0.50
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.94	0.50
1:C:238:ARG:HD3	1:C:239:GLY:O	2.11	0.50
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.47	0.49
6:D:505:BTB:H62	6:D:505:BTB:O8	2.12	0.49
4:A:503:H44:H12	4:A:503:H44:C14	2.43	0.49
1:C:265:PRO:HA	1:C:268:VAL:HG23	1.94	0.49
1:D:139:LYS:NZ	11:D:607:HOH:O	2.44	0.49
1:C:275:ILE:C	1:C:277:HIS:H	2.21	0.48
1:A:244:TRP:CZ2	1:A:300:PRO:HG3	2.48	0.48
1:A:202:ARG:HD2	1:A:206:GLU:OE2	2.14	0.48
1:C:147:GLU:O	1:C:151:GLN:NE2	2.27	0.48
1:D:321:GLU:OE2	6:D:505:BTB:O4	2.32	0.48
6:B:505:BTB:O4	6:B:505:BTB:H82	2.14	0.47
1:C:124:LEU:HD11	1:C:154:GLU:HG2	1.97	0.47
1:D:70:ARG:HD2	1:D:79:ILE:HD13	1.97	0.47
1:B:127:ALA:O	1:B:131:ILE:HG12	2.14	0.47
6:B:505:BTB:H61	11:B:761:HOH:O	2.14	0.47
1:A:234:ARG:HA	1:A:238:ARG:HH12	1.79	0.47
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.49	0.47
1:C:233:GLN:NE2	11:C:604:HOH:O	2.28	0.47
1:B:298:GLU:OE1	6:B:506:BTB:H42	2.14	0.47
6:A:506:BTB:H11	6:A:506:BTB:H51	1.47	0.47
6:C:506:BTB:HO3	6:C:506:BTB:HO4	1.54	0.47
1:D:301:GLU:HB3	1:D:303:PHE:CE1	2.50	0.47
1:A:382:CYS:HA	6:A:505:BTB:H11	1.96	0.46
1:C:75:GLU:CD	1:D:370:PRO:HG2	2.40	0.46
1:C:128:ARG:HH11	1:C:128:ARG:HB2	1.79	0.46
6:B:505:BTB:O4	6:B:505:BTB:C8	2.63	0.46
1:B:143:SER:O	1:B:147:GLU:HG2	2.16	0.46
4:C:503:H44:H18	4:C:503:H44:H12	1.98	0.46
1:C:235:CYS:SG	1:C:238:ARG:HD2	2.55	0.46
1:A:224:LEU:HB2	1:A:416:THR:HB	1.97	0.46
6:B:505:BTB:H51	6:B:505:BTB:H32	1.66	0.46
1:A:244:TRP:CD1	1:A:479:PRO:HG2	2.51	0.46
1:D:312:GLU:CD	1:D:329:ARG:HH21	2.24	0.46
1:C:92:GLY:N	1:D:96:PRO:O	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.98	0.45
1:A:387:THR:HA	1:A:394:TRP:CD1	2.52	0.45
1:A:432:GLU:HG2	1:A:436:LYS:HE2	1.98	0.45
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.51	0.45
2:D:501:HEM:C4D	4:D:503:H44:H19	2.52	0.45
1:D:250:ARG:HD2	1:D:250:ARG:HA	1.75	0.45
1:D:361:GLU:OE1	4:D:503:H44:N07	2.46	0.45
1:C:67:LYS:HB3	1:C:67:LYS:HE2	1.79	0.44
1:C:89:GLN:HG3	1:C:90:GLN:H	1.83	0.44
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.31	0.44
1:D:397:LYS:NZ	11:D:612:HOH:O	2.50	0.44
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.52	0.44
1:A:463:GLU:HB3	1:B:103:LEU:HD12	1.99	0.44
6:A:505:BTB:H72	6:A:505:BTB:H12	1.68	0.44
6:A:506:BTB:O4	6:A:506:BTB:O3	2.16	0.44
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.77	0.44
1:B:247:GLN:HB2	1:B:250:ARG:HD3	2.00	0.44
1:B:139:LYS:N	1:B:139:LYS:HD2	2.33	0.44
1:D:93:PRO:HG3	1:D:106:PRO:HB3	1.99	0.44
4:D:503:H44:C12	4:D:503:H44:C05	2.96	0.44
1:A:336:VAL:HG23	4:A:503:H44:H26	1.98	0.44
6:D:506:BTB:H31	11:D:615:HOH:O	2.18	0.43
1:A:255:ARG:HE	1:A:255:ARG:HB2	1.62	0.43
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.53	0.43
1:D:247:GLN:HB2	1:D:250:ARG:HD3	1.99	0.43
1:B:244:TRP:CH2	1:B:300:PRO:HG3	2.53	0.43
2:B:501:HEM:C4D	4:B:503:H44:H19	2.53	0.43
1:C:387:THR:HA	1:C:394:TRP:CD1	2.53	0.43
1:B:357:TYR:CD2	1:B:362:ILE:HD11	2.53	0.43
2:B:501:HEM:HHC	2:B:501:HEM:CBB	2.46	0.43
1:D:122:GLN:N	1:D:122:GLN:CD	2.75	0.43
1:D:128:ARG:HB2	1:D:128:ARG:NH1	2.33	0.43
1:D:214:HIS:CD2	1:D:214:HIS:C	2.96	0.43
1:C:163:TYR:OH	1:C:344:GLY:O	2.35	0.43
1:B:90:GLN:HB2	1:B:468:PHE:CD2	2.52	0.43
6:B:505:BTB:H72	6:B:505:BTB:H11	1.46	0.43
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.90	0.42
1:B:229:THR:O	1:B:351:ALA:HA	2.18	0.42
1:B:258:ASP:OD1	1:B:258:ASP:N	2.49	0.42
1:B:124:LEU:HD21	1:B:154:GLU:HA	2.01	0.42
1:A:89:GLN:HG3	1:A:90:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLU:OE1	6:A:506:BTB:O8	2.27	0.42
6:B:506:BTB:H42	6:B:506:BTB:H72	1.81	0.42
6:D:506:BTB:H51	6:D:506:BTB:H11	1.71	0.42
1:A:89:GLN:NE2	1:A:90:GLN:OE1	2.53	0.42
4:B:503:H44:C12	4:B:503:H44:C05	2.97	0.42
1:A:129:ASP:HA	11:A:624:HOH:O	2.20	0.42
1:B:326:LEU:HB3	1:B:328:LEU:HG	2.02	0.42
1:A:357:TYR:CD2	1:A:362:ILE:HD11	2.54	0.42
1:C:368:CYS:SG	1:C:376:LEU:HD13	2.59	0.42
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.55	0.42
1:C:150:LEU:HB2	1:C:151:GLN:NE2	2.34	0.41
1:C:306:PRO:HA	1:C:307:PRO:HD3	1.90	0.41
1:B:202:ARG:HG3	1:B:206:GLU:OE2	2.20	0.41
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.55	0.41
1:C:426[A]:SER:OG	5:C:504:ACT:H2	2.20	0.41
6:C:506:BTB:H51	6:C:506:BTB:H11	1.52	0.41
4:A:503:H44:C12	4:A:503:H44:C05	2.97	0.41
6:D:505:BTB:H72	6:D:505:BTB:H11	1.66	0.41
1:C:428:MET:HG3	1:C:458:PRO:HB2	2.03	0.41
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.35	0.41
1:D:90:GLN:HB3	1:D:468:PHE:CD2	2.56	0.41
1:D:104:VAL:O	1:D:106:PRO:HD3	2.20	0.41
1:D:279:TRP:CD1	1:D:290:PRO:HG3	2.56	0.41
1:A:361:GLU:OE1	4:A:503:H44:N07	2.48	0.41
1:C:218:ALA:O	1:C:224:LEU:HA	2.21	0.41
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.61	0.40
1:B:455:SER:HA	1:B:460:PHE:CG	2.56	0.40
1:D:429:LYS:HA	1:D:429:LYS:HD2	1.87	0.40
1:B:358:MET:HE3	1:B:360:THR:OG1	2.21	0.40
1:D:309:LEU:HD12	1:D:309:LEU:HA	1.95	0.40
1:A:170:LEU:HD11	1:A:230:VAL:HG11	2.02	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	397/441 (90%)	388 (98%)	8 (2%)	1 (0%)	37	35
1	B	401/441 (91%)	391 (98%)	9 (2%)	1 (0%)	44	42
1	C	397/441 (90%)	382 (96%)	14 (4%)	1 (0%)	37	35
1	D	400/441 (91%)	387 (97%)	13 (3%)	0	100	100
All	All	1595/1764 (90%)	1548 (97%)	44 (3%)	3 (0%)	44	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	ARG
1	C	276	GLN
1	A	239	GLY

