



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:39 AM BST

PDB ID : 6PP3  
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 7-(3-(Aminomethyl)-4-(pyridin-2-ylmethoxy)phenyl)-4-methylquinolin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2019-07-05  
Resolution : 1.95 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

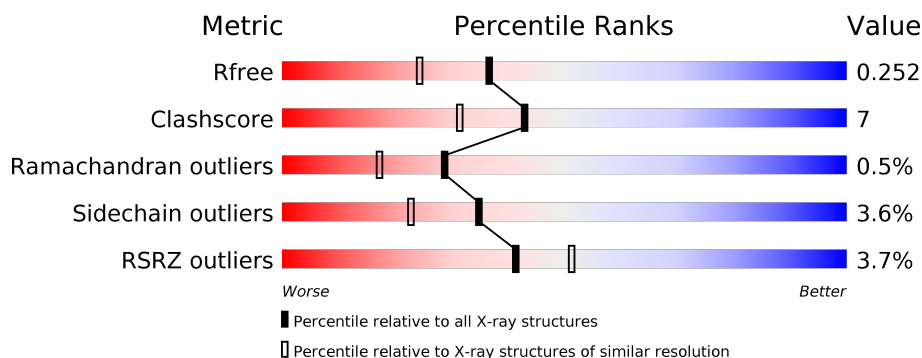
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on 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>10%</div> <div> <div>68%</div> <div>21%</div> <div>• 9%</div> </div> </div>
1	B	440	<div> <div>%</div> <div> <div>75%</div> <div>15%</div> <div>• 9%</div> </div> </div>
1	C	440	<div> <div>2%</div> <div> <div>81%</div> <div>9%</div> <div>• 9%</div> </div> </div>
1	D	440	<div> <div>80%</div> <div>11%</div> <div>9%</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13906 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.

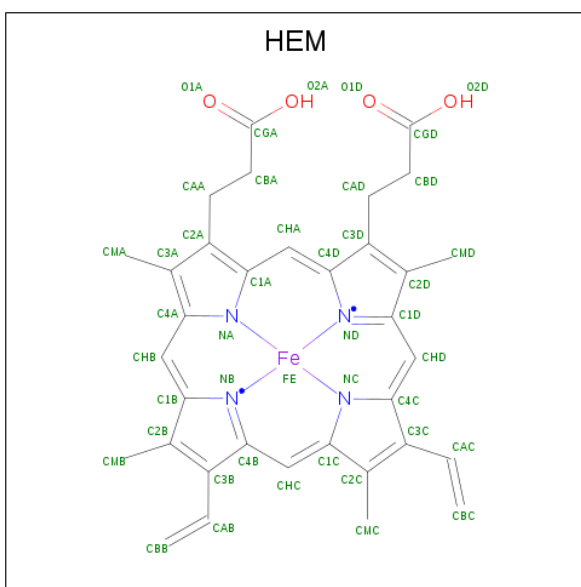
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	2	0
			3215	2047	566	586	16			
1	B	402	Total	C	N	O	S	0	4	0
			3225	2054	566	589	16			
1	C	401	Total	C	N	O	S	0	2	0
			3209	2044	563	586	16			
1	D	401	Total	C	N	O	S	0	2	0
			3206	2042	563	585	16			

There are 4 discrepancies between the modelled and reference sequences:

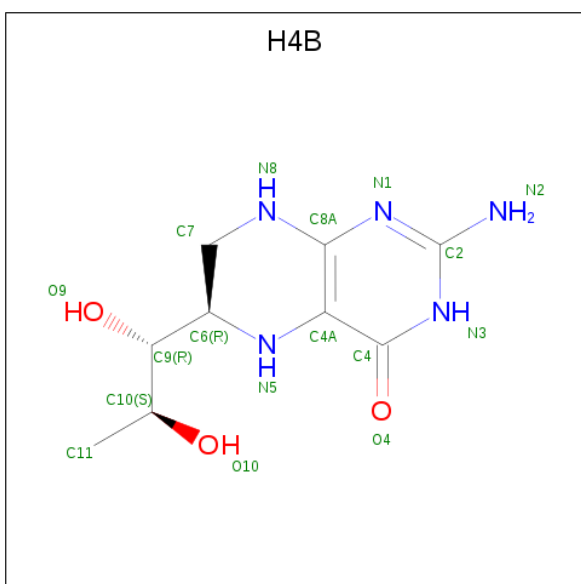
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



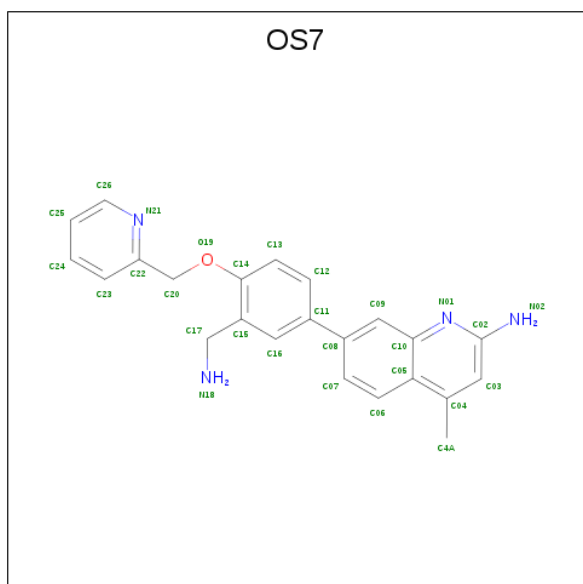
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



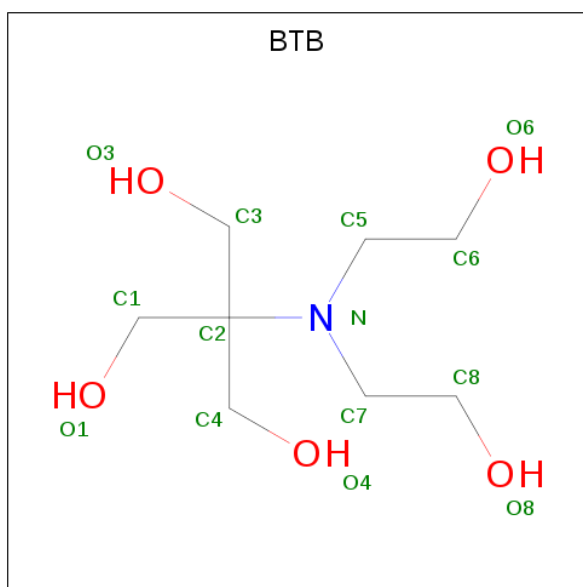
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-{3-(aminomethyl)-4-[(pyridin-2-yl)methoxy]phenyl}-4-methylquinolin-2-amine (three-letter code: OS7) (formula: C<sub>23</sub>H<sub>22</sub>N<sub>4</sub>O) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	23	4	1		
4	B	1	Total	C	N	O	0	0
			28	23	4	1		
4	C	1	Total	C	N	O	0	0
			28	23	4	1		
4	D	1	Total	C	N	O	0	0
			28	23	4	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	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	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 ZINC ION (three-letter code: ZN) (formula: Zn).

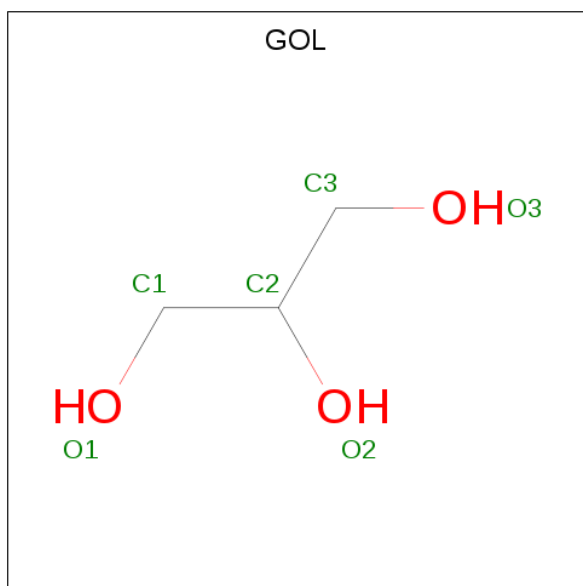
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: 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		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

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

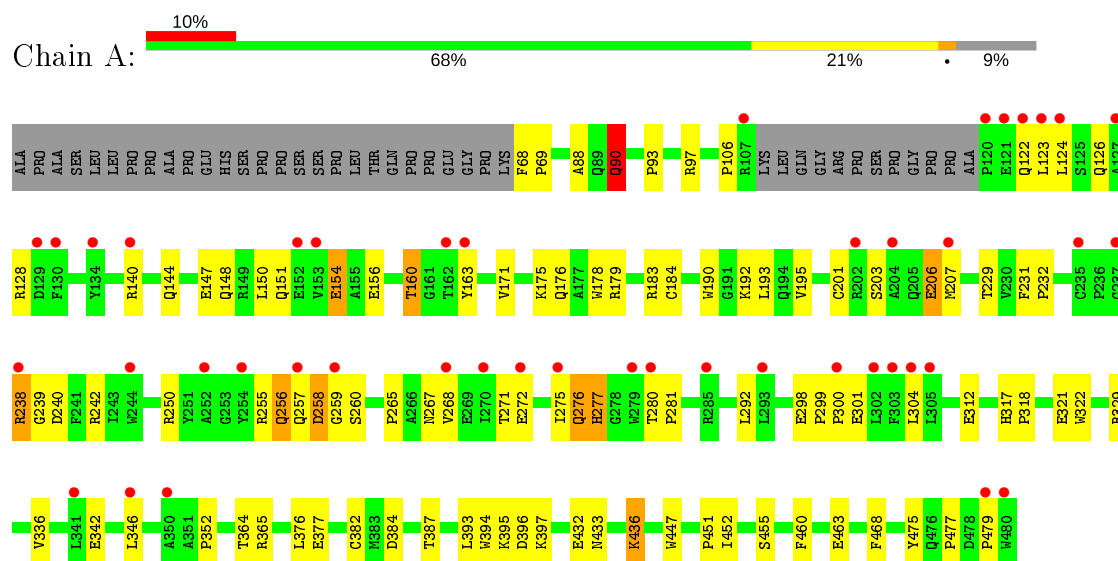
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	66	Total 66	O 66	0	0
10	B	168	Total 168	O 168	0	0
10	C	121	Total 121	O 121	0	0
10	D	168	Total 168	O 168	0	0

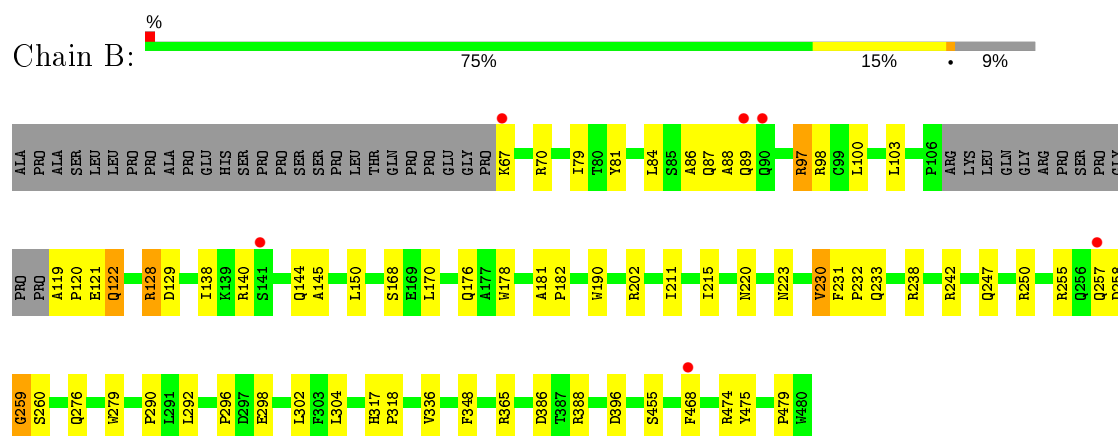
### 3 Residue-property plots

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.