### 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	341/374 (91%)	324 (95%)	17 (5%)	20	18
1	B	344/374 (92%)	334 (97%)	10 (3%)	37	39
1	C	341/374 (91%)	325 (95%)	16 (5%)	22	20
1	D	343/374 (92%)	338 (98%)	5 (2%)	60	66
All	All	1369/1496 (92%)	1321 (96%)	48 (4%)	31	31

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	89	GLN
1	A	121	GLU
1	A	122	GLN
1	A	139	LYS

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Mol	Chain	Res	Type
1	A	141	SER
1	A	147	GLU
1	A	200	ASP
1	A	202	ARG
1	A	203	SER
1	A	234	ARG
1	A	256	GLN
1	A	257	GLN
1	A	291	LEU
1	A	308	GLU
1	A	309	LEU
1	A	329	ARG
1	B	67	LYS
1	B	90	GLN
1	B	128	ARG
1	B	202	ARG
1	B	302	LEU
1	B	326	LEU
1	B	342	GLU
1	B	378	ASP
1	B	389	THR
1	B	429	LYS
1	C	79	ILE
1	C	89	GLN
1	C	122	GLN
1	C	125	SER
1	C	128	ARG
1	C	129	ASP
1	C	139	LYS
1	C	147	GLU
1	C	202	ARG
1	C	209	THR
1	C	256	GLN
1	C	272	GLU
1	C	275	ILE
1	C	291	LEU
1	C	321	GLU
1	C	329	ARG
1	D	122	GLN
1	D	128	ARG
1	D	144	GLN
1	D	255	ARG

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Mol	Chain	Res	Type
1	D	257	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	164	GLN
1	A	257	GLN
1	B	408	HIS
1	C	233	GLN
1	D	276	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 36 ligands modelled in this entry, 9 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	$\# Z  > 2$
3	H4B	A	502	-	16,18,18	0.99	0	14,26,26	2.48	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	C	507	-	5,5,5	0.39	0	5,5,5	0.41	0
3	H4B	B	502	-	16,18,18	0.80	0	14,26,26	2.47	7 (50%)
2	HEM	A	501	1	42,50,50	1.47	5 (11%)	46,82,82	1.77	10 (21%)
2	HEM	C	501	1	42,50,50	1.52	6 (14%)	46,82,82	1.72	12 (26%)
4	H44	D	503	-	35,35,35	1.18	6 (17%)	29,46,46	2.50	8 (27%)
5	ACT	A	504	-	3,3,3	1.11	0	3,3,3	0.80	0
5	ACT	B	504	-	3,3,3	1.22	0	3,3,3	1.06	0
2	HEM	B	501	1	42,50,50	1.48	5 (11%)	46,82,82	1.77	9 (19%)
3	H4B	C	502	-	16,18,18	0.90	0	14,26,26	2.33	5 (35%)
2	HEM	D	501	1	42,50,50	1.53	8 (19%)	46,82,82	1.93	15 (32%)
6	BTB	A	506	-	13,13,13	0.51	0	7,16,16	0.74	0
6	BTB	C	506	-	13,13,13	0.36	0	7,16,16	0.53	0
4	H44	A	503	-	35,35,35	1.34	6 (17%)	29,46,46	2.23	6 (20%)
4	H44	C	503	-	35,35,35	1.27	6 (17%)	29,46,46	2.22	5 (17%)
6	BTB	D	505	9	13,13,13	0.34	0	7,16,16	0.51	0
5	ACT	D	504	-	3,3,3	1.19	0	3,3,3	1.63	1 (33%)
7	GOL	A	507	-	5,5,5	0.33	0	5,5,5	0.43	0
6	BTB	B	505	9	13,13,13	0.38	0	7,16,16	0.57	0
6	BTB	B	506	-	13,13,13	0.50	0	7,16,16	1.11	1 (14%)
3	H4B	D	502	-	16,18,18	0.79	0	14,26,26	2.49	5 (35%)
6	BTB	D	506	-	13,13,13	0.50	0	7,16,16	0.63	0
4	H44	B	503	-	35,35,35	1.24	5 (14%)	29,46,46	2.57	9 (31%)
7	GOL	D	507	-	5,5,5	0.36	0	5,5,5	0.38	0
5	ACT	C	504	-	3,3,3	0.94	0	3,3,3	1.23	1 (33%)
6	BTB	C	505	-	13,13,13	0.60	0	7,16,16	1.05	0
6	BTB	A	505	9	13,13,13	0.42	0	7,16,16	0.57	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
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
7	GOL	C	507	-	-	2/4/4/4	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
2	HEM	A	501	1	-	0/12/54/54	-
2	HEM	C	501	1	-	2/12/54/54	-
4	H44	D	503	-	-	4/15/23/23	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	1	-	0/12/54/54	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
2	HEM	D	501	1	-	1/12/54/54	-
6	BTB	C	506	-	-	4/21/21/21	-
6	BTB	A	506	-	-	8/21/21/21	-
4	H44	A	503	-	-	5/15/23/23	0/4/4/4
4	H44	C	503	-	-	3/15/23/23	0/4/4/4
6	BTB	D	505	9	-	3/21/21/21	-
7	GOL	A	507	-	-	4/4/4/4	-
6	BTB	B	505	9	-	4/21/21/21	-
6	BTB	B	506	-	-	11/21/21/21	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
6	BTB	D	506	-	-	5/21/21/21	-
4	H44	B	503	-	-	6/15/23/23	0/4/4/4
7	GOL	D	507	-	-	2/4/4/4	-
6	BTB	C	505	-	-	8/21/21/21	-
6	BTB	A	505	9	-	4/21/21/21	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-4.14	1.34	1.40
2	A	501	HEM	C3C-C2C	-3.83	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.38	1.35	1.40
2	B	501	HEM	C3C-CAC	3.36	1.55	1.47
2	D	501	HEM	C3C-CAC	3.33	1.55	1.47
4	A	503	H44	C11-N07	-3.33	1.34	1.41
2	A	501	HEM	C3C-CAC	3.32	1.55	1.47
2	C	501	HEM	C3C-CAC	3.26	1.55	1.47
2	D	501	HEM	CAB-C3B	3.23	1.56	1.47
2	C	501	HEM	CAB-C3B	3.22	1.56	1.47
4	A	503	H44	C31-N27	-3.15	1.35	1.41
2	A	501	HEM	CAB-C3B	3.12	1.55	1.47
4	B	503	H44	C06-N07	-3.08	1.32	1.38
2	D	501	HEM	C3C-C2C	-3.03	1.36	1.40
4	C	503	H44	C06-N07	-3.02	1.33	1.38
2	D	501	HEM	C3C-C4C	2.98	1.45	1.41
4	A	503	H44	C06-N07	-2.96	1.33	1.38
2	C	501	HEM	FE-NB	2.95	2.14	1.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	H44	C31-N27	-2.91	1.35	1.41
2	C	501	HEM	C3C-C4C	2.83	1.45	1.41
4	A	503	H44	C26-N27	-2.82	1.33	1.38
4	A	503	H44	C05-C06	2.82	1.50	1.46
4	B	503	H44	C25-C26	2.81	1.50	1.46
4	B	503	H44	C31-N27	-2.70	1.36	1.41
4	C	503	H44	C11-N07	-2.70	1.36	1.41
2	B	501	HEM	C3C-C4C	2.67	1.45	1.41
2	B	501	HEM	CAB-C3B	2.67	1.54	1.47
4	C	503	H44	C25-C26	2.63	1.49	1.46
2	A	501	HEM	C3C-C4C	2.62	1.45	1.41
2	D	501	HEM	CHA-C4D	2.60	1.41	1.34
4	C	503	H44	C26-N27	-2.56	1.33	1.38
2	B	501	HEM	CMD-C2D	2.55	1.56	1.50
4	D	503	H44	C31-N27	-2.53	1.36	1.41
4	D	503	H44	C25-C26	2.49	1.49	1.46
4	D	503	H44	C05-C06	2.48	1.49	1.46
4	B	503	H44	C26-N27	-2.47	1.34	1.38
4	D	503	H44	C06-N07	-2.46	1.34	1.38
4	A	503	H44	C25-C26	2.42	1.49	1.46
4	C	503	H44	C05-C06	2.38	1.49	1.46
4	B	503	H44	C05-C06	2.31	1.49	1.46
2	D	501	HEM	CMB-C2B	2.25	1.55	1.50
2	D	501	HEM	C3B-C2B	-2.19	1.32	1.37
4	D	503	H44	C11-N07	-2.18	1.37	1.41
2	C	501	HEM	CMB-C2B	2.17	1.55	1.50
2	D	501	HEM	C1A-CHA	-2.07	1.35	1.41
2	A	501	HEM	CMB-C2B	2.03	1.54	1.50
4	D	503	H44	C26-N27	-2.03	1.34	1.38