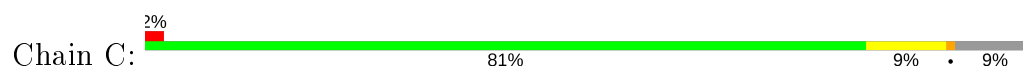
- Molecule 1: Nitric oxide synthase, endothelial

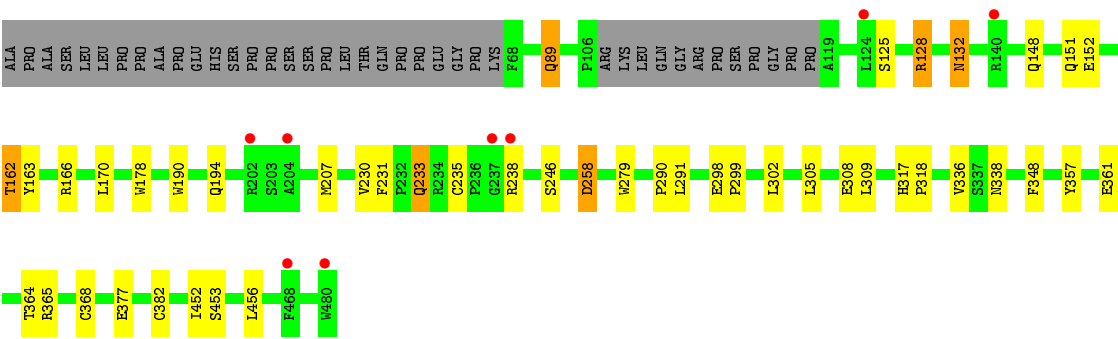


- Molecule 1: Nitric oxide synthase, endothelial

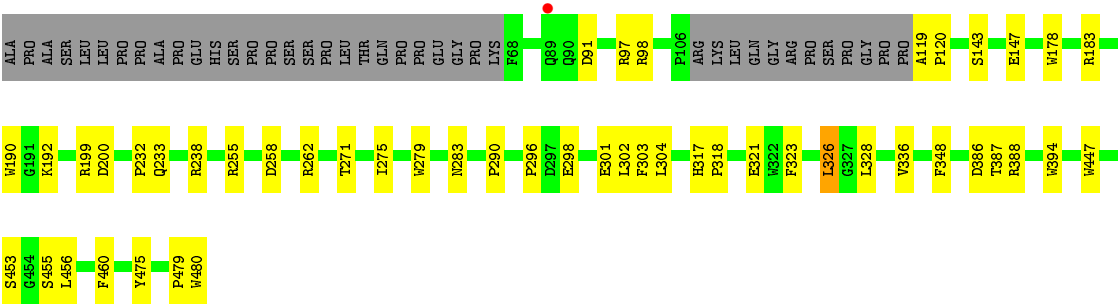
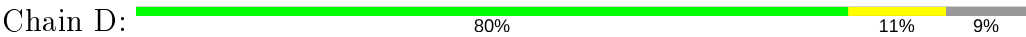


- Molecule 1: Nitric oxide synthase, endothelial





● 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, $\alpha$ , $\beta$ , $\gamma$	59.87Å 152.08Å 108.58Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	49.86 – 1.95 49.86 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.86-1.95) 99.8 (49.86-1.95)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.211 , 0.260 0.202 , 0.252	Depositor DCC
$R_{free}$ test set	7064 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13906	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, CL, OS7, GD, BTB, HEM

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	0.35	0/3313	0.51	0/4513
1	B	0.41	0/3329	0.56	0/4536
1	C	0.37	0/3307	0.51	0/4507
1	D	0.44	0/3304	0.57	0/4503
All	All	0.39	0/13253	0.54	0/18059

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	3215	0	3118	62	0
1	B	3225	0	3131	47	0
1	C	3209	0	3109	25	1
1	D	3206	0	3108	27	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	1	0
3	A	17	0	15	1	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	1	0
3	D	17	0	15	0	0
4	A	28	0	0	1	0
4	B	28	0	0	2	0
4	C	28	0	0	4	0
4	D	28	0	0	1	0
5	A	42	0	56	7	0
5	B	70	0	93	10	1
5	C	14	0	19	3	0
5	D	28	0	37	6	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	0	0
7	C	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	2	0	0	0	0
9	D	1	0	0	0	0
10	A	66	0	0	2	0
10	B	168	0	0	0	0
10	C	121	0	0	1	0
10	D	168	0	0	4	0
All	All	13906	0	12867	178	1

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 7.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLN:HA	1:B:259:GLY:H	1.38	0.87
1:C:128:ARG:O	1:C:132:ASN:ND2	2.13	0.81
1:A:147:GLU:O	1:A:151:GLN:NE2	2.15	0.79
1:A:312:GLU:OE2	1:A:329:ARG:NH1	2.14	0.78
1:A:322:TRP:CD1	5:A:504:BTB:H62	2.21	0.76
1:A:433:ASN:HA	1:A:436:LYS:HE3	1.69	0.71
1:D:119:ALA:N	10:D:602:HOH:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:509:BTB:H12	1:C:382:CYS:HA	1.74	0.70
1:C:258:ASP:OD1	1:C:258:ASP:N	2.25	0.70
1:B:298:GLU:OE2	5:B:505:BTB:N	2.26	0.69
1:D:336:VAL:HG21	4:D:503:OS7:C07	2.22	0.68
1:B:336:VAL:HG21	4:B:503:OS7:C07	2.24	0.68
5:D:504:BTB:H61	10:D:728:HOH:O	1.92	0.67
2:A:501:HEM:HHC	2:A:501:HEM:HBB2	1.74	0.67
1:A:321:GLU:CD	1:A:321:GLU:H	2.03	0.62
1:C:336:VAL:HG21	4:C:503:OS7:C07	2.29	0.62
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.82	0.62
1:A:336:VAL:HG21	4:A:503:OS7:C07	2.29	0.61
1:D:91:ASP:OD1	10:D:601:HOH:O	2.16	0.61
1:B:119:ALA:HB1	1:B:122:GLN:HE21	1.65	0.61
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.84	0.60
1:A:150:LEU:HB2	1:A:151:GLN:NE2	2.16	0.60
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.86	0.58
1:B:257:GLN:HA	1:B:259:GLY:N	2.13	0.57
1:A:377:GLU:OE1	5:A:505:BTB:H11	2.05	0.57
1:A:384:ASP:OD1	5:A:504:BTB:O3	2.21	0.57
1:B:121:GLU:OE1	1:B:122:GLN:NE2	2.38	0.56
1:C:235:CYS:SG	1:C:238:ARG:NH2	2.79	0.56
2:D:501:HEM:HHC	2:D:501:HEM:HBB2	1.87	0.56
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.18	0.55
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.24	0.55
1:A:258:ASP:N	1:A:258:ASP:OD1	2.40	0.54
1:C:364:THR:O	1:C:368:CYS:HB2	2.07	0.54
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.43	0.54
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.90	0.54
1:B:138:ILE:HG13	1:B:140:ARG:HB2	1.91	0.53
1:B:386:ASP:OD1	1:B:388:ARG:HG2	2.10	0.52
1:D:326:LEU:HB3	1:D:328:LEU:HG	1.90	0.52
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.91	0.52
1:B:144:GLN:NE2	1:B:145:ALA:H	2.08	0.52
1:A:124:LEU:HD23	1:A:128:ARG:NE	2.24	0.52
1:A:148:GLN:O	1:A:151:GLN:HG2	2.10	0.51
1:C:298:GLU:HG3	1:C:299:PRO:HD2	1.91	0.51
1:A:382:CYS:HA	5:A:504:BTB:H11	1.92	0.51
1:C:162:THR:OG1	1:C:163:TYR:N	2.43	0.51
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.93	0.51
5:B:510:BTB:H12	1:C:377:GLU:OE1	2.10	0.51
1:D:238:ARG:HG2	1:D:296:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:ASP:OD1	1:D:388:ARG:NH1	2.44	0.51
1:B:122:GLN:H	1:B:122:GLN:CD	2.13	0.51
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.46	0.51
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.46	0.50
5:D:505:BTB:O1	5:D:505:BTB:O4	2.13	0.50
1:A:97:ARG:NH2	1:B:86:ALA:O	2.34	0.50
1:A:124:LEU:O	1:A:128:ARG:HG3	2.11	0.50
1:A:156:GLU:O	1:A:160:THR:OG1	2.30	0.50
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.24	0.49
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.47	0.49
1:B:70:ARG:HD2	1:B:79:ILE:HD13	1.93	0.49
1:B:170:LEU:HD21	1:B:230:VAL:HG11	1.93	0.49
1:B:89:GLN:NE2	1:B:129:ASP:OD2	2.46	0.49
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.94	0.49
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.48	0.48
1:A:242:ARG:NH1	1:A:477:PRO:O	2.39	0.48
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.48	0.48
1:B:468:PHE:CZ	1:B:474:ARG:HD2	2.49	0.48
1:C:279:TRP:CG	1:C:290:PRO:HG3	2.49	0.48
5:B:505:BTB:H51	5:B:505:BTB:O3	2.10	0.48
1:C:361:GLU:OE2	4:C:503:OS7:N02	2.46	0.47
1:D:387:THR:HA	1:D:394:TRP:CD1	2.49	0.47
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.96	0.47
1:A:124:LEU:HD23	1:A:128:ARG:HE	1.78	0.47
1:D:119:ALA:N	1:D:120:PRO:HD3	2.30	0.47
1:A:451:PRO:HB2	1:B:455:SER:OG	2.15	0.47
1:C:148:GLN:HE22	1:C:166:ARG:NH2	2.12	0.47
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.96	0.47
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.97	0.47
1:A:364:THR:HG21	1:A:452:ILE:HG23	1.96	0.46
1:A:90:GLN:HB2	1:A:468:PHE:CE2	2.50	0.46
5:B:510:BTB:O1	5:B:510:BTB:O3	2.23	0.46
2:C:501:HEM:HBA2	4:C:503:OS7:C12	2.45	0.46
1:D:262:ARG:HD3	1:D:283:ASN:O	2.16	0.46
1:C:279:TRP:HB2	1:C:302:LEU:HD11	1.97	0.46
1:D:479:PRO:HD2	1:D:480:TRP:CZ3	2.51	0.46
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.51	0.46
1:B:242:ARG:CZ	1:B:479:PRO:HG3	2.45	0.46
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.51	0.46
1:C:291:LEU:HD11	1:C:305:LEU:HD21	1.97	0.46
1:A:154:GLU:HG3	1:A:154:GLU:H	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:TRP:CE3	1:D:190:TRP:HA	2.50	0.46
5:D:504:BTB:H51	5:D:504:BTB:H32	1.65	0.46
1:A:275:ILE:C	1:A:277:HIS:H	2.19	0.45
2:C:501:HEM:HHC	2:C:501:HEM:HBB2	1.98	0.45
5:D:505:BTB:H32	5:D:505:BTB:H51	1.31	0.45
1:A:256:GLN:HB3	1:A:258:ASP:H	1.80	0.45
1:B:258:ASP:O	1:B:260:SER:N	2.49	0.45
1:A:176:GLN:OE1	1:A:179:ARG:NH1	2.44	0.45
1:A:393:LEU:O	1:A:397:LYS:HG3	2.16	0.45
1:B:100:LEU:HB3	1:B:103:LEU:HD22	1.99	0.45
1:A:229:THR:O	1:A:352:PRO:HD2	2.17	0.45
1:A:455:SER:HA	1:A:460:PHE:CG	2.52	0.45
1:B:211:ILE:O	1:B:215:ILE:HG13	2.17	0.45
1:A:267:ASN:O	1:A:271:THR:OG1	2.20	0.44
1:B:84:LEU:HD12	1:B:87:GLN:HG3	1.98	0.44
1:A:242:ARG:CZ	1:A:479:PRO:HD3	2.46	0.44
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.52	0.44
1:A:201:CYS:SG	1:A:206:GLU:HB3	2.58	0.44
1:A:258:ASP:O	1:A:260:SER:N	2.51	0.44
1:A:97:ARG:HG2	1:B:88:ALA:HB3	2.00	0.44
1:B:298:GLU:OE1	5:B:505:BTB:H31	2.18	0.44
5:C:504:BTB:H41	5:C:504:BTB:H51	1.57	0.44
1:A:265:PRO:HA	1:A:268:VAL:HG23	1.99	0.44
1:B:336:VAL:HG21	4:B:503:OS7:C06	2.48	0.44
1:D:298:GLU:OE1	5:D:505:BTB:H42	2.17	0.44
1:A:275:ILE:HD11	1:A:281:PRO:HB3	2.00	0.44
1:A:88:ALA:HB3	1:B:97:ARG:HH11	1.82	0.44
5:C:504:BTB:H71	5:C:504:BTB:H32	1.54	0.44
1:D:143:SER:O	1:D:147:GLU:HG2	2.18	0.44
1:D:279:TRP:HB2	1:D:302:LEU:HD21	1.99	0.43
1:A:140:ARG:NH1	10:A:601:HOH:O	2.36	0.43
1:A:93:PRO:HG3	1:A:106:PRO:HB3	2.00	0.43
1:C:246:SER:HA	1:C:338:ASN:HB3	2.01	0.43
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.83	0.43
1:D:301:GLU:HB3	1:D:303:PHE:CE1	2.54	0.43
1:D:475:TYR:HA	10:D:689:HOH:O	2.18	0.43
1:A:276:GLN:O	1:A:277:HIS:ND1	2.28	0.43
1:A:123:LEU:HD11	1:A:346:LEU:HD23	2.00	0.43
5:A:504:BTB:H81	5:A:504:BTB:H52	1.65	0.43
1:A:203:SER:H	1:A:206:GLU:HB2	1.83	0.43
1:C:357:TYR:HA	4:C:503:OS7:N02	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:505:BTB:H72	5:A:505:BTB:H41	1.44	0.43
1:C:207:MET:HG3	1:C:231:PHE:CZ	2.54	0.43
1:A:178:TRP:CE3	1:A:190:TRP:HA	2.54	0.42
1:A:68:PHE:HA	1:A:69:PRO:HD3	1.83	0.42
5:B:509:BTB:H12	5:B:509:BTB:H51	1.68	0.42
1:A:163:TYR:CE1	1:A:346:LEU:HD21	2.54	0.42
1:B:250:ARG:HD2	1:B:250:ARG:HA	1.86	0.42
5:B:504:BTB:H12	5:B:504:BTB:H72	1.85	0.42
1:A:88:ALA:O	1:B:97:ARG:NH1	2.36	0.42
1:B:128:ARG:NH1	1:B:128:ARG:HB2	2.33	0.42
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.32	0.42
5:B:510:BTB:H42	5:B:510:BTB:H72	1.81	0.42
1:A:238:ARG:HH21	1:A:240:ASP:HA	1.85	0.42
1:C:170:LEU:HD11	1:C:230:VAL:HG11	2.01	0.42
1:A:171:VAL:HG22	1:A:195:VAL:HB	2.02	0.42
1:A:342:GLU:HA	1:A:346:LEU:O	2.20	0.42
1:B:67:LYS:HE3	1:B:67:LYS:HB2	1.86	0.42
1:C:364:THR:HG21	1:C:452:ILE:HG23	2.01	0.42
5:A:506:BTB:H11	5:A:506:BTB:H72	1.60	0.41
1:D:271:THR:O	1:D:275:ILE:HG12	2.20	0.41
1:A:184:CYS:HB2	2:A:501:HEM:ND	2.35	0.41
1:A:475:TYR:OH	2:A:501:HEM:O1D	2.15	0.41
1:B:120:PRO:HD2	1:B:121:GLU:OE2	2.21	0.41
1:D:199:ARG:O	1:D:232:PRO:HG3	2.21	0.41
1:A:376:LEU:HD21	1:A:395:LYS:HB3	2.03	0.41
1:B:468:PHE:HZ	1:B:474:ARG:HH11	1.69	0.41
1:A:231:PHE:HB3	1:A:232:PRO:CD	2.51	0.41
1:A:387:THR:HA	1:A:394:TRP:CD1	2.56	0.41
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.95	0.41
1:B:220:ASN:HB3	1:B:223:ASN:O	2.20	0.41
1:B:365:ARG:HH12	3:B:502:H4B:C4	2.34	0.41
1:C:194:GLN:NE2	10:C:622:HOH:O	2.54	0.41
1:D:183:ARG:HD3	1:D:447:TRP:CD2	2.55	0.41
1:D:455:SER:HA	1:D:460:PHE:CG	2.56	0.41
1:B:128:ARG:HD3	1:B:150:LEU:HD22	2.03	0.41
1:B:231:PHE:HB3	1:B:232:PRO:HD2	2.03	0.41
5:B:509:BTB:H72	5:B:509:BTB:H41	1.56	0.41
1:B:279:TRP:HB2	1:B:302:LEU:HD21	2.01	0.40
1:D:479:PRO:HD2	1:D:480:TRP:CE3	2.56	0.40
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.93	0.40
1:A:463:GLU:HB3	1:B:103:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:HD3	1:B:81:TYR:CZ	2.56	0.40
1:D:323:PHE:O	1:D:326:LEU:HB2	2.21	0.40
1:A:298:GLU:HG2	10:A:636:HOH:O	2.22	0.40
1:A:175:LYS:HG2	1:A:193:LEU:HB3	2.03	0.40
1:A:298:GLU:HB3	1:A:299:PRO:HD2	2.04	0.40
1:C:178:TRP:CE3	1:C:190:TRP:HA	2.57	0.40
5:C:504:BTB:H82	5:C:504:BTB:O6	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLU:OE2	5:B:505:BTB:O3[2_842]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	399/440 (91%)	373 (94%)	20 (5%)	6 (2%)	10	3
1	B	402/440 (91%)	393 (98%)	8 (2%)	1 (0%)	47	38
1	C	399/440 (91%)	385 (96%)	13 (3%)	1 (0%)	41	30
1	D	399/440 (91%)	392 (98%)	7 (2%)	0	100	100
All	All	1599/1760 (91%)	1543 (96%)	48 (3%)	8 (0%)	29	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	239	GLY
1	B	259	GLY

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Mol	Chain	Res	Type
1	A	90	GLN
1	A	276	GLN
1	A	255	ARG
1	A	259	GLY
1	C	89	GLN

### 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	343/373 (92%)	322 (94%)	21 (6%)	18	7
1	B	345/373 (92%)	333 (96%)	12 (4%)	36	24
1	C	342/373 (92%)	332 (97%)	10 (3%)	42	31
1	D	342/373 (92%)	335 (98%)	7 (2%)	55	48
All	All	1372/1492 (92%)	1322 (96%)	50 (4%)	35	23

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	122	GLN
1	A	126	GLN
1	A	154	GLU
1	A	160	THR
1	A	192	LYS
1	A	206	GLU
1	A	207	MET
1	A	238	ARG
1	A	250	ARG
1	A	256	GLN
1	A	257	GLN
1	A	258	ASP
1	A	272	GLU
1	A	277	HIS
1	A	280	THR

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Mol	Chain	Res	Type
1	A	301	GLU
1	A	304	LEU
1	A	396	ASP
1	A	432	GLU
1	A	436	LYS
1	B	97	ARG
1	B	98	ARG
1	B	122	GLN
1	B	128	ARG
1	B	168[A]	SER
1	B	168[B]	SER
1	B	176	GLN
1	B	202	ARG
1	B	230	VAL
1	B	255	ARG
1	B	276	GLN
1	B	396	ASP
1	C	89	GLN
1	C	125	SER
1	C	128	ARG
1	C	132	ASN
1	C	151	GLN
1	C	162	THR
1	C	233	GLN
1	C	258	ASP
1	C	308	GLU
1	C	309	LEU
1	D	97	ARG
1	D	98	ARG
1	D	192	LYS
1	D	200	ASP
1	D	255	ARG
1	D	258	ASP
1	D	326	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	122	GLN
1	C	89	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 35 ligands modelled in this entry, 10 are monoatomic - leaving 25 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	$\# Z  > 2$
5	BTB	A	504	9	13,13,13	0.48	0	7,16,16	1.11	1 (14%)
3	H4B	D	502	-	16,18,18	0.89	1 (6%)	11,26,26	2.53	5 (45%)
7	GOL	A	508	-	5,5,5	0.36	0	5,5,5	0.30	0
2	HEM	B	501	1	27,50,50	1.98	5 (18%)	17,82,82	2.10	5 (29%)
5	BTB	D	504	9	13,13,13	0.41	0	7,16,16	0.34	0
7	GOL	C	506	-	5,5,5	0.39	0	5,5,5	0.27	0
5	BTB	C	504	-	13,13,13	0.43	0	7,16,16	0.44	0
5	BTB	D	505	-	13,13,13	0.59	0	7,16,16	0.96	0
2	HEM	D	501	1	27,50,50	1.73	4 (14%)	17,82,82	1.68	4 (23%)
2	HEM	A	501	1	27,50,50	1.85	4 (14%)	17,82,82	1.70	4 (23%)
4	OS7	B	503	-	31,31,31	0.94	2 (6%)	42,43,43	1.95	10 (23%)
3	H4B	B	502	-	16,18,18	0.92	0	11,26,26	2.56	6 (54%)
5	BTB	B	505	-	13,13,13	0.42	0	7,16,16	0.54	0
3	H4B	A	502	-	16,18,18	0.96	1 (6%)	11,26,26	2.57	5 (45%)
5	BTB	B	509	9	13,13,13	0.36	0	7,16,16	0.94	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BTB	B	506	-	13,13,13	0.38	0	7,16,16	0.41	0
4	OS7	C	503	-	31,31,31	0.78	0	42,43,43	1.51	6 (14%)
2	HEM	C	501	1	27,50,50	1.96	5 (18%)	17,82,82	1.89	5 (29%)
4	OS7	A	503	-	31,31,31	0.82	1 (3%)	42,43,43	1.60	8 (19%)
5	BTB	A	505	-	13,13,13	0.46	0	7,16,16	0.60	0
4	OS7	D	503	-	31,31,31	0.88	2 (6%)	42,43,43	1.71	8 (19%)
3	H4B	C	502	-	16,18,18	0.93	0	11,26,26	2.64	4 (36%)
5	BTB	B	504	9	13,13,13	0.36	0	7,16,16	0.43	0
5	BTB	A	506	-	13,13,13	0.33	0	7,16,16	0.44	0
5	BTB	B	510	-	13,13,13	0.84	1 (7%)	7,16,16	1.11	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
5	BTB	A	504	9	-	6/21/21/21	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
7	GOL	A	508	-	-	4/4/4/4	-
2	HEM	B	501	1	-	0/6/54/54	-
5	BTB	D	504	9	-	6/21/21/21	-
7	GOL	C	506	-	-	2/4/4/4	-
5	BTB	C	504	-	-	2/21/21/21	-
5	BTB	D	505	-	-	12/21/21/21	-
2	HEM	D	501	1	-	0/6/54/54	-
2	HEM	A	501	1	-	1/6/54/54	-
4	OS7	B	503	-	-	9/11/11/11	0/4/4/4
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
5	BTB	B	505	-	-	4/21/21/21	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
5	BTB	B	509	9	-	3/21/21/21	-
5	BTB	B	506	-	-	6/21/21/21	-
4	OS7	C	503	-	-	8/11/11/11	0/4/4/4
2	HEM	C	501	1	-	0/6/54/54	-
4	OS7	A	503	-	-	8/11/11/11	0/4/4/4
5	BTB	A	505	-	-	13/21/21/21	-
4	OS7	D	503	-	-	7/11/11/11	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
5	BTB	B	504	9	-	1/21/21/21	-
5	BTB	A	506	-	-	6/21/21/21	-
5	BTB	B	510	-	-	5/21/21/21	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C2B	-5.19	1.33	1.40
2	C	501	HEM	C3B-C2B	-4.64	1.33	1.40
2	A	501	HEM	C3B-C2B	-4.34	1.34	1.40
2	C	501	HEM	C3B-CAB	4.01	1.56	1.47
2	A	501	HEM	C3B-CAB	3.86	1.55	1.47
2	C	501	HEM	C3C-CAC	3.84	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.84	1.35	1.40
2	D	501	HEM	C3C-CAC	3.82	1.55	1.47
2	B	501	HEM	C3C-CAC	3.79	1.55	1.47
2	B	501	HEM	C3B-CAB	3.79	1.55	1.47
2	A	501	HEM	C3C-C2C	-3.69	1.35	1.40
2	D	501	HEM	C3B-C2B	-3.68	1.35	1.40
2	A	501	HEM	C3C-CAC	3.67	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.57	1.35	1.40
2	D	501	HEM	C3B-CAB	3.53	1.55	1.47
2	D	501	HEM	C3C-C2C	-3.12	1.36	1.40
4	B	503	OS7	C02-N01	2.54	1.36	1.33
2	C	501	HEM	CAA-C2A	2.29	1.55	1.52
4	B	503	OS7	C05-C10	-2.28	1.38	1.42
4	D	503	OS7	C02-N01	2.25	1.36	1.33
3	A	502	H4B	C4-C4A	-2.21	1.38	1.41
4	D	503	OS7	C05-C10	-2.08	1.39	1.42
5	B	510	BTB	C3-C2	-2.07	1.50	1.53
3	D	502	H4B	C7-C6	2.04	1.54	1.52
2	B	501	HEM	CMD-C2D	2.03	1.55	1.51
4	A	503	OS7	C02-N01	2.02	1.36	1.33