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	H44	C23-C22-S21	-7.68	106.75	112.98
4	D	503	H44	C23-C22-S21	-7.55	106.86	112.98
4	B	503	H44	C03-C02-S01	-7.54	106.86	112.98
4	C	503	H44	C23-C22-S21	-7.46	106.92	112.98
4	C	503	H44	C03-C02-S01	-7.43	106.95	112.98
4	A	503	H44	C23-C22-S21	-7.26	107.08	112.98
4	D	503	H44	C03-C02-S01	-7.19	107.14	112.98
3	A	502	H4B	C8A-C4A-C4	6.55	120.46	114.50
4	A	503	H44	C03-C02-S01	-5.97	108.13	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBA-CAA-C2A	-5.80	102.78	112.54
3	B	502	H4B	C8A-C4A-C4	5.59	119.59	114.50
3	C	502	H4B	C8A-C4A-C4	5.50	119.50	114.50
2	D	501	HEM	CBA-CAA-C2A	-5.32	103.59	112.54
3	D	502	H4B	C8A-C4A-C4	4.94	119.00	114.50
2	B	501	HEM	CBA-CAA-C2A	-4.68	104.66	112.54
2	A	501	HEM	C4B-CHC-C1C	4.08	127.95	122.56
2	C	501	HEM	C4B-CHC-C1C	4.07	127.93	122.56
3	D	502	H4B	C2-N3-C4	4.02	121.56	115.96
3	D	502	H4B	N1-C2-N3	-3.99	119.36	125.48
2	D	501	HEM	C4B-CHC-C1C	3.96	127.78	122.56
4	B	503	H44	C15-C17-N18	-3.85	100.67	112.79
3	B	502	H4B	C2-N3-C4	3.77	121.21	115.96
2	B	501	HEM	C4B-CHC-C1C	3.76	127.51	122.56
4	A	503	H44	C31-N27-C26	-3.75	119.78	128.41
3	A	502	H4B	C2-N3-C4	3.72	121.14	115.96
2	B	501	HEM	C4C-CHD-C1D	3.66	127.39	122.56
2	C	501	HEM	C3B-C2B-C1B	3.56	109.09	106.41
3	C	502	H4B	C2-N3-C4	3.48	120.81	115.96
4	D	503	H44	C15-C17-N18	-3.48	101.84	112.79
4	D	503	H44	C17-C15-C14	-3.46	113.87	120.94
4	B	503	H44	C17-C15-C14	-3.41	113.98	120.94
4	B	503	H44	C31-N27-C26	-3.39	120.62	128.41
2	D	501	HEM	C3B-C2B-C1B	3.27	108.87	106.41
3	C	502	H4B	N1-C2-N3	-3.22	120.55	125.48
3	A	502	H4B	N1-C2-N3	-3.18	120.60	125.48
3	B	502	H4B	N1-C2-N3	-3.10	120.73	125.48
3	D	502	H4B	N2-C2-N1	3.08	121.83	117.22
2	D	501	HEM	CMC-C2C-C3C	3.07	130.81	124.68
4	C	503	H44	C31-N27-C26	-3.06	121.38	128.41
4	A	503	H44	C38-C37-C34	-3.02	106.03	112.83
2	B	501	HEM	CMC-C2C-C3C	2.97	130.62	124.68
4	D	503	H44	C17-N18-C38	2.96	123.62	113.20
2	C	501	HEM	CBA-CAA-C2A	-2.95	107.57	112.54
2	B	501	HEM	CMA-C3A-C4A	-2.90	124.20	128.46
3	D	502	H4B	C2-N1-C8A	2.90	121.49	114.59
2	C	501	HEM	C1B-NB-C4B	2.86	108.59	105.21
2	A	501	HEM	C3B-C4B-NB	-2.80	107.46	109.47
2	B	501	HEM	C1B-NB-C4B	2.77	108.48	105.21
4	B	503	H44	C17-N18-C38	2.76	122.91	113.20
2	C	501	HEM	CBD-CAD-C3D	-2.75	104.94	112.53
4	A	503	H44	C11-N07-C06	-2.74	122.10	128.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C4D-ND-C1D	2.73	108.44	105.21
5	D	504	ACT	O-C-CH3	-2.67	111.58	122.53
2	D	501	HEM	C3B-C4B-NB	-2.65	107.56	109.47
4	C	503	H44	C17-N18-C38	2.64	122.50	113.20
2	D	501	HEM	CAD-CBD-CGD	-2.64	106.66	113.67
2	D	501	HEM	C3D-C4D-ND	-2.60	107.32	110.17
4	D	503	H44	C31-N27-C26	-2.60	122.42	128.41
2	B	501	HEM	C4D-ND-C1D	2.60	108.28	105.21
4	A	503	H44	C17-N18-C38	2.59	122.31	113.20
2	D	501	HEM	CHD-C1D-ND	2.55	127.18	124.44
2	A	501	HEM	C3B-C2B-C1B	2.55	108.33	106.41
3	B	502	H4B	O10-C10-C9	-2.52	105.60	109.77
2	A	501	HEM	CBD-CAD-C3D	-2.52	105.58	112.53
4	D	503	H44	C38-C37-C34	-2.51	107.18	112.83
2	C	501	HEM	C3B-C4B-NB	-2.50	107.67	109.47
2	C	501	HEM	C4D-ND-C1D	2.48	108.14	105.21
2	A	501	HEM	C3D-C4D-ND	-2.42	107.52	110.17
2	A	501	HEM	CAD-C3D-C2D	-2.42	123.34	127.87
2	C	501	HEM	C4A-C3A-C2A	2.41	108.67	107.00
4	C	503	H44	C11-N07-C06	-2.41	122.87	128.41
3	C	502	H4B	C2-N1-C8A	2.40	120.30	114.59
3	B	502	H4B	C2-N1-C8A	2.39	120.27	114.59
2	B	501	HEM	C3B-C2B-C1B	2.38	108.20	106.41
2	D	501	HEM	CHA-C4D-ND	2.36	127.29	124.37
2	D	501	HEM	C1B-NB-C4B	2.36	108.00	105.21
2	C	501	HEM	CMC-C2C-C3C	2.34	129.37	124.68
3	B	502	H4B	N2-C2-N1	2.33	120.72	117.22
2	C	501	HEM	C4C-CHD-C1D	2.28	125.57	122.56
2	D	501	HEM	C2D-C1D-ND	-2.27	107.28	109.90
2	A	501	HEM	C1B-NB-C4B	2.25	107.87	105.21
4	B	503	H44	C14-C15-C16	2.24	121.64	118.55
2	B	501	HEM	C3D-C4D-ND	-2.24	107.72	110.17
2	C	501	HEM	C3D-C4D-ND	-2.22	107.74	110.17
6	B	506	BTB	O1-C1-C2	-2.21	106.21	111.40
2	D	501	HEM	C4A-C3A-C2A	2.18	108.51	107.00
3	A	502	H4B	C2-N1-C8A	2.17	119.75	114.59
2	D	501	HEM	CMB-C2B-C3B	-2.17	123.17	128.43
2	C	501	HEM	C2B-C1B-NB	-2.16	107.36	109.84
3	C	502	H4B	N2-C2-N3	2.16	120.46	117.22
3	A	502	H4B	C4A-C4-N3	-2.15	118.47	123.91
2	D	501	HEM	CAB-C3B-C2B	-2.13	121.52	128.43
4	D	503	H44	C11-N07-C06	-2.12	123.53	128.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CMC-C2C-C3C	2.07	128.81	124.68
4	B	503	H44	C13-C12-C11	2.06	122.10	119.73
4	B	503	H44	C11-N07-C06	-2.04	123.72	128.41
5	C	504	ACT	O-C-CH3	-2.04	114.18	122.53
2	A	501	HEM	C4D-ND-C1D	2.02	107.60	105.21
3	B	502	H4B	C4A-C4-N3	-2.00	118.85	123.91