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	H4B	C4-C4A-C8A	6.46	120.31	114.57
3	A	502	H4B	C4-C4A-C8A	5.92	119.83	114.57
2	B	501	HEM	CBA-CAA-C2A	-5.43	102.48	112.49
4	B	503	OS7	C05-C10-N01	-5.35	117.13	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	H4B	C4-C4A-C8A	5.25	119.23	114.57
4	B	503	OS7	C04-C05-C10	5.09	120.77	118.01
3	B	502	H4B	C4-C4A-C8A	4.85	118.88	114.57
4	D	503	OS7	C05-C10-N01	-4.69	117.83	122.81
2	C	501	HEM	CBA-CAA-C2A	-4.59	104.02	112.49
4	B	503	OS7	O19-C14-C15	4.50	121.66	115.78
4	D	503	OS7	C04-C05-C10	4.44	120.41	118.01
2	D	501	HEM	CBA-CAA-C2A	-4.29	104.57	112.49
4	A	503	OS7	O19-C14-C15	4.15	121.20	115.78
4	C	503	OS7	O19-C14-C15	4.05	121.08	115.78
4	A	503	OS7	C04-C05-C10	4.04	120.20	118.01
4	D	503	OS7	O19-C14-C15	3.98	120.98	115.78
4	A	503	OS7	C05-C10-N01	-3.92	118.66	122.81
4	C	503	OS7	C04-C05-C10	3.90	120.12	118.01
4	C	503	OS7	C05-C10-N01	-3.88	118.70	122.81
3	B	502	H4B	C4-N3-C2	3.52	121.53	115.93
3	B	502	H4B	N3-C2-N1	-3.52	119.90	125.42
2	B	501	HEM	CAA-CBA-CGA	3.36	118.31	112.67
3	D	502	H4B	C4-N3-C2	3.32	121.21	115.93
4	B	503	OS7	C03-C04-C05	3.29	121.02	117.78
4	D	503	OS7	C03-C04-C05	3.17	120.91	117.78
3	A	502	H4B	C4-N3-C2	3.13	120.90	115.93
3	C	502	H4B	C4-N3-C2	3.08	120.82	115.93
2	C	501	HEM	CBD-CAD-C3D	-3.08	106.80	112.48
4	B	503	OS7	C07-C08-C11	-3.05	116.07	121.36
2	B	501	HEM	CAD-CBD-CGD	-2.96	107.70	112.67
3	A	502	H4B	N3-C2-N1	-2.94	120.80	125.42
3	D	502	H4B	N3-C2-N1	-2.92	120.84	125.42
2	A	501	HEM	CBA-CAA-C2A	-2.92	107.11	112.49
2	B	501	HEM	CMC-C2C-C3C	2.91	130.12	124.68
3	C	502	H4B	N3-C2-N1	-2.89	120.88	125.42
2	D	501	HEM	CBD-CAD-C3D	-2.85	107.22	112.48
2	D	501	HEM	CMC-C2C-C3C	2.84	129.99	124.68
2	C	501	HEM	CMA-C3A-C4A	-2.82	124.14	128.46
4	D	503	OS7	C26-N21-C22	2.80	121.26	117.42
2	A	501	HEM	CMA-C3A-C4A	-2.76	124.22	128.46
2	A	501	HEM	CAD-CBD-CGD	-2.75	108.05	112.67
4	B	503	OS7	C26-N21-C22	2.75	121.18	117.42
3	B	502	H4B	C2-N1-C8A	2.66	120.51	114.54
5	A	504	BTB	O3-C3-C2	2.56	118.46	111.44
4	A	503	OS7	O19-C14-C13	-2.52	118.53	123.97
4	B	503	OS7	N02-C02-N01	2.51	120.33	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CBD-CAD-C3D	-2.50	107.86	112.48
3	D	502	H4B	C2-N1-C8A	2.50	120.15	114.54
4	C	503	OS7	C26-N21-C22	2.50	120.84	117.42
3	A	502	H4B	C2-N1-C8A	2.45	120.02	114.54
4	B	503	OS7	C09-C08-C11	2.44	126.62	121.05
4	B	503	OS7	C09-C10-N01	2.43	122.42	118.72
3	C	502	H4B	C2-N1-C8A	2.42	119.97	114.54
4	A	503	OS7	C07-C08-C11	-2.39	117.21	121.36
3	D	502	H4B	C4-C4A-N5	2.38	121.12	119.12
4	A	503	OS7	C26-N21-C22	2.30	120.56	117.42
5	B	509	BTB	O3-C3-C2	2.29	117.70	111.44
4	D	503	OS7	C09-C10-N01	2.27	122.18	118.72
4	C	503	OS7	O19-C14-C13	-2.26	119.08	123.97
3	B	502	H4B	N2-C2-N1	2.22	120.71	117.25
4	A	503	OS7	C03-C04-C05	2.22	119.96	117.78
4	B	503	OS7	C04-C03-C02	-2.16	117.36	119.72
3	A	502	H4B	N2-C2-N3	2.15	120.59	117.25
2	D	501	HEM	CMA-C3A-C4A	-2.14	125.18	128.46
2	C	501	HEM	CMC-C2C-C3C	2.13	128.65	124.68
3	B	502	H4B	C4-C4A-N5	2.12	120.90	119.12
2	C	501	HEM	C4C-C3C-C2C	2.09	108.36	106.90
4	C	503	OS7	C03-C04-C05	2.07	119.82	117.78
4	D	503	OS7	N02-C02-N01	2.07	119.97	118.26
2	A	501	HEM	C4A-C3A-C2A	2.05	108.42	107.00
4	D	503	OS7	C04-C03-C02	-2.05	117.48	119.72
4	A	503	OS7	C08-C09-C10	-2.05	119.65	121.44

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	BTB	C1-C2-C3-O3
5	A	504	BTB	N-C2-C3-O3
7	A	508	GOL	C1-C2-C3-O3
5	D	504	BTB	O1-C1-C2-C3
5	D	504	BTB	O1-C1-C2-C4
5	D	504	BTB	O1-C1-C2-N
5	D	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4
5	D	504	BTB	N-C2-C4-O4
7	C	506	GOL	O1-C1-C2-C3
5	C	504	BTB	C8-C7-N-C5

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Mol	Chain	Res	Type	Atoms
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
5	D	505	BTB	C1-C2-N-C7
5	D	505	BTB	C3-C2-N-C7
5	D	505	BTB	C4-C2-N-C7
5	D	505	BTB	C8-C7-N-C5
5	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	C4-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	B	509	BTB	C1-C2-C3-O3
5	B	509	BTB	C4-C2-C3-O3
5	B	509	BTB	N-C2-C3-O3
5	B	506	BTB	O1-C1-C2-C3
5	B	506	BTB	O1-C1-C2-C4
5	B	506	BTB	O1-C1-C2-N
5	B	506	BTB	C1-C2-C3-O3
5	B	506	BTB	C4-C2-C3-O3
5	B	506	BTB	N-C2-C3-O3
5	A	505	BTB	O1-C1-C2-C4
5	A	505	BTB	O1-C1-C2-N
5	A	505	BTB	C1-C2-C3-O3
5	A	505	BTB	C4-C2-C3-O3
5	A	505	BTB	N-C2-C3-O3
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-C7
5	A	506	BTB	C1-C2-C3-O3
5	A	506	BTB	C4-C2-C3-O3
5	A	506	BTB	N-C2-C3-O3
5	A	506	BTB	C1-C2-C4-O4
5	A	506	BTB	C3-C2-C4-O4
5	A	506	BTB	N-C2-C4-O4
5	B	510	BTB	C1-C2-C3-O3
5	B	510	BTB	C4-C2-C3-O3
5	B	510	BTB	N-C2-C3-O3
4	C	503	OS7	C07-C08-C11-C12
4	C	503	OS7	C09-C08-C11-C16

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Mol	Chain	Res	Type	Atoms
4	C	503	OS7	C07-C08-C11-C16
4	C	503	OS7	C09-C08-C11-C12
4	A	503	OS7	C07-C08-C11-C16
4	A	503	OS7	C09-C08-C11-C16
4	A	503	OS7	C09-C08-C11-C12
4	A	503	OS7	C07-C08-C11-C12
4	B	503	OS7	C07-C08-C11-C16
4	B	503	OS7	C09-C08-C11-C16
4	B	503	OS7	C07-C08-C11-C12
4	D	503	OS7	C09-C08-C11-C16
4	D	503	OS7	C07-C08-C11-C16
4	D	503	OS7	C07-C08-C11-C12
4	B	503	OS7	C09-C08-C11-C12
4	D	503	OS7	C09-C08-C11-C12
5	A	505	BTB	N-C5-C6-O6
4	B	503	OS7	C14-C15-C17-N18
4	C	503	OS7	C14-C15-C17-N18
4	A	503	OS7	C14-C15-C17-N18
7	A	508	GOL	O1-C1-C2-C3
2	A	501	HEM	C2A-CAA-CBA-CGA
7	A	508	GOL	O2-C2-C3-O3
7	C	506	GOL	O1-C1-C2-O2
4	B	503	OS7	C13-C14-O19-C20
4	B	503	OS7	C15-C14-O19-C20
5	C	504	BTB	N-C7-C8-O8
5	B	505	BTB	N-C5-C6-O6
4	A	503	OS7	C13-C14-O19-C20
5	A	504	BTB	N-C5-C6-O6
7	A	508	GOL	O1-C1-C2-O2
4	D	503	OS7	C14-C15-C17-N18
4	A	503	OS7	C15-C14-O19-C20
4	C	503	OS7	C13-C14-O19-C20
5	A	504	BTB	C4-C2-C3-O3
5	A	505	BTB	O1-C1-C2-C3
5	A	504	BTB	O1-C1-C2-N
5	A	504	BTB	C4-C2-N-C7
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C3-C2-N-C5
5	D	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C5
5	B	510	BTB	O1-C1-C2-N
4	D	503	OS7	C13-C14-O19-C20