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	H44	C34-C37-C38-N18
4	C	503	H44	C34-C37-C38-N18
4	D	503	H44	C34-C37-C38-N18
6	A	505	BTB	O1-C1-C2-C3
6	A	505	BTB	O1-C1-C2-C4
6	A	505	BTB	O1-C1-C2-N
6	A	506	BTB	C1-C2-C4-O4
6	A	506	BTB	N-C2-C4-O4
6	B	505	BTB	C1-C2-C4-O4
6	B	505	BTB	C3-C2-C4-O4
6	B	505	BTB	N-C2-C4-O4
6	B	506	BTB	C1-C2-C3-O3
6	B	506	BTB	C4-C2-C3-O3
6	B	506	BTB	N-C2-C3-O3
6	B	506	BTB	C1-C2-N-C5
6	B	506	BTB	C1-C2-N-C7
6	B	506	BTB	C3-C2-N-C5
6	B	506	BTB	C3-C2-N-C7
6	B	506	BTB	C4-C2-N-C5
6	B	506	BTB	C4-C2-N-C7
6	C	505	BTB	C1-C2-C3-O3
6	C	505	BTB	C4-C2-C3-O3
6	C	505	BTB	N-C2-C3-O3
6	C	506	BTB	C1-C2-C4-O4
6	C	506	BTB	C3-C2-C4-O4
6	C	506	BTB	N-C2-C4-O4
6	D	506	BTB	C4-C2-C3-O3
6	D	506	BTB	N-C2-C3-O3
7	A	507	GOL	O1-C1-C2-C3
7	A	507	GOL	C1-C2-C3-O3
7	C	507	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	D	507	GOL	C1-C2-C3-O3
6	D	505	BTB	N-C5-C6-O6
7	C	507	GOL	O1-C1-C2-O2
4	B	503	H44	C34-C37-C38-N18
6	B	506	BTB	N-C7-C8-O8
4	D	503	H44	C15-C17-N18-C38
6	A	506	BTB	N-C7-C8-O8
6	C	506	BTB	N-C7-C8-O8
6	D	506	BTB	N-C5-C6-O6
6	D	506	BTB	N-C7-C8-O8
7	A	507	GOL	O1-C1-C2-O2
7	D	507	GOL	O2-C2-C3-O3
2	C	501	HEM	C4B-C3B-CAB-CBB
7	A	507	GOL	O2-C2-C3-O3
4	C	503	H44	C36-C31-N27-C26
4	A	503	H44	C36-C31-N27-C26
4	A	503	H44	C32-C31-N27-C26
4	C	503	H44	C32-C31-N27-C26
6	C	505	BTB	N-C7-C8-O8
6	A	506	BTB	C3-C2-C4-O4
4	B	503	H44	C36-C31-N27-C26
4	B	503	H44	C32-C31-N27-C26
6	C	505	BTB	N-C5-C6-O6
2	C	501	HEM	C2A-CAA-CBA-CGA
6	B	505	BTB	N-C7-C8-O8
4	A	503	H44	C25-C26-N27-C31
6	A	506	BTB	C3-C2-N-C7
6	A	506	BTB	C4-C2-N-C7
6	C	505	BTB	O1-C1-C2-N
6	D	505	BTB	C1-C2-N-C5
4	D	503	H44	N06-C06-N07-C11
6	C	505	BTB	O1-C1-C2-C3
6	C	505	BTB	C3-C2-C4-O4
4	B	503	H44	C25-C26-N27-C31
4	B	503	H44	C15-C17-N18-C38
6	A	505	BTB	N-C5-C6-O6
6	B	506	BTB	N-C5-C6-O6
4	D	503	H44	C37-C38-N18-C17
2	D	501	HEM	C4B-C3B-CAB-CBB
6	D	506	BTB	C1-C2-C3-O3
6	A	506	BTB	C1-C2-N-C5
6	A	506	BTB	C3-C2-N-C5

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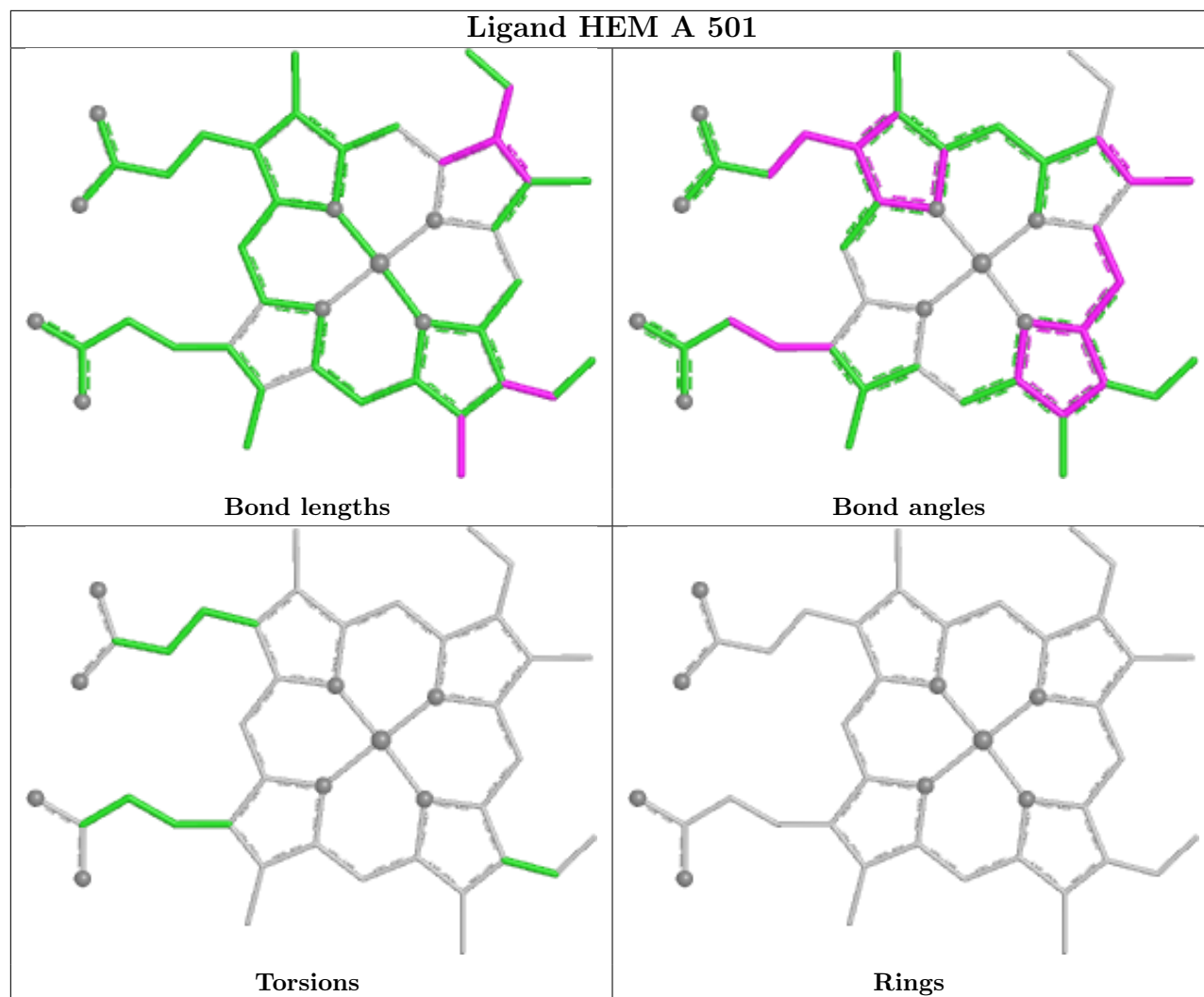
Mol	Chain	Res	Type	Atoms
6	D	505	BTB	C3-C2-N-C5
4	A	503	H44	N06-C06-N07-C11
4	B	503	H44	N06-C06-N07-C11