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Mol	Chain	Res	Type	Atoms
5	B	504	BTB	N-C5-C6-O6
4	C	503	OS7	C22-C20-O19-C14
4	C	503	OS7	C15-C14-O19-C20
4	D	503	OS7	C15-C14-O19-C20
4	B	503	OS7	O19-C20-C22-N21
4	A	503	OS7	C16-C15-C17-N18
4	B	503	OS7	O19-C20-C22-C23
5	B	510	BTB	O1-C1-C2-C4

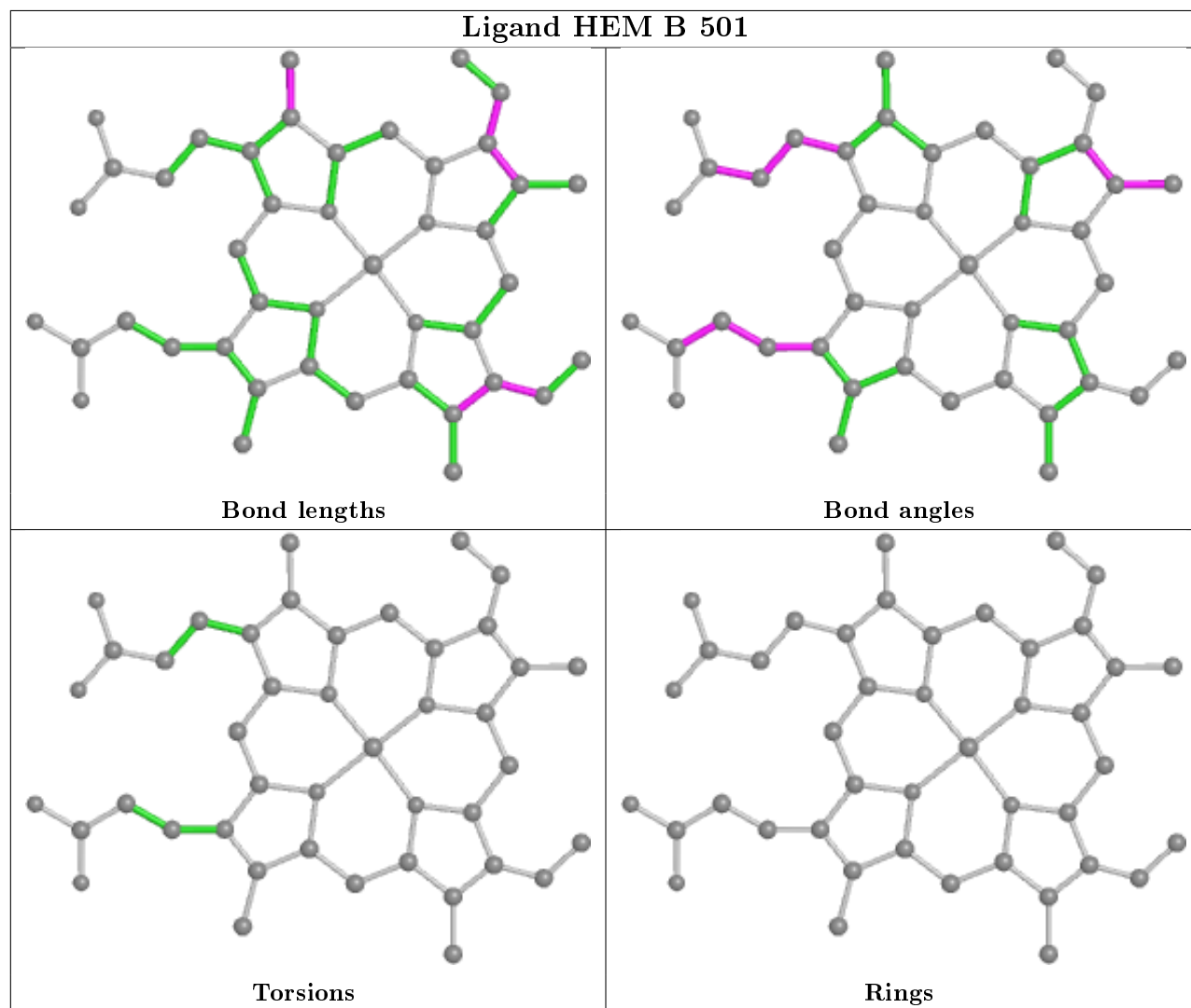
There are no ring outliers.

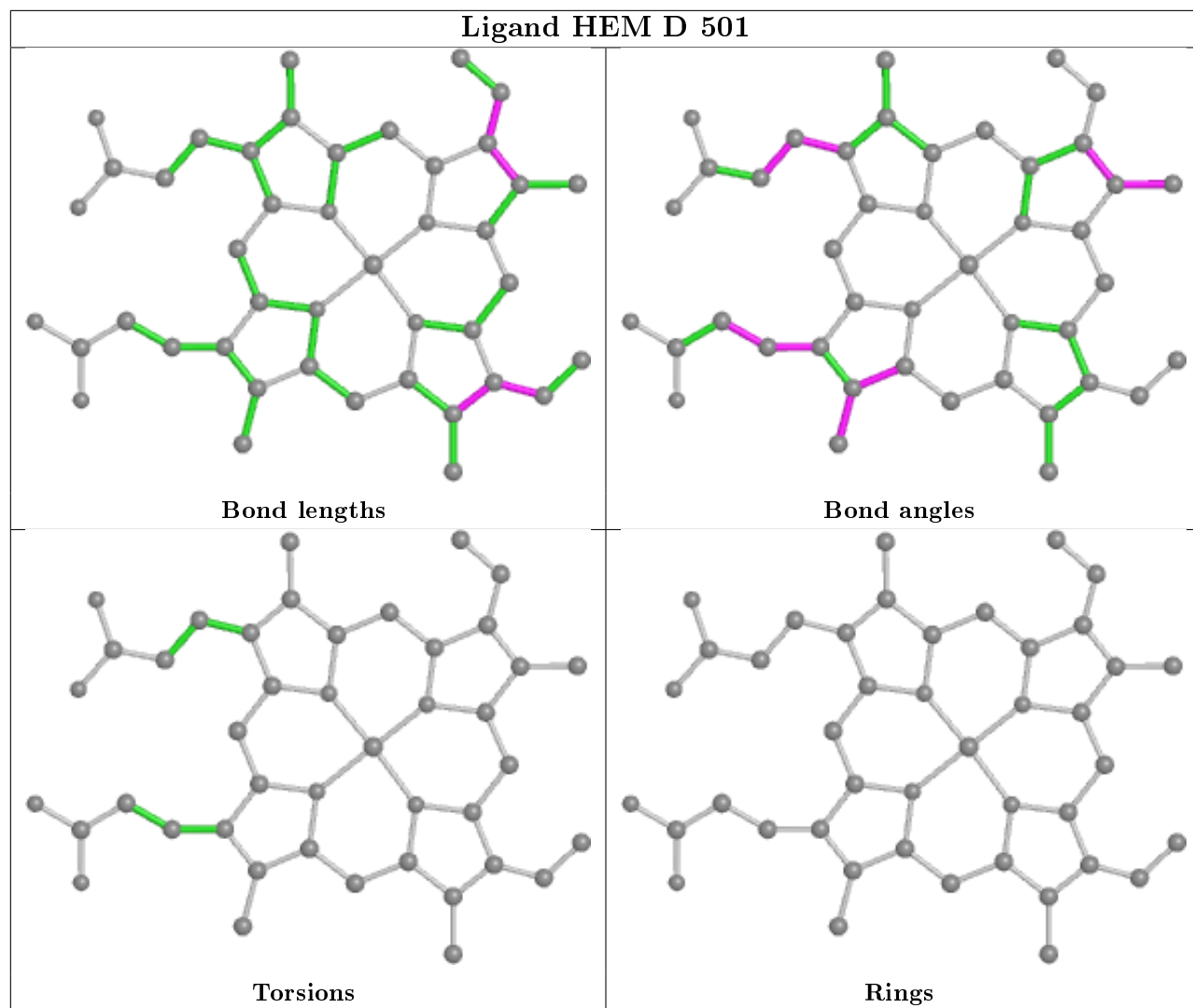
21 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	BTB	4	0
2	B	501	HEM	3	0
5	D	504	BTB	3	0
5	C	504	BTB	3	0
5	D	505	BTB	3	0
2	D	501	HEM	1	0
2	A	501	HEM	3	0
4	B	503	OS7	2	0
3	B	502	H4B	1	0
5	B	505	BTB	3	1
3	A	502	H4B	1	0
5	B	509	BTB	3	0
4	C	503	OS7	4	0
2	C	501	HEM	3	0
4	A	503	OS7	1	0
5	A	505	BTB	2	0
4	D	503	OS7	1	0
3	C	502	H4B	1	0
5	B	504	BTB	1	0
5	A	506	BTB	1	0
5	B	510	BTB	3	0

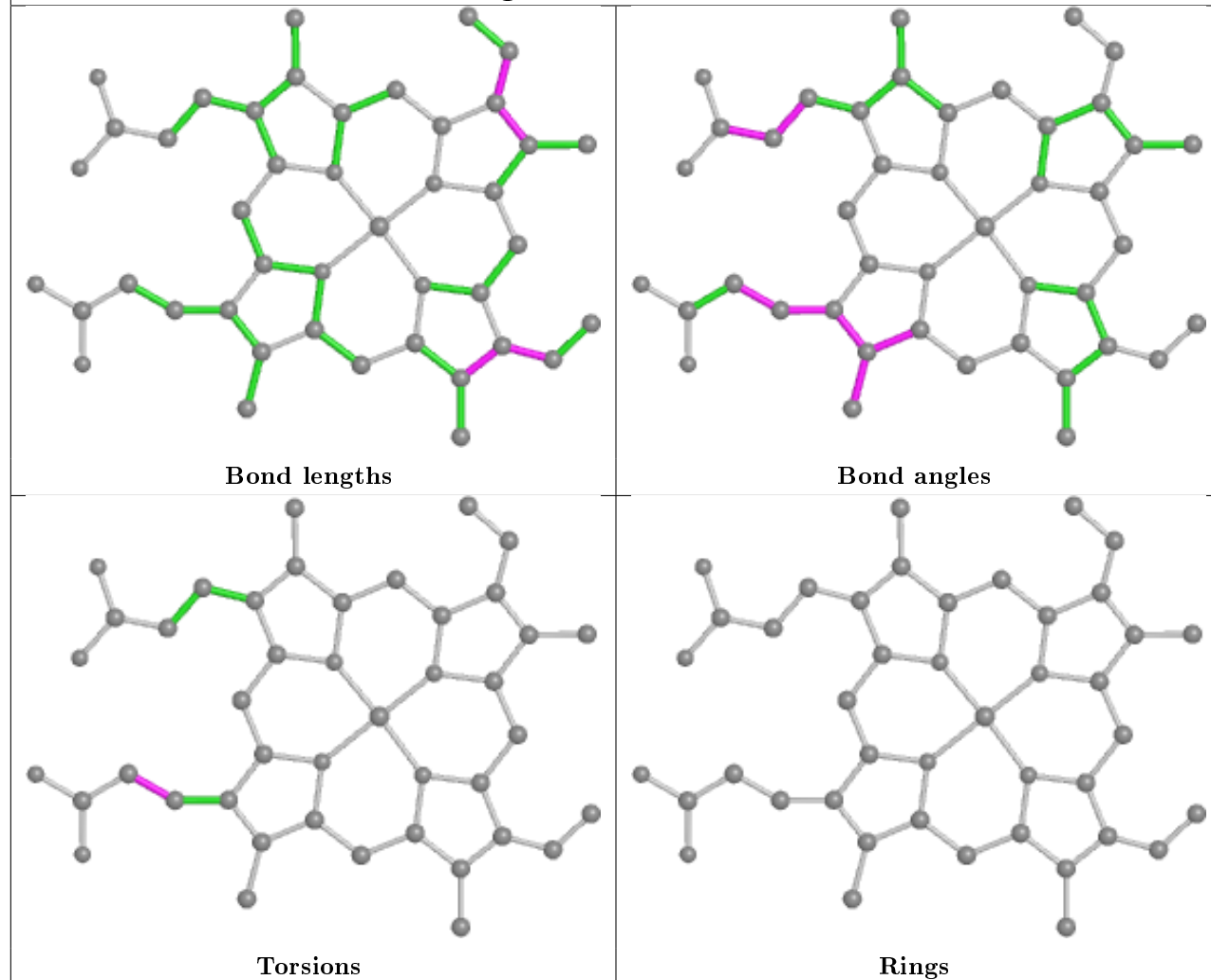
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