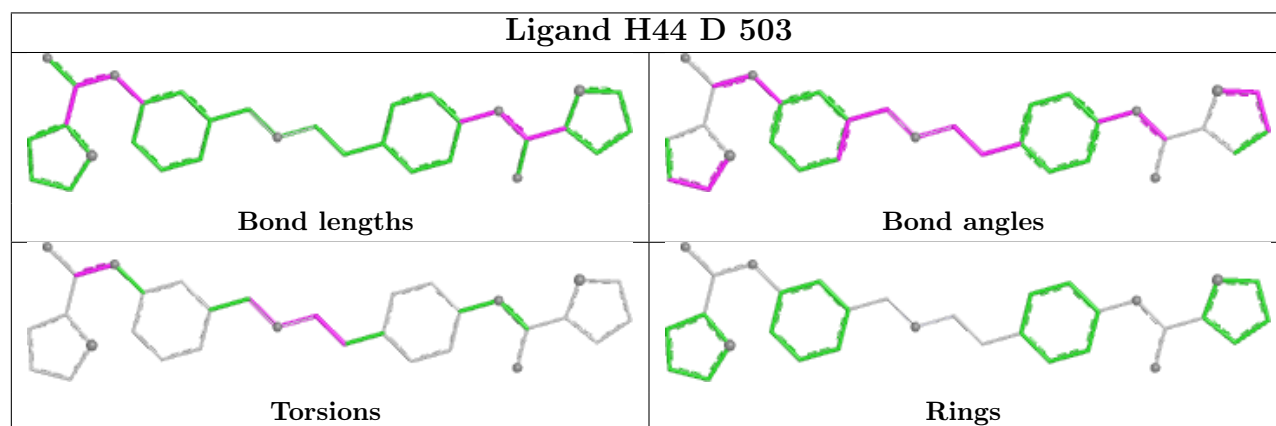
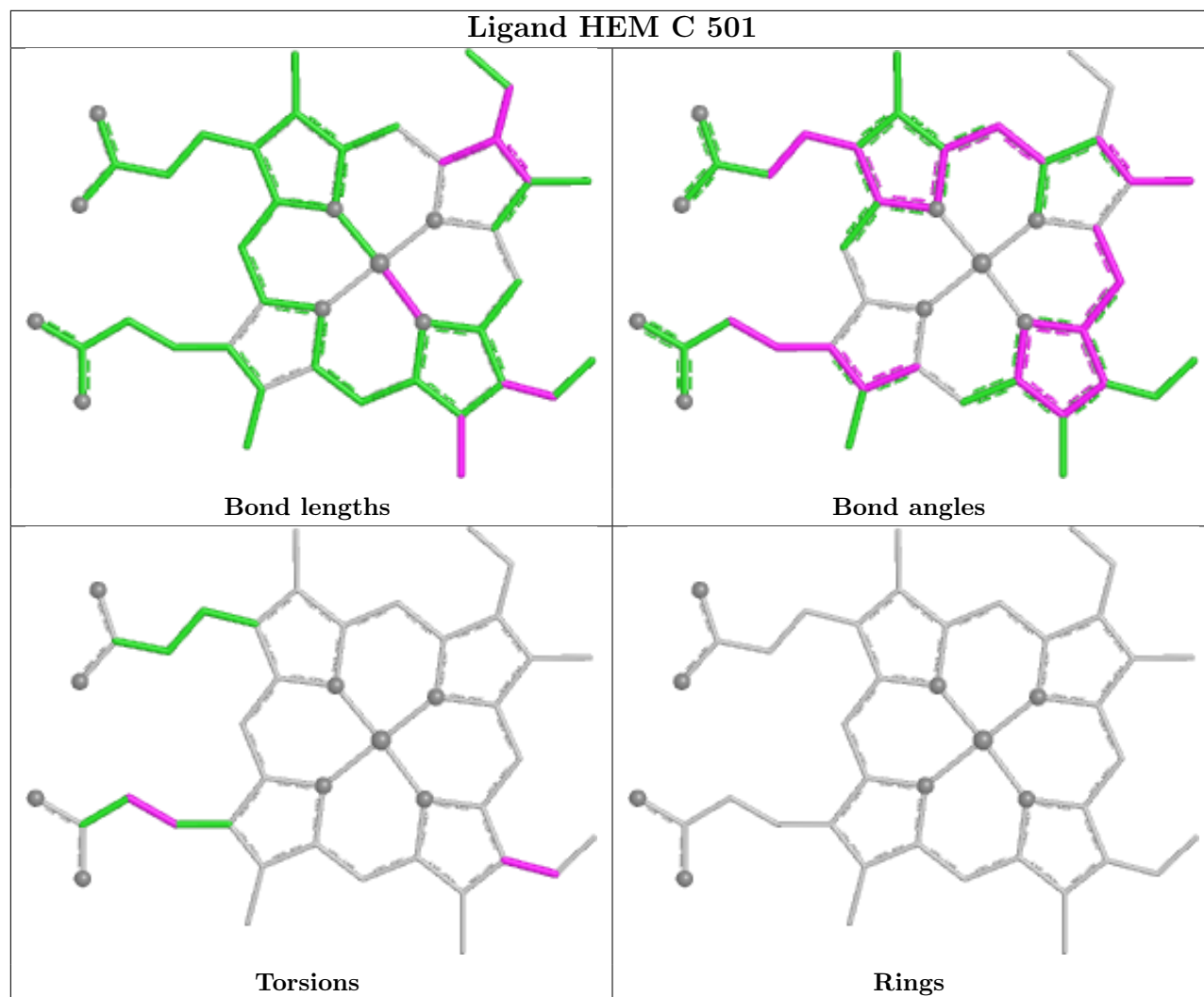
There are no ring outliers.

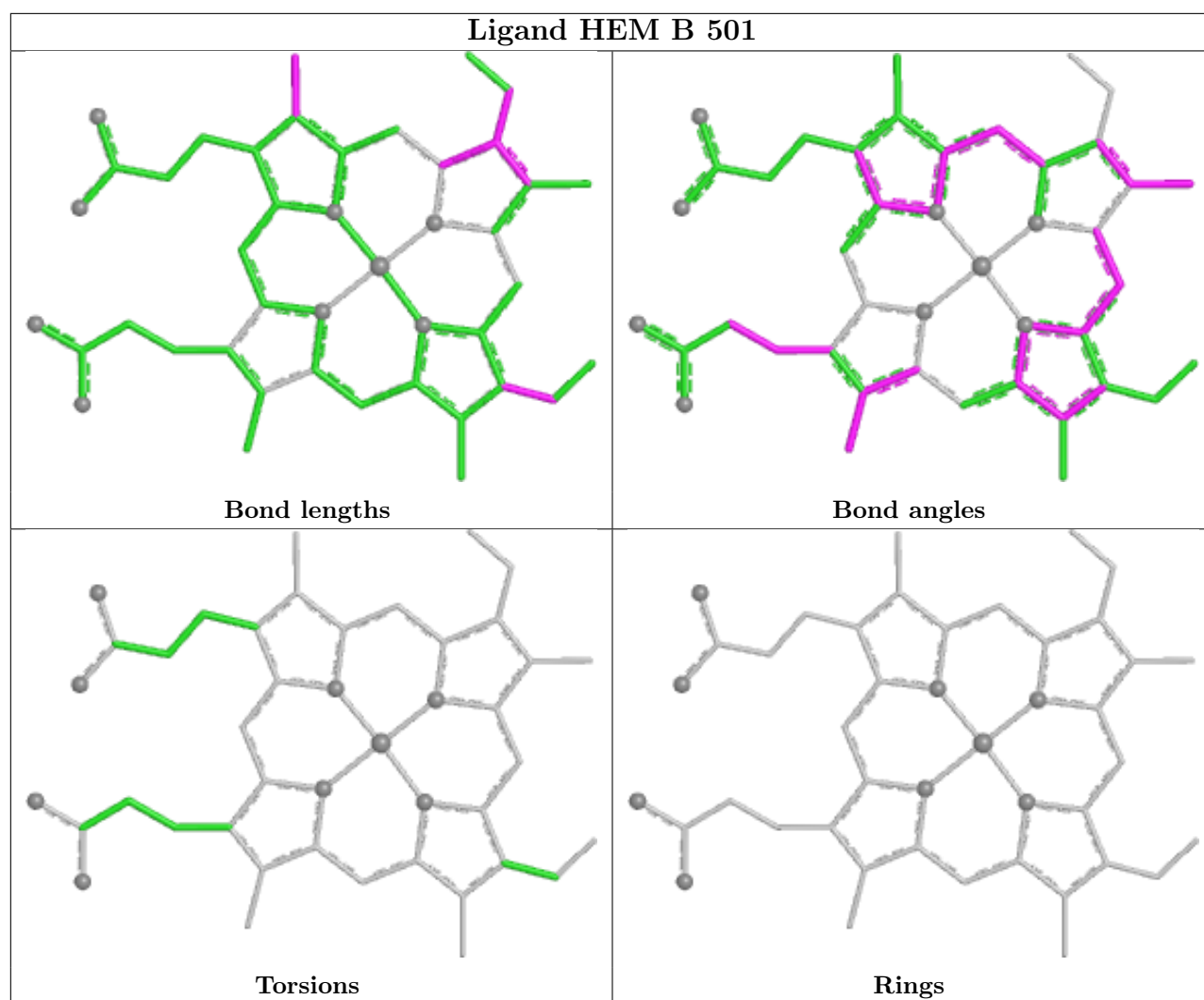
20 monomers are involved in 51 short contacts:

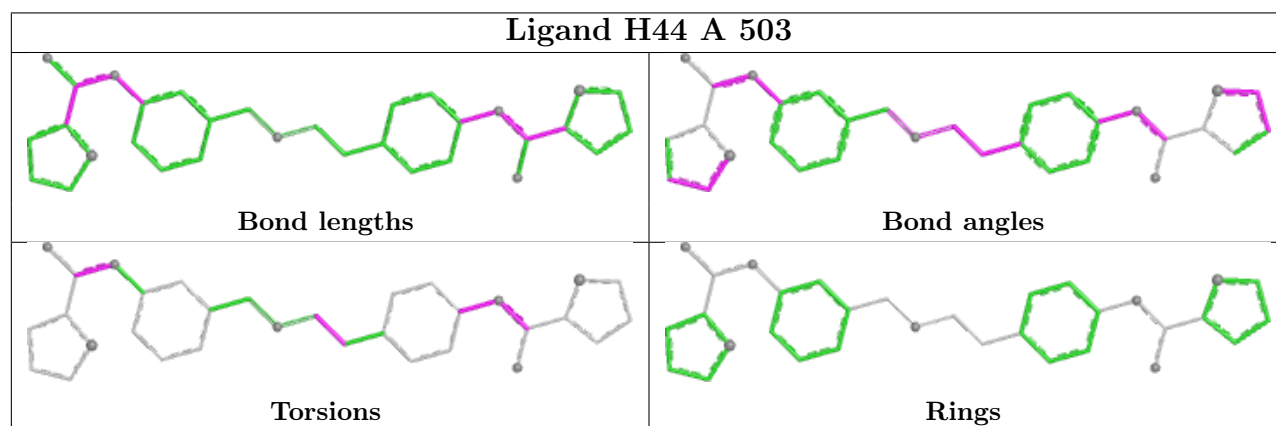
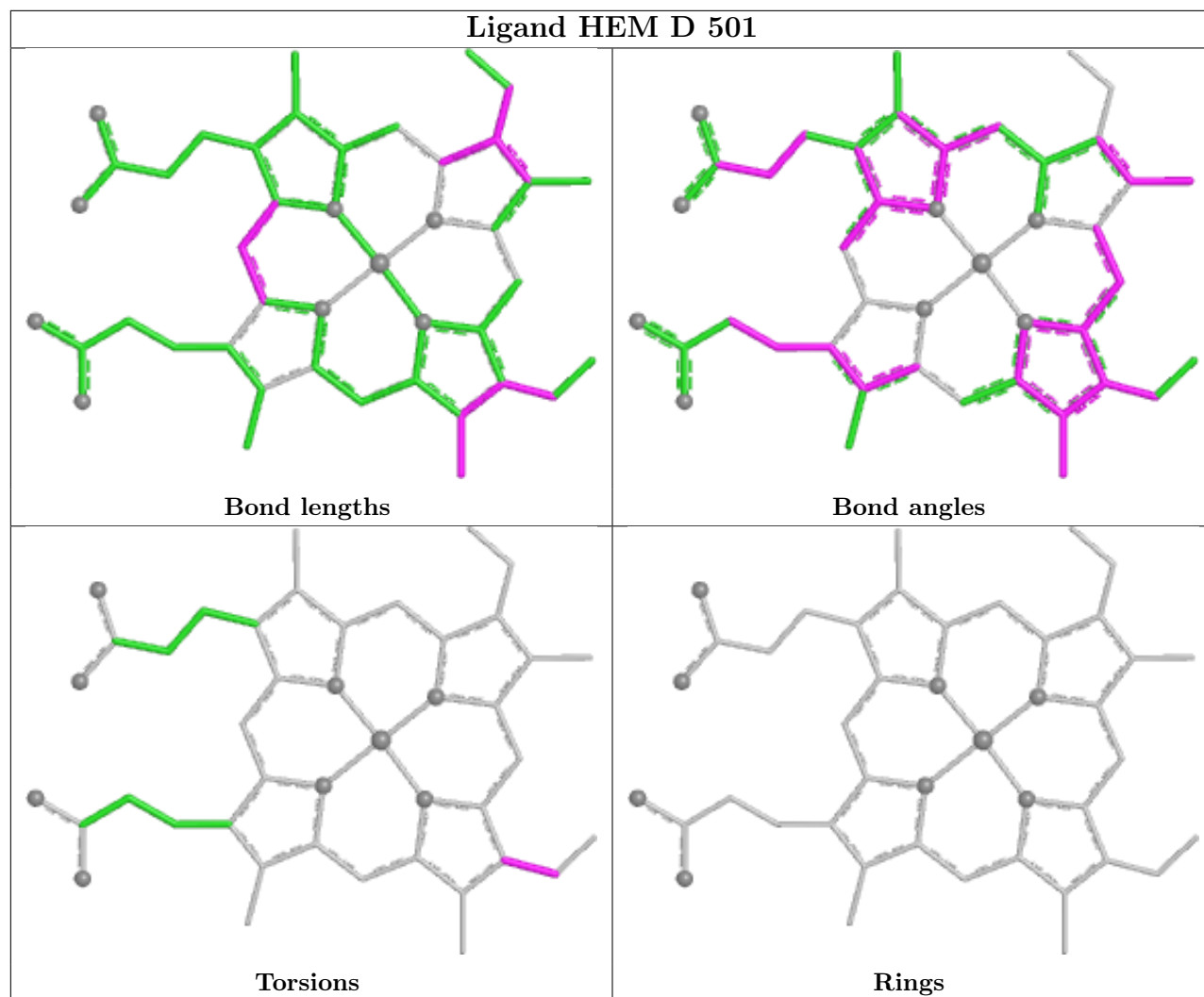
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	H4B	2	0
3	B	502	H4B	1	0
2	A	501	HEM	2	0
2	C	501	HEM	3	0
4	D	503	H44	3	0
2	B	501	HEM	4	0
2	D	501	HEM	3	0
6	A	506	BTB	3	0
6	C	506	BTB	2	0
4	A	503	H44	5	0
4	C	503	H44	1	0
6	D	505	BTB	3	0
6	B	505	BTB	6	0
6	B	506	BTB	3	0
3	D	502	H4B	1	0
6	D	506	BTB	3	0
4	B	503	H44	2	0
5	C	504	ACT	1	0
6	C	505	BTB	1	0
6	A	505	BTB	4	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.

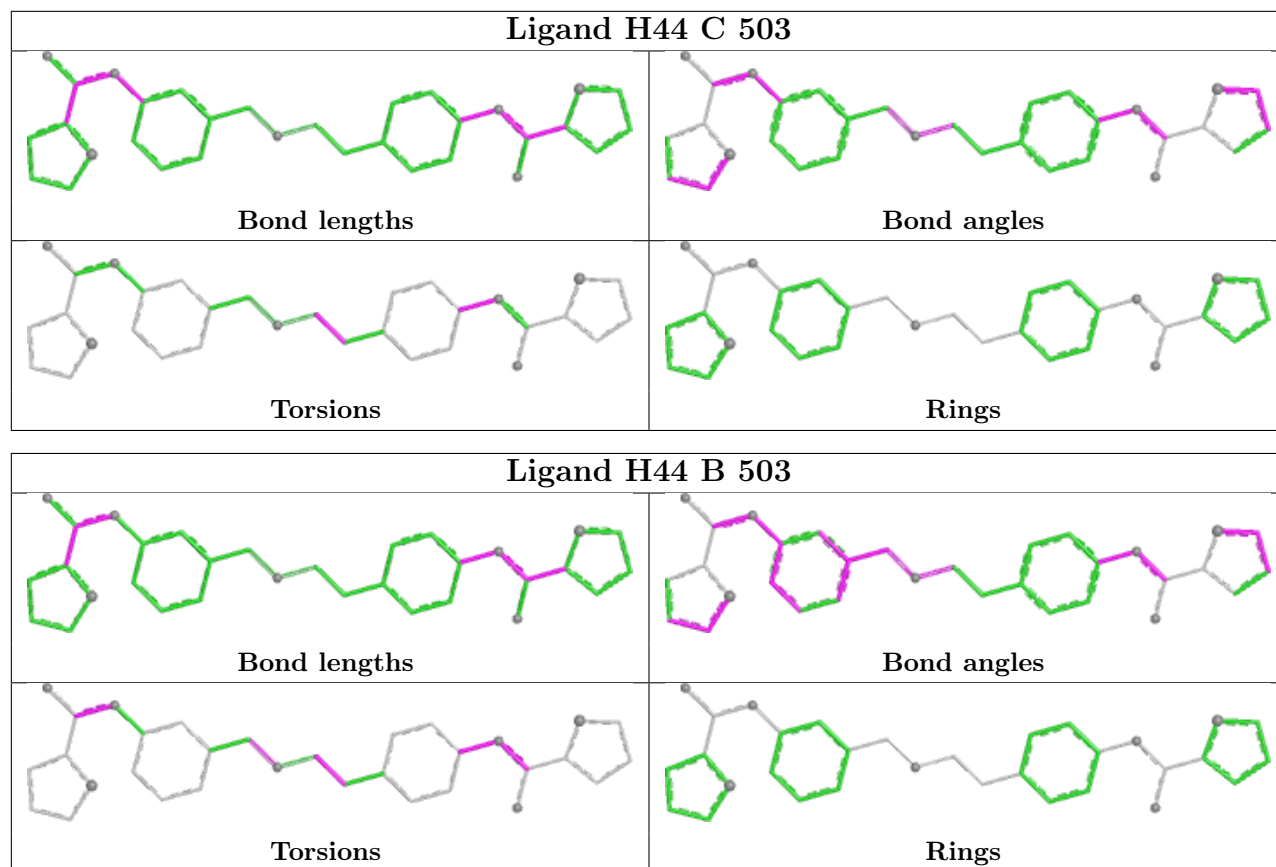












## 5.7 Other polymers [i](#)

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 [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	400/441 (90%)	-1.35	0	100   100	18, 41, 80, 109	1 (0%)
1	B	403/441 (91%)	-1.63	0	100   100	14, 30, 56, 109	2 (0%)
1	C	400/441 (90%)	-0.89	1 (0%)	90   89	18, 50, 101, 124	1 (0%)
1	D	402/441 (91%)	-1.58	0	100   100	15, 31, 62, 111	2 (0%)
All	All	1605/1764 (90%)	-1.36	1 (0%)	92   91	14, 36, 85, 124	6 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	153	VAL	2.3