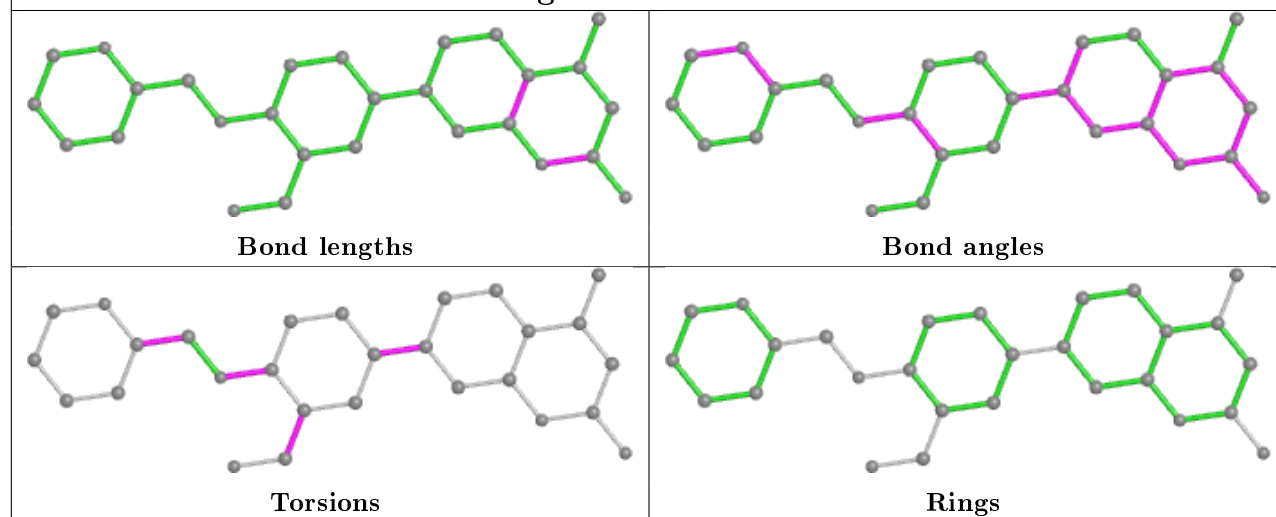




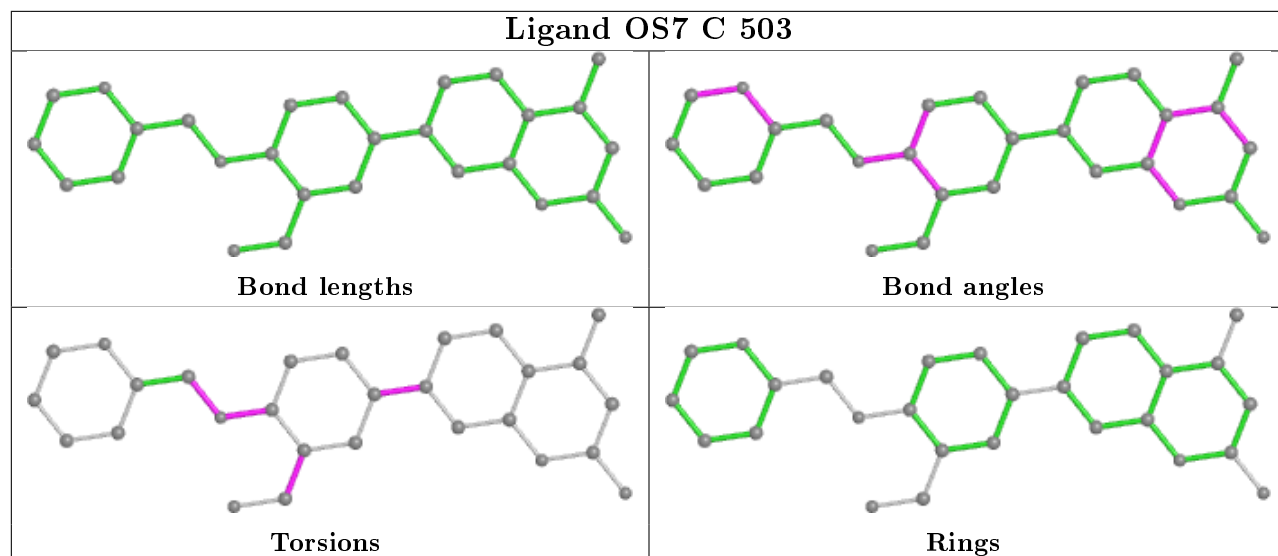
## Ligand HEM A 501



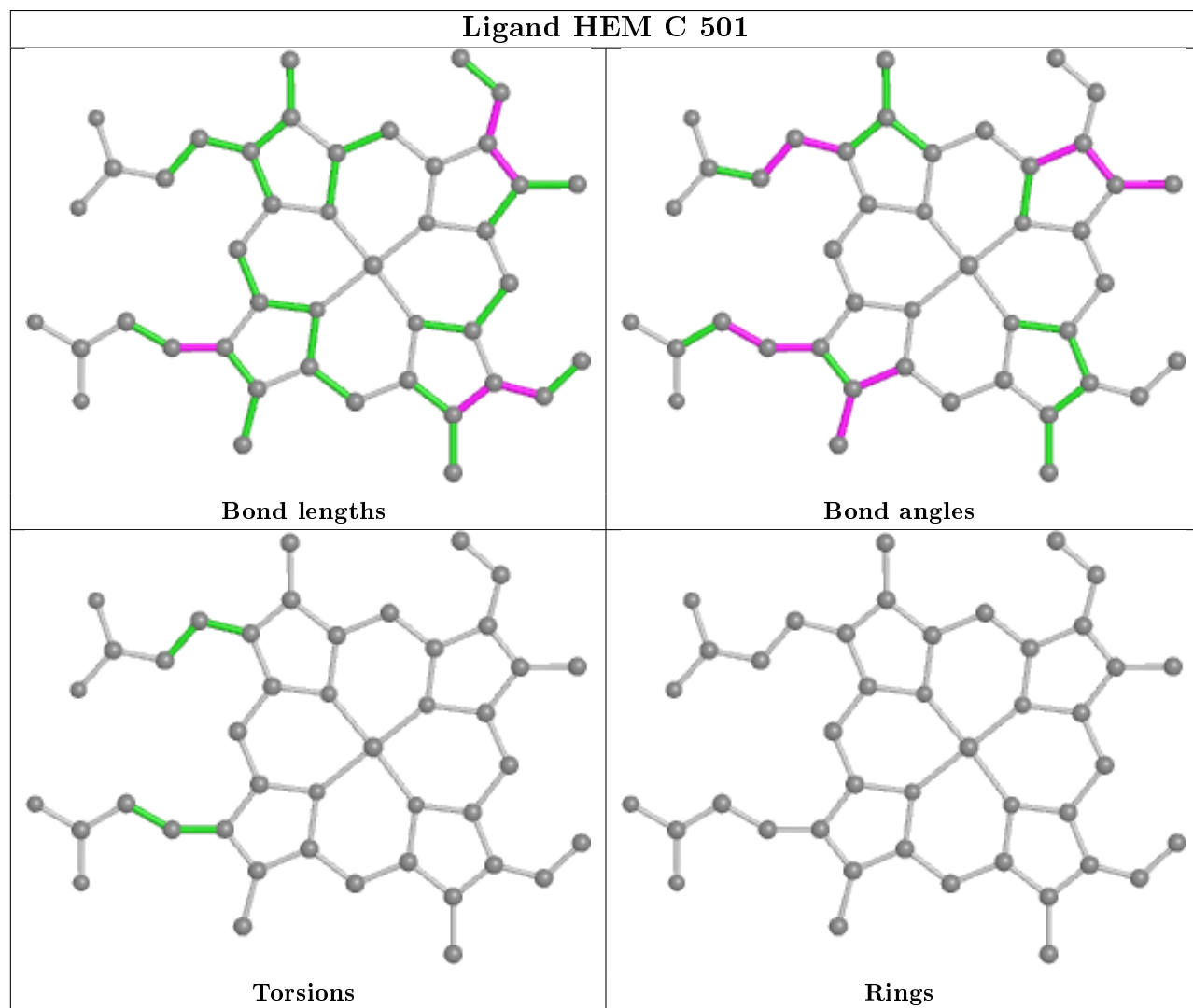
## Ligand OS7 B 503

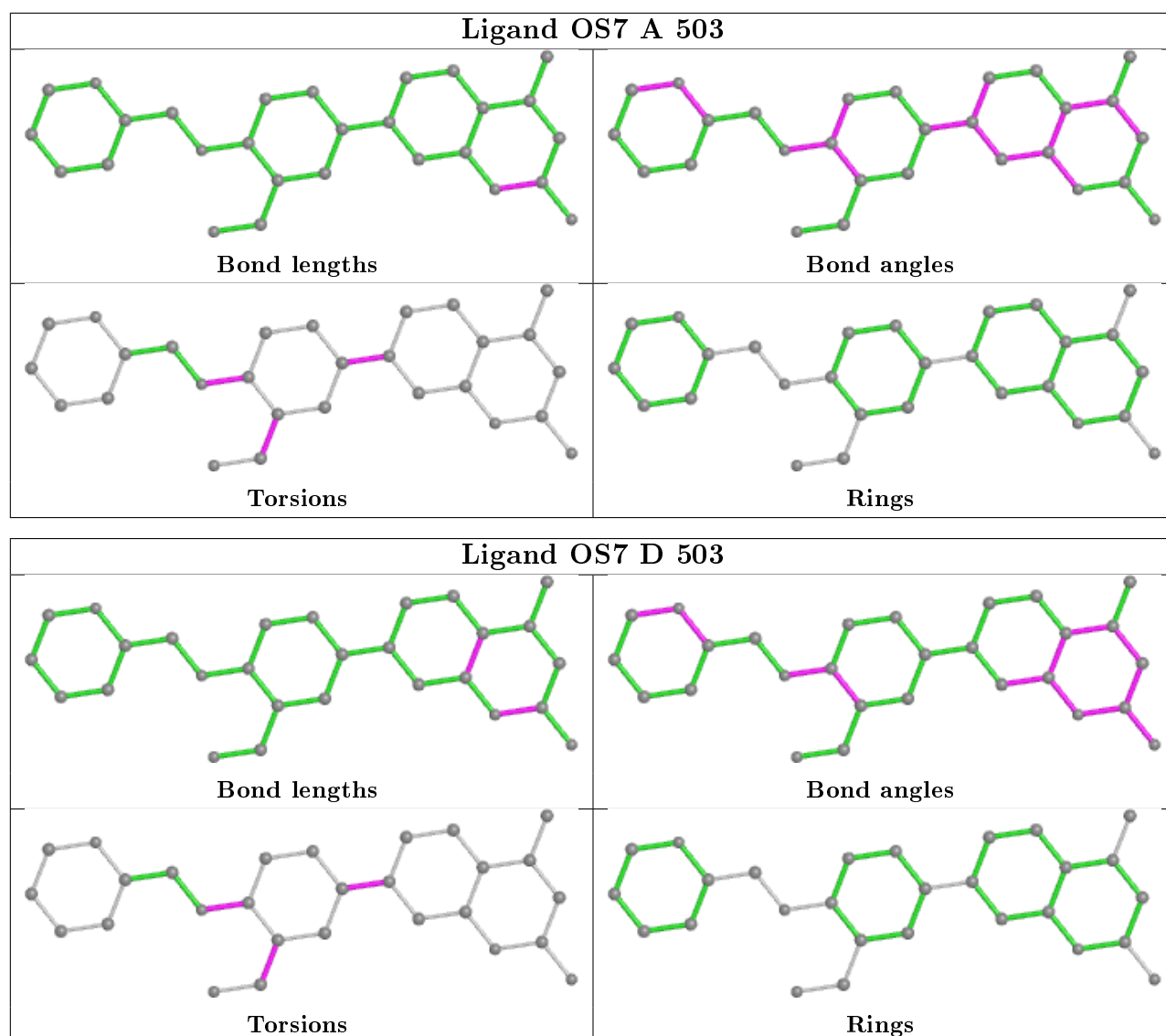


## Ligand OS7 C 503



## Ligand HEM C 501





## 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	401/440 (91%)	0.65	44 (10%) 5 9	31, 66, 122, 156	0
1	B	402/440 (91%)	0.08	6 (1%) 73 81	27, 42, 78, 111	0
1	C	401/440 (91%)	0.23	8 (1%) 65 73	30, 54, 98, 137	0
1	D	401/440 (91%)	0.01	1 (0%) 95 97	27, 40, 65, 126	0
All	All	1605/1760 (91%)	0.24	59 (3%) 41 51	27, 49, 102, 156	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	480	TRP	6.7
1	A	259	GLY	5.7
1	C	238	ARG	5.7
1	A	153	VAL	5.5
1	A	120	PRO	5.3
1	A	204	ALA	5.2
1	A	304	LEU	4.6
1	A	163	TYR	4.5
1	A	238	ARG	4.2
1	A	293	LEU	4.2
1	A	130	PHE	4.0
1	C	237	GLY	3.9
1	A	305	LEU	3.9
1	A	121	GLU	3.8
1	A	107	ARG	3.8
1	A	280	THR	3.8
1	A	127	ALA	3.7
1	A	244	TRP	3.7
1	B	141[A]	SER	3.6
1	A	303	PHE	3.6
1	D	89	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	202	ARG	3.6
1	A	275	ILE	3.3
1	A	237	GLY	3.1
1	A	341	LEU	3.1
1	A	207	MET	3.1
1	A	346	LEU	3.0
1	A	123	LEU	3.0
1	A	162	THR	3.0
1	B	90	GLN	2.9
1	A	140	ARG	2.8
1	A	279	TRP	2.8
1	A	129	ASP	2.8
1	C	124	LEU	2.7
1	A	257	GLN	2.7
1	A	124	LEU	2.7
1	A	350	ALA	2.7
1	C	468	PHE	2.7
1	C	480	TRP	2.7
1	A	300	PRO	2.6
1	A	152	GLU	2.6
1	A	235	CYS	2.5
1	A	254	TYR	2.5
1	B	67	LYS	2.5
1	A	252	ALA	2.4
1	A	122	GLN	2.4
1	B	257	GLN	2.4
1	A	302	LEU	2.3
1	A	202	ARG	2.3
1	A	479	PRO	2.3
1	A	272	GLU	2.3
1	A	270	ILE	2.2
1	C	140	ARG	2.2
1	A	285	ARG	2.2
1	C	204	ALA	2.1
1	B	89	GLN	2.1
1	A	268	VAL	2.0
1	A	134	TYR	2.0
1	B	468	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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
5	BTB	B	506	14/14	0.74	0.17	82,98,104,106	0
4	OS7	B	503	28/28	0.77	0.25	49,87,108,110	0
4	OS7	A	503	28/28	0.79	0.23	59,104,108,111	0
4	OS7	C	503	28/28	0.80	0.23	69,87,97,102	0
4	OS7	D	503	28/28	0.81	0.20	44,79,101,104	0
5	BTB	A	506	14/14	0.83	0.17	98,107,113,114	0
5	BTB	C	504	14/14	0.84	0.11	70,97,104,106	0
5	BTB	D	504	14/14	0.85	0.17	39,67,89,90	0
7	GOL	C	506	6/6	0.90	0.16	57,68,75,81	0
5	BTB	B	505	14/14	0.91	0.17	44,69,80,83	0
5	BTB	B	504	14/14	0.91	0.12	31,58,76,77	0
5	BTB	A	505	14/14	0.91	0.18	63,71,80,83	0
5	BTB	D	505	14/14	0.92	0.18	48,68,96,99	0
7	GOL	A	508	6/6	0.92	0.13	58,79,84,88	0
8	CL	A	509	1/1	0.94	0.09	58,58,58,58	0
9	GD	A	510	1/1	0.94	0.11	94,94,94,94	0
3	H4B	B	502	17/17	0.95	0.11	35,41,48,49	0
3	H4B	C	502	17/17	0.95	0.13	35,47,56,60	0
5	BTB	B	510	14/14	0.95	0.19	32,63,73,76	0
5	BTB	A	504	14/14	0.96	0.11	38,73,82,83	0
3	H4B	A	502	17/17	0.96	0.12	43,50,65,75	0
2	HEM	A	501	43/43	0.97	0.14	42,58,75,78	0
5	BTB	B	509	14/14	0.97	0.12	25,66,74,76	0
3	H4B	D	502	17/17	0.97	0.08	31,39,45,48	0
8	CL	B	507	1/1	0.97	0.08	54,54,54,54	0
8	CL	C	507	1/1	0.97	0.05	65,65,65,65	0
8	CL	D	506	1/1	0.97	0.09	55,55,55,55	0
2	HEM	C	501	43/43	0.98	0.13	31,43,67,79	0
9	GD	B	511	1/1	0.98	0.12	84,84,84,84	0
2	HEM	D	501	43/43	0.98	0.12	24,34,45,51	0
2	HEM	B	501	43/43	0.99	0.12	21,33,47,67	0
6	ZN	A	507	1/1	0.99	0.14	46,46,46,46	0

*Continued on next page...*

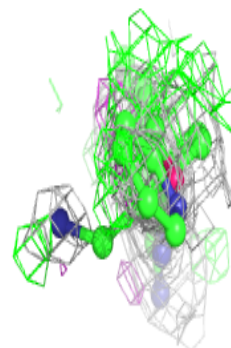
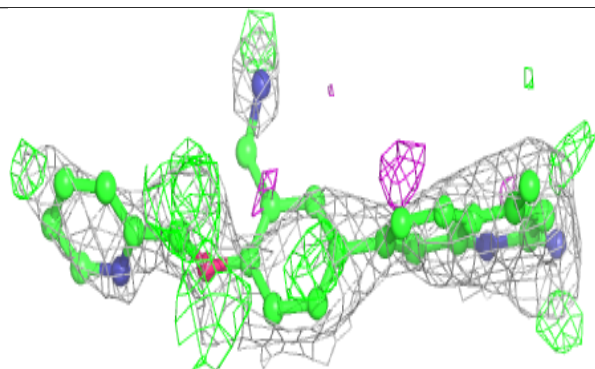
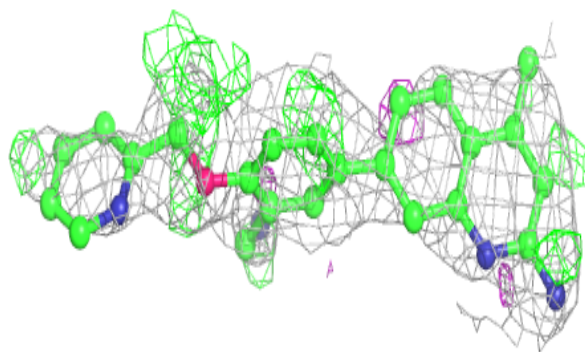
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	GD	D	507	1/1	0.99	0.15	48,48,48,48	0
9	GD	B	508	1/1	0.99	0.17	47,47,47,47	0
6	ZN	C	505	1/1	1.00	0.13	36,36,36,36	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.

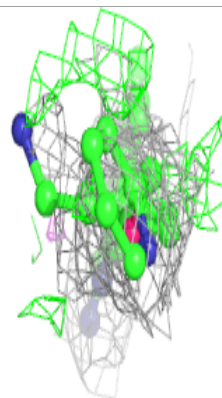
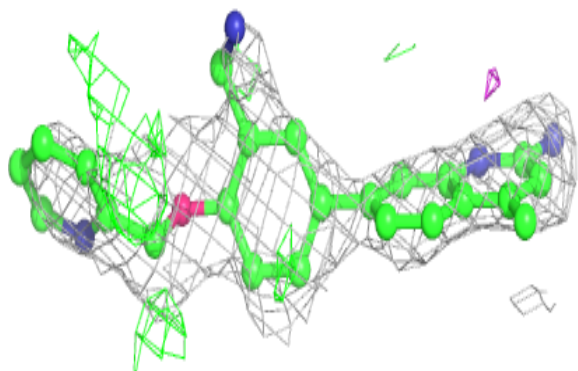
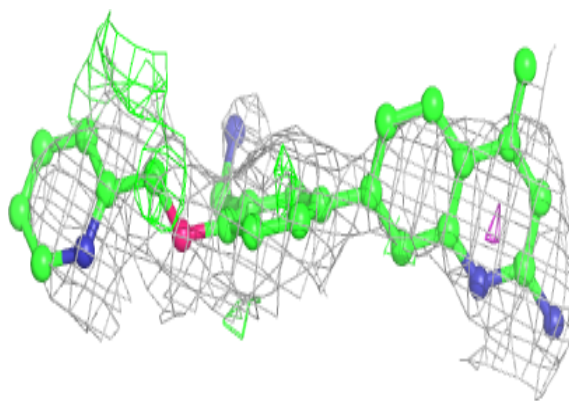
**Electron density around OS7 B 503:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