### 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
7	GOL	C	507	6/6	0.95	0.07	65,71,83,86	0

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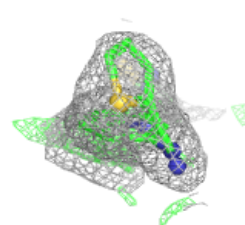
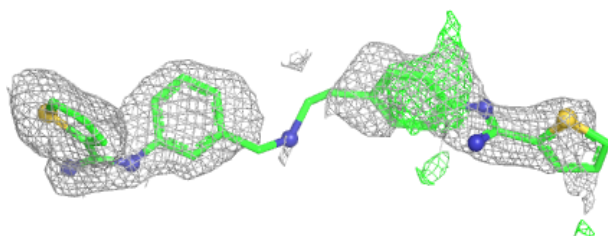
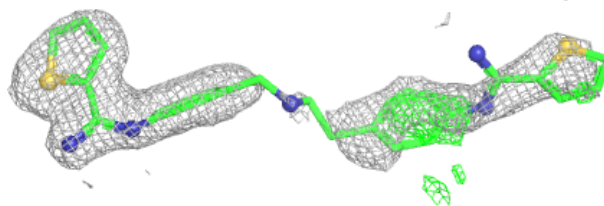
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	D	507	6/6	0.95	0.05	66,68,68,71	0
6	BTB	B	506	14/14	0.97	0.06	66,74,81,81	0
4	H44	C	503	32/32	0.98	0.08	30,78,110,112	0
6	BTB	C	505	14/14	0.98	0.06	57,71,77,83	0
6	BTB	C	506	14/14	0.98	0.04	61,74,83,83	0
6	BTB	D	506	14/14	0.98	0.04	53,68,73,74	0
7	GOL	A	507	6/6	0.98	0.04	43,56,59,60	0
6	BTB	A	505	14/14	0.98	0.06	50,63,69,71	0
6	BTB	A	506	14/14	0.98	0.04	47,63,72,74	0
4	H44	A	503	32/32	0.99	0.06	21,65,109,112	0
4	H44	B	503	32/32	0.99	0.06	13,56,117,121	0
3	H4B	B	502	17/17	0.99	0.03	19,25,30,31	0
6	BTB	D	505	14/14	0.99	0.04	25,51,68,76	0
4	H44	D	503	32/32	0.99	0.06	18,54,121,123	0
3	H4B	C	502	17/17	0.99	0.03	27,36,45,48	0
3	H4B	D	502	17/17	0.99	0.02	15,28,34,38	0
6	BTB	B	505	14/14	0.99	0.04	30,53,66,73	0
9	GD	A	509	1/1	0.99	0.04	141,141,141,141	0
2	HEM	A	501	43/43	1.00	0.02	16,31,39,41	0
2	HEM	B	501	43/43	1.00	0.02	9,17,27,40	0
5	ACT	A	504	4/4	1.00	0.06	35,49,56,61	0
5	ACT	B	504	4/4	1.00	0.04	42,47,52,53	0
5	ACT	C	504	4/4	1.00	0.03	26,40,50,54	0
5	ACT	D	504	4/4	1.00	0.04	26,39,47,57	0
2	HEM	C	501	43/43	1.00	0.03	24,40,48,53	0
2	HEM	D	501	43/43	1.00	0.02	8,18,27,37	0
8	CL	A	508	1/1	1.00	0.03	39,39,39,39	0
8	CL	B	507	1/1	1.00	0.03	36,36,36,36	0
8	CL	C	508	1/1	1.00	0.02	54,54,54,54	0
8	CL	D	508	1/1	1.00	0.02	37,37,37,37	0
3	H4B	A	502	17/17	1.00	0.02	19,27,37,37	0
9	GD	B	508	1/1	1.00	0.01	47,47,47,47	0
9	GD	D	509	1/1	1.00	0.01	41,41,41,41	0
10	ZN	A	510	1/1	1.00	0.01	28,28,28,28	0
10	ZN	C	509	1/1	1.00	0.01	34,34,34,34	0

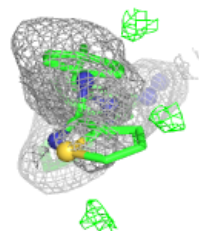
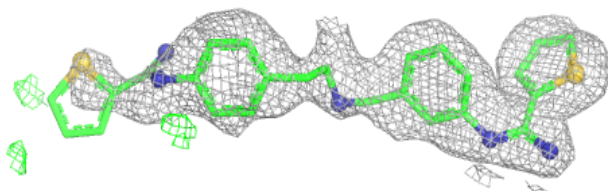
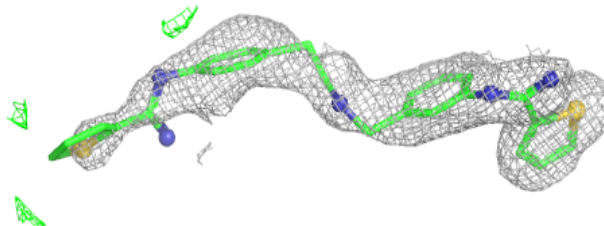
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around H44 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)

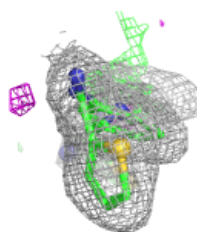
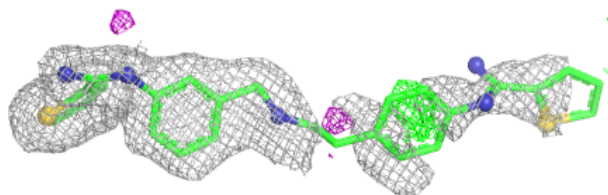
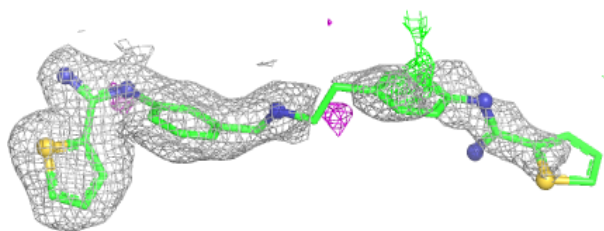
**Electron density around H44 A 503:**

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

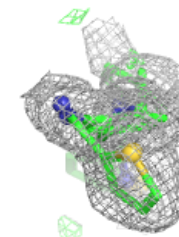
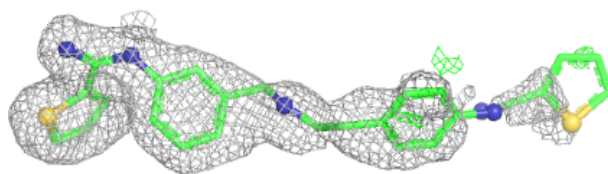
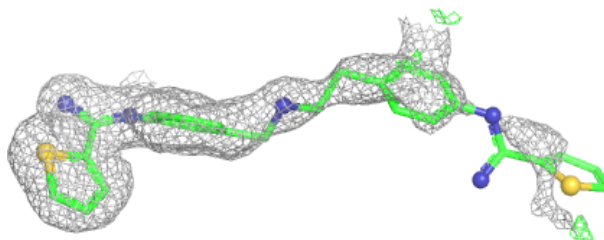


**Electron density around H44 B 503:**

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

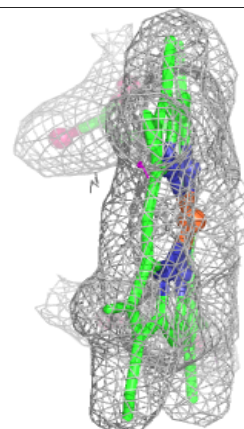
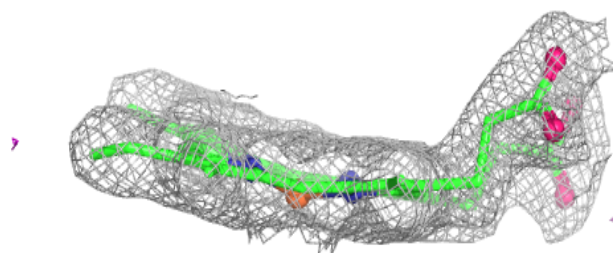
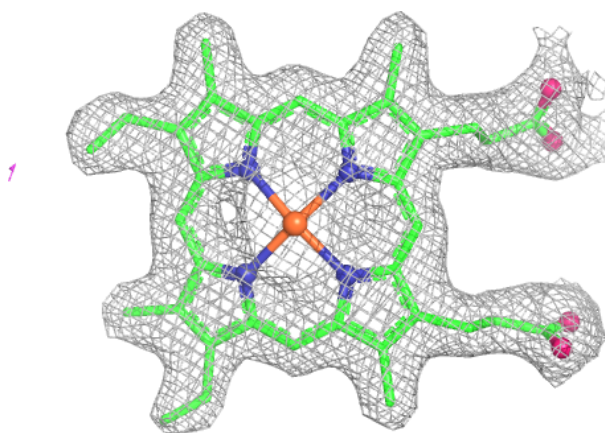
**Electron density around H44 D 503:**