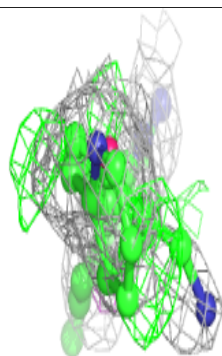
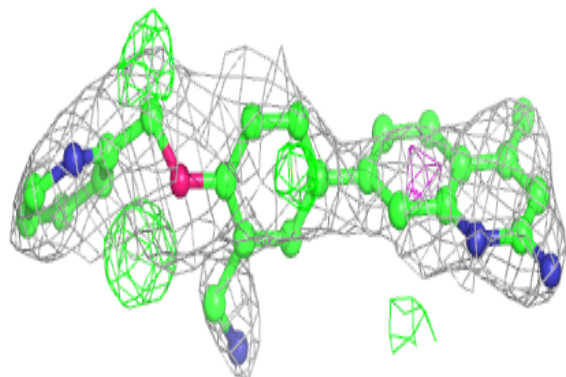
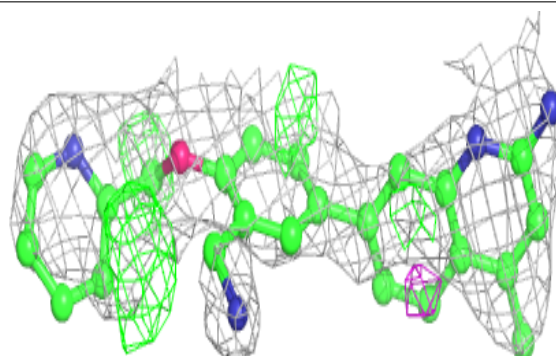


**Electron density around OS7 A 503:**

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

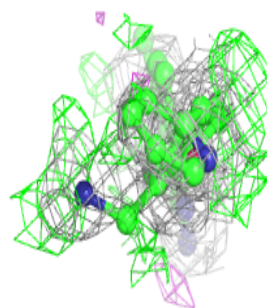
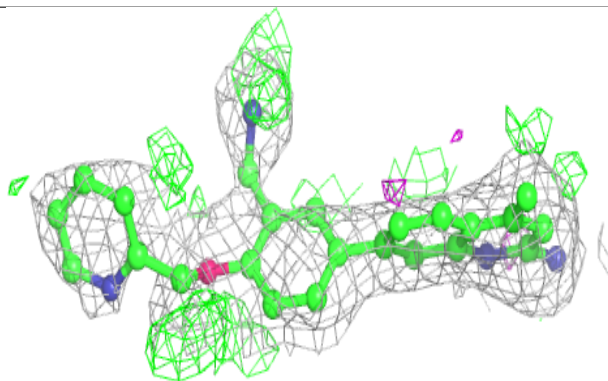
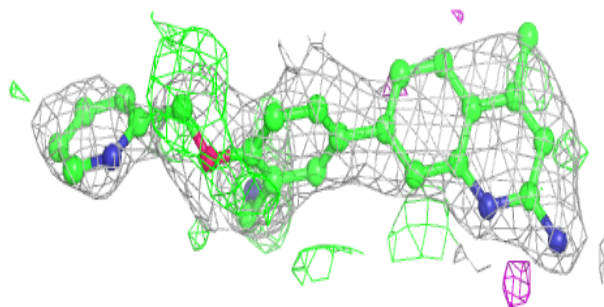
**Electron density around OS7 C 503:**

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



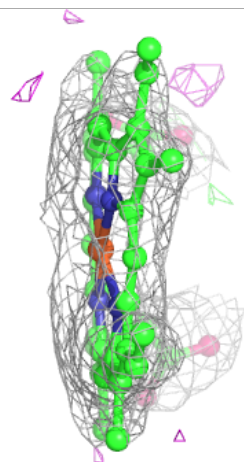
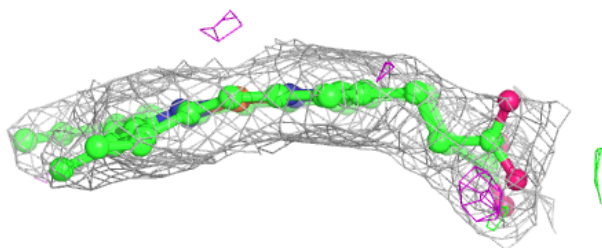
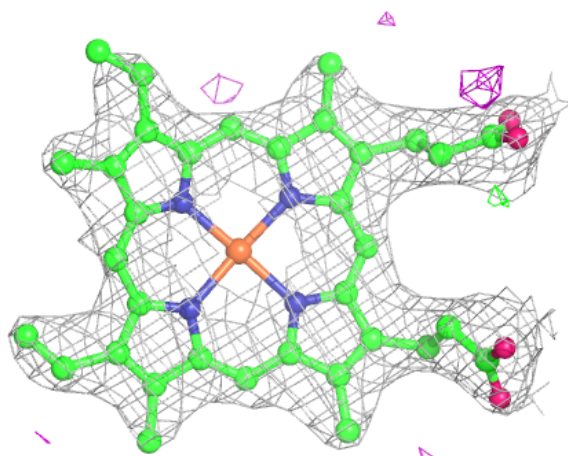
**Electron density around OS7 D 503:**

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



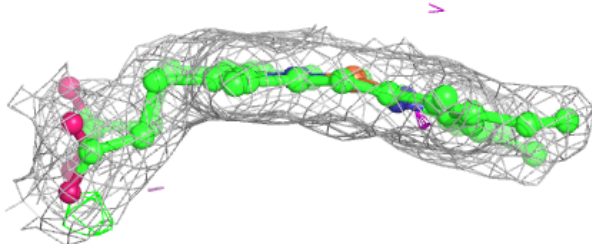
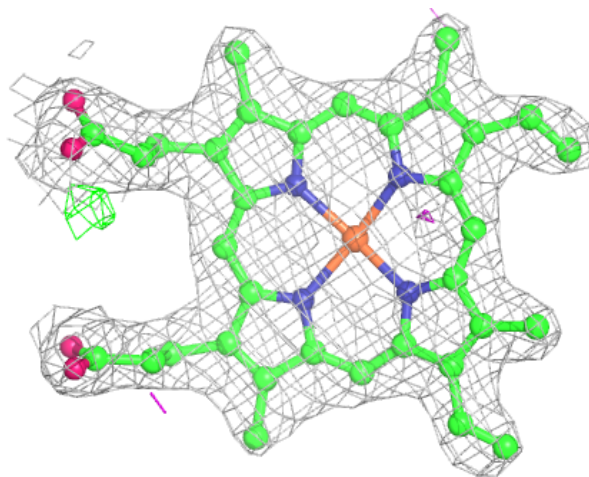
**Electron density around HEM A 501:**

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



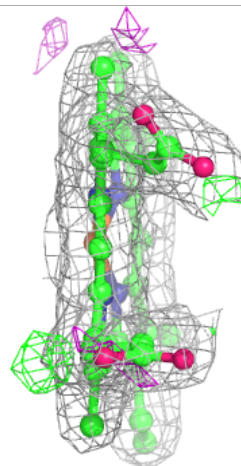
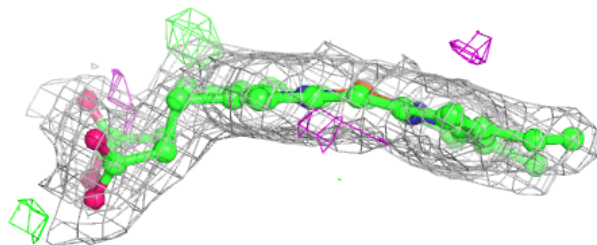
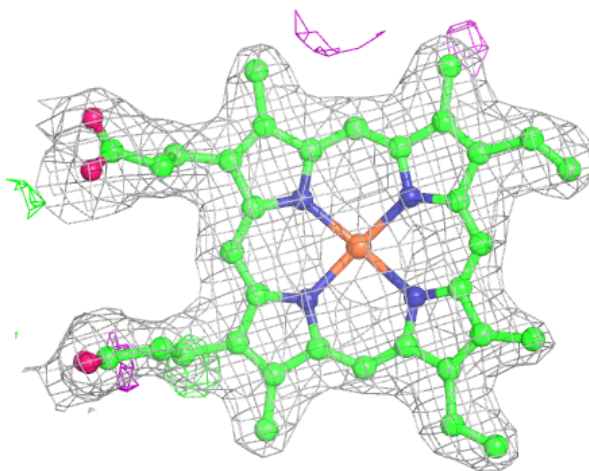
**Electron density around HEM C 501:**

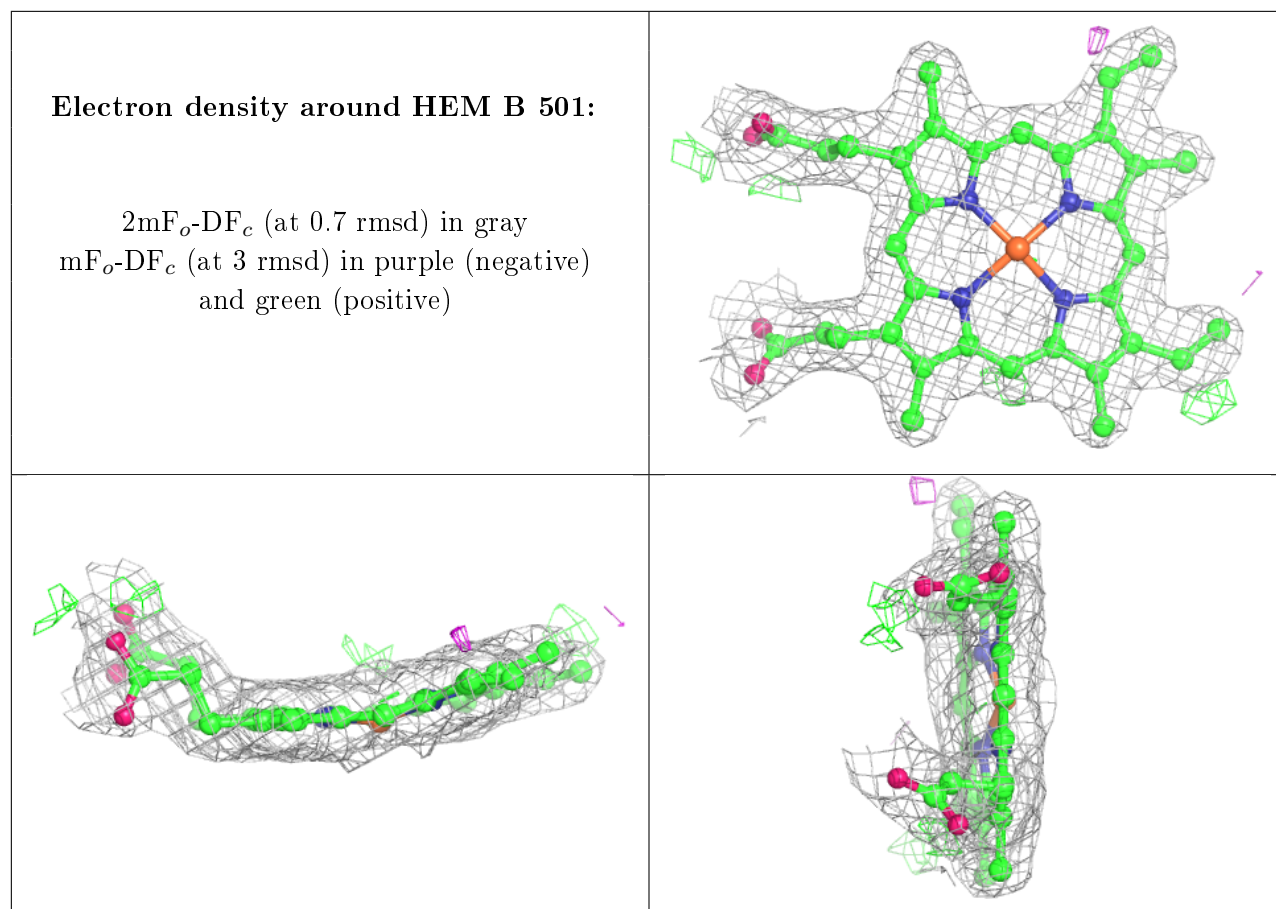
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM D 501:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.