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



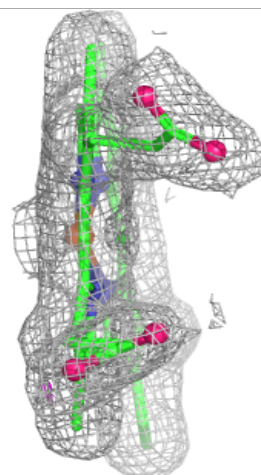
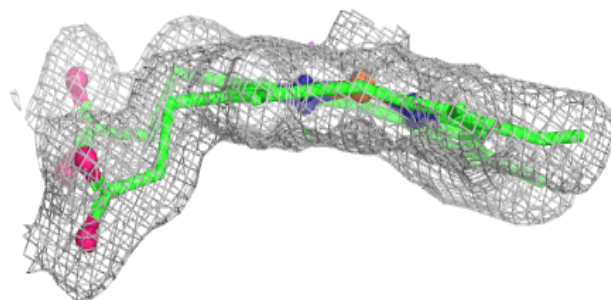
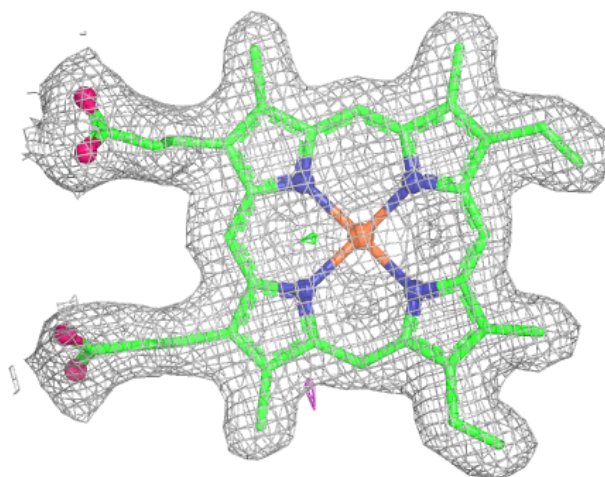
**Electron density around HEM A 501:**

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



**Electron density around HEM B 501:**

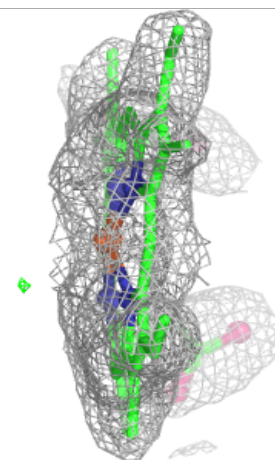
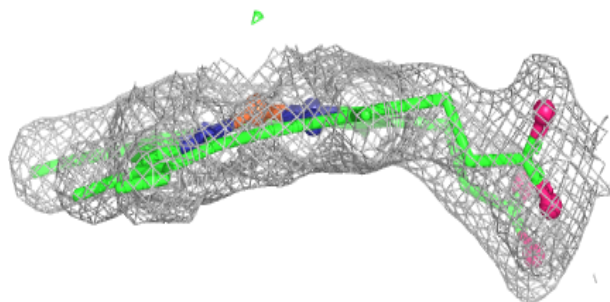
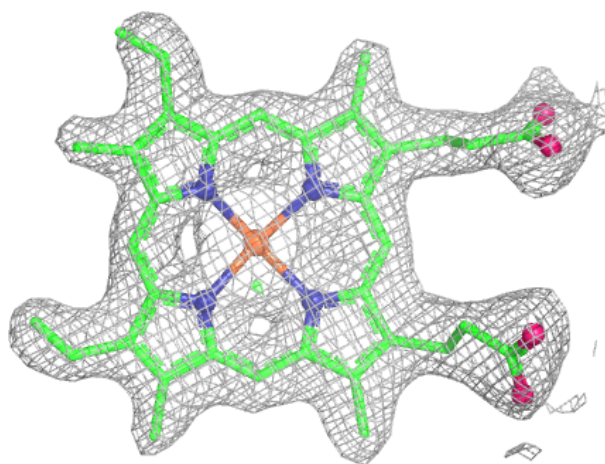
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



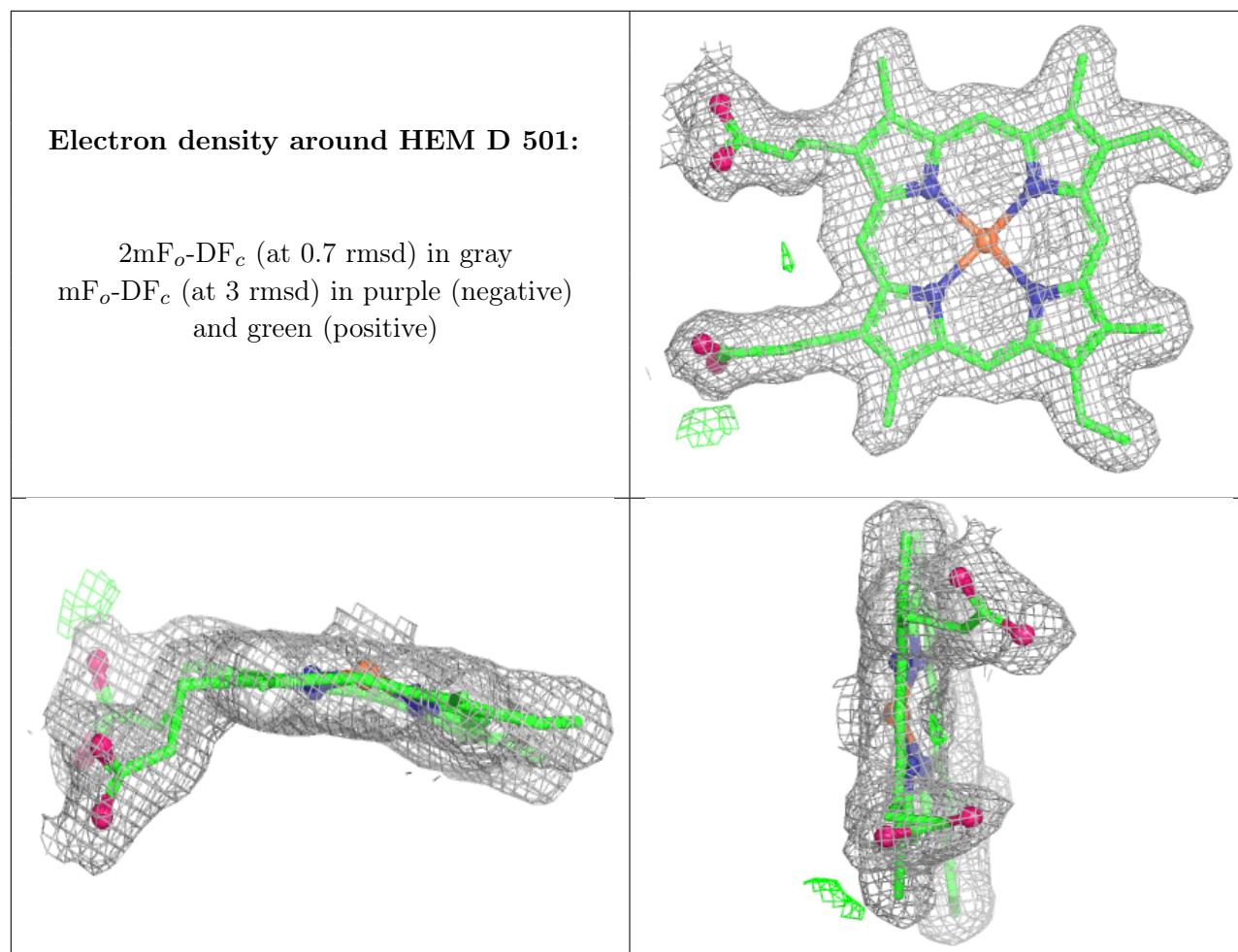


**Electron density around HEM C 501:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